The *OPAL* Framework

Version 2024.2

WRITTEN BY

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Chapter 1

Preliminary note

This is the manual for *OPAL* 2024.2 which is still under development. Use at your own risc.

New feature might not yet be documented or something is already documented but not yet implemented.

Chapter 2

Abstract

OPAL is a parallel open source tool for charged-particle optics in linear accelerators and rings, including 3D space charge. Using the *MAD* language with extensions, *OPAL* can run on a laptop as well as on the largest high performance computing systems. *OPAL* is built from the ground up as a parallel application exemplifying the fact that high performance computing is the third leg of science, complementing theory and experiment.

The *OPAL* framework makes it easy to add new features in the form of new *C++* classes. *OPAL* comes in the following flavours:

OPAL-cycl tracks particles with 3D space charge including neighbouring turns in cyclotrons and FFAs with time as the independent variable.

OPAL-t models beam lines, linacs, rf-photo injectors and complete XFELs.

OPAL-map map tracking (experimental, no space charge yet)

It should be noted that not all features of *OPAL* are available in all flavours.

Chapter 3

Introduction

3.1 History

Using the *MAD* language with extensions, *OPAL* is derived from *MAD9P* and is based on the *CLASSIC* [1] class library, which was started in 1995 by an international collaboration. IPPL (Independent Parallel Particle Layer) is the framework which provides parallel particles and fields using data parallel approach. IPPL was inspired by the POOMA [6].

OPAL-t can be used to model guns, injectors, ERLs and complete XFELs.

3.2 Parallel Processing Capabilities

OPAL is built to harness the power of parallel processing for an improved quantitative understanding of particle accelerators. This goal can only be achieved with detailed 3D modelling capabilities and a sufficient number of simulation particles to obtain meaningful statistics on various quantities of the particle ensemble such as emittance, slice emittance, halo extension etc.

The following example is exemplifying this fact:

Distribution	**Particles**	**Mesh**	**Greens Function**	**Time steps**
Gauss 3D	10^8	1024^3	Integrated	10

Table 1: Parameters Parallel Performance Example

Figure 1 shows the parallel efficiency time as a function of used cores for a test example with parameters given in Table 1. The data were obtained on a Cray XT5 at the Swiss Center for Scientific Computing.

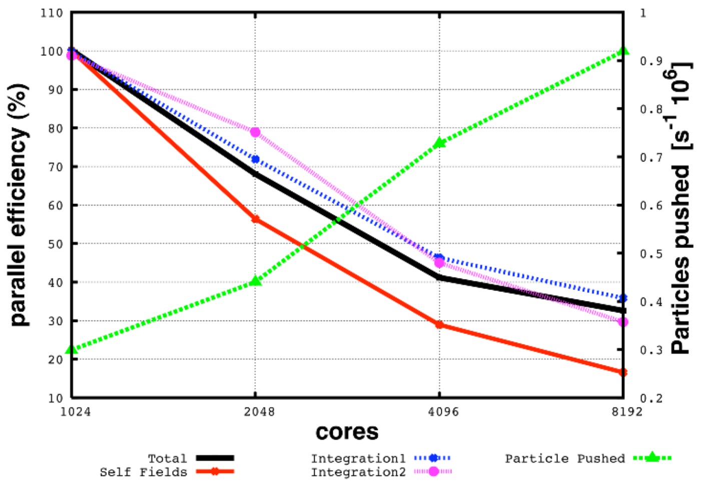


Figure 1: Parallel efficiency and particles pushed per μs as a function of cores

3.3 Quality Management

Documentation and quality assurance are given our highest attention since we are convinced that adequate documentation is a key factor in the usefulness of a code like *OPAL* to study present and future particle accelerators. Using tools such as a source code version control system (git), source code documentation using Doxygen (found here) and the extensive user manual you are now enjoying, we are committed to providing users as well as co-developers with state-of-the-art documentation to *OPAL*.

One example of an non trivial test-example is the PSI DC GUN. In Figure 2 the comparison between *Impact-t* and *OPAL-t* is shown. This example is part of the regression test suite that is run every night. The input file is found in Examples of Particle Accelerators and Beamlines.

Misprints and obscurity are almost inevitable in a document of this size. Comments and *active contributions* from readers are therefore most welcome. They may be sent to Andreas Adelmann.

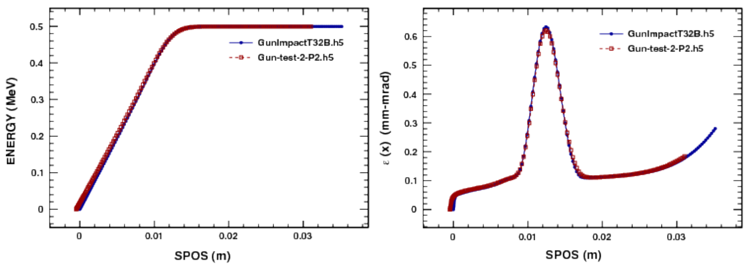


Figure 2: Comparison of energy and emittance in x between *Impact-t* and *OPAL-t*

3.4 Output

The phase space is stored in the H5hut file-format [3] and can be analyzed using e.g. H5root [4], [5]. The frequency of the data output (phase space and some statistical quantities) can be controlled using the (see Option Statement), with the flag `PSDUMPFREQ`. The file is named like in input file but with the extension *.h5*.

A SDDS compatible ASCII file with statistical beam parameters is written to a file with extension .stat. The frequency with which this data is written can be controlled with the OPTION statement with the flag `STATDUMPFREQ`.

For postprocessing we recommend to use the pyOPALTools Python package which contains many tools for pre- and postprocessing, and analysing and plotting output data.

In addition to the output files, note that important information is displayed on the *stdout* i.e. the *terminal*. The user is advised to consult the stdout frequently.

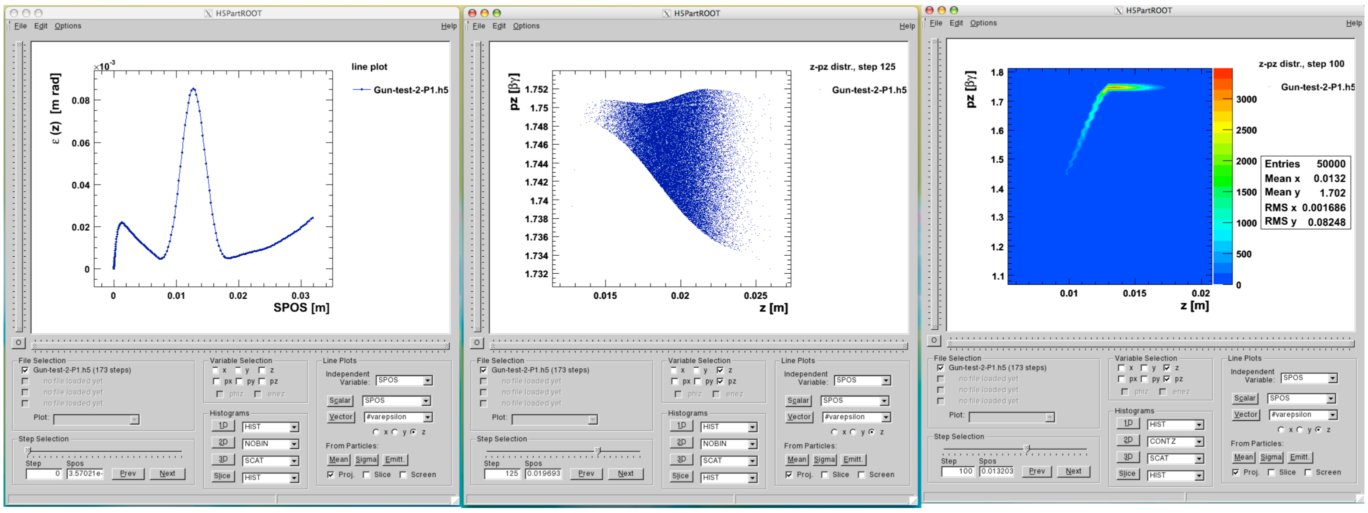


Figure 3: H5root enables a variety of data analysis and post processing task on *OPAL* data

3.5 Change History

See Release Notes for a detailed list of changes in *OPAL*.

3.6 Known Issues and Limitations

See the issue list in the repository.

See also pitfalls and limitations.

3.7 Acknowledgments

The contributions of various individuals and groups are acknowledged in the relevant chapters, however a few individuals have or had considerable influence on the development of *OPAL*, namely Chris Iselin, John Jowett, Julian Cummings, Ji Qiang, Robert Ryne and Stefan Adam. For the H5root visualization tool credits go to Thomas Schietinger.

The following individuals are acknowledged for past contributions: Christian Baumgarten, J. Scott Berg, Yuanjie Bi, David Bruhwiler, Chris Cortes, Martin Duy Tat, Philippe Ganz, Colwyn Gulliford, Yves Ineichen, Tulin Kaman, Christopher Mayes, Xiaoying Pang, Valeria Rizzoglio, Chuan Wang, Jianjun Yang, Hao Zha.

3.8 Citation

Please cite *OPAL* in the following way:

```
@ARTICLE{2019arXiv190506654A,
       author = {{Adelmann}, Andreas and {Calvo}, Pedro and {Frey}, Matthias and
         {Gsell}, Achim and {Locans}, Uldis and {Metzger-Kraus}, Christof and
         {Neveu}, Nicole and {Rogers}, Chris and {Russell}, Steve and
         {Sheehy}, Suzanne and {Snuverink}, Jochem and {Winklehner}, Daniel},
        title = "{OPAL a Versatile Tool for Charged Particle Accelerator ↩
           Simulations}",
      journal = {arXiv e-prints},
     keywords = {Physics - Accelerator Physics},
         year = "2019",
        month = "May",
          eid = {arXiv:1905.06654},
        pages = {arXiv:1905.06654},
archivePrefix = {arXiv},
       eprint = {1905.06654},
 primaryClass = {physics.acc-ph},
       adsurl = {https://ui.adsabs.harvard.edu/abs/2019arXiv190506654A},
      adsnote = {Provided by the SAO/NASA Astrophysics Data System}
}
```

3.9 References

[1] F. C. Iselin, *The classic project*, Tech. Rep. CERN/SL/96-061, European Organization for Nuclear Research (1996).

[2] J. Qiang et al., *A three-dimensional quasi-static model for high brightness beam dynamics simulation*, Tech. Rep. LBNL-59098, Lawrence Berkeley National Laboratory (2005).

[3] M. Howison et al., *H5hut: A High-Performance I/O Library for Particle-based Simulations*, in 2010 IEEE International Conference on Cluster Computing Workshops and Posters, vol. 1, pp. 1–8 (Heraklion, Crete, 2010).

[4] *H5root: a ROOT Based Graphical User Interface for H5hut*.

[5] T. Schietinger, *H5PartROOT - A visualization and post-processing tool for accelerator simulations*, in Proceedings of the 10th International Computational Accelerator Physics conference (ICAP09), pp. 343-346 (San Francisco, CA, USA, 2009).

[6] R. Günther, *Parallel Object-Oriented Methods and Applications* (2005).

Chapter 4

Conventions

4.1 Physical Units

Throughout the computations, *OPAL* internally uses international units, as defined by SI (Système International), for all physical quantities (see Table 2). However, some elements and field maps are defined in other units in the input file, as is specified in their corresponding description in the Manual.

Quantity	**Dimension**
Length	m (meters)
Angle	rad (radians)
Quadrupole coefficient	Tm^{-1}
Multipole coefficient, 2n poles	Tm^{-n+1}
Electric voltage	MV (Megavolts)
Electric field strength	MVm^{-1}
Frequency	MHz (Megahertz)
Particle energy	MeV or eV
Particle mass	MeVc^{-2}
Particle momentum	$\beta\gamma$ or eV (see Units)
Beam current	A (Amperes)
Particle charge	e (elementary charges)
Impedances	MΩ (Megaohms)
Emittances (normalized and geometric	mrad
RF power	MW (Megawatts)

Table 2: Physical Units

4.2 Symbols used

Symbol	**Definition**
X	Ellipse axis along the x dimension [m]. $X = R$ for circular beams.
Y	Ellipse axis along the y dimension [m]. $Y = R$ for circular beams.
R	Beam radius for circular beam [m].
R^*	Effective beam radius for elliptical beam: $R^* = (X+Y)/2$ [m].
σ_x	Rms beam size in x: $\sigma_x = \langle x^2\rangle^{1/2}$ [m]. $\sigma_x = X/2$ for elliptical or circular beams (X=Y=R).
σ_y	Rms beam size in y: $\sigma_y = \langle y^2\rangle^{1/2}$ [m]. $\sigma_y = Y/2$ for elliptical or circular beams (X=Y=R).
σ_i	Rms beam size in x (i=1) or y (i=2): $\sigma = \langle x^2\rangle^{1/2}$ or $\langle y^2\rangle^{1/2}$ [m].
σ_L	Rms beam size in the Larmor frame for cylindrical symmetric beam and external fields [m]: $\sigma_L = \sigma_x = \sigma_y$.
σ_r	Rms beam size in r for a circular beam: $\sigma_r = \langle r^2\rangle^{1/2} = R/\sqrt{2}$ [m].
σ^*	Average rms size for elliptical beam: $\sigma^* = (\sigma_x + \sigma_y)/2$ [m].
θ_r	Larmor angle [rad]
$\dot{\theta}_r$	Time derivative of Larmor angle: $\dot{\theta}_r = -eB_z/2m\gamma$ [rad/sec].
z_s	Longitudinal position of a particular beam slice [m].
z_h, z_t	Position of the head & tail of a beam bunch [m].
ζ	Used to label the position of a beam slice in the beam [m]. For bunched beams: $\zeta = z_s - z_t$.
ξ	Used to label the position of a slice image charge [m]. For bunched beams: $\xi = z_h + z_t$.
K	Focusing function of cylindrical symmetric external fields: $K = -\frac{\partial F_r}{\partial r}$ [N/m].
K_i	Focusing function in x_i direction: $K_i = -\frac{\partial F_{x_i}}{\partial x_i}$ [N/m].
I_0	Alfven current: $I_0 = e/4\pi\varepsilon_0 mc^3$ [A].
I	Beam current [A].
$I(\zeta)$	Slice beam current [A].
k_p	Beam perveance: $k_p = I(\zeta)/2I_0$
$g(\zeta)$	Form factor used in slice analysis of bunched beams.

Table 3: List of Symbols used and their definition.

4.3 Elegant Multipole Conversion

OPAL-t uses gradient in T/m so the conversion is dB_y/dx=0.29979/(E[GeV])*dBy/dx[T/m])

A Python code for conversion:

```
 def k1tog(k1, E = 45):
    """convert K1 to gradient, E in MeV"""
    g = 3.335E-3 * E * k1
    return g
// EOF
```

Chapter 5

Pitfalls and Limitations

A loose collection of pitfalls that may be difficult to avoid in particular for new users but also experienced user might profit from this list.

5.1 Hard Edge Fields

Fields that feature steps like hard edge fringe fields are strongly advised not to be used. In sector magnets where particles have different path lengths inside the magnet they are kicked 1, 2 or even more steps more (or less) depending on position and momentum. Combine it with big time steps and you'll observe strange effects like splitting beams.

5.2 Very Short Active Elements / Big Time Steps

This is similar to the problem with hard edge fields. This concerns elements that model electromagnetic devices whose lengths are very short and comparable to the time step. In this case a split of the bunch can be observed which is caused by the fact that some particles are kicked more often than others. The length of the time step should then be decreased to reduce this effect.

Chapter 6

Tutorial

This chapter will provide a jump start describing some of the most common used features of *OPAL*. The complete set of examples can be found and downloaded at https://gitlab.psi.ch/OPAL/src/wikis/home. All examples are requiring a small amount of computing resources and run on a single core, but can be used efficiently on up to 8 cores. *OPAL* scales in the weak sense, hence for a higher concurrency one has to increase the problem size i.e. number of macro particles and the grid size, which is beyond this tutorial.

6.1 The Simulation Cycle

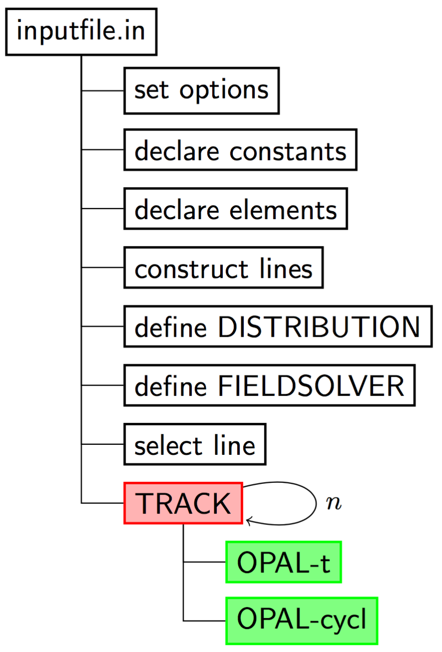


Figure 4: The simulation cycle

6.2 Starting *OPAL*

The name of the application is `opal`. When called without any argument an interactive session is started.

```
\$ opal
Ippl> CommMPI: Parent process waiting for children ...
Ippl> CommMPI: Initialization complete.
>                ____  _____       ___
>               / __ \|  __ \ /\   | |
>              | |  | | |__) /  \  | |
>              | |  | |  ___/ /\ \ | |
>              | |__| | |  / ____ \| |____
>               \____/|_| /_/    \_\______|
OPAL >
OPAL > This is OPAL (Object Oriented Parallel Accelerator Library) Version 2.0.0 ...
OPAL >
OPAL > Please send cookies, goodies or other motivations (wine and beer ... )
OPAL > to the OPAL developers opal@lists.psi.ch
OPAL >
OPAL > Time: 16.43.23 date: 30/05/2017
OPAL > Reading startup file "/Users/adelmann/init.opal".
OPAL > Finished reading startup file.
==>
```

One can exit from this session with the command `QUIT;` (including the semicolon).

For batch runs *OPAL* accepts the command line arguments shown in Table 4:

Argument	**Values**	**Function**
--input	<file >	The input file. Using "--input" is optional. Instead the input file can be provided either as first or as last argument.
--info	0 – 5	Controls the amount of output to the command line. 0 means no or scarce output, 5 means a lot of output. Default: 1.
--warn	0 – 5	Controls the amount of output warning message. Default: 1.
--restart	-1 – <Integer>	Restarts from given step in file with saved phase space. Per default *OPAL* tries to restart from a file <file>.h5 where <file>is the input file without extension. -1 stands for the last step in the file. If no other file is specified to restart from and if the last step of the file is chosen, then the new data is appended to the file. Otherwise the data from this particular step is copied to a new file and all new data appended to the new file.
--restartfn	<file>	A file in H5hut format from which *OPAL* should restart.
--help		Displays a summary of all command-line arguments and then quits.
--help-command	<command>	Display the help for the *OPAL* command <command> and all the information about their attributes.
--version		Prints the curent version of *OPAL* installed.
--version-full		Prints the version of *OPAL* with additional informations.
--git-revision		Print the revision hash of the repository.
--summary		Print IPPL lib summary at start.
--time		Show total time used in execution.
--notime		Do not show timing info (default).
--commlib <x>	mpi or serial	Selects a parallel comm. library.

Table 4: Command line arguments

Example:

```
opal input.in --restartfn input.h5 --restart -1 --info 3
```

6.3 Auto-phase Example

This is a partially complete example. First we have to set *OPAL* in `AUTOPHASE` mode, as described in Option Statement and for example set the nominal phase to -3.5°). The way how *OPAL* is computing the phases is explained in Appendix Auto-phasing Algorithm.

```
Option, AUTOPHASE=4;

REAL FINSS_RGUN_phi= (-3.5/180*Pi);
```

The cavity would be defined like

```
FINSS_RGUN: RFCavity, L = 0.17493, VOLT = 100.0,
    FMAPFN = "FINSS-RGUN.dat",
    ELEMEDGE = 0.0, TYPE = STANDING, FREQ = 2998.0,
    LAG = FINSS_RGUN_phi;
```

with `FINSS_RGUN_phi` defining the off crest phase. Now a normal `TRACK` command can be executed. A file containing the values of maximum phases is created, and has the format like:

```
1
FINSS_RGUN
2.22793
```

with the first entry defining the number of cavities in the simulation.

6.4 Examples of Particle Accelerators and Beamlines

6.4.1 Laser emission, OBLA (SwissFEL test facility) 4 MeV Gun and Beamline

LaserEmission-1.in

All supplementary files can be found in the laser emission regression test.

6.4.2 PSI Injector II Cyclotron

Injector II is a separated sector cyclotron specially designed for pre-acceleration (inject: 870 keV, extract: 72 MeV) of high intensity proton beam for Ring cyclotron. It has 4 sector magnets, two double-gap acceleration cavities (represented by 2 single-gap cavities here) and two single-gap flat-top cavities.

Following is an input file of **Single Particle Tracking mode** for PSI Injector II cyclotron.

Injector2.in

The supplementary files should be placed in the same directory.

- Cav1.dat
- Cav3.dat
- ZYKL9Z.NAR
- scdist.opal
- spdist.opal
- tdist.opal

To run *OPAL* on a single node, just use this command:

```
opal Injector2.in
```

Here shows some pictures using the resulting data from single particle tracking using *OPAL-cycl*.

Left plot of Figure 5 shows the accelerating orbit of reference particle. After 106 turns, the energy increases from 870 keV at the injection point to 72.16 MeV at the deflection point.

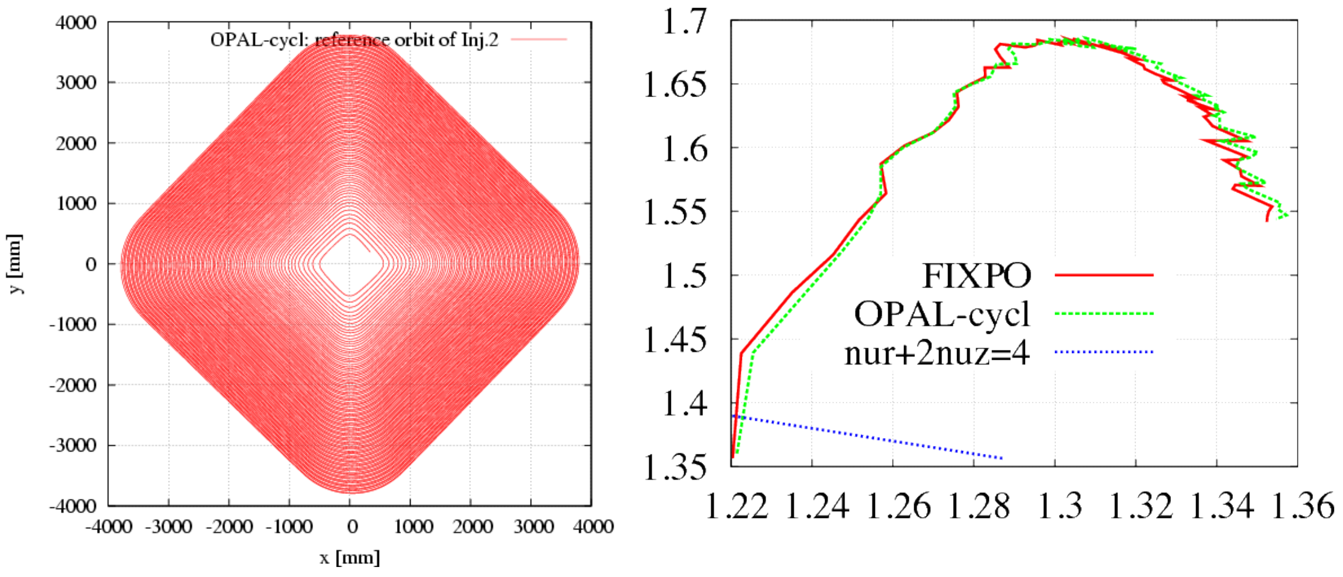


Figure 5: Reference orbit(left) and tune diagram(right) in Injector II

From theoretic view, there should be an eigen ellipse for any given energy in stable area of a fixed accelerator structure. Only when the initial phase space shape matches its eigen ellipse, the oscillation of beam envelop amplitude will get minimal and the transmission efficiency get maximal. We can calculate the eigen ellipse by single particle tracking using betatron oscillation property of off-centered particle as following: track an off-centered particle and record its coordinates and momenta at the same azimuthal position for each revolution. Figure 6 shows the eigen ellipse at symmetric line of sector magnet for energy of 2 MeV in Injector II.

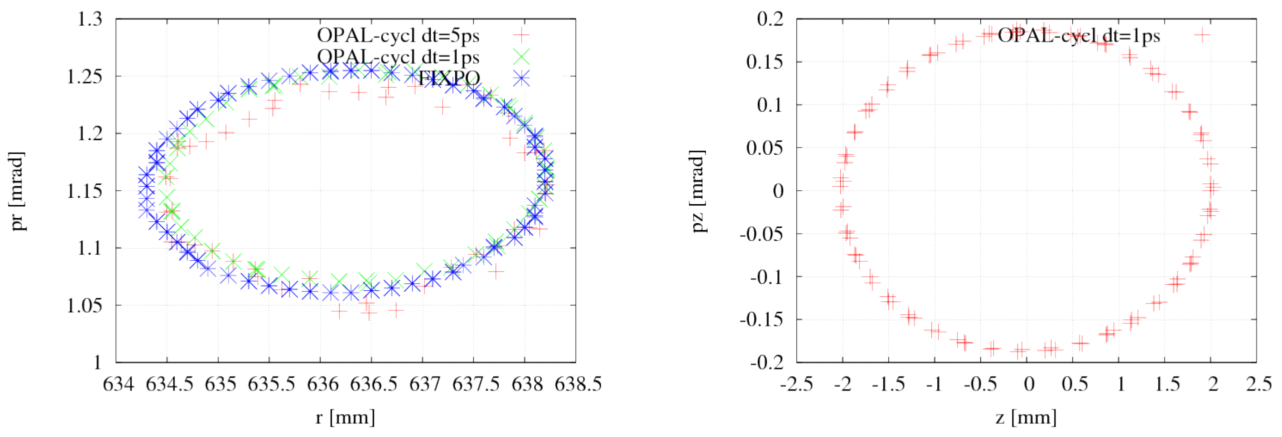


Figure 6: Radial and vertical eigenellipse at 2 MeV of Injector II

Right plot of Figure 5 shows very good agreement of the tune diagram by *OPAL-cycl* and FIXPO. The trivial discrepancy should come from the methods they used. In FIXPO, the tune values are obtained according to the crossing points of the initially displaced particle. Meanwhile, in *OPAL-cycl*, the Fourier analysis method is used to manipulate orbit difference between the reference particle and an initially displaced particle. The frequency point with the biggest amplitude is the betatron tune value at the given energy.

Following is the input file for single bunch tracking with space charge effects in Injector II.

Injector2-sc.in

For the supplementary files see above, Section 6.4.2

To run *OPAL* on single node, just use this command:

```
opal Injector2-sc.in
```

To run *OPAL* on N nodes in parallel environment interactively, use this command instead:

```
mpirun -np N opal Injector2-sc.in
```

If restart a job from the last step of an existing *.h5* file, add a new argument like this:

```
mpirun -np N opal Injector2-sc.in --restart -1
```

Figure 7 and Figure 8 are simulation results, shown by H5root code.

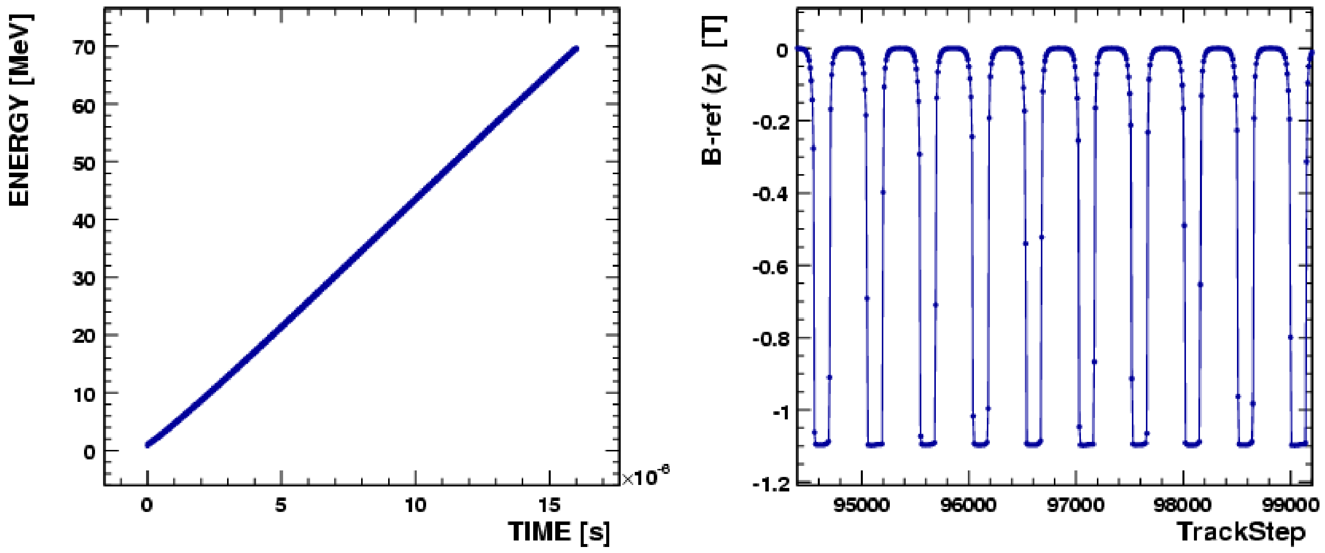


Figure 7: Energy vs. time (left) and external B field vs. track step (Right, only show for about 2 turns)

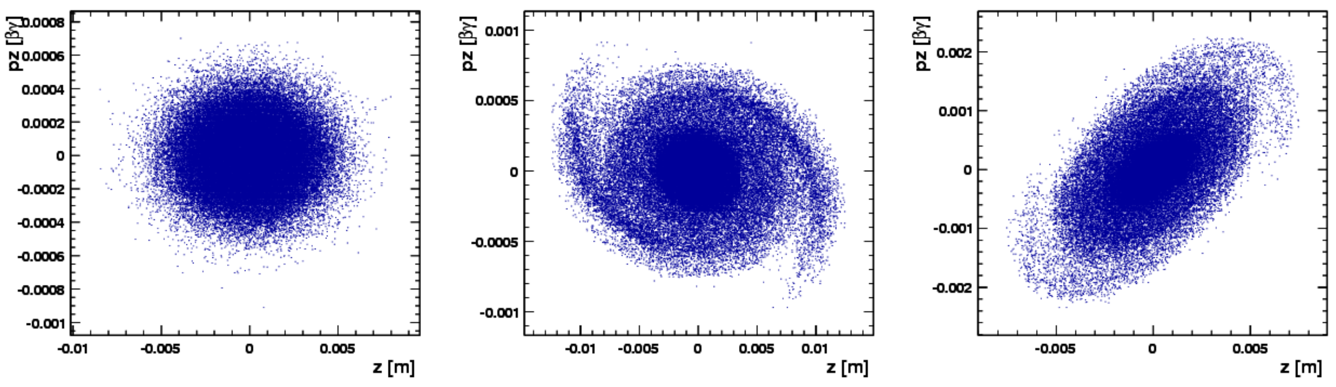


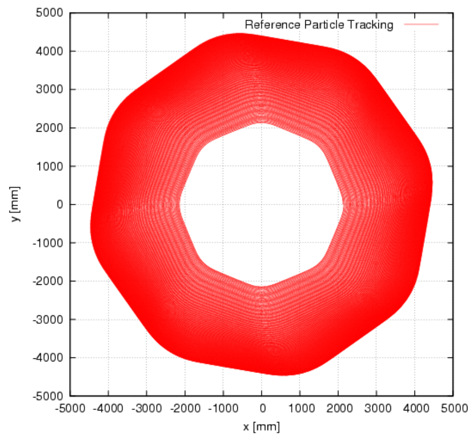
Figure 8: Vertical phase at different energy from left to right: 0.87 MeV, 15 MeV and 35 MeV

6.4.3 PSI Ring Cyclotron

From the view of numerical simulation, the difference between Injector II and Ring cyclotron comes from two aspects:

B Field The structure of Ring is totally symmetric, the field on median plain is periodic along azimuthal direction, *OPAL-cycl* take this advantage to only store field data to save memory.

RF Cavity In the Ring, all the cavities are typically single gap with some parallel displacement from its radial position.*OPAL-cycl* have an argument `PDIS` to manipulate this issue.



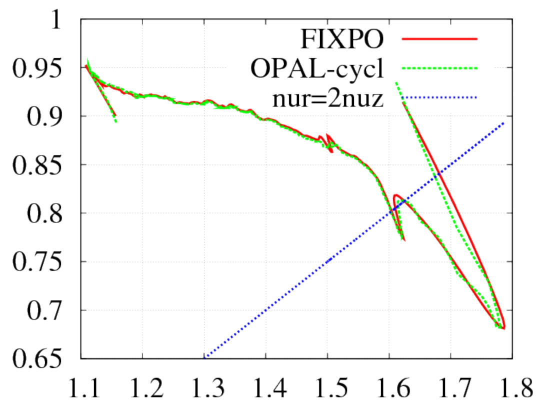


Figure 9: Reference orbit(left) and tune diagram(right) in Ring cyclotron

Figure 9 shows a single particle tracking result and tune calculation result in the PSI Ring cyclotron. Limited by size of the user guide, we don't plan to show too much details as in Injector II.

6.5 Translate Old to New Distribution Commands

As of *OPAL* 1.2, the distribution command see Chapter Distribution was changed significantly. Many of the changes were internal to the code, allowing us to more easily add new distribution command options. However, other changes were made to make creating a distribution easier, clearer and so that the command attributes were more consistent across distribution types. Therefore, we encourage our users to refer to when creating any new input files, or if they wish to update existing input files.

With the new distribution command, we did attempt as much as possible to make it backward compatible so that existing *OPAL* input files would still work the same as before, or with small modifications. In this section of the manual, we will give several examples of distribution commands that will still work as before, even though they have antiquated command attributes. We will also provide examples of commonly used distribution commands that need small modifications to work as they did before.

An important point to note is that it is very likely you will see small changes in your simulation even when the new distribution command is nominally generating particles in exactly the same way. This is because random number generators and their seeds will likely not be the same as before. These changes are only due to *OPAL* using a different sequence of numbers to create your distribution, and not because of errors in the calculation. (Or at least we hope not.)

6.5.1 `GUNGAUSSFLATTOPTH` and `ASTRAFLATTOPTH` Distribution Types

The GUNGAUSSFLATTOPTH and ASTRAFLATTOPTH distribution types are two common types previously implemented to simulate electron beams emitted from photocathodes in an electron photoinjector. These are no longer explicitly supported and are instead now defined as specialized sub-types of the distribution type `FLATTOP`. That is, the *emitted* distributions represented by `GUNGAUSSFLATTOPTH` and `ASTRAFLATTOPTH` can now be easily reproduced by using the `FLATTOP` distribution type and we would encourage use of the new command structure.

Having said this, however, old input files that use the `GUNGAUSSFLATTOPTH` and `ASTRAFLATTOPTH` distribution types will still work as before, with the following exception. Previously, *OPAL* had a Boolean `OPTION` command `FINEEMISSION` (default value was `TRUE`). This `OPTION` is no longer supported. Instead you will need to set the distribution attribute Table 28 to a value that is 10 $\times$ the value of the distribution attribute Table 26 in order for your simulation to behave the same as before.

6.5.2 `FROMFILE`, `GAUSS` and `BINOMIAL` Distribution Types

The FROMFILE, GAUSS and BINOMIAL distribution types have changed from previous versions of *OPAL*. However, legacy distribution commands should work as before as long as the momentum units are converted to the current convention (see section on units).

6.5.3 Change in Momentum Units

Input momentum can be given without units i.e. as $\beta\gamma$, or in eV/c. Up until *OPAL* 2.2, eV was used instead of eV/c, but this was changed since eV is a unit of energy rather than momentum. To adapt old files with momentum in eV, such that they can work for the newer *OPAL* versions, the following formula can be used:

$$P[eV/c]c = mc^2\sqrt{(\frac{P[eV]}{mc^2}+1)^2-1}$$

and you will need to set the distribution attribute INPUTMOUNITS to:

```
INPUTMOUNITS = EVOVERC
```

Chapter 7

OPAL-t

7.1 Introduction

OPAL-t is a fully three-dimensional program to track in time, relativistic particles taking into account space charge forces, self-consistently in the electrostatic approximation, and short-range longitudinal and transverse wake fields. *OPAL-t* is one of the few codes that is implemented using a parallel programming paradigm from the ground up. This makes *OPAL-t* indispensable for high statistics simulations of various kinds of existing and new accelerators. It has a comprehensive set of beamline elements, and furthermore allows arbitrary overlap of their fields, which gives *OPAL-t* a capability to model both the standing wave structure and traveling wave structure. Beside IMPACT-T it is the only code making use of space charge solvers based on an integrated Green [7], [8], [9] function to efficiently and accurately treat beams with large aspect ratio, and a shifted Green function to efficiently treat image charge effects of a cathode [10], [7], [8],[9]. For simulations of particles sources i.e. electron guns *OPAL-t* uses the technique of energy binning in the electrostatic space charge calculation to model beams with large energy spread. In the very near future a parallel Multigrid solver taking into account the exact geometry will be implemented.

7.2 Variables in *OPAL-t*

OPAL-t uses the following canonical variables to describe the motion of particles. The physical units are listed in square brackets.

X Horizontal position x of a particle relative to the axis of the element [m].

PX $\beta_x\gamma$ Horizontal canonical momentum [Units].

Y Vertical position y of a particle relative to the axis of the element [m].

PY $\beta_y\gamma$ Vertical canonical momentum [Units].

Z Longitudinal position z of a particle in floor co-ordinates [m].

PZ $\beta_z\gamma$ Longitudinal canonical momentum [Units].

The independent variable is **t** [s].

7.3 Integration of the Equation of Motion

OPAL-t integrates the relativistic Lorentz equation

$$\frac{\mathrm{d}\gamma\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}[\mathbf{E}_{ext} + \mathbf{E}_{sc} + \mathbf{v} \times (\mathbf{B}_{ext} + \mathbf{B}_{sc})]$$

where γ is the relativistic factor, q is the charge, and m is the rest mass of the particle. **E** and **B** are abbreviations for the electric field $\mathbf{E}(\mathbf{x},t)$ and magnetic field $\mathbf{B}(\mathbf{x},t)$. To update the positions and momenta *OPAL-t* uses the Boris-Buneman algorithm [11].

7.4 Positioning of Elements

Since *OPAL* version 2.0 of *OPAL* elements can be placed in space using 3D coordinates `X`, `Y`, `Z`, `THETA`, `PHI` and `PSI`, see Common Attributes for all Elements. The old notation using `ELEMEDGE` is still supported. *OPAL-t* then computes the position in 3D using `ELEMDGE`, `ANGLE` and `DESIGNENERGY`. It assumes that the trajectory consists of straight lines and segments of circles. Fringe fields are ignored. For cases where these simplifications aren't justifiable the user should use 3D positioning. For a simple switchover *OPAL* writes a file *_3D.opal* where all elements are placed in 3D.

Beamlines containing guns should be supplemented with the element `SOURCE`. This allows *OPAL* to distinguish the cases and adjust the initial energy of the reference particle.

Prior to *OPAL* version 2.0 elements needed only a defined length. The transverse extent was not defined for elements except when combined with 2D or 3D field maps. An aperture had to be designed to give elements a limited extent in transverse direction since elements now can be placed freely in three-dimensional space. See Common Attributes for all Elements for how to define an aperture.

7.5 Coordinate Systems

The motion of a charged particle in an accelerator can be described by relativistic Hamilton mechanics. A particular motion is that of the reference particle, having the central energy and traveling on the so-called reference trajectory. Motion of a particle close to this fictitious reference particle can be described by linearized equations for the displacement of the particle under study, relative to the reference particle. In *OPAL-t*, the time t is used as independent variable instead of the path length s. The relation between them can be expressed as

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{ds}}\frac{\mathrm{ds}}{\mathrm{d}t} = \beta c \frac{\mathrm{d}}{\mathrm{ds}}.$$

7.5.1 Global Cartesian Coordinate System

We define the global cartesian coordinate system, also known as floor coordinate system with K, a point in this coordinate system is denoted by $(X,Y,Z) \in K$. In Figure 10 of the accelerator is uniquely defined by the sequence of physical elements in K. The beam elements are numbered $e_0,\ldots,e_i,\ldots e_n$.

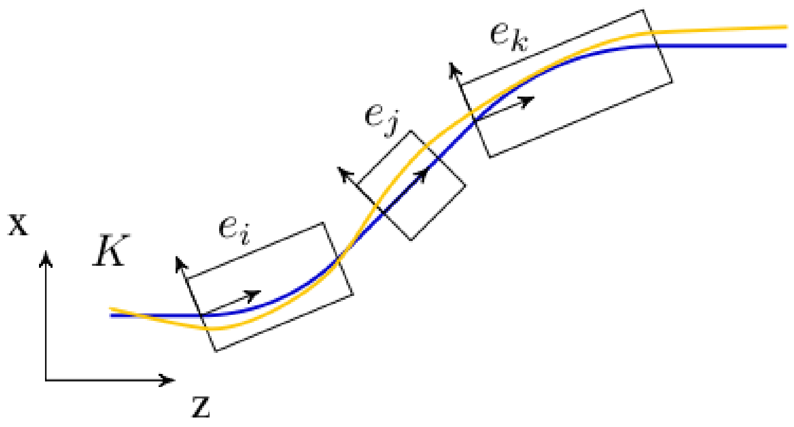


Figure 10: Illustration of local and global coordinates.

7.5.2 Local Cartesian Coordinate System

A local coordinate system K'_i is attached to each element e_i. This is simply a frame in which $(0,0,0)$ is at the entrance of each element. For an illustration see Figure 10. The local reference system $(x,y,z) \in K'_n$ may thus be referred to a global Cartesian coordinate system $(X,Y,Z) \in K$.

The local coordinates (x_i, y_i, z_i) at element e_i with respect to the global coordinates (X,Y,Z) are defined by three displacements (X_i, Y_i, Z_i) and three angles $(\Theta_i, \Phi_i, \Psi_i)$.

Ψ is the roll angle about the global Z-axis. Φ is the yaw angle about the global Y-axis. Lastly, Θ is the pitch angle about the global X-axis. All three angles form right-handed screws with their corresponding axes. The angles (Θ, Φ, Ψ) are the Tait-Bryan angles [12].

The displacement is described by a vector $\mathbf{v}$ and the orientation by a unitary matrix $\mathscr{W}$. The column vectors of $\mathscr{W}$ are unit vectors spanning the local coordinate axes in the order (x,y,z). $\mathbf{v}$ and $\mathscr{W}$ have the values:

$$\mathbf{v} = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \qquad \mathscr{W} = \mathscr{S}\mathscr{T}\mathscr{U}$$

where

$$\mathscr{S} = \begin{pmatrix} \cos\Theta & 0 & \sin\Theta \\ 0 & 1 & 0 \\ -\sin\Theta & 0 & \cos\Theta \end{pmatrix}, \quad \mathscr{T} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & \sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{pmatrix}, \quad \mathscr{U} = \begin{pmatrix} \cos\Psi & -\sin\Psi & 0 \\ \sin\Psi & \cos\Psi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We take the vector $\mathbf{r}_i$ to be the displacement and the matrix $\mathscr{S}_i$ to be the rotation of the local reference system at the exit of the element i with respect to the entrance of that element.

Denoting with i a beam line element, one can compute $\mathbf{v}_i$ and $\mathscr{W}_i$ by the recurrence relations

$$\mathbf{v}_i = \mathscr{W}_{i-1}\mathbf{r}_i + \mathbf{v}_{i-1}, \qquad \mathscr{W}_i = \mathscr{W}_{i-1}\mathscr{S}_i,$$

where $\mathbf{v}_0$ corresponds to the origin of the `LINE` and $\mathscr{W}_0$ to its orientation. In *OPAL-t* they can be defined using either `X`, `Y`, `Z`, `THETA`, `PHI` and `PSI` or `ORIGIN` and `ORIENTATION`, see Simple Beam Lines.

7.5.3 Space Charge Coordinate System

In order to calculate space charge in the electrostatic approximation, we introduce a co-moving coordinate system K_{sc}, in which the origin coincides with the mean position of the particles and the mean momentum is parallel to the z-axis.

7.5.4 Curvilinear Coordinate System

In order to compute statistics of the particle ensemble, K_s is introduced. The accompanying tripod (Dreibein) of the reference orbit spans a local curvilinear right handed system (x,y,s). The local s-axis is the tangent to the reference orbit. The two other axes are perpendicular to the reference orbit and are labelled x (in the bend plane) and y (perpendicular to the bend plane).

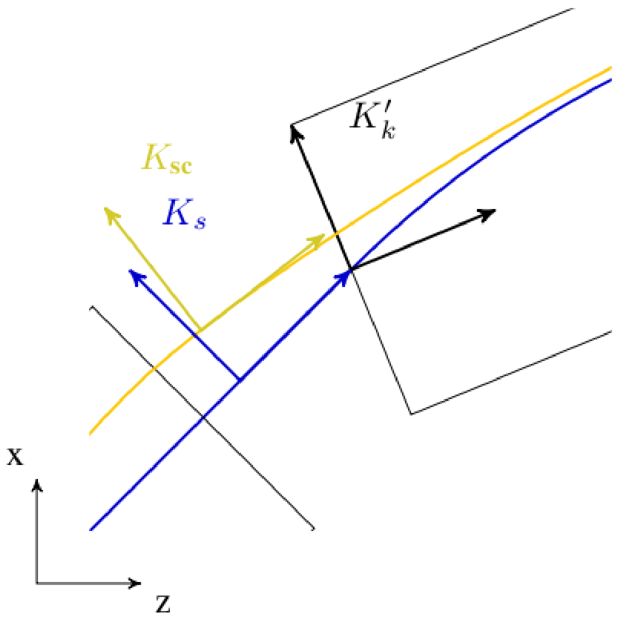


Figure 11: Illustration of K_{sc} and K_s

Both coordinate systems are described in Figure 11.

7.5.5 Design or Reference Orbit

The reference orbit consists of a series of straight sections and circular arcs and is **computed** by the Orbit Threader i.e. deduced from the element placement in the floor coordinate system.

7.5.6 Compatibility Mode

To facilitate the change for users we will provide a compatibility mode. The idea is that the user does not have to change the input file. Instead *OPAL-t* will compute the positions of the elements. For this it uses the bend angle and chord length of the dipoles and the position of the elements along the trajectory. The user can choose whether effects due to fringe fields are considered when computing the path length of dipoles or not. The option to toggle *OPAL-t*'s behavior is called `IDEALIZED`. *OPAL-t* assumes per default that provided `ELEMEDGE` for elements downstream of a dipole are computed without any effects due to fringe fields.

Elements that overlap with the fields of a dipole have to be handled separately by the user to position them in 3D.

We split the positioning of the elements into two steps. In a first step we compute the positions of the dipoles. Here we assume that their fields don't overlap. In a second step we can then compute the positions and orientations of all other elements.

The accuracy of this method is good for all elements except for those that overlap with the field of a dipole.

7.5.7 Orbit Threader and Autophasing

The `OrbitThreader` integrates a design particle through the lattice and setups up a multi map structure (`IndexMap`). Furthermore when the reference particle hits an rf-structure for the first time then it auto-phases the rf-structure, see Appendix Auto-phasing Algorithm. The multi map structure speeds up the search for elements that influence the particles at a given position in 3D space by minimizing the looping over elements when integrating an ensemble of particles. For each time step, `IndexMap` returns a set of elements $\mathscr{S}_e \subset e_0 \dots e_n$ in case of the example given in Figure 10. An implicit drift is modelled as an empty set $\emptyset$.

7.6 Flow Diagram of *OPAL-t*

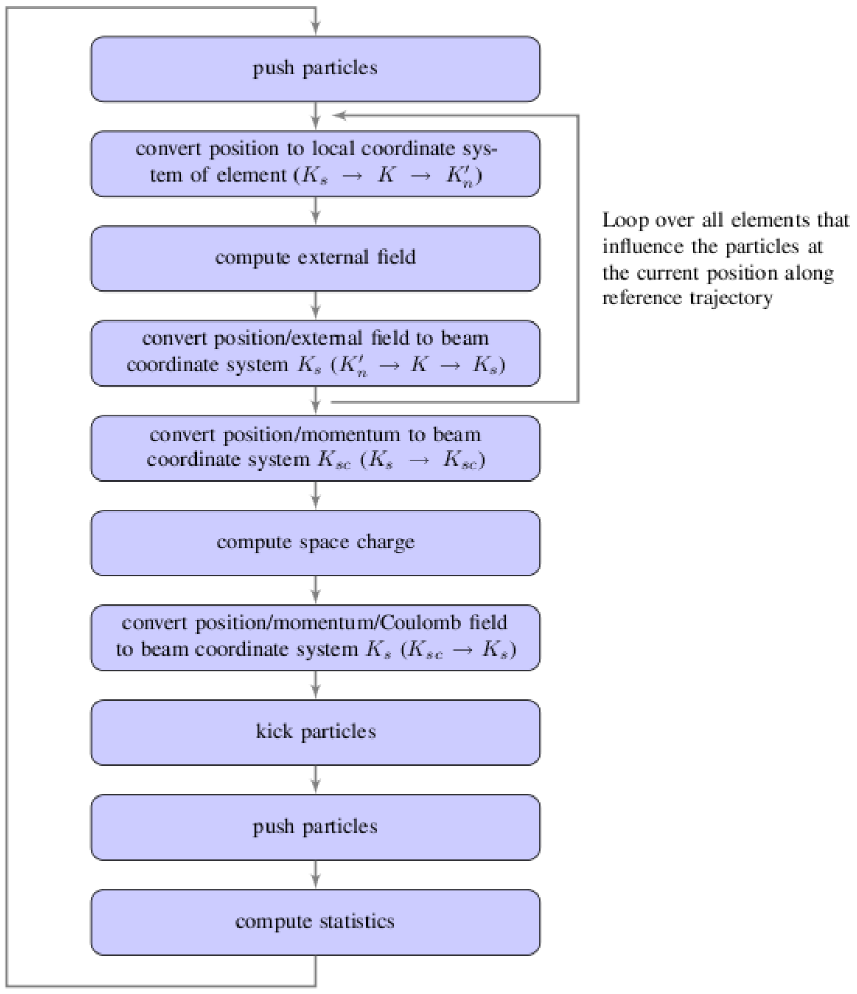

push particles
convert position to local coordinate system of element ($K_s \rightarrow K \rightarrow K'_n$)
compute external field
convert position/external field to beam coordinate system K_s ($K'_n \rightarrow K \rightarrow K_s$)
convert position/momentum to beam coordinate system K_{sc} ($K_s \rightarrow K_{sc}$)
compute space charge
convert position/momentum/Coulomb field to beam coordinate system K_s ($K_{sc} \rightarrow K_s$)
kick particles
push particles
compute statistics
Loop over all elements that influence the particles at the current position along reference trajectory

Figure 12: Schematic workflow of *OPAL-t*'s execute method.

A regular time step in *OPAL-t* is sketched in Figure 12. In order to compute the coordinate system transformation from the reference coordinate system K_s to the local coordinate systems K'_n we join the transformation from floor coordinate system K to K'_n to the transformation from K_s to K. All computations of rotations which are involved in the computation of coordinate system transformations are performed using quaternions. The resulting quaternions are then converted to the appropriate matrix representation before applying the rotation operation onto the particle positions and momenta.

As can be seen from Figure 12 the integration of the trajectories of the particles are integrated and the computation of the statistics of the six-dimensional phase space are performed in the reference coordinate system.

7.7 Output

In addition to the progress report that *OPAL-t* writes to the standard output (stdout) it also writes different files for various purposes.

7.7.1 Statistics output

This file is used to log the statistical properties of the bunch in the ASCII variant of the SDDS format [13]. It can be viewed with the SDDS Tools [14] or GNUPLOT. The frequency with which the statistics are computed and written to file can be controlled With the option `STATDUMPFREQ` (see Option Statement). The name of the output file is *<input_file_name >.stat*. The information that is stored are found in Table 5. Additionally, more statistical information about the beam can be saved. The option `COMPUTEPERCENTILES` allow whether the 68.27 (1 sigma for normal distribution), the 95.45 (2 sigmas), the 99.73 (3 sigmas) and the 99.994 (4 sigmas) percentiles for the beam size and the normalized emittance should be computed (see Table 6)). Whereas, `DUMPBEAMMATRIX` control whether to write the 6-dimensional beam matrix (upper triangle only) to statatistic file (see Table 7)).

Column Nr.	Name	Units	Meaning
1	t	ns	Time
2	s	m	Path length
3	numParticles	1	Number of macro particles
4	charge	C	Bunch charge
5	energy	MeV	Mean bunch energy
6	rms_x	m	RMS beamsize in x
7	rms_y	m	RMS beamsize in y
8	rms_s	m	RMS beamsize in s
9	rms_px	1	RMS beamsize normalised momentum in x
10	rms_py	1	RMS beamsize normalised momentum in y
11	rms_ps	1	RMS beamsize normalised momentum in s
12	emit_x	mrad	Normalized emittance in x
13	emit_y	mrad	Normalized emittance in y
14	emit_s	mrad	Normalized emittance in s
15	mean_x	m	X-component of mean position relative to reference particle
16	mean_y	m	Y-component of mean position relative to reference particle
17	mean_s	m	S-component of mean position relative to reference particle
18	ref_x	m	X-component of reference particle in floor coordinate system
19	ref_y	m	Y-component of reference particle in floor coordinate system
20	ref_z	m	Z-component of reference particle in floor coordinate system
21	ref_px	1	X-component of normalized momentum of reference particle in floor coordinate system
22	ref_py	1	Y-component of normalized momentum of reference particle in floor coordinate system
23	ref_pz	1	Z-component of normalized momentum of reference particle in floor coordinate system
24	max_x	m	Max beamsize in x-direction
25	max_y	m	Max beamsize in y-direction
26	max_s	m	Max beamsize in s-direction
27	xpx	1	Correlation between x-components of positions and momenta
28	ypy	1	Correlation between y-components of positions and momenta
29	zpz	1	Correlation between s-components of positions and momenta
30	Dx	m	Dispersion in x-direction
31	DDx	1	Derivative of dispersion in x-direction
32	Dy	m	Dispersion in y-direction
33	DDy	1	Derivative of dispersion in y-direction
34	Bx_ref	T	X-component of magnetic field at reference particle
35	By_ref	T	Y-component of magnetic field at reference particle
36	Bz_ref	T	Z-component of magnetic field at reference particle
37	Ex_ref	MVm^-1	X-component of electric field at reference particle
38	Ey_ref	MVm^-1	Y-component of electric field at reference particle
39	Ez_ref	MVm^-1	Z-component of electric field at reference particle
40	dE	MeV	Energy spread of the bunch
41	dt	ns	Size of time step
42	partsOutside	1	Number of particles outside $n \times gma$ of beam, where n is controlled with `BEAMHALOBOUNDARY` (see Option Statement)
43	DebyeLength	m	Debye length in the boosted frame
44	plasmaParameter	1	Plasma parameter that gives no. of particles in a Debye sphere
45	temperature	K	Temperature of the beam
46	rmsDensity	1	RMS number density of the beam

Table 5: Data stored in statistics output file in *OPAL-t*.

Name	**Units**	**Meaning**
68_Percentile_x	m	68.27 percentile (1 sigma of normal distribution) of x-component of position
68_Percentile_y	m	68.27 percentile (1 sigma of normal distribution) of y-component of position
68_Percentile_z	m	68.27 percentile (1 sigma of normal distribution) of z-component of position
95_Percentile_x	m	95.45 percentile (2 sigma of normal distribution) of x-component of position
95_Percentile_y	m	95.45 percentile (2 sigma of normal distribution) of y-component of position
95_Percentile_z	m	95.45 percentile (2 sigma of normal distribution) of z-component of position
99_Percentile_x	m	99.73 percentile (3 sigma of normal distribution) of x-component of position
99_Percentile_y	m	99.73 percentile (3 sigma of normal distribution) of y-component of position
99_Percentile_z	m	99.73 percentile (3 sigma of normal distribution) of z-component of position
99_99_Percentile_x	m	99.994 percentile (4 sigma of normal distribution) of x-component of position
99_99_Percentile_y	m	99.994 percentile (4 sigma of normal distribution) of y-component of position
99_99_Percentile_z	m	99.994 percentile (4 sigma of normal distribution) of z-component of position
normalizedEps68Percentile_x	m	x-component of normalized emittance at 68 percentile (1 sigma of normal distribution)
normalizedEps68Percentile_y	m	y-component of normalized emittance at 68 percentile (1 sigma of normal distribution)
normalizedEps68Percentile_z	m	z-component of normalized emittance at 68 percentile (1 sigma of normal distribution)
normalizedEps95Percentile_x	m	x-component of normalized emittance at 95 percentile (2 sigma of normal distribution)
normalizedEps95Percentile_y	m	y-component of normalized emittance at 95 percentile (2 sigma of normal distribution)
normalizedEps95Percentile_z	m	z-component of normalized emittance at 95 percentile (2 sigma of normal distribution)
normalizedEps99Percentile_x	m	x-component of normalized emittance at 99 percentile (3 sigma of normal distribution)
normalizedEps99Percentile_y	m	y-component of normalized emittance at 99 percentile (3 sigma of normal distribution)
normalizedEps99Percentile_z	m	z-component of normalized emittance at 99 percentile (3 sigma of normal distribution)
normalizedEps99_99Percentile_x	m	x-component of normalized emittance at 99.99 percentile (4 sigma of normal distribution)
normalizedEps99_99Percentil_y	m	y-component of normalized emittance at 99.99 percentile (4 sigma of normal distribution)
normalizedEps99_99Percentil_z	m	z-component of normalized emittance at 99.99 percentile (4 sigma of normal distribution)

Table 6: Additional data stored in statistics output file if `COMPUTEPERCENTILES=TRUE`.

Name	Units	Meaning
S11	m2	Element 1,1 of 6D beam matrix
S12	m	Element 1,2 of 6D beam matrix
S13	m2	Element 1,3 of 6D beam matrix
S14	m	Element 1,4 of 6D beam matrix
S15	m2	Element 1,5 of 6D beam matrix
S16	m	Element 1,6 of 6D beam matrixn
S22	1	Element 2,2 of 6D beam matrix
S23	m	Element 2,3 of 6D beam matrix
S24	1	Element 2,4 of 6D beam matrixn
S25	m	Element 2,5 of 6D beam matrix
S26	1	Element 2,6 of 6D beam matrix
S33	m2	Element 3,3 of 6D beam matrix
S34	m	Element 3,4 of 6D beam matrix
S35	m2	Element 3,5 of 6D beam matrix
S36	m	Element 3,6 of 6D beam matrix
S44	1	Element 4,4 of 6D beam matrix
S45	m	Element 4,5 of 6D beam matrix
S46	1	Element 4,6 of 6D beam matrix
S55	m2	Element 5,5 of 6D beam matrix
S56	m	Element 5,6 of 6D beam matrix
S66	1	Element 6,6 of 6D beam matrix

Table 7: Additional data stored in statistics output file if `DUMPBEAMMATRIX=TRUE`.

7.7.2 Monitor statistics output

OPAL-t computes the statistics of the bunch for every `MONITOR` that it passes. The name of the output file is *data/<input_file_name >_Monitors.stat*. The information that is written can be found in the following table.

Column Nr.	Name	Units	Meaning
1	name	a string	Name of the monitor
2	s	m	Position of the monitor in path length
3	t	ns	Time at which the reference particle pass
4	numParticles	1	Number of macro particles
5	rms_x	m	Standard deviation of the x-component of the particles positions
6	rms_y	m	Standard deviation of the y-component of the particles positions
7	rms_s	m	Standard deviation of the s-component of the particles positions (only nonvanishing when type of `MONITOR` is `TEMPORAL`)
8	rms_t	ns	Standard deviation of the passage time of the particles (zero if type is of `MONITOR` is `TEMPORAL`
9	rms_px	1	Standard deviation of the x-component of the particles momenta
10	rms_py	1	Standard deviation of the y-component of the particles momenta
11	rms_ps	1	Standard deviation of the s-component of the particles momenta
12	emit_x	mrad	X-component of the normalized emittance
13	emit_y	mrad	Y-component of the normalized emittance
14	emit_s	mrad	S-component of the normalized emittance
15	mean_x	m	X-component of mean position relative to reference particle
16	mean_y	m	Y-component of mean position relative to reference particle
17	mean_s	m	S-component of mean position relative to reference particle
18	mean_t	ns	Mean time at which the particles pass
19	ref_x	m	X-component of reference particle in floor coordinate system
20	ref_y	m	Y-component of reference particle in floor coordinate system
21	ref_z	m	Z-component of reference particle in floor coordinate system
22	ref_px	1	X-component of normalized momentum of reference particle in floor coordinate system
23	ref_py	1	Y-component of normalized momentum of reference particle in floor coordinate system
24	ref_pz	1	Z-component of normalized momentum of reference particle in floor coordinate system
25	max_x	m	Max beamsize in x-direction
26	max_y	m	Max beamsize in y-direction
27	max_s	m	Max beamsize in s-direction
28	xpx	1	Correlation between x-components of positions and momenta
29	ypy	1	Correlation between y-components of positions and momenta
40	zpz	1	Correlation between s-components of positions and momenta

Table 8: Data stored in `MONITOR` statistics output file in *OPAL-t*.

7.7.3 Input file transcription

OPAL-t copies the input file into this file and replaces all occurrences of `ELEMEDGE` with the corresponding position using `X`, `Y`, `Z`, `THETA`, `PHI` and `PSI`. The name of the output file is *data/<input_file_name >_3D.opal*.

7.7.4 Element positions output files

7.7.4.1 *data/<input_file_name >_ElementPositions.txt*

OPAL-t stores for every element the position of the entrance and the exit. Additionally the reference trajectory inside dipoles is stored. On the first column the name of the element is written prefixed with `BEGIN: ",` END: " and ``MID: " respectively. The remaining columns store the z-component then the x-component and finally the y-component of the position in floor coordinates.

7.7.4.2 *data/<input_file_name >_ElementPositions.py*

This Python script can be used to generate visualizations of the beam line in different formats. Beside an ASCII file that can be printed using GNUPLOT a VTK file and an HTML file can be generated. The VTK file can then be opened in e.g. ParaView [15], [16] or VisIt [17]. The HTML file can be opened in any modern web browser. Both the VTK and the HTML output are three-dimensional. For the ASCII format on the other hand you have provide the normal of a plane onto which the beam line is projected.

The script is not directly executable. Instead one has to pass it as argument to `python`:

```
python myinput_ElementPositions.py --export-web
```

The following arguments can be passed

- `-h` or `--help` for a short help
- `--export-vtk` to export to the VTK format
- `--export-web` to export for the web
- `--background r g b` to specify background color of web canvas where `0` $\Leftarrow$ `r|g|b` $\Leftarrow$ `1`
- `--project-to-plane` to project the beam line to the plane (default zx plane)
- `--normal x y z` specify the normal for projection with the components `x`, `y` and `z`

7.7.4.3 *data/<input_file_name >_ElementPositions.sdds*

This file can be used when plotting the statistics of the bunch to indicate the positions of the magnets. It is written in the SDDS format. The information that is written can be found in the following table.

Column Nr.	Name	Units	Meaning
1	s	m	The position in path length
2	dipole	0.333	Whether the field of a dipole is present
3	quadrupole	1	Whether the field of a quadrupole is present
4	sextupole	0.5	Whether the field of a sextupole is present
5	octupole	0.25	Whether the field of a octupole is present
6	decapole	1	Whether the field of a decapole is present
7	multipole	1	Whether the field of a general multipole is present
8	solenoid	1	Whether the field of a solenoid is present
9	rfcavity	± 1	Whether the field of a cavity is present
10	monitor	1	Whether a monitor is present
11	element_names	a string	The names of the elements that are present

Table 9: Data stored in the element position output file in *OPAL-t*.

In the example below this file is used to indicate the positions of dipoles and quadrupoles in a plot of RMS x

```
plot '70MeV_Gantry2.stat' u 2:6 w l t 'rms x'
repl 'data/70MeV_Gantry2_ElementPositions.sdds' u 1:(-$2/0.45 + 1.6) w l axis x1y2 lc 2 t ' ↩
    Dipole'
repl 'data/70MeV_Gantry2_ElementPositions.sdds' u 1:(-$2/0.45 - 1.6) w l axis x1y2 lc 2  ↩
    notitle
repl 'data/70MeV_Gantry2_ElementPositions.sdds' u 1:(-$3 + 1.6) w l axis x1y2 lc 3 t ' ↩
    Quadrupole'
repl 'data/70MeV_Gantry2_ElementPositions.sdds' u 1:(-$3 - 1.6) w l axis x1y2 lc 3 notitle
set xrange[32:]
set y2range[-1.2:1.2]
```

This produces a plot as found in 13

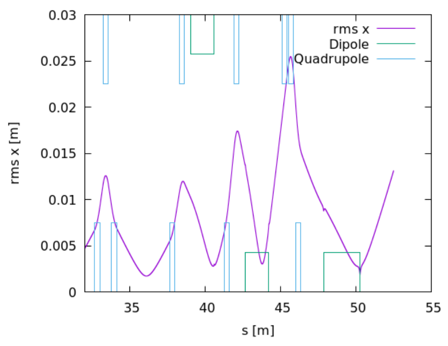


Figure 13: Plot of RMS x supplemented with an indicator of the element positions

7.7.5 Reference particle trajectory output

The trajectory of the reference particle is stored in this ASCII file. The name of the output file is *data/<input_file_name >_DesignPath.dat*. The content of the columns are listed in the following table.

Column Nr.	Name	Units	Meaning
1		m	Position in path length
2		m	X-component of position in floor coordinates
3		m	Y-component of position in floor coordinates
4		m	Z-component of position in floor coordinates
5		1	X-component of momentum in floor coordinates
6		1	Y-component of momentum in floor coordinates
7		1	Z-component of momentum in floor coordinates
8		MV mˆ-1	X-component of electric field at position
9		MV mˆ-1	Y-component of electric field at position
10		MV mˆ-1	Z-component of electric field at position
11		T	X-component of magnetic field at position
12		T	Y-component of magnetic field at position
13		T	Z-component of magnetic field at position
14		MeV	Kinetic energy
15		s	Time

Table 10: Data stored in the reference particle output file in *OPAL-t*.

7.8 Multiple Species

In the present version only one particle species can be defined see Chapter Beam Command, however due to the underlying general structure, the implementation of a true multi species version of *OPAL* should be simple to accomplish.

7.9 Multipoles in different Coordinate systems

In the following sections there are three models presented for the fringe field of a multipole. The first one deals with a straight multipole, while the second one treats a curved multipole, both starting with a power expansion for the magnetic field. The last model tries to be different by starting with a more compact functional form of the field which is then adapted to straight and curved geometries.

7.9.1 Fringe field models

(for a straight multipole)

Most accelerator modeling codes use the hard-edge model for magnets - constant Hamiltonian. Real magnets always have a smooth transition at the edges - fringe fields. To obtain a multipole description of a field we can apply the theory of analytic functions.

$$\begin{aligned} \nabla \cdot \mathbf{B} = 0 \Rightarrow \exists \quad \mathbf{A} \quad \text{with} \quad \mathbf{B} = \nabla \times \mathbf{A} \\ \nabla \times \mathbf{B} = 0 \Rightarrow \exists \quad V \quad \text{with} \quad \mathbf{B} = -\nabla V \end{aligned}$$

Assuming that A has only a non-zero component A_s we get

$$B_x = -\frac{\partial V}{\partial x} = \frac{\partial A_s}{\partial y}$$

$$B_y = -\frac{\partial V}{\partial y} = -\frac{\partial A_s}{\partial x}$$

These equations are just the Cauchy-Riemann conditions for an analytic function $\tilde{A}(z) = A_s(x,y) + iV(x,y)$. So the complex potential is an analytic function and can be expanded as a power series

$$\tilde{A}(z) = \sum_{n=0}^{\infty} \kappa_n z^n, \quad \kappa_n = \lambda_n + i\mu_n$$

with λ_n, μ_n being real constants. It is practical to express the field in cylindrical coordinates (r, φ, s)

$$\begin{aligned} x = r\cos\varphi \quad y = r\sin\varphi \\ z^n = r^n(\cos n\varphi + i\sin n\varphi) \end{aligned}$$

From the real and imaginary parts of equation () we obtain

$$\begin{aligned} V(r,\varphi) &= \sum_{n=0}^{\infty} r^n(\mu_n \cos n\varphi + \lambda_n \sin n\varphi) \\ A_s(r,\varphi) &= \sum_{n=0}^{\infty} r^n(\lambda_n \cos n\varphi - \mu_n \sin n\varphi) \end{aligned}$$

Taking the gradient of $-V(r,\varphi)$ we obtain the multipole expansion of the azimuthal and radial field components, respectively

$$\begin{aligned} B_\varphi &= -\frac{1}{r}\frac{\partial V}{\partial \varphi} = -\sum_{n=0}^{\infty} nr^{n-1}(\lambda_n \cos n\varphi - \mu_n \sin n\varphi) \\ B_r &= -\frac{\partial V}{\partial r} = -\sum_{n=0}^{\infty} nr^{n-1}(\mu_n \cos n\varphi + \lambda_n \sin n\varphi) \end{aligned}$$

Furthermore, we introduce the normal multipole coefficient b_n and skew coefficient a_n defined with the reference radius r_0 and the magnitude of the field at this radius B_0 (these coefficients can be a function of s in a more general case as it is presented further on).

$$b_n = -\frac{n\lambda_n}{B_0} r_0^{n-1} \qquad a_n = \frac{n\mu_n}{B_0} r_0^{n-1}$$

$$\begin{aligned} B_\varphi(r,\varphi) &= B_0 \sum_{n=1}^{\infty} (b_n \cos n\varphi + a_n \sin n\varphi) \left(\frac{r}{r_0}\right)^{n-1} \\ B_r(r,\varphi) &= B_0 \sum_{n=1}^{\infty} (-a_n \cos n\varphi + b_n \sin n\varphi) \left(\frac{r}{r_0}\right)^{n-1} \end{aligned}$$

To obtain a model for the fringe field of a straight multipole, a proposed starting solution for a non-skew magnetic field is

$$V = \sum_{n=1}^{\infty} V_n(r,z) \sin n\varphi$$

$$V_n = \sum_{k=0}^{\infty} C_{n,k}(z) r^{n+2k}$$

It is straightforward to derive a relation between coefficients

$$\nabla^2 V = 0 \Rightarrow \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V_n}{\partial r}\right) + \frac{\partial^2 V_n}{\partial z^2} = \frac{n^2 V_n}{r^2} = 0$$

$$V_n = \sum_{k=0}^{\infty} C_{n,k}(z) r^{n+2k}$$

$$\Rightarrow \sum_{k=0}^{\infty}\left[r^{n+2(k-1)}\left[(n+2k)^2 - n^2\right]C_{n,k}(z) + r^{n+2k}\frac{\partial^2 C_{n,k}(z)}{\partial z^2}\right] = 0$$

By identifying the term in front of the same powers of r we obtain the recurrence relation

$$C_{n,k}(z) = -\frac{1}{4k(n+k)}\frac{d^2 C_{n,k-1}}{dz^2}, k = 1,2,\ldots$$

The solution of the recursion relation becomes

$$C_{n,k}(z) = (-1)^k \frac{n!}{2^{2k}k!(n+k)!}\frac{d^{2k}C_{n,0}(z)}{dz^{2k}}$$

Therefore

$$V_n = -\left(\sum_{k=0}^{\infty}(-1)^{k+1}\frac{n!}{2^{2k}k!(n+k)!}C_{n,0}^{(2k)}(z)r^{2k}\right)r^n$$

The transverse components of the field are

$$B_r = \sum_{n=1}^{\infty} g_{rn} r^{n-1}\sin n\varphi$$

$$B_\varphi = \sum_{n=1}^{\infty} g_{\varphi n} r^{n-1}\cos n\varphi$$

where the following gradients determine the entire potential and can be deduced from the function $C_{n,0}(z)$ once the harmonic n is fixed.

$$g_{rn}(r,z) = \sum_{k=0}^{\infty}(-1)^{k+1}\frac{n!(n+2k)}{2^{2k}k!(n+k)!}C_{n,0}^{(2k)}(z)r^{2k}$$

$$g_{\varphi n}(r,z) = \sum_{k=0}^{\infty}(-1)^{k+1}\frac{n!n}{2^{2k}k!(n+k)!}C_{n,0}^{(2k)}(z)r^{2k}$$

The z-directed component of the filed can be expressed in a similar form

$$B_z = -\frac{\partial V}{\partial z} = \sum_{n=1}^{\infty} g_{zn} r^n \sin n\varphi$$

$$g_{zn} = \sum_{k=0}^{\infty}(-1)^{k+1}\frac{n!}{2^{2k}k!(n+k)!}C_{n,0}^{2k+1} r^{2k}$$

The gradient functions $g_{rn}, g_{\varphi n}, g_{zn}$ are obtained from

$$B_{r,n} = -\frac{\partial V_n}{\partial r}\sin n\varphi = g_{rn} r^{n-1}\sin n\varphi$$

$$B_{\varphi,n} = -\frac{n}{r}V_n \cos n\varphi = g_{\varphi n} r^{n-1}\cos n\varphi$$

$$B_{z,n} = -\frac{\partial V_n}{\partial z}\sin n\varphi = g_{zn} r^n \sin n\varphi$$

One preferred model to approximate the gradient profile on the central axis is the k-parameter Enge function

$$C_{n,0}(z) = \frac{G_0}{1 + exp[P(d(z))]}, \quad G_0 = \frac{B_0}{r_0^{n-1}}$$

$$P(d) = C_0 + C_1\left(\frac{d}{\lambda}\right) + C_2\left(\frac{d}{\lambda}\right)^2 + \ldots + C_{k-1}\left(\frac{d}{\lambda}\right)^{k-1}$$

where $d(z)$ is the distance to the field boundary and λ characterizes the fringe field length.

7.9.2 Fringe field of a curved multipole

(fixed radius)

We consider the Frenet-Serret coordinate system $(\hat{\mathbf{x}}, \hat{\mathbf{s}}, \hat{\mathbf{z}})$ with the radius of curvature ρ constant and the scale factor $h_s = 1 + x/\rho$. A conversion to these coordinates implies that

$$\nabla \cdot \mathbf{B} = \frac{1}{h_s}\left[\frac{\partial(h_s B_x)}{\partial x} + \frac{\partial B_s}{\partial s} + \frac{\partial(h_s B_z)}{\partial z}\right]$$

$$\nabla \times \mathbf{B} = \frac{1}{h_s}\left[\frac{\partial B_z}{\partial s} - \frac{\partial(h_s B_s)}{\partial z}\right]\hat{\mathbf{x}} + \left[\frac{\partial B_x}{\partial z} - \frac{\partial B_z}{\partial x}\right]\hat{\mathbf{s}} + \frac{1}{h_s}\left[\frac{\partial(h_s B_s)}{\partial x} - \frac{\partial B_x}{\partial s}\right]\hat{\mathbf{z}}$$

To simplify the problem, consider multipoles with mid-plane symmetry, i.e.

$$b_z(z) = B_z(-z) \qquad B_x(z) = -B_x(-z) \qquad B_s(z) = -B_s(-z)$$

The most general form of the expansion is

$$B_z = \sum_{i,k=0}^{\infty} b_{i,k} x^i z^{2k}$$

$$B_x = z \sum_{i,k=0}^{\infty} a_{i,k} x^i z^{2k}$$

$$B_s = z \sum_{i,k=0}^{\infty} c_{i,k} x^i z^{2k}$$

EQUATION 7.1: General form

Maxwell's equations $\nabla \cdot \mathbf{B} = 0$ and $\nabla \times \mathbf{B} = 0$ in the above coordinates yield

$$\frac{\partial}{\partial x}((1+x/\rho)B_x) + \frac{\partial B_s}{\partial s} + (1+x/\rho)\frac{\partial B_z}{\partial z} = 0$$

$$\frac{\partial B_z}{\partial s} = (1+x/\rho)\frac{\partial B_s}{\partial z}$$

$$\frac{\partial B_x}{\partial z} = \frac{\partial B_z}{\partial s}$$

$$\frac{\partial B_x}{\partial s} = \frac{\partial}{\partial x}((1+x/\rho)B_s)$$

EQUATION 7.2: Maxwell equations

The substitution of Equation 7.1 into Maxwell's equations allows for the derivation of recursion relations. Equation 7.2 gives

$$\sum_{i,k=0}^{\infty} a_{i,k}(2k+1)x^i z^{2k} = \sum_{i,k=0}^{\infty} b_{i,k} i x^{i-1} z^{2k}$$

Equating the powers in $x^i z^{2k}$

$$a_{i,k} = \frac{i+1}{2k+1} b_{i+1,k}$$

EQUATION 7.3: a factors

A similar result is obtained from Equation 7.2

$$\sum_{i,k=0}^{\infty} \partial_s b_{i,k} x^i z^{2k} = \left(1+\frac{x}{\rho}\right) \sum_{i,k=0}^{\infty} c_{i,k}(2k+1) x^i z^{2k}$$
$$\Rightarrow c_{i,k} + \frac{1}{\rho} c_{i-1,k} = \frac{1}{2k+1} \partial_s b_{i,k}$$

EQUATION 7.4: c factors

The last equation from $\nabla \times \mathbf{B} = 0$ should be consistent with the two recursion relations obtained. Equation 7.2 implies

$$\sum_{i,k=0}^{\infty} \left[\frac{i+1}{\rho} c_{i,k} x^i + c_{i,k} i x^{i-1}\right] z^{k+1} = \sum_{i,k=0}^{\infty} \partial_s a_{i,k} x^i z^{2k}$$

$$\Rightarrow \frac{\partial_s a_{i,k}}{i+1} = \frac{1}{\rho} c_{i,k} + c_{i+1,k}$$

This results follows directly from Equation 7.3 and Equation 7.4; therefore the relations are consistent. Furthermore, the last required relations is obtained from the divergence of $\mathbf{B}$

$$\sum_{i,k=0}^{\infty} \left[\frac{a_{i,k} x^i z^{2k+1}}{\rho} + i a_{i,k} x^{i-1} z^{2k+1} + \frac{i a_{i,k} x^i z^{2k+1}}{\rho} + \partial_s c_{i,k} x^i z^{2k+1} + 2k b_{i,k} x^i z^{2k-1}\right] = 0$$

$$\Rightarrow \partial_s c_{i,k} + \frac{2(k+1)}{\rho} b_{i-1,k+1} + 2(k+1) b_{i,k+1} + \frac{1}{\rho} a_{i,k} + (i+1) a_{i+1,k} + \frac{1}{\rho} a_{i,k} = 0$$

Using the relation (Equation 7.3) to replace the a coefficients with b's we arrive at

$$\partial_s c_{i,k} + \frac{(i+1)^2}{\rho(2k+1)} b_{i+1,k} + \frac{(i+1)(i+2)}{2k+1} b_{i+2,k} + \frac{2(k+1)}{\rho} b_{i-1,k+1} + 2(k+1) b_{i,k+1} = 0$$

All the coefficients above can be determined recursively provided the field B_z can be measured at the mid-plane in the form

$$B_z(z=0) = B_{0,0} + B_{1,0}x + B_{2,0}x^2 + B_{3,0}x^3 + \dots$$

where $B_{i,0}$ are functions of s and they can model the fringe field for each multipole term x^n. As an example, for a dipole magnet, the $B_{1,0}$ function can be model as an Enge function or *tanh*.

7.9.3 Fringe field of a curved multipole

(variable radius of curvature)

The difference between this case and the above is that ρ is now a function of s, $\rho(s)$. We can obtain the same result starting with the same functional forms for the field (Equation 7.1). The result of the previous section also holds in this case since no derivative $\frac{\partial}{\partial s}$ is applied to the scale factor h_s. If the radius of curvature is set to be proportional to the dipole filed observed by some reference particle that stays in the centre of the dipole

$$\rho(s) \propto B(z=0, x=0, s) = B_x(z=0, x=0) = b_{0,0}(s)$$

7.9.4 Fringe field of a multipole

This is a different, more compact treatment The derivation is more clear if we gather the variables together in functions. We assume again mid-plane symmetry and that the z-component of the field in the mid-plane has the form

$$B_z(x, z=0, s) = T(x)S(s)$$

where $T(s)$ is the transverse field profile and $S(s)$ is the fringe field. One of the requirements of the symmetry is that $B_z(z) = B_z(-z)$ which using a scalar potential ψ requires $\frac{\partial\psi}{\partial z}$ to be an even function in z. Therefore, ψ is an odd function in z and can be written as

$$\psi = zf_0(x,s) + \frac{z^3}{3!}f_1(x,s) + \frac{z^5}{5!}f_3(x,s) + \ldots$$

The given transverse profile requires that $f_0(x,s) = T(x)S(s)$, while $\nabla^2\psi = 0$ follows from Maxwell's equations as usual, more explicitly

$$\frac{\partial}{\partial x}\left(h_s\frac{\partial\psi}{\partial x}\right) + \frac{\partial}{\partial s}\left(\frac{1}{h_s}\frac{\partial\psi}{\partial s}\right) + \frac{\partial}{\partial z}\left(h_s\frac{\partial\psi}{\partial z}\right) = 0$$

For a straight multipole $h_s = 1$. Laplace's equation becomes

$$\sum_{n=0}\frac{z^{2n+1}}{(2n+1)!}\left[\partial_x^2 f_n(x,s) + \partial_s^2 f_n(x,s)\right] + \sum_{n=1} f_n(x,s)\frac{z^{n-1}}{(n-1)!} = 0$$

By equating powers of z we obtain the recursion relation

$$f_{n+1}(x,s) = -\left(\partial_x^2 + \partial_s^2\right)f_n(x,s)$$

The general expression for any $f_n(x,s)$ is then obtained from the mid-plane field by

$$f_n(x,s) = (-1)^n\left(\partial_x^2 + \partial_s^2\right)^n f_0(x,s)$$

$$f_n(x,s) = (-1)^n\sum_{i=0}^{n}\binom{n}{i}T^{(2i)}(x)S^{(2n-2i)}(s)$$

For a curved multipole of constant radius $h_s = 1 + \frac{x}{\rho}$ with $\rho = const$. The corresponding Laplace's equation is

$$\left(\frac{1}{\rho h_s}\partial_x + \partial_x^2 + \partial_z^2 + \frac{\partial_s^2}{h_s^2}\right)\psi = 0$$

Again we substitute with the functional form of the potential to get the recursion

$$f_{n+1}(x,s) = -\left[\frac{1}{\rho + x}\partial_x + \partial_x^2 + \frac{\partial_s^2}{(1+x/\rho)^2}\right]f_n(x,s)$$

$$f_{n+1}(x,s) = (-1)^n\left[\frac{1}{\rho + x}\partial_x + \partial_x^2 + \frac{\partial_s^2}{(1+x/\rho)^2}\right]^n f_0(x,s)$$

Finally consider what changes for $\rho = \rho(s)$. Laplace's equation is

$$\left[\frac{1}{\rho h_s}\partial_x + \partial_x^2 + \partial_z^2 + \frac{\partial_s^2}{h_s^2} + \frac{x}{\rho^2 h_s^3}(\partial_s\rho)\partial_s\right]\psi = 0$$

The last step is again the substitution to get

$$f_{n+1}(x,s) = -\left[\frac{\partial_x}{\rho h_s} + \partial_x^2 + \partial_z^2 + \frac{1}{h_s^2}\partial_s^2 + \frac{x}{\rho^2 h_s^3}(\partial_s\rho)\partial_s\right]f_n(x,s)$$

$$f_n(x,s) = (-1)^n\left[\frac{\partial_x}{\rho h_s} + \partial_x^2 + \partial_z^2 + \frac{\partial_s^2}{h_s^2} + \frac{x}{\rho^2 h_s^3}(\partial_s\rho)\partial_s\right]^n f_0(x,s)$$

If the radius of curvature is proportional to the dipole field in the centre of the multipole (the dipole component of the transverse field is a constant $T_{dipole}(x) = B_0$ and

$$\rho(s) = B_0 \times S(s)$$

This expression can be replaced in ([eq.40]) to obtain a more explicit equation.

7.10 References

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Chapter 8

OPAL-cycl

8.1 Introduction

OPAL-cycl, as one of the flavors of the *OPAL* framework, is a fully three-dimensional parallel beam dynamics simulation program dedicated to future high intensity cyclotrons and FFAs. It tracks multiple particles which takes into account the space charge effects. For the first time in the cyclotron community, *OPAL-cycl* has the capability of tracking multiple bunches simultaneously and take into account the beam-beam effects of the radially neighboring bunches (we call it neighboring bunch effects for short) by using a self-consistent numerical simulation model.

Apart from the multi-particle simulation mode, *OPAL-cycl* also has two other serial tracking modes for conventional cyclotron machine design. One mode is the single particle tracking mode, which is a useful tool for the preliminary design of a new cyclotron. It allows one to compute basic parameters, such as reference orbit, phase shift history, stable region, and matching phase ellipse. The other one is the tune calculation mode, which can be used to compute the betatron oscillation frequency. This is useful for evaluating the focusing characteristics of a given magnetic field map.

In addition, the widely used plugin elements, including collimator, radial profile probe, septum, trim-coil field and charge stripper, are currently implemented in *OPAL-cycl*. These functionalities are very useful for designing, commissioning and upgrading of cyclotrons and FFAs.

8.2 Tracking modes

According to the number of particles defined by the argument `NPART` in `BEAM` (see Chapter Beam Command), *OPAL-cycl* works in one of the following three operation modes automatically.

8.2.1 Single Particle Tracking mode

In this mode, only one particle is tracked, either with acceleration or not. Working in this mode, *OPAL-cycl* can be used as a tool during the preliminary design phase of a cyclotron.

The 6D parameters of a single particle in the initial local frame must be read from a file. To do this, in the *OPAL* input file, the command line `DISTRIBUTION` (see Chapter Distribution) should be defined like this:

```
Dist1: DISTRIBUTION, TYPE=fromfile, FNAME="PartDatabase.dat";
```

where the file *PartDatabase.dat* should have two lines:

```
1
0.001 0.001   0.001   0.001   0.001  0.001
```

The number in the first line is the total number of particles. In the second line the data represents x, p_x, y, p_y, z, p_z in the local reference frame. Their units are described in Units.

Please don't try to run this mode in parallel environment. You should believe that a single processor of the 21^{st} century is capable of doing the single particle tracking.

8.2.2 Tune Calculation mode

In this mode, two particles are tracked, one with all data is set to zero is the reference particle and another one is an off-centering particle which is off-centered in both r and z directions. Working in this mode, *OPAL-cycl* can calculate the betatron oscillation frequency ν_r and ν_z for different energies to evaluate the focusing characteristics for a given magnetic field.

Like the single particle tracking mode, the initial 6D parameters of the two particles in the local reference frame must be read from a file, too. In the file should has three lines:

```
2
0.0    0.0    0.0    0.0    0.0    0.0
0.001  0.0    0.0    0.0    0.001   0.0
```

When the total particle number equals 2, this mode is triggered automatically. Only the element `CYCLOTRON` in the beam line is used and other elements are omitted if any exists.

Please don't try to run this mode in parallel environment, either.

8.2.3 Multi-particle tracking mode

In this mode, large scale particles can be tracked simultaneously, either with space charge or not, either single bunch or multi-bunch, either serial or parallel environment, either reading the initial distribution from a file or generating a typical distribution, either running from the beginning or restarting from the last step of a former simulation.

Because this is the main mode as well as the key part of *OPAL-cycl*, we will describe this in detail in Section 8.8.

8.3 Variables in *OPAL-cycl*

OPAL-cycl uses the following canonical variables to describe the motion of particles:

X Horizontal position x of a particle in given global Cartesian coordinates [m].

PX Horizontal canonical momentum [Units].

Y Longitudinal position y of a particle in global Cartesian coordinates [m].

PY Longitudinal canonical momentum [Units].

Z Vertical position z of a particle in global Cartesian coordinates [m].

PZ Vertical canonical momentum [Units].

The independent variable is: **t** [s].

8.3.1 The initial distribution in the local reference frame

The initial distribution of the bunch, either read from file or generated by a distribution generator (see Chapter Distribution), is specified in the local reference frame of the *OPAL-cycl* Cartesian coordinate system (see Section 8.3). At the beginning of the run, the 6 phase space variables (x, y, z, p_x, p_y, p_z) are transformed to the global Cartesian coordinates (X, Y, Z, PX, PY, PZ) using the starting coordinates r_0 (`RINIT`), ϕ_0 (`PHIINIT`), and z_0 (`ZINIT`), and the starting momenta p_{total} (defined by the beam energy specified in the Beam Command), p_{r0} (PRINIT), and p_{z0} (PZINIT) of the reference particle, defined in the CYCLOTRON element. Note that $p_{\phi 0}$ is calculated automatically from p_{total}, p_{r0}, and p_{z0}.

$$\begin{aligned} X &= x\cos(\phi_0) - y\sin(\phi_0) + r_0\cos(\phi_0) \\ Y &= x\sin(\phi_0) + y\cos(\phi_0) + r_0\sin(\phi_0) \\ Z &= z + z_0 \end{aligned}$$

$$\begin{aligned} PX &= (p_x + p_{r0})\cos(\phi_0) - (p_y + p_{\phi 0})\sin(\phi_0) \\ PY &= (p_x + p_{r0})\sin(\phi_0) + (p_y + p_{\phi 0})\cos(\phi_0) \\ PZ &= p_z + p_{z0} \end{aligned}$$

8.4 Field Maps

In *OPAL-cycl*, the magnetic field on the median plane is read from an ASCII type file. The field data should be stored in the cylinder coordinates frame (because the field map on the median plane of the cyclotron is usually measured in this frame).

With respect to the external magnetic field map two possible situations can be considered: in the first situation, the measured field map data is loaded by the tracker. In most cases, only the vertical field, B_z, can be measured on the median plane ($z = 0$). by using measurement equipment. Since the magnetic field outside the median plane is required to compute trajectories with $z \neq 0$, the field needs to be expanded in the z direction. According to the approach given by Gordon and Taivassalo [18] by using a magnetic potential and measured B_z on the median plane at the point (r, θ, z) in cylindrical polar coordinates, the third order field can be written as:

$$\begin{aligned} B_r(r,\theta,z) &= z\frac{\partial B_z}{\partial r} - \frac{1}{6}z^3 C_r, \\ B_\theta(r,\theta,z) &= \frac{z}{r}\frac{\partial B_z}{\partial \theta} - \frac{1}{6}\frac{z^3}{r}C_\theta, \\ B_z(r,\theta,z) &= B_z - \frac{1}{2}z^2 C_z, \end{aligned}$$

EQUATION 8.1: Derivative of magnetic field

where $B_z \equiv B_z(r, \theta, 0)$ and

$$\begin{aligned} C_r &= \frac{\partial^3 B_z}{\partial r^3} + \frac{1}{r}\frac{\partial^2 B_z}{\partial r^2} - \frac{1}{r^2}\frac{\partial B_z}{\partial r} + \frac{1}{r^2}\frac{\partial^3 B_z}{\partial r \partial \theta^2} - 2\frac{1}{r^3}\frac{\partial^2 B_z}{\partial \theta^2}, \\ C_\theta &= \frac{1}{r}\frac{\partial^2 B_z}{\partial r \partial \theta} + \frac{\partial^3 B_z}{\partial r^2 \partial \theta} + \frac{1}{r^2}\frac{\partial^3 B_z}{\partial \theta^3}, \\ C_z &= \frac{1}{r}\frac{\partial B_z}{\partial r} + \frac{\partial^2 B_z}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 B_z}{\partial \theta^2}. \end{aligned}$$

EQUATION 8.2: Coefficients for derivatives with 5-point Lagrange formula

All the partial differential coefficients are computed from the median plane data by interpolation using Lagrange's 5-point formula.

In the other situation, 3D magnetic field data for the region of interest is calculated numerically by building a 3D model using commercial software, such as TOSCA, ANSOFT and ANSYS during the design phase of a new cyclotron. If the field on the median plane is calculated, the field off the median plane can be obtained using the same expansion approach as the measured field map as described above. In this case the calculated field will be more accurate, especially at large distances from the median plane i.e. a full 3D field map can be calculated.

In the current version, we implemented three specific type field-read functions *Cyclotron::getFieldFromFile()* of the median plane fields. Which function is used is controlled by the parameters `TYPE` of `CYCLOTRON` in the input file.

8.4.1 CARBONCYCL type

If `TYPE=CARBONCYCL`, the program requires the B_z data which is stored in a sequence shown in Figure 14.

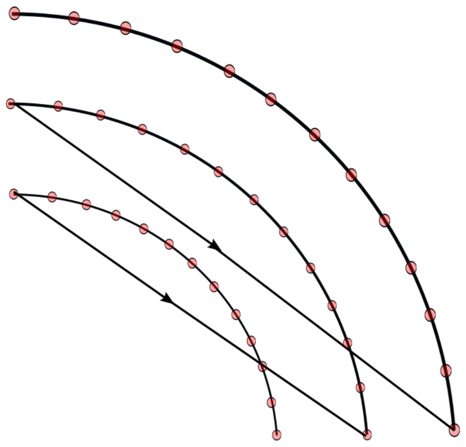

Figure 14: 2D field map on the median plane with primary direction corresponding to the azimuthal direction, secondary direction to the radial direction

We need to add 6 parameters at the header of a plain B_z [kG] data file, namely, r_{min} [mm], Δr [mm], θ_{min} [°], $\Delta\theta$ [°], N_θ (total data number in each arc path of azimuthal direction) and N_r (total path number along radial direction). If Δr or $\Delta\theta$ is decimal, one can set its negative opposite number. For instance, if $\Delta\theta = \frac{1}{3}°$, the fourth line of the header should be set to -3.0. Example showing the above explained format:

```
3.0e+03
10.0
0.0
-3.0
300
161
1.414e-03  3.743e-03  8.517e-03  1.221e-02  2.296e-02
3.884e-02  5.999e-02  8.580e-02  1.150e-01  1.461e-01
1.779e-01  2.090e-01  2.392e-01  2.682e-01  2.964e-01
3.245e-01  3.534e-01  3.843e-01  4.184e-01  4.573e-01
                        ...
```

The number of values per column is arbitrary.

8.4.2 CYCIAE type

If `TYPE=CYCIAE`, the program requires data format given by ANSYS10.0. This function is originally for the 100 MeV cyclotron of CIAE, whose isochronous fields is numerically computed by ANSYS. The median plane fields data is output by reading the APDL (ANSYS Parametric Design Language) script during the post-processing phase (you may need to do minor changes to adapt your own cyclotron model):

```
/post1
resume,solu,db
csys,1
nsel,s,loc,x,0
nsel,r,loc,y,0
nsel,r,loc,z,0
PRNSOL,B,COMP

CSYS,1
rsys,1

*do,count,0,200
   path,cyc100_Ansys,2,5,45
   ppath,1,,0.01*count,0,,1
   ppath,2,,0.01*count/sqrt(2),0.01*count/sqrt(2),,1

   pdef,bz,b,z
   paget,data,table

   *if,count,eq,0,then
      /output,cyc100_ANSYS,dat
      *STATUS,data,,,5,5
      /output
   *else
      /output,cyc100_ANSYS,dat,,append
      *STATUS,data,,,5,5
      /output
   *endif
*enddo
finish
```

By running this in ANSYS, you can get a fields file with the name *cyc100_ANSYS.data*. You need to put 6 parameters at the header of the file, namely, r_{min} [mm], Δr [mm], θ_{min} [°], $\Delta\theta$ [°], N_θ(total data number in each arc path of azimuthal direction) and N_r(total path number along radial direction). If Δr or $\Delta\theta$ is decimal, one can set its negative opposite number. This is useful if the decimal is unlimited. For instance, if $\Delta\theta = \frac{1}{3}^\circ$, the fourth line of the header should be -3.0. In other words, the fields are stored in the following format:

```
0.0
10.0
0.0e+00
1.0e+00
90
201
 PARAMETER STATUS- DATA  ( 336 PARAMETERS DEFINED)
                  (INCLUDING    17 INTERNAL PARAMETERS)

      LOCATION                VALUE
        1       5       1   0.537657876
        2       5       1   0.538079473
        3       5       1   0.539086731
                    ...
       44       5       1   0.760777286
       45       5       1   0.760918663
       46       5       1   0.760969074

 PARAMETER STATUS- DATA  ( 336 PARAMETERS DEFINED)
                  (INCLUDING    17 INTERNAL PARAMETERS)

      LOCATION                VALUE
        1       5       1   0.704927299
        2       5       1   0.705050993
        3        5        1    0.705341275
                           ...
```

8.4.3 BANDRF type

BANDRF fieldmap TYPE allows to read both the magnetic field and the electric field from the CYCLOTRON element. The magnetic field data (B_z) are stored in the same format as CARBONCYCL. Regarding the electric field, the 3D RF field-map can be read from H5Hut type file (*.h5part* file extension) making use of a conversion tool integrated into *OPAL*: *ascii2h5block*. For the details about its usage, please see Read 3D RF field-map. The electric field map can be imported from some field files, which can be optionally superposed, providing different meshing specifications for the field map. This is useful for modeling the central region electric fields which usually has complicated shapes. Please note that in this case, the E field is treated as a part of CYCLOTRON element, rather than an independent RFCAVITY element.

8.4.4 RING type

If TYPE=RING, the program requires the data format like PSI format field file *ZYKL9Z.NAR* and *SO3AV.NAR*, which was given by the measurement. We add 4 parameters at the header of the file, namely, r_{min} [mm], Δr [mm], $\theta_{min}[^\circ]$, $\Delta\theta[^\circ]$. If Δr or $\Delta\theta$ is decimal, one can set its negative opposite number. This is useful if the decimal is unlimited. For instance, if $\Delta\theta = \frac{1}{3}^\circ$, the fourth line of the header should be -3.0.

```
1900.0
20.0
0.0
-3.0
 LABEL=S03AV
 CFELD=FIELD      NREC=  141       NPAR=    3
 LPAR=    7       IENT=    1       IPAR=    1
              3              141              135               30               8
              8               70
 LPAR= 1089       IENT=    2       IPAR=    2
 0.100000000E+01 0.190000000E+04 0.200000000E+02 0.000000000E+00 0.333333343E+00
 0.506500015E+02 0.600000000E+01 0.938255981E+03 0.100000000E+01 0.240956593E+01
 0.282477260E+01 0.340503168E+01 0.419502926E+01 0.505867147E+01 0.550443363E+01
 0.570645094E+01 0.579413509E+01 0.583940887E+01 0.586580372E+01 0.588523722E+01
                           ...
```

8.4.5 3D field-map

It is additionally possible to load 3D field-maps for tracking through *OPAL-cycl*. 3D field-maps are loaded by sequentially adding new field elements to a line, as is done in *OPAL-t*. It is not possible to add RF cavities while operating in this mode. In order to define ring parameters such as initial ring radius a RINGDEFINITION type is loaded into the line, followed by one or more SBEND3D elements.

```
ringdef: RINGDEFINITION, HARMONIC_NUMBER=6, LAT_RINIT=2350.0, LAT_PHIINIT=0.0,
         LAT_THETAINIT=0.0, BEAM_PHIINIT=0.0, BEAM_PRINIT=0.0,
         BEAM_RINIT=2266.0, SYMMETRY=4.0, RFFREQ=0.2;

triplet: SBEND3D, FMAPFN="fdf-tosca-field-map.table", LENGTH_UNITS=10., FIELD_UNITS=-1e-4;

l1: Line = (ringdef, triplet, triplet);
```

The field-map with file name *fdf-tosca-field-map.table* is loaded, which is a file like

```
      422280       422280       422280           1
 1 X [LENGU]
 2 Y [LENGU]
 3 Z [LENGU]
 4 BX [FLUXU]
 5 BY [FLUXU]
 6 BZ [FLUXU]
 0
 194.01470 0.0000000 80.363520 0.68275932346E-07 -5.3752492577 0.28280706805E-07
 194.36351 0.0000000 79.516210 0.42525693524E-07 -5.3827955117 0.17681348191E-07
 194.70861 0.0000000 78.667380 0.19766168358E-07 -5.4350026348 0.82540823165E-08
<continues>
```

The header parameters are ignored - user supplied parameters `LENGTH_UNITS` and `FIELD_UNITS` are used. Fields are supplied on points in a grid in (r, y, ϕ). Positions and field elements are specified by Cartesian coordinates (x, y, z).

8.4.6 User's own field-map

You should revise the function or write your own function according to the instructions in the code to match your own field format if it is different to above types. For more detail about the parameters of `CYCLOTRON`, please refer to Cyclotron.

8.5 RF field

8.5.1 Read RF voltage profile

The RF cavities are treated as straight lines with infinitely narrow gaps and the electric field is a δ function plus a transit time correction. The two-gap cavity is treated as two independent single-gap cavities. The spiral gap cavity is not implemented yet. For more detail about the parameters of cyclotron cavities, see Cyclotron.

The voltage profile of a cavity gap is read from ASCII file. Here is an example:

```
6
0.00      0.15      2.40
0.20      0.65      2.41
0.40      0.98      0.66
0.60      0.88     -1.59
0.80      0.43     -2.65
1.00     -0.05     -1.71
```

The number in the first line means 6 sample points and in the following lines the three values represent the normalized distance to the inner edge of the cavity, the normalized voltage and its derivative respectively.

8.5.2 Read 3D RF field-map

The 3D RF field-map can be read from H5Hut type file for `TYPE=BANDRF`. To generate the *h5part* field files, it is necessary to use the *ascii2h5block* conversion tool. This tool is available after compiling *OPAL* with `ENABLE_BANDRF=ON`. This program builds h5part field files from ASCII file output of ANSYS or OPERA 3D field data. The command to use it should be like:

```
ascii2h5block efield.txt hfield.txt ehfout
```

The ASCII input files must be adapted for an adequate conversion. The first row of each input field map that you wish to combine should specify the grid size in each direction, that is integers with the amount of steps (or different values) in x, y and z. The first three columns contains the spatial coordinates specified in meters, and the last three columns store the field data. Positions and field are supplied on points in a Cartesian coordinates grid:[(x, y, z)]. Example showing the requiered format for ASCII file:

```
101 101 11
-0.110000   -0.018000   -0.006000   37.341814   226.620820    -319049.189111
-0.109200   -0.018000   -0.006000   56.839707   209.995240    303511.031113
-0.108400   -0.018000   -0.006000   -28.180696  37.248050     -292542.457735
-0.107600   -0.018000   -0.00600    8.412707    89.317296     -283046.136227
                        ...
```

8.6 Particle Tracking and Acceleration

The precision of the tracking methods is vital for the entire simulation process, especially for long distance tracking jobs. *OPAL-cycl* uses a fourth order Runge-Kutta algorithm and the second order Leap-Frog scheme. The fourth order Runge-Kutta algorithm needs four external magnetic field evaluations in each time step τ. During the field interpolation process, for an arbitrary given point the code first interpolates Formula B_z for its counterpart on the median plane and then expands to this given point using Equation 8.1.

After each time step i, the code detects whether the particle crosses any one of the RF cavities during this step. If it does, the time point t_c of crossing is calculated and the particle return back to the start point of step i. Then this step is divided into three sub-steps: first, the code tracks this particle for $t_1 = \tau - (t_c - t_{i-1})$; then it calculates the voltage and adds momentum kick to the particle and refreshes its relativistic parameters β and γ; and then tracks it for $t_2 = \tau - t_1$.

8.7 Space Charge

OPAL-cycl uses the same solvers as *OPAL-t* to calculate the space charge effects see Chapter Field Solver.

Typically, the space charge field is calculated once per time step. This is no surprise for the second order Boris-Buneman time integrator (leapfrog-like scheme) which has per default only one force evaluation per step. The fourth order Runge-Kutta integrator keeps the space charge field constant for one step, although there are four external field evaluations. There is an experimental multiple-time-stepping (MTS) variant of the Boris-Buneman/leapfrog-method, which evaluates space charge only every N^th step, thus greatly reducing computation time while usually being still accurate enough.

8.8 Multi-bunch Mode

The neighboring bunches problem is motivated by the fact that for high intensity cyclotrons with small turn separation, single bunch space charge effects are not the only contribution. Along with the increment of beam current, the mutual interaction of neighboring bunches in radial direction becomes more and more important, especially at large radius where the distances between neighboring bunches get increasingly small and even they can overlap each other. One good example is PSI 590 MeV Ring cyclotron with a current of about 2 mA in CW operation and the beam power amounts to 1.2 MW. An upgrade project for Ring is in process with the goal of 1.8 MW CW on target by replacing four old aluminum resonators by four new copper cavities with peak voltage increasing from about 0.7 MW to above 0.9 MW. After upgrade, the total turn number is reduced from 200 turns to less than 170 turns. Turn separation is increased a little bit, but still are at the same order of magnitude as the radial size of the bunches. Hence once the beam current increases from 2 mA to 3 mA, the mutual space charge effects between radially neighboring bunches can have significant impact on beam dynamics. In consequence, it is important to cover neighboring bunch effects in the simulation to quantitatively study its impact on the beam dynamics.

In *OPAL-cycl*, we developed a new fully consistent algorithm of multi-bunch simulation. We implemented two working modes, namely , `AUTO` and `FORCE`. In the first mode, only a single bunch is tracked and accelerated at the beginning, until the radial neighboring bunch effects become an important factor to the bunches' behavior. Then the new bunches will be injected automatically to take these effects into account. In this way, we can save time and memory, and more important, we can get higher precision for the simulation in the region where neighboring bunch effects are important. In the other mode, multi-bunch simulation starts from the injection points.

In the space charge calculation for multi-bunch, the computation region covers all bunches. Because the energy of the bunches is quite different, it is inappropriate to use only one particle rest frame and a single Lorentz transformation any more. So the particles are grouped into different energy bins and in each bin the energy spread is relatively small. We apply Lorentz transforming, calculate the space charge fields and apply the back Lorentz transforming for each bin separately. Then add the field data together. Each particle has a ID number to identify which energy bin it belongs to.

8.9 Input

All the three working modes of *OPAL-cycl* use an input file written in *MAD* language which will be described in detail in the following chapters.

For the **Tune Calculation mode**, one additional auxiliary file with the following format is needed.

```
72.000 2131.4   -0.240
74.000 2155.1   -0.296
76.000 2179.7   -0.319
78.000 2204.7   -0.309
80.000 2229.6   -0.264
82.000 2254.0   -0.166
84.000 2278.0    0.025
```

In each line the three values represent energy E, radius r and P_r for the SEO (Static Equilibrium Orbit) at starting point respectively and their units are MeV, mm and mrad.

A bash script *tuning.sh* is shown on the next page, to execute *OPAL-cycl* for tune calculations.

tuning.sh

To start execution, just run *tuning.sh* which uses the input file *testcycl.in* and the auxiliary file *FIXPO* SEO_. The output file is *plotdata* from which one can plot the tune diagram.

8.10 Output

OPAL-cycl writes out several output files, some specific to the Tracking mode (see following sections).

8.10.1 Statistics output

See OPAL-t Statistics output. The only difference is in the cyclotron coordinate convention. The z (or s) coordinate refers to the vertical direction and y corresponds to the longitudinal or beam travel direction. In addition, *OPAL-cycl* includes some extra data, as is described in the following table.

Name	**Units**	**Meaning**
R0_x	m	X-component of position of particle with ID 0 (only when run serial)
R0_y	m	Y-component of position of particle with ID 0 (only when run serial)
R0_s	m	S-component of position of particle with ID 0 (only when run serial)
P0_x	m	X-component of momentum of particle with ID 0 (only when run serial)
P0_y	m	Y-component of momentum of particle with ID 0 (only when run serial)
P0_s	m	S-component of momentum of particle with ID 0 (only when run serial)
halo_x	1	Halo in x
halo_y	1	Halo in y
halo_z	1	Halo in z
azimuth	deg	Azimuth in global coordinates

Table 11: Additional data stored in statistics output file in *OPAL-cycl*.

8.10.2 Single Particle Tracking mode

The intermediate phase space data is stored in an ASCII file which can be used to plot the orbit. The file's name is combined by input file name (without extension) and *-trackOrbit.dat*. The data are stored in the global Cartesian coordinates. The frequency of the data output can be set using the option `SPTDUMPFREQ` of OPTION statement.

The phase space data per `STEPSPERTURN` (a parameter in the `TRACK` command) steps is stored in an ASCII file. The file's is named *<input_file_name >-afterEachTurn.dat*. The data is stored in the global cylindrical coordinate system. Please note that if the field map is ideally isochronous, the reference particle of a given energy take exactly one revolution in `STEPSPERTURN` steps; Otherwise, the particle may not go through a full 360° in `STEPSPERTURN` steps.

There are 3 ASCII files which store the phase space data around 0, $\pi/8$ and $\pi/4$ azimuths. Their names are the combinations of input file name (without extension) and *-Angle0.dat*, *-Angle1.dat* and *-Angle2.dat* respectively. The data is stored in the global cylindrical coordinate system, which can be used to check the property of the closed orbit.

8.10.3 Tune calculation mode

The tunes ν_r and ν_z of each energy are stored in a ASCII file named *tuningresult*.

8.10.4 Multi-particle tracking mode

The intermediate phase space data of all particles and some interesting parameters, including RMS envelop size, RMS emittance, external field, time, energy, length of path, number of bunches and tracking step, are stored in the H5hut file-format [19] and can be analyzed using H5root [20], [21]. The frequency of the data output can be set using the `PSDUMPFREQ` option of OPTION statement. The file is named *<input_file_name >.h5*. This output can be switched on or off with the option `ENABLEHDF5`.

The intermediate phase space data of central particle (with ID of 0) and an off-centering particle (with ID of 1) are stored in an ASCII file. The file is named *<input_file_name >-trackOrbit.dat*. The frequency of the data output can be set using the `SPTDUMPFREQ` option of OPTION statement.

8.10.5 Field maps

The magnetic field map read by *OPAL* could be saved into an output file called *gnu.out*. This file stores the magnetic field B_z data in the median plane in cylindrical coordinates following the sequence shown in Figure 14. This output file is available in the cyclotron field types `CARBONCYCL`, `BANDRF`, `FFA` and `AVFEQ`.

In case of `CARBONCYCL` or `BANDRF` an additional output field file an additional output field file is saved (*eb.out*), storing three vectors with the position, electric field and the magnetic field.

Writing these output files is enabled when *OPAL* is run on single node, and it can be switched on or off with the `INFO` option of OPTION statement.

Moreover, `DUMPFIELDS` and `DUMPEMFIELDS` routines (see Chapter Field Output) can be employed to write out the external field used in *OPAL-cycl* in a different grid than the input field maps.

8.11 Matched Distribution

In order to run matched distribution simulation one has to specify a periodic accelerator. The function call also needs the symmetry of the machine as well as a field map. The user then specifies the emittance $\pi\ mm\ mrad$.

```
/*
 * specify periodic accelerator
 */
l1 = ...

/*
 * try finding a matched distribution
 */
Dist1:DISTRIBUTION, TYPE=GAUSSMATCHED, LINE=l1, FMAPFN=...,
                    MAGSYM=..., EX = ..., EY = ..., ET = ...;
```

8.11.1 Example

Simulation of the PSI Ring Cyclotron at 580 MeV and current 2.2 mA. The program finds a matched distribution followed by a bunch initialization according to the matched covariance matrix. The matched distribution algorithm works with normalized emittances, i.e. normalized by the lowest energy of the machine. The printed emittances, however, are the geometric emittances. In addition, it has to be paid attention that the computation is based on $(x, x', y, y', z, \delta)$ instead of (x, p_x, y, p_y, z, p_z). Since the particles are represented in the latter coordinate system, the corresponding transformation has to be applied to obtain the rms emittances that are given in the output.

8.11.1.1 Input file

matchedDistribution.in

All supplementary files can be found in the matched distribution regression test.

8.11.1.2 Output

matchedDistribution.output

8.12 References

[18] M. M. Gordon and V. Taivassalo, *Nonlinear Effects of Focusing Bars Used in the Extraction Systems of Superconducting Cyclotrons*, IEEE Trans. Nucl. Sci. 32, 2447 (1985).

[19] M. Howison et al., *H5hut: A High-Performance I/O Library for Particle-based Simulations*, in 2010 IEEE International Conference on Cluster Computing Workshops and Posters, vol. 1, pp. 1–8 (Heraklion, Crete, 2010).

[20] *H5root: a ROOT Based Graphical User Interface for H5hut*

[21] T. Schietinger, *H5PartROOT - A visualization and post-processing tool for accelerator simulations*, in Proceedings of the 10th International Computational Accelerator Physics conference (ICAP09), pp. 343-346 (San Francisco, CA, USA, 2009).

Chapter 9

OPAL-map

9.1 Introduction

OPAL-map is a map tracking beam optics code. This type computes maps for each beam line element to describe the action of the system.

The map creation is done by applying the Lie Operator on the element Hamiltonian and calculated in the Truncated Power Series Algebra (TPSA)[22]. The TPSA is a Differential Algebra (DA), which uses the Taylor expansion as the equivalent function. In *OPAL-map* the TPSA gets provided from the own *OPAL* DA package.

In contrast to time t dependent tracking codes, as OPAL-t, map tracking codes use the longitudinal bunch position s as independent variable. Furthermore, map tracking codes do not use numerical integrators for the determination of the particle trajectory, which can be a computationally very expensive.

The main advantage in map tracking codes lies in the ”map” itself. These do not only contain valuable information about the beam line, but also can be accumulated to reduce the computational effort in the particle tracking.

9.2 Variables in *OPAL-map*

For in and outputs, the units as in `Variables in OPAL-t` are used.

OPAL-map uses an Frenet-Serret coordinate system, referring on a reference particle. This particle has the ideal properties, ergo follows the design path. The following canonical variables to describe the motion of particles. The physical units are listed in square brackets.

X Horizontal position x of a particle relative to the reference particle [m].

PX $\frac{p_x}{P_0}$ Normalized horizontal canonical momentum [1]. (Where p_x is the momentum of the particle and P_0 is the momentum of the reference particle)

Y Vertical position y of a particle relative to the reference particle [m].

PY $\frac{p_y}{P_0}$ Normalized vertical canonical momentum [1].

Z Longitudinal position z of a particle relative to the reference particle [m].

DELTA $\frac{E}{P_0 c} - \frac{1}{\beta_0}$ Energy derivation [1]. (Where E is the total energy of the particle and $\beta_0 = \frac{u}{c}$ the speed relative to the speed of light c of the reference particle)

The independent variable is position of the reference particle **s** [m].

9.3 Principle of Map Tracking

The particle motion gets calculated by applying the map on the particle parameter.

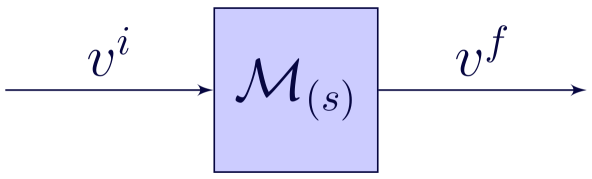

Figure 15: Flow chart of map tracking.

$$v^f = \mathscr{M} \circ v^i$$

Where v denotes the final (v^f) and initial (v^i) six dimensional phase space vector of each particle. $\mathscr{M}$ is the map. This map can represent either a beam element slice, the whole element, a beam line section or the whole system.

9.3.1 Creation of map

The creation of the element map is based on the Hamiltonian Mechanic, more specifically on the Lie Operator.

$$H = T + V$$
$$\frac{d\mathbf{q_i}}{ds} = \frac{\partial H}{\partial p_i}, \frac{d\mathbf{p_i}}{ds} = -\frac{\partial H}{\partial q_i}$$

Here H, the time dependent Hamiltonian represents the total energy, consisting of the kinetic T and potential V energy. The lower equations are the Hamiltonian equations of motion, where the momenta p_i and the positions q_i form the canonical pairs. Using canonical transformations, the Hamiltonian can be adjusted to use the path length s as independent and the particle parameters as dependent variable(s).

Introducing the Lie operator, which acts similar to a "waiting" Poisson Bracket:

$$:f := [f, \circ] = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial \circ}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial \circ}{\partial q_i} \right)$$

If a function $f := f\left(\mathbf{q}_{(\mathbf{s})}, \mathbf{p}_{(\mathbf{s})}\right)$ describes one of the phase space variables v its total derivative to the independent variable, combined with the Hamiltonian equations of motions, is similar to the Lie operator times the indepedent variable, i. e. s.

$$\frac{df}{ds} = \sum_{i=1}^{n} \left(\frac{dq_i}{ds} \frac{\partial f}{\partial q_i} + \frac{dp_i}{ds} \frac{\partial f}{\partial p_i} \right)$$
$$\frac{df}{ds} = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} \right) \equiv - :H: f$$

The integral over the independent variable $\int \cdot ds$:

$$f(s) = e^{-:H:s} f(s_0)$$
$$\mathscr{M} = e^{-:H:s}$$

Where $e^{-:H:s}$ is the Lie expansion.

9.3.2 Implementation of map tracking

For the derivative of the Hamiltonian, a Differential Algebra (DA) was used, in particular the Truncated Power Series Algebra (TPSA). This algebra uses the Taylor expansion as the equivalent function, which also is responsible for its name by creating truncated power series. Just form the definition of the Taylor expansion, it can be seen that a finite, to the order Ω, expansion is an approximation of the actual function, due to the error term $\mathscr{O}\left(\mathbf{v}^{\Omega+1}(\Delta s)\right)$.

$$f = \mathscr{M} = \sum_{n=0}^{\Omega} \frac{f^{(n)}}{n!} \left(\mathbf{v}(\Delta s)\right)^n + \mathscr{O}\left(\mathbf{v}^{\Omega+1}(\Delta s)\right)$$

In *OPAL-map* the Hamiltonian gets Taylor expanded and its map derived (`Creation of Map`) in the TPSA using the *OPAL* DA package. The truncation length gets defined in `TRACK` setting the `MAP_ORDER` attribute.

```
TRACK, LINE= QUADTEST, BEAM=BEAM1, MAXSTEPS=10000, DT=1.0e-10, ZSTOP=4.0, MAP_ORDER=2;
```

9.4 Additional Parameter in *OPAL-map*

Attribute Name	**set in**	**Default Value**	**Units**	**Description**
`MAP_ORDER`	`TRACK`	1	[ ]	defines the map order (= order TPSA - 1).
`NSlices`	beam line element	1	[ ]	defines the number of steps inside the element.

Table 12: Additional Parameter.

9.4.1 Limitations

OPAL-map is the new flavour of *OPAL* and currently just contains the fundamental beam line elements:

- Drift (`Drift`),
- Dipole (`Sbend`),
- Quadrupole (`Quadrupole`)

9.5 Example

FODO lattice: MAP-FODO.in

Input distribution (to be put in directory `data`): FODO_DIST.dat

To `RUN` *OPAL-map*, the `METHOD` attribute gets set to `THICK`.

```
RUN, METHOD = "THICK", BEAM=BEAM1, FIELDSOLVER=FS1, DISTRIBUTION=DIST1;
```

The maximal order of the beam line maps get defined with the `MAP_ORDER` attribute.

```
TRACK, LINE= QUADTEST, BEAM=BEAM1, MAXSTEPS=10000, DT=1.0e-10, ZSTOP=4.0, MAP_ORDER=2;
```

As an optional parameter for the beam line elements `NSlices=<x>` provides the opportunity to split one element in `<x>` smaller steps. Otherwise, the default value is defined with `1`.

```
D1:  DRIFT,          L=1.,                ELEMEDGE=0.000, NSLICES=10;
QP1: QUADRUPOLE,     L=0.3,  K1= 8.64195, ELEMEDGE=1.000, NSLICES=15;
```

9.6 Output

In addition to the progress report that *OPAL-map* writes to the standard output (stdout) it also writes different files for various purposes.

9.6.1 Statistics output

The file structure is analogous to OPAL-t Statistics output file.

9.6.2 *data/<input_file_name >.dispersion*

OPAL-map computes the dispersion of the beam line according to:

$$\begin{pmatrix} \eta_i \\ \eta_{p_i} \end{pmatrix}_{s_1} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \cdot \begin{pmatrix} \eta_i \\ \eta_{p_i} \end{pmatrix}_{s_0} + \begin{pmatrix} R_{16} \\ R_{26} \end{pmatrix}$$

where R is the Transfermatrix and η is the dispersion.

Column Nr.	Name	Units	Meaning
1	position	m	Longitudinal position
2	η_x	m	Spatial dispersion in x
3	η_{px}	1	Momentum dispersion in x
4	η_y	m	Spatial dispersion in x
5	η_{py}	1	Momentum dispersion in y positions

9.6.3 *data/<input_file_name >.map*

Here the transfer map of the whole beamline gets printed. Its format is analogous to a DA- `FVPs` (src/Classic/FixedAlgebra), where the polynomials (DA- `FTPs`) get represented in a 6 dimensional vector. The first number describes the coefficient and the following 6 the variables of the monomial.

Column Nr.	Name	Units	Meaning
1	coefficient	1	coefficient of monomial
2	x	1	x in monomial
3	p_x	1	p_x in monomial
4	y	1	y in monomial
5	p_y	1	p_y in monomial
6	z	1	z in monomial
7	δ	1	δ in monomial

9.7 References

[22] M. Berz, *Modern map methods in particle beam physics*, Academic Press (1999).

Chapter 10

Command Format

All flavors of *OPAL* using the same input language the *MAD* language. The language dialect here is ajar to *MAD9*, for hard core *MAD8* users there is a conversion guide.

It is the first time that machines such as cyclotrons, proton and electron linacs can be described within the same language in the same simulation framework.

10.1 Statements and Comments

Input for *OPAL* is free format, and the line length is not limited. During reading, input lines are normally printed on the echo file, but this feature can be turned off for long input files. The input is broken up into tokens (words, numbers, delimiters etc.), which form a sequence of commands, also known as statements. Each statement must be terminated by a semicolon (`;`), and long statements can be continued on any number of input lines. White space, like blank lines, spaces, tabs, and newlines are ignored between tokens. Comments can be introduced with two slashes (`//`) and any characters following the slashes on the same line are ignored.

The C convention for comments is also accepted. The comment delimiters can be nested; this allows to "comment out" sections of input.

In the following descriptions, words in `lower case` stand for syntactic units which are to be replaced by actual text. `UPPER CASE` is used for keywords or names. These must be entered as shown. Ellipses (`...`) are used to indicate repetition.

The general format for a command is

```
keyword,attribute,...,attribute;
label:keyword,attribute,...,attribute;
```

It has three parts:

1. The `label` is required for a definition statement. Its must be an identifier (see Section 10.2) and gives a name to the stored command.
2. The `keyword` identifies the action desired. It must be an identifier (see Section 10.2).
3. Each `attribute` is entered in one of the forms

   ```
   attribute-name
   attribute-name=attribute-value
   attribute-name:=attribute-value
   ```

   and serves to define data for the command, where:

   - The `attribute-name` selects the attribute, it must be an identifier (see Section 10.2).

- The `attribute-value` gives it a value (see Section 10.3). When the attribute value is a constant or an expression preceded by the delimiter = it is evaluated immediately and the result is assigned to the attribute as a constant. When the attribute value is an expression preceded by the delimiter := the expression is retained and re-evaluated whenever one of its operands changes.

  Each attribute has a fixed attribute type (see Section 10.3). The `attribute-value` can only be left out for logical attributes, this implies a `true` value.

When a command has a `label`, *OPAL* keeps the command in memory. This allows repeated execution of the same command by entering its label only:

```
label;
```

or to re-execute the command with modified attributes:

```
label,attribute,...,attribute;
```

If the label of such a command appears together with new attributes, *OPAL* makes a copy of the stored command, replaces the attributes entered, and then executes the copy:

```
QF:QUADRUPOLE,L=1,K1=0.01; // first definition of QF
QF,L=2;                    // redefinition of QF

MATCH;
...
LMD:LMDIF,CALLS=10;            // first execution of LMD
LMD;                           // re-execute LMD with
                               // the same attributes
LMD,CALLS=100,TOLERANCE=1E-5;  // re-execute LMD with
                               // new attributes
ENDMATCH;
```

10.2 Identifiers or Labels

An identifier refers to a keyword, an element, a beam line, a variable, an array, etc.

A label begins with a letter, followed by an arbitrary number of letters, digits, periods (`.`), underscores (_). Other special characters can be used in a label, but the label must then be enclosed in single or double quotes. It makes no difference which type of quotes is used, as long as the same are used at either end. The preferred form is double quotes. The use of non-numeric characters is however strongly discouraged, since it makes it difficult to subsequently process an _OPAL_ output with another program.

When a name is not quoted, it is converted to upper case; the resulting name must be unique. An identifier can also be generated from a string expression (see Section 10.4).

10.3 Command Attribute Types

An object attribute is referred to by the syntax

```
object-name->attribute-name
```

If the attribute is an array (see Section 10.13), one of its components is found by the syntax

```
object-name->attribute-name[index]
```

The following types of command attributes are available in *OPAL*:

String	Section 10.4
Logical	Section 10.5
Real expression	Section 10.6
Deferred expression	Section 10.8.5
Place	Section 10.9.1
Range	Section 10.9.2
Constraint	Section 10.10
Variable Reference	Section 10.11
Regular expression	Section 10.12
Array	Section 10.13
Array of logical	Section 10.13.1
Array of real	Section 10.13.2
Array of string	Section 10.13.3
Array of token lists	Section 10.13.4

See also:

Operators	Table 16
Functions	Table 17
Real functions of arrays	Table 20
Operand	Section 10.8
Random generators	Section 10.8.5

10.4 String Attributes

A string attribute makes alphanumeric information available, e.g. a title, file name, element class name, or an option. It can contain any characters, enclosed in single (`'`) or double (`"`) quotes. However, if it contains a quote, this character must be doubled. Strings can be concatenated using the `&` operator (see Table 13). An operand in a string can also use the function `STRING` (see Table 14). String values can occur in string arrays (see Section 10.13).

Operator	**Meaning**	**result type**	**operand types**
`X & Y`	concatenate the strings `X` and `Y`. String concatenations are always evaluated immediately when read.	string	string,string

Table 13: String Operator in *OPAL*

Function	**Meaning**	**result type**	**argument type**
`STRING(X)`	return string representation of the value of the numeric expression `X`	string	real

Table 14: String Function in *OPAL*

Examples:

```
TITLE,"This is a title for the program run ""test""";
CALL,FILE="save";

REAL X=1;
STRING L2=LEP&STRING(X+1);
```

The second example converts the value of the expression `X+1` to a string and appends it to `LEP`, giving the string `LEP2`.

10.4.1 Predefined String Attributes

OPAL recognizes some specific string names using a list of predefined strings. Consequentially, attributes of type `PredefinedString` should only accept strings that are contained in a predefined set of strings according to their internal description. If the provided string is not contained in the predefined set, an exception is thrown, since this string is marked as a protected keyword and cannot be used to name an object. Most of the string attributes in *OPAL* have been defined based on `PredefinedString` to prevent the user from entering variable names that are used internally for another functionality. All these predefined string attributes do not have to be enclosed in quotes, unlike regular strings. The list of accepted strings as well as the default value, if any, are added to the `--help-command` message (see Table 4).

10.5 Logical Expressions

Many commands in *OPAL* require the setting of logical values (flags) to represent the on/off state of an option. A logical value is represented by one of the values `TRUE` or `FALSE`, or by a logical expression. A logical expression can occur in logical arrays (see Section 10.13.1).

A logical expression has the same format and operator precedence as a logical expression in C. It is built from logical operators (see Table 15) and logical operands:

```
relation      ::= "TRUE" |
                  "FALSE" |
                  real-expr rel-operator real-expr

rel-operator  ::= "==" | "!=" | "<" | ">" | ">=" | "<="

and-expr      ::= relation | and-expr "&&" relation

logical-expr  ::= and-expr | logical-expr "||" and-expr
```

Operator	**Meaning**	**result type**	**operand type**
`X` < `Y`	true, if `X` is less than `Y`	logical	real,real
`X` <= `Y`	true, if `X` is not greater than `Y`	logical	real,real
`X` > `Y`	true, if `X` is greater than `Y`	logical	real,real
`X` >= `Y`	true, if `X` is not less than `Y`	logical	real,real
`X` == `Y`	true, if `X` is equal to `Y`	logical	real,real
`X` != `Y`	true, if `X` is not equal to `Y`	logical	real,real
`X` && `Y`	true, if both `X` and `Y` are true	logical	logical,logical
`X` || `Y`	true, if at least one of `X` and `Y` is true	logical	logical,logical

Table 15: Logical Operators in *OPAL*

Example:

```
OPTION,ECHO=TRUE; // output echo is desired
```

When a logical attribute is not entered, its default value is always `FALSE`. When only its name is entered, the value is set to `TRUE`:

```
OPTION,ECHO;       // same as above
```

Example of a logical expression:

```
X>10 && Y<20 || Z==15
```

10.6 Real Expressions

To facilitate the definition of interdependent quantities, any real value can be entered as an arithmetic expression. When a value used in an expression is redefined by the user or changed in a matching process, the expression is re-evaluated. Expression definitions may be entered in any order. *OPAL* evaluates them in the correct order before it performs any computation. At evaluation time all operands used must have values assigned. A real expression can occur in real arrays (see Section 10.13.2).

A real expression is built from operators (see Table 16) and operands (see Section 10.8):

```
real-ref  ::= real-variable |
              real-array "[" index "]" |
              object "->" real-attribute |
              object "->" real-array-attribute "[" index "]" |

table-ref ::= table "@" place "->" column-name

primary   ::= literal-constant |
              symbolic-constant |
              "#" |
              real-ref |
              table-ref |
              function-name "(" arguments ")" |
              (real-expression)

factor    ::= primary |
              factor "^" primary

term      ::= factor |
              term "*" factor |
              term "/" factor

real-expr ::= term |
              "+" term |
              "-" term |
              real-expr "+" term |
              real-expr "-" term |
```

It may contain functions (see Table 17), Parentheses indicate operator precedence if required. Constant sub-expressions are evaluated immediately, and the result is stored as a constant.

10.7 Operators

An expression can be formed using operators (see Table 16) and functions (see Table 17) acting on operands (see Section 10.8).

Operator	Meaning	result type	operand type(s)
	Real operators with one operand		
`+ X`	unary plus, returns `X`	real	real
`- X`	unary minus, returns the negative of `X`	real	real
	Real operators with two operands		
`X + Y`	add `X` to `Y`	real	real,real
`X - Y`	subtract `Y` from `X`	real	real,real
`X * Y`	multiply `X` by `Y`	real	real,real
`X / Y`	divide `X` by `Y`	real	real,real
`X ^ Y`	power, return `X` raised to the power `Y`	real	real,real

Table 16: Real Operators in *OPAL*

Function	Meaning	result type	argument type(s)
Real functions with no arguments			
`RANF()`	random number, uniform distribution in [0,1)	real	-
`GAUSS()`	random number, Gaussian distribution with $\mu = 0$ and $\sigma = 1$	real	-
`GETEKIN()`	returns the kinetic energy of the bunch (MeV)	real	-
`USER0()`	random number, user-defined distribution	real	-
Real functions with one argument			
`TRUNC(X)`	truncate `X` towards zero (discard fractional part)	real	real
`ROUND(X)`	round `X` to nearest integer	real	real
`FLOOR(X)`	return largest integer not greater than `X`	real	real
`CEIL(X)`	return smallest integer not less than `X`	real	real
`SIGN(X)`	return sign of `X` (+1 for `X` positive, -1 for `X` negative, 0 for `X` zero)	real	real
`SQRT(X)`	return square root of `X`	real	real
`LOG(X)`	return natural logarithm of `X`	real	real
`EXP(X)`	return exponential to the base *e* of `X`	real	real
`SIN(X)`	return trigonometric sine of `X`	real	real
`COS(X)`	return trigonometric cosine of `X`	real	real
`ABS(X)`	return absolute value of `X`	real	real
`TAN(X)`	return trigonometric tangent of `X`	real	real
`ASIN(X)`	return inverse trigonometric sine of `X`	real	real
`ACOS(X)`	return inverse trigonometric cosine of `X`	real	real
`ATAN(X)`	return inverse trigonometric tangent of `X`	real	real
`TGAUSS(X)`	random number, Gaussian distribution with σ=1, truncated at `X`	real	real
`USER1(X)`	random number, user-defined distribution with one parameter	real	real
`EVAL(X)`	evaluate the argument immediately and transmit it as a constant	real	real
Real functions with two arguments			
`ATAN2(X,Y)`	return inverse trigonometric tangent of `Y/X`	real	real,real
`MAX(X,Y)`	return the larger of `X`, `Y`	real	real,real
`MIN(X,Y)`	return the smaller of `X`, `Y`	real	real,real
`MOD(X,Y)`	return the largest value less than `Y` which differs from `X` by a multiple of `Y`	real	real,real
`USER2(X,Y)`	random number, user-defined distribution with two parameters	real	real,real

Table 17: Real Functions in *OPAL*

Function	Meaning	result type	operand type
`VMAX(X,Y)`	return largest array component	real	real array
`VMIN(X,Y)`	return smallest array component	real	real array
`VRMS(X,Y)`	return rms value of an array	real	real array
`VABSMAX(X,Y)`	return absolute largest array component	real	real array

Table 18: Real Functions of Arrays in *OPAL*

Care must be used when an ordinary expression contains a random generator. It may be re-evaluated at unpredictable times, generating a new value. However, the use of a random generator in an assignment expression is safe. Examples:

```
D:DRIFT,L=0.01*RANF();     // a drift space with rand. length,
                           // may change during execution.
REAL P=EVAL(0.001*TGAUSS(X));  // Evaluated once and stored as a constant.
```

10.8 Operands in Expressions

A real expression may contain the operands listed in the following subsections.

10.8.1 Literal Constants

Numerical values are entered like FORTRAN constants. Real values are accepted in INTEGER or REAL format. The use of a decimal exponent, marked by the letter `D` or `E`, is permitted.

Examples:

```
1, 10.35, 5E3, 314.1592E-2
```

10.8.2 Symbolic constants

OPAL recognizes a few built-in mathematical and physical constants (see <<tab_constant>). Their names must not be used for user-defined labels. Additional symbolic constants may be defined to simplify their repeated use in statements and expressions.

***OPAL* name**	**Mathematical symbol**	**Value**	**Unit**
`PI`	π	3.14159265358979323846	1
`TWOPI`	2π	6.28318530717958647692	1
`RADDEG`	$180/\pi$	57.29577951308232087685	rad/deg
`DEGRAD`	$\pi/180$	0.01745329251994329576922	deg/rad
`E`	e	2.7182818284590452354	1
`EMASS`	m_e	0.51099895000e-03	GeV
`MUMASS`	m_μ	0.1056583755	GeV
`PMASS`	m_p	0.93827208816	GeV
`DMASS`	m_d	2.013553212745 * `AMU`	GeV
`HMMASS`	m_{hm}	1.00837 * `AMU`	GeV
`H2PMASS`	m_{h2p}	2.01510 * `AMU`	GeV
`ALPHAMASS`	m_α	4.001506179127 * `AMU`	GeV
`CMASS`	m_c	11.9967074146787 * `AMU`	GeV
`XEMASS`	m_{xe}	128.87494026 * `AMU`	GeV
`UMASS`	m_u	237.999501 * `AMU`	GeV
`CLIGHT`	c	299792458	m/s
`AMU`		0.93149410242	GeV
OPALVERSION		120	for 1.2.0
`RANK`		$0 \ldots N_p - 1$	1

Table 19: Predefined Symbolic Constants

Here the `RANK` represents the MPI-Rank of the process and N_p the total number of MPI processes.

10.8.3 Variable labels

Often a set of numerical values depends on a common variable parameter. Such a variable must be defined as a global variable by one of

```
REAL X=expression;
REAL X:=expression;
VECTOR X=vector-expression;
VECTOR X:=vector-expression;
```

When such a variable is used in an expression, *OPAL* uses the current value of the variable. When the value is a constant or an expression preceded by the delimiter = it is evaluated immediately and the result is assigned to the variable as a constant. When the value is an expression preceded by the delimiter := the expression is retained and re-evaluated whenever one of its operands changes. Example:

```
REAL L=1.0;
REAL X:=L;
D1:DRIFT,L:=X;
D2:DRIFT,L:=2.0-X;
```

When the value of `X` is changed, the lengths of the drift spaces are recalculated as `X` and `2-X` respectively.

10.8.4 Element or command attributes

In arithmetic expressions the attributes of physical elements or commands can occur as operands. They are named respectively by

```
element-name->attribute-name
command-name->attribute-name
```

If they are arrays, they are denoted by

```
element-name->attribute-name[index]
command-name->attribute-name[index]
```

Values are assigned to attributes in element definitions or commands.

Example:

```
D1:DRIFT,L=1.0;
D2:DRIFT,L=2.0-D1->L;
```

`D1`→`L` refers to the length `L` of the drift space `D1`.

10.8.5 Deferred Expressions and Random Values

Definition of random machine imperfections requires evaluation of expressions containing random functions. These are not evaluated like other expressions before a command begins execution, but sampled as required from the distributions indicated when errors are generated. Such an expression is known as a **deferred expression**. Its value cannot occur as an operand in another expression.

10.9 Element Selection

Many *OPAL* commands allow for the possibility to process or display a subset of the elements occurring in a beam line or sequence. This is not yet available in *OPAL-t* and *OPAL-cycl*.

10.9.1 Element Selection

A `place` denotes a single element, or the position **following** that element. It can be specified by one of the choices

object-name[index] The name `object-name` is the name of an element, line or sequence, and the integer `index` is its occurrence count in the beam line. If the element is unique, `[index]` can be omitted.

#S denotes the position before the first physical element in the **full** beam line. This position can also be written `#0`.

#E denotes the position after the last physical element in the **full** beam line.

Either form may be qualified by one or more beam line names, as described by the formal syntax:

```
place ::= element-name |
          element-name "[" integer "]" |
          "#S" |
          "#E" |
          line-name "::" place
```

An omitted index defaults to one. Examples: assume the following definitions:

```
M: MARKER;
S: LINE=(C,M,D);
L: LINE=(A,M,B,2*S,A,M,B);
   SURVEY,LINE=L
```

The line `L` is equivalent to the sequence of elements

```
A,M,B,C,M,D,C,M,D,A,M,B
```

Some possible `place` definitions are:

C[1] The first occurrence of element `C`.

#S The beginning of the line `L`.

M[2] The second marker `M` at top level of line `L`, i. e. the marker between second `A` and the second `B`.

#E The end of line `L`

S[1]::M[1] The marker `M` nested in the first occurrence of `S`.

10.9.2 Range Selection

A `range` in a beam line (see Chapter Beam Lines) is selected by the following syntax:

```
range ::= place |
          place "/" place
```

This denotes the range of elements from the first`place` to the second `place`. Both positions are included. A few special cases are worth noting:

- When `place1` refers to a `LINE` (see Chapter Beam Lines), the range starts at the **beginning** of this line.
- When `place2` refers to a `LINE` (see Chapter Beam Lines), the range ends at the **ending** of this line.
- When both `place` specifications refer to the same object, then the second can be omitted. In this case, and if `place` refers to a `LINE` (see Chapter Beam Lines) the range contains the whole of the line.

Examples: Assume the following definitions:

```
M: MARKER;
S: LINE=(C,M,D);
L: LINE=(A,M,B,2*S,A,M,B);
```

The line L is equivalent to the sequence of elements

```
A,M,B,C,M,D,C,M,D,A,M,B
```

Examples for `range` selections:

#S/#E The full range or `L`.

A[1]/A[2] `A[1]` through `A[2]`, both included.

S::M/S[2]::M From the marker `M` nested in the first occurrence of `S`, to the marker `M` nested in the second occurrence of `S`.

S[1]/S[2] Entrance of first occurrence of `S` through exit of second occurrence of `S`.

10.10 Constraints

Please note this is not yet available in *OPAL-t* and *OPAL-cycl*.

In matching it is desired to specify equality constraints, as well as lower and upper limits for a quantity. *OPAL* accepts the following form of constraints:

```
constraint          ::= array-expr constraint-operator array-expr

constraint-operator ::= "==" | "<" | ">"
```

10.11 Variable Names

A variable name can have one of the formats:

```
   variable name ::= real variable |
                     object"->"real attribute
```

The first format refers to the value of the global variable (see Section 10.8.3), the second format refers to a named `attribute` of the named `object`. `object` can refer to an element or a command

10.12 Regular Expressions

Some commands allow selection of items via a `regular-expression`. Such a pattern string **must** be enclosed in single or double quotes; and the case of letters is significant. The meaning of special characters follows the standard UNIX usage:

. Stands for a single arbitrary character,

[letter...letter] Stands for a single character occurring in the bracketed string, Example: `[abc]` denotes the choice of one of `a,b,c`.

[character-character] Stands for a single character from a range of characters, Example: `[a-zA-Z]` denotes the choice of any letter.

***** Allows zero or more repetitions of the preceding item, Example: `[A-Z]*` denotes a string of zero or more upper case letters.

\character Removes the special meaning of `character`, Example: `\*` denotes a literal asterisk.

All other characters stand for themselves. The pattern

```
"[A-Za-z][A-Za-z0-9_']*"
```

illustrates all possible unquoted identifier formats (see Section 10.2). Since identifiers are converted to lower case, after reading they will match the pattern

```
"[a-z][a-z0-9_']*"
```

Examples for pattern use:

```
SELECT,PATTERN="D.."
SELECT,PATTERN="K.*QD.*\.R1"
```

The first command selects all elements whose names have exactly three characters and begin with the letter `D`. The second command selects definitions beginning with the letter `K`, containing the string `QD`, and ending with the string `.R1`. The two occurrences of `.*` each stand for an arbitrary number (including zero) of any character, and the occurrence `\.` stands for a literal period.

10.13 Arrays

An attribute array is a set of values of the same attribute type (see Section 10.3). Normally an array is entered as a list in braces:

```
{value,...,value}
```

The list length is only limited by the available storage. If the array has only one value, the braces (``) can be omitted:

```
value
```

10.13.1 Logical Arrays

For the time being, logical arrays can only be given as a list. The formal syntax is:

```
logical-array ::= "{" logical-list "}"

logical-list  ::= logical-expr |
                  logical-list "," logical-expr
```

Example:

```
{true,true,a==b,false,x>y && y>z,true,false}
```

10.13.2 Real Arrays

Real arrays have the following syntax:

```
array-ref     ::= array-variable |
                  object "->" array-attribute |

table-ref     ::= "ROW" "(" table "," place ")" |
                  "ROW" "(" table "," place "," column-list ")"
                  "COLUMN" "(" table "," column ")" |
                  "COLUMN" "(" table "," column "," range ")"

columns       ::= column |
                  "{" column-list "}"

column-list   ::= column |
                  column-list "," column

column        ::= string

real-list     ::= real-expr |
                  real-list "," real-expr

index-select  ::= integer |
                  integer "," integer |
                  integer "," integer "," integer

array-primary ::= "{" real-list "}" |
                  "TABLE" "(" index-select "," real-expr ")" |
                  array-ref |
                  table-ref |
                  array-function-name "(" arguments ")" |
                  (array-expression)

array-factor  ::= array-primary |
                  array-factor "^" array-primary

array-term    ::= array-factor |
                  array-term "*" array-factor |
                  array-term "/" array-factor

array-expr    ::= array-term |
                  "+" array-term |
                  "-" array-term |
                  array-expr "+" array-term |
                  array-expr "-" array-term |
```

Function	**Meaning**	**result type**	**argument type**
`TRUNC(X)`	truncate `X` towards zero (discard fractional part)	real array	real array
`ROUND(X)`	round `X` to nearest integer	real array	real array
`FLOOR(X)`	return largest integer not greater than `X`	real array	real array
`CEIL(X)`	return smallest integer not less than `X`	real array	real array
`SIGN(X)`	return sign of `X` (+1 for `X` positive, -1 for `X` negative, 0 for `X` zero)	real array	real array
`SQRT(X)`	return square root of `X`	real array	real array
`LOG(X)`	return natural logarithm of `X`	real array	real array
`EXP(X)`	return exponential to the base *e* of `X`	real array	real array
`SIN(X)`	return trigonometric sine of `X`	real array	real array
`COS(X)`	return trigonometric cosine of `X`	real array	real array
`ABS(X)`	return absolute value of `X`	real array	real array
`TAN(X)`	return trigonometric tangent of `X`	real array	real array
`ASIN(X)`	return inverse trigonometric sine of `X`	real array	real array
`ACOS(X)`	return inverse trigonometric cosine of `X`	real array	real array
`ATAN(X)`	return inverse trigonometric tangent of `X`	real array	real array
`TGAUSS(X)`	random number, Gaussian distribution with σ=1, truncated at `X`	real array	real array
`USER1(X)`	random number, user-defined distribution with one parameter	real array	real array
`EVAL(X)`	evaluate the argument immediately and transmit it as a constant	real array	real array

Table 20: Real Array Functions in *OPAL* (acting component-wise)

Example:

```
{a,a+b,a+2*b}
```

There are also three functions allowing the generation of real arrays:

TABLE Generate an array of expressions:

```
TABLE(n2,expression)    // implies
                        // TABLE(1:n2:1,expression)
TABLE(n1:n2,expression) // implies
                        // TABLE(n1:n2:1,expression)
TABLE(n1:n2:n3,expression)
```

These expressions all generate an array with `n2` components. The components selected by `n1:n2:n3` are filled from the given `expression`; a C pseudo-code for filling is

```
int i;
for (i = n1; i <= n2; i += n3) a[i] = expression(i);
```

In each generated expression the special character hash sign (#) is replaced by the current value of the index i.

Example:

```
// an array with 9 components, evaluates to
// {1,4,7,10,13}:
table(5:9:2,3*#+1) // equivalent to
                   // {0,0,0,0,16,0,22,0,28}
```

ROW Generate a table row:

```
ROW(table,place)             // implies all columns
ROW(table,place,column list)
```

This generates an array containing the named (or all) columns in the selected place.

COLUMN Generate a table column:

```
COLUMN(table,column)         // implies all rows
COLUMN(table,column,range)
```

This generates an array containing the selected (or all) rows of the named column.

10.13.3 String Arrays

String arrays can only be given as lists of single values. For permissible values String values see Section 10.4.

Example:

```
{A, "xyz", A & STRING(X)}
```

10.13.4 Token List Arrays

Token list arrays are always lists of single token lists.

Example:

```
{X:12:8,Y:12:8}
```

Chapter 11

Control Statements

11.1 Getting Help

11.1.1 HELP Command

A user who is uncertain about the attributes of a command should try the command `HELP`, which has three formats:

```
HELP;                   // Give help on the "HELP" command
HELP,NAME=label;        // List funct. and attr. types of
                        // "label"
HELP,label;             // Shortcut for the second format
```

`label` is an identifier (see Identifiers or Labels). If it is non-blank, *OPAL* prints the function of the object `label` and lists its attribute types. Entering `HELP` alone displays help on the `HELP` command.

Examples:

```
HELP;
HELP,NAME=FIELDSOLVER;
HELP,FIELDSOLVER;
```

11.2 STOP / QUIT Statement

The statement

```
STOP or QUIT;
```

terminates execution of the *OPAL* program, or, when the statement occurs in a `CALL` file (see Section 11.7.1), returns to the calling file. Any statement following the `STOP` or `QUIT` statement is ignored.

11.3 OPTION Statement

The `OPTION` command controls global command execution and sets a few global quantities. Each of the settings options are listed in Table 21 with their corresponding default values.

```
OPTION, VERSION=integer, ECHO=logical,INFO=logical,TRACE=logical,
        WARN=logical, SEED=real, PSDUMPFREQ=integer,
        STATDUMPFREQ=integer, SPTDUMFREQ=integer,
        REPARTFREQ=integer, REBINFREQ=integer, TELL=logical;
```

VERSION Used to indicate for which version of *OPAL* the input file is written. The major and minor versions of *OPAL* and of the input file have to match. The patch version of *OPAL* must be greater or equal to the patch version of the input file. If the version doesn't fulfill above criteria *OPAL* stops immediately and prints instructions on how to convert the input file. Starting with version 1.6.0 of *OPAL* the option `VERSION` is mandatory in the *OPAL* input file. The format is `Mmmpp` where `M` stands for the major, `m` for the minor and `p` for the patch version. For version 1.6.0 of *OPAL* `VERSION` should read `10600`.

The next five logical flags activate or deactivate execution options:

ECHO Controls printing of an echo of input lines on the standard error file. Its default value is false.

INFO If this option is turned off, *OPAL* suppresses all information messages. It also affects the *gnu.out* and *eb.out* files in case of *OPAL-cycl* simulations (see OPAL-cycl output field maps). The level of information showed is controlled with `--info` command line (see Table 4) Its default value is true.

TELL If true, the current option settings are listed. Must be the last option in the input file in order to render correct results. Its default value is false.

TRACE If true, print execution trace. Must be the first option in the inputfile in order to render correct results. Its default value is false.

WARN If this option is turned off, *OPAL* suppresses all warning messages. Its default value is true.

The remaining options (ordered alphabetically) are used to control diverse *OPAL* features:

AMR Enable adaptive mesh refinement (see AMR Solver). Its default value is false.

AMR_REGRID_FREQ Defines after how many steps an AMR regrid is performed. Its default value is 10.

AMR_YT_DUMP_FREQ The frequency to dump grid and particle data for AMR. Its default value is 10.

ASCIIDUMP If true, instead of HDF5, ASCII output is generated for the following elements: Collimator, Geometry, Monitor, Probe, Stripper, Vacuum and global losses. Its default value is false.

AUTOPHASE Defines how accurate the search for the phase at which the maximal energy is gained should be. The higher this number the more accurate the phase will be. If it is set to 0 then the auto-phasing algorithm isn't run. Its default value is 6.

BEAMHALOBOUNDARY Defines in terms of sigma where the halo starts. Only used in *OPAL-cycl*. Its default value is 0.0.

BOUNDPDESTROYFQ The frequency to delete particles which are too far away from the center of beam. Only used in *OPAL-cycl*. Its default value is 10.

CLOTUNEONLY If set to true, stop after closed orbit finder and tune calculation. Only used in *OPAL-cycl*. Its default value is false.

COMPUTEPERCENTILES If true, the 68 (1 sigmas for normal distribution), the 95 (2 sigmas), the 99.7 (3 sigmas) and the 99.99 (4 sigmas) percentiles of the bunch size and the normalized emittance are calculated. The data are stored into *.stat* output file and loss file in HDF5 format (*.h5*). The calculation is performed whenever the number of particles exceeds 100. Its default value is false.

CSRDUMP If true the electric csr field component, E_z, line density and the derivative of the line density is written into the *data* directory. The first line gives the average position of the beam bunch. Subsequent lines list z position of longitudinal mesh (with respect to the head of the beam bunch), E_z, line density and the derivative of the line density. Note that currently the line density derivative needs to be scaled by the inverse of the mesh spacing to get the correct value. The CSR field is dumped at each time step of the calculation. Each text file is named "Bend Name" (from input file) + "-CSRWake" + "time step number in that bend (starting from 1)" + ".txt". Its default value is false.

CZERO If true the distributions are generated such that the centroid is exactly zero and not statistically dependent. Its default value is false.

DELPARTFREQ The frequency to delete particles in *OPAL-cycl*. Its default value is 1.

DUMPBEAMMATRIX If true, the 6-dimensional beam matrix (upper triangle only) is stored in the statistics output file (*.stat*). Its default value is false.

EBDUMP If true the electric and magnetic field on the particle is saved each time a phase space is written. Its default value is false.

ENABLEHDF5 If true (default), HDF5 read and write is enabled.

ENABLEVTK If true (default), VTK write of geometry voxel mesh is enabled.

HALOSHIFT Constant parameter to shift halo value. Its default value is 0.0.

IDEALIZED Instructs to use the hard edge model for the calculation of the path length in *OPAL-t*. The path length is computed to place the elements in the three-dimensional space from `ELEMEDGE`. Its default value is false.

LOGBENDTRAJECTORY Save the reference trajectory inside dipoles in an ASCII file. For each dipole a separate file is written to the directory *data/*. Its default value is false.

MEMORYDUMP If true, it writes the memory consumption of every core to a SDDS file (*.mem*). The write frequency corresponds to `STATDUMPFREQ`. Its default value is false.

MINBINEMITTED The number of bins that have to be emitted before the bin are squashed into a single bin. Its default value is 10.

MINSTEPFORREBIN The number of steps into the simulation before the bins are squashed into a single bin. This should be used instead of the global variable of the same name. Its default value is 200.

MTSSUBSTEPS Only used for multiple-time-stepping (`MTS`) integrator in *OPAL-cycl*. Specifies how many sub-steps for external field integration are done per step. Making less steps per turn and increasing this value is the recommended way to reduce space charge solve frequency. Its default value is 1.

NLHS Number of stored old solutions for extrapolating the new starting vector. Default value is 1 and just the last solution is used.

NUMBLOCKS Maximum number of vectors in the Krylov space for `ITSOLVER=CG` or `ITSOLVER=GMRES` (see FIELDSOLVER command). Its default value is 0.

PSDUMPFREQ Defines after how many time steps the phase space is dumped into the H5hut file (*.h5*). It also controls the frequency of phase space printed on the standard output. Its default value is 10.

PSDUMPEACHTURN Control option of phase space dumping. If true, dump phase space after each turn. For the time being, this is only use for multi-bunch simulation in *OPAL-cycl*. Its default value is false.

PSDUMPFRAME Control option that defines the frame in which the phase space data is written for *.h5* and *.stat* files. Beware that the data is written in a given time step. Most accelerator physics quantities are defined at a given s-step where s is distance along the reference trajectory. For non-isochronous accelerators, particles at a given time step can be quite a long way away from the reference particle, yielding unexpected results. Currently only available for *OPAL-cycl*. In *OPAL-t* the phase-space is always written in the frame of the reference particle.

- `GLOBAL`: data is written in the global Cartesian frame;
- `BUNCH_MEAN`: data is written in the bunch mean frame or;
- `REFERENCE`: data is written in the frame of the reference particle.

REBINFREQ Defines after how many time steps we update the energy Bin ID of each particle. For the time being. Only available for multi-bunch simulation in *OPAL-cycl*. Its default value is 100.

RECYCLEBLOCKS Number of vectors in the recycle space for `ITSOLVER=CG` or `ITSOLVER=GMRES` (see FIELDSOLVER command). Its default value is 0.

REMOTEPARTDEL Artificially delete remote particles if their distances to the beam centroid is larger than `REMOTEPARTDEL` times of the beam rms size. In *OPAL-t* only the longitudinal component of the particles is considered. In *OPAL-cycl* all components are considered if the the value is negative (further on using its absolute value) and only the transverse components if the value is positive. Its default value is 0.0, i.e. no particles are deleted.

REPARTFREQ Defines after how many time steps we do particles repartition to balance the computational load of the computer nodes. Its default value is 10.

RHODUMP If true the scalar ρ field is saved each time a phase space is written. There exists a reader in Visit with versions greater or equal 1.11.1. Its default value is false.

RNGTYPE The name (see String Attributes) of a random number generator can be provided. The default random number generator (RANDOM) is a portable 48-bit generator. Three quasi random generators are available: `HALTON`, `SOBOL` and `NIEDERREITER`. For details see the GSL reference manual (18.5).

SCSOLVEFREQ If the space charge field is slowly varying w.r.t. external fields, this option allows to change the frequency of space charge calculation, i.e. the space charge forces are evaluated every `SCSOLVEFREQ` step and then reused for the following steps. Affects integrators `LF2` and `RK4` of *OPAL-cycl*. Its default value is 1. Note: as the multiple-time-stepping (`MTS`) integrator maintains accuracy much better with reduced space charge solve frequency, this option should probably not be used anymore.

SEED Selects a particular sequence of random values. A `SEED` value is an integer in the range [0...999999999] (default: 123456789). `SEED` can be an expression. If `SEED` = -1, the time is used as seed and the generator is not portable anymore. See also Deferred Expressions and Random Values.

SPTDUMPFREQ Defines after how many time steps we dump the phase space of single particle in *OPAL-cycl*. It is always useful to record the trajectory of reference particle or some specified particle for primary study. Its default value is 1.

STATDUMPFREQ Defines after how many time steps we dump statistical data, such as RMS beam emittance, to the *.stat* file. Its default value is 10.

AMR	= FALSE	AMR_REGRID_FREQ	= 10	AMR_YT_DUMP_FREQ	= 10
ASCIIDUMP	= FALSE	AUTOPHASE	= 6	BEAMHALOBOUNDARY	= 0.0
BOUNDPDESTROYFQ	= 10	CLOTUNEONLY	= FALSE	COMPUTEPERCENTILES	= FALSE
CSRDUMP	= FALSE	CZERO	= FALSE	DELPARTFREQ	= 1
DUMPBEAMMATRIX	= FALSE	EBDUMP	= FALSE	ECHO	= FALSE
ENABLEHDF5	= TRUE	ENABLEVTK	= TRUE	HALOSHIFT	= 0.0
IDEALIZE	= FALSE	INFO	= TRUE	LOGBENDTRAJECTORY	= FALSE
MEMORYDUMP	= FALSE	MINBINEMITTED	= 10	MINSTEPFORREBIN	= 200
MTSSUBSTEPS	= 1	NLHS	= 1	NUMBLOCKS	= 0
PSDUMPEACHTURN	= FALSE	PSDUMPFRAME	= GLOBAL	PSDUMPFREQ	= 10
RECYCLEBLOCKS	= 0	REBINFREQ	= 100	REMOTEPARTDEL	= 0.0
REPARTFREQ	= 10	RHODUMP	= FALSE	RNGTYPE	= RANDOM
SCSOLVEFREQ	= 1	SEED	= 123456789	SPTDUMPFREQ	= 1
STATDUMPFREQ	= 10	TELL	= FALSE	TRACE	= FALSE
VERSION	= none	WARN	= TRUE		

Table 21: Default settings for Options

11.4 Parameter Statements

11.4.1 Variable Definitions

OPAL recognizes several types of variables.

11.4.1.1 Real Scalar Variables

```
REAL variable-name=real-expression;
```

For backward compatibility the program also accepts the form

```
REAL variable-name:=real-expression;
```

This statement creates a new global variable `variable-name` and discards any old variable with the same name. Its value depends on all quantities occurring in real-expression (see Real Expressions). Whenever an operand changes in `real-expression`, a new value is calculated. The definition may be thought of as a mathematical equation. However, *OPAL* is not able to solve the equation for a quantity on the right-hand side.

An assignment in the sense of the FORTRAN or C languages can be achieved by using the `EVAL` function (see Section 11.4.4).

A reserved variable is the value `P0` which is used as the global reference momentum for normalizing all magnetic field coefficients. Example:

```
REAL GEV=100;
P0=GEV;
```

Circular definitions are not allowed:

```
X=X+1;    // X cannot be equal to X+1
REAL A=B;
REAL B=A; // A and B are equal, but of unknown value
```

However, redefinitions by assignment are allowed:

```
X=EVAL(X+1);
```

11.4.1.2 Real Vector Variables

```
REAL VECTOR variable-name=vector-expression;
```

In old version of *OPAL* (before 1.6.0) the keyword `REAL` was optional, now it is mandatory!

This statement creates a new global variable `variable-name` and discards any old variable with the same name. Its value depends on all quantities occurring in vector-expression (see Arrays) on the right-hand side. Whenever an operand changes in `vector-expression`, a new value is calculated. The definition may be thought of as a mathematical equation. However, *OPAL* is not able to solve the equation for a quantity on the right-hand side.

Example:

```
REAL VECTOR A = TABLE(10, #);
REAL VECTOR B = { 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 };
```

Circular definitions are not allowed, but redefinitions by assignment are allowed.

11.4.1.3 Logical Variables

```
BOOL variable-name=logical-expression;
```

This statement creates a new global variable `variable-name` and discards any old variable with the same name. Its value depends on all quantities occurring in logical-expression (see Logical Expressions). Whenever an operand changes in `logical-express` a new value is calculated. The definition may be thought of as a mathematical equation. However, *OPAL* is not able to solve the equation for a quantity on the right-hand side.

Example:

```
BOOL FLAG = X != 0;
```

Circular definitions are not allowed, but redefinitions by assignment are allowed.

11.4.2 Symbolic Constants

OPAL recognizes a few build-in built-in mathematical and physical constants (see Table 19). Additional constants can be defined by the command

```
REAL CONST label:CONSTANT=<real-expression>;
```

which defines a constant with the name `label`. The keyword `REAL` is optional, and `label` must be unique. An existing symbolic constant can never be redefined. The `real-expression` is evaluated at the time the `CONST` definition is read, and the result is stored as the value of the constant.

Example:

```
CONST IN=0.0254; // conversion of inches to meters
```

11.4.3 Vector Values

A vector of expressions is established by a statement

```
REAL VECTOR vector-name=vector-expression;
```

The keyword `REAL` is optional. It creates a new global vector `vector-name` and discards any old vector with the same name. Its value depends on all quantities occurring in vector-expression (see Arrays). Whenever an operand changes in `vector-expression`, a new value is calculated. The definition may be thought of as a mathematical equation. However, *OPAL* is not able to solve the equation for a quantity on the right-hand side.

Example:

```
VECTOR A_AMPL={2.5e-3,3.4e-2,0,4.5e-8};
VECTOR A_ON=TABLE(10,1);
```

Circular definitions are not allowed.

11.4.4 Assignment to Variables

A value is assigned to a variable or vector by using the function `EVAL(real- expression)`. When seen, this function is immediately evaluated and replaced by the result treated like a constant.

```
variable-name=EVAL(real-expression);
```

This statement acts like a FORTRAN or C assignment. The `real-expression` or `vector-expression` is **evaluated**, and the result is assigned as a constant to the variable or vector on the left-hand side. Finally the expression is discarded. The `EVAL` function can also be used within an expression, e. g.:

```
vector-name=TABLE(range,EVAL(real-expression));
vector-name={...,EVAL(real-expression),...);
```

A sequence like the following is permitted:

```
...                 // some definitions
REAL X=0;           // create variable X with value
                    // zero
WHILE (X <= 0.10) {
  VALUE, VALUE={X};
  X=EVAL(X+.01);    // increment variable X by 0.01
                    // CANNOT use: X=X+.01;
}
```

11.4.5 VALUE: Output of Expressions

The statement

```
VALUE,VALUE=expression-vector;
```

evaluates a set of expressions using the most recent values of any operands and prints the results on the standard error file.

Example:

```
REAL A=4;
VALUE,VALUE=TABLE(5,#*A);
REAL P1=5;
REAL P2=7;
VALUE,VALUE={P1,P2,P1*P2-3};
```

These commands give the results:

```
value: TABLE(1:5:1,(#*A)) = {4, 8, 12, 16, 20}
value: {P1,P2,P1*P2-3} = {5, 7, 32}
```

This commands serves mainly for printing one or more quantities which depend on matched attributes. It also allows use of *OPAL* as a programmable calculator. One may also tabulate functions.

11.5 Miscellaneous Commands

11.5.1 ECHO Statement

The `ECHO` statement has two formats:

```
ECHO,MESSAGE=message;
ECHO,message;            // shortcut
```

`message` is a string value (see String Attributes). It is immediately transmitted to the `ECHO` stream.

11.5.2 SYSTEM: Execute System Command

The command `SYSTEM` allows to execute operating system commands on a single core. After execution of the system command, successful or not, control returns to *OPAL*. It has two formats:

```
SYSTEM,CMD=string;
SYSTEM,string;          // shortcut
```

The string (see String Attributes) `string` must be a valid operating system command.

Most UNIX commands can be issued directly.

Example:

```
SYSTEM,"ls -l"
```

causes a listing of the current directory in long form on the terminal.

The `SYSTEM` command can also be used to execute an external script.

Below is an example that generates a random seed with python. The python script gen_seed.py is called with the `SYSTEM` command. This scripts writes the seed to a file gen_seed.opal that can be read with the `CALL` command.

```
SYSTEM, "python gen_seed.py";
CALL, "gen_seed.opal";
```

11.5.3 PSYSTEM: Execute System Command in Parallel

Also the command PSYSTEM allows to execute operating system commands. But contrary to the command SYSTEM this command is executed on all cores.

11.6 TITLE Statement

The TITLE statement has three formats:

```
TITLE,STRING=page-header;   // define new page header
TITLE,page-header;          // shortcut for first format
TITLE,STRING="";            // clear page header
```

page-header is a string value (see String Attributes). It defines the page header which will be used as a title for subsequent output pages. Before the first TITLE statement is encountered, the page header is empty. It can be redefined at any time.

11.7 File Handling

11.7.1 CALL Statement

The CALL command has two formats:

```
CALL,FILE=file-name;
CALL,file-name;
```

file-name is a string (see String Attributes). The statement causes the input to switch to the named file. Input continues on that file until a STOP or an end of file is encountered. Example:

```
CALL,FILE="structure";
CALL,"structure";
```

11.7.2 init.opal

Before entering the main input file, the file $HOME/init.opal is executed (if present). It can be thought of as a CALL, FILE=$HOME/init.opal statement at the start of the input file. This init file can be used to avoid writing the same lines in every input file. For example one can set some OPTION, define a MACRO, or define some physics constants.

Note that one should be well aware of the contents of the init.opal file as otherwise it might lead to confusion when switching to a different computer where the file is not present. Therefore, it might be advisable to use an explicit CALL statement instead.

Example:

```
// this is a init.opal file
// all OPAL runs will use the same OPTIONs
OPTION, ECHO=FALSE;
OPTION, INFO=FALSE;              //psdump and statdump are in time steps
OPTION, PSDUMPFREQ = 10000000;   //How often 6d info is dumped to _.h5_
OPTION, STATDUMPFREQ = 10;       //How often beam stats dumped to _.stat_
OPTION, BOUNDPDESTROYFQ=10;      //Delete lost particles, if any
OPTION, AUTOPHASE=4;             //Always leave this on, unless doing a phase scan
OPTION, VERSION=20000;
```

11.8 IF: Conditional Execution

Conditional execution can be requested by an `IF` statement. It allows usages similar to the C language `if` statement:

```
IF (logical) statement;
IF (logical) statement; ELSE statement;
IF (logical) { statement-group; }
IF (logical) { statement-group; }
  ELSE { statement-group; }
```

Note that all statements must be terminated with semicolons (`;`), but there is no semicolon after a closing brace. The statement or group of statements following the `IF` is executed if the condition is satisfied. If the condition is false, and there is an `ELSE`, the statement or group following the `ELSE` is executed.

11.9 WHILE: Repeated Execution

Repeated execution can be requested by a `WHILE` statement. It allows usages similar to the C language `while` statement:

```
WHILE (logical) statement;
WHILE (logical) { statement-group; }
```

Note that all statements must be terminated with semicolons (`;`), but there is no semicolon after a closing brace. The condition is re-evaluated in each iteration. The statement or group of statements following the `WHILE` is repeated as long as the condition is satisfied. Of course some variable(s) must be changed within the `WHILE` group to allow the loop to terminate.

11.10 MACRO: Macro Statements (Subroutines)

Subroutine-like commands can be defined by a `MACRO` statement. It allows usages similar to C language function call statements. A macro is defined by one of the following statements:

```
name(formals): MACRO { token-list }
name(): MACRO { token-list }
```

A macro may have formal arguments, which will be replaced by actual arguments at execution time. An empty formals list is denoted by `()`. Otherwise the `formals` consist of one or more names, separated by commas. The `token-list` consists of input tokens (strings, names, numbers, delimiters etc.) and is stored unchanged in the definition.

A macro is executed by one of the statements:

```
name(actuals);
name();
```

Each actual consists of a set of tokens which replaces all occurrences of the corresponding formal name. The actuals are separated by commas. Examples:

```
// macro definitions:
SHOWIT(X): MACRO {
   VALUE,VALUE={X};
}
DOIT(): MACRO {
   DYNAMIC,LINE=RING,FILE="DYNAMIC.OUT";
}
KS(X,Y): MACRO {
   Y = 3e-3*X+0.5e-3;
}

// macro calls:
```

```
SHOWIT(PI);
DOIT();
REAL X = 2;
REAL Y;
KS(X, Y);
SHOWIT(Y);
```

Chapter 12

Elements

12.1 Element Input Format

All physical elements are defined by statements of the form

```
label:keyword, attribute,..., attribute
```

where

label Is the name to be given to the element (in the example QF), it is an identifier (see Identifiers or Labels).

keyword Is a keyword (see Identifiers or Labels), it is an element type keyword (in the example `QUADRUPOLE`),

attribute normally has the form

```
attribute-name=attribute-value
```

attribute-name selects the attribute from the list defined for the element type `keyword` (in the example `L` and `K1`). It must be an identifier (see Identifiers or Labels).

attribute-value gives it a value (see Command Attribute Types) (in the example `1.8` and `0.015832`).

Omitted attributes are assigned a default value, normally zero.

Example:

```
QF: QUADRUPOLE, L=1.8, K1=0.015832;
```

12.2 Common Attributes for all Elements

The following attributes are allowed on all elements:

TYPE A string value (see String Attributes). It specifies an "engineering type" and can be used for element selection.

APERTURE A string value (see String Attributes) which describes the element aperture. All but the last attribute of the aperture have units of meter, the last one is optional and is a positive real number. Possible choices are

- `APERTURE`="SQUARE(a,f)" has a square shape of width and height `a`,
- `APERTURE`="RECTANGLE(a,b,f)" has a rectangular shape of width `a` and height `b`,
- `APERTURE`="CIRCLE(d,f)" has a circular shape of diameter `d`,

- `APERTURE`="ELLIPSE(a,b,f)" has an elliptical shape of major `a` and minor `b`.

  The option `SQUARE(a, f)` is equivalent to `RECTANGLE(a, a, f)` and `CIRCLE(d, f)` is equivalent to `ELLIPSE(d, d, f)`. The size of the exit aperture is scaled by a factor f. For $f < 1$ the exit aperture is smaller than the entrance aperture, for $f = 1$ they are the same and for $f > 1$ the exit aperture is bigger.

  Dipoles have `GAP` and `HGAP` which define an aperture and hence do not recognise `APERTURE`. The aperture of the dipoles has rectangular shape of height `GAP` and width `HGAP`. In longitudinal direction it is bent such that its center coincides with the circular segment of the reference particle when ignoring fringe fields. Between the beginning of the fringe field and the entrance face and between the exit face and the end of the exit fringe field the rectangular shape has width and height that are twice of what they are inside the dipole.

  Default aperture for all other elements is a circle of 1.0m.

L The length of the element (default: 0m).

ELEMEDGE The edge of an element is specified in s coordinates in meters. This edge corresponds to the origin of the local coordinate system and is the physical start of the element. (Note that in general the fields will extend in front of this position.) The physical end of the element is determined by `ELEMEDGE` and its physical length. (Note again that in general the fields will extend past the physical end of the element.)

X X-component of the position of the element relative to the position of the first beamline which it is part of and which uses absolute positioning.

Y Y-component of the position of the element relative to the position of the first beamline which it is part of and which uses absolute positioning.

Z Z-component of the position of the element relative to the position of the first beamline which it is part of and which uses absolute positioning.

THETA Rotation angle of the element about the y-axis relative to the orientation of the first beamline which it is part of and which uses absolute positioning.

PHI Rotation angle of the element about the x-axis relative to the orientation of the first beamline which it is part of and which uses absolute positioning.

PSI Rotation angle of the element about the z-axis relative to the orientation of the first beamline which it is part of and which uses absolute positioning.

DX Error on x-component of position of element. Doesn't affect the design trajectory.

DY Error on y-component of position of element. Doesn't affect the design trajectory.

DZ Error on z-component of position of element. Doesn't affect the design trajectory.

DTHETA Error on angle `THETA`. Doesn't affect the design trajectory.

DPHI Error on angle `PHI`. Doesn't affect the design trajectory.

DPSI Error on angle `PSI`. Doesn't affect the design trajectory.

WAKEF Attach wakefield that was defined using the `WAKE` command.

PARTICLEMATTERINTERACTION Attach a handler for particle-matter interaction (see Chapter Particle Matter Interaction).

OUTFN The file name into which the element should write the collected data. The user must only provide the output name without the extension. The extension will be set according to the OPTION statements. If this attribute is empty, the file will be named as the element label.

DELETEONTRANSVERSEEXIT Particles that exit elements on their sides get deleted in *OPAL-t*. The user can control this behavior by setting this attribute. If its value is `TRUE` then particles that exit on the sides are deleted (default), with `FALSE` they are kept.

All elements can have arbitrary additional attributes which are defined in the respective section.

12.3 Drift Spaces

```
label: DRIFT, TYPE=string, APERTURE=string, L=real;
```

A `DRIFT` space has no additional attributes. Examples:

```
DR1:DRIFT, L=1.5;
DR2:DRIFT, L=DR1->L, TYPE=DRF;
```

The length of `DR2` will always be equal to the length of `DR1`. The reference system for a drift space is a Cartesian coordinate system. This is a restricted feature of *OPAL-t*. In *OPAL-t* drifts are implicitly given, if no field is present.

12.4 Bending Magnets

Bending magnets refer to dipole fields that bend particle trajectories. Currently *OPAL* supports the following different bend elements: `RBEND`, (valid in *OPAL-t*, see Section 12.4.1), `SBEND` (valid in *OPAL-t*, see Section 12.4.3), `RBEND3D`, (valid in *OPAL-t*, see Section 12.4.2) and `SBEND3D` (valid in *OPAL-cycl*, see Section 12.4.7).

Describing a bending magnet can be somewhat complicated as there can be many parameters to consider: bend angle, bend radius, entrance and exit angles etc. Therefore we have divided this section into several parts:

1. Section 12.4.1 and Section 12.4.3 describe the geometry and attributes of the *OPAL-t* bend elements `RBEND` and `SBEND`.
2. Section 12.4.4 describes how to implement an `RBEND` or `SBEND` in an *OPAL-t* simulation.
3. Section 12.4.7 is self contained. It describes how to implement an `SBEND3D` element in an *OPAL-cycl* simulation.

Figure 16 illustrates a general rectangular bend (`RBEND`) with a positive bend angle α. The entrance edge angle, E_1, is positive in this example. An `RBEND` has parallel entrance and exit pole faces, so the exit angle, E_2, is uniquely determined by the bend angle, α, and E_1 ($E_2 = \alpha - E_1$). For a positively charge particle, the magnetic field is directed out of the page.

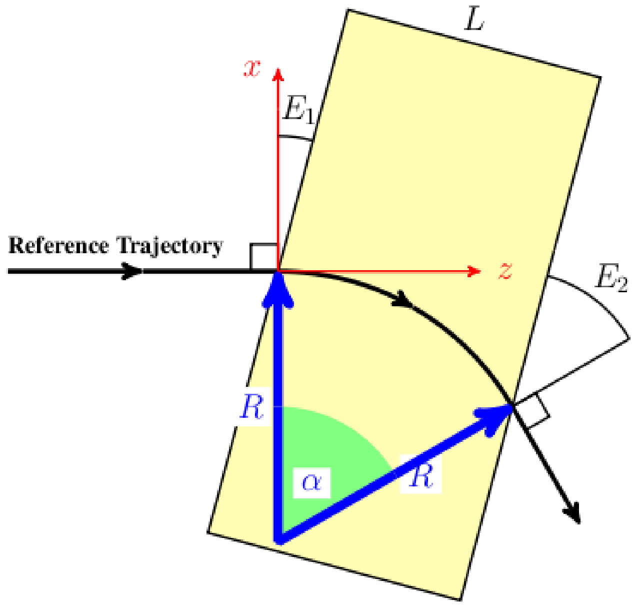

Figure 16: Illustration of a general rectangular bend (`RBEND`) with a positive bend angle α.

12.4.1 RBend (*OPAL-t*)

An `RBEND` is a rectangular bending magnet. The key property of an `RBEND` is that it has parallel pole faces. Figure 16 shows an `RBEND` with a positive bend angle and a positive entrance edge angle.

L Physical length of magnet (meters, see Figure 16).

GAP Full vertical gap of the magnet (meters).

HAPERT Non-bend plane aperture of the magnet (meters). (Defaults to one half the bend radius.)

ANGLE Bend angle (radians). Field amplitude of bend will be adjusted to achieve this angle. (Note that for an `RBEND`, the bend angle must be less than $\frac{\pi}{2}+E1$, where `E1` is the entrance edge angle.)

K0 Field amplitude in y direction (Tesla). If the `ANGLE` attribute is set, `K0` is ignored.

K0S Field amplitude in x direction (Tesla). If the `ANGLE` attribute is set, `K0S` is ignored.

K1 Field gradient index of the magnet, $K_1 = -\frac{R}{B_y}\frac{\partial B_y}{\partial x}$, where R is the bend radius as defined in Figure 16. Not supported in *OPAL-t* any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (radians). Figure 16 shows the definition of a positive entrance edge angle. (Note that the exit edge angle is fixed in an `RBEND` element to $\mathrm{E2} = \mathrm{ANGLE} - \mathrm{E1}$).

DESIGNENERGY Energy of the reference particle (MeV). The reference particle travels approximately the path shown in Figure 16.

FMAPFN Name of the field map for the magnet. Currently maps of type 1DProfile1 can be used. The default option for this attribute is `FMAPN` = `1DPROFILE1-DEFAULT` (see Section 12.4.6). The field map is used to describe the fringe fields of the magnet (see 1DProfile1).

12.4.2 RBend3D (*OPAL-t*)

An `RBEND3D3D` is a rectangular bending magnet. The key property of an `RBEND3D` is that it has parallel pole faces. Figure 16 shows an `RBEND3D` with a positive bend angle and a positive entrance edge angle.

L Physical length of magnet (meters, see Figure 16).

GAP Full vertical gap of the magnet (meters).

HAPERT Non-bend plane aperture of the magnet (meters). (Defaults to one half the bend radius.)

ANGLE Bend angle (radians). Field amplitude of bend will be adjusted to achieve this angle. (Note that for an `RBEND3D`, the bend angle must be less than $\frac{\pi}{2}+E1$, where `E1` is the entrance edge angle.)

K0 Field amplitude in y direction (Tesla). If the `ANGLE` attribute is set, `K0` is ignored.

K0S Field amplitude in x direction (Tesla). If the `ANGLE` attribute is set, `K0S` is ignored.

K1 Field gradient index of the magnet, $K_1 = -\frac{R}{B_y}\frac{\partial B_y}{\partial x}$, where R is the bend radius as defined in Figure 16. Not supported in *OPAL-t* any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (radians). Figure 16 shows the definition of a positive entrance edge angle. (Note that the exit edge angle is fixed in an `RBEND3D` element to $\mathrm{E2} = \mathrm{ANGLE} - \mathrm{E1}$).

DESIGNENERGY Energy of the reference particle (MeV). The reference particle travels approximately the path shown in Figure 16.

FMAPFN Name of the field map for the magnet. Currently maps of type 1DProfile1 can be used. The default option for this attribute is `FMAPN` = `1DPROFILE1-DEFAULT` (see Section 12.4.6). The field map is used to describe the fringe fields of the magnet (see 1DProfile1).

Figure 17 illustrates a general sector bend(`SBEND`) with a positive bend angle α. In this example the entrance and exit edge angles E_1 and E_2 have positive values. For a positively charge particle, the magnetic field is directed out of the page.

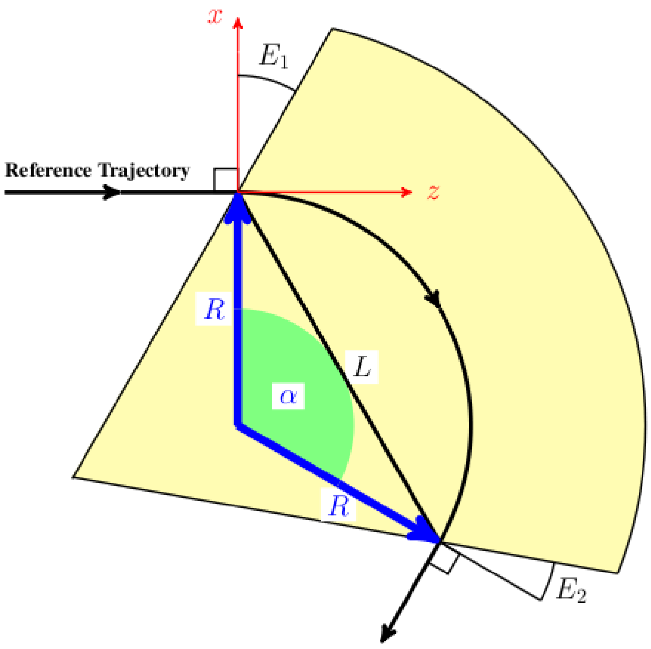

Figure 17: Illustration of a general sector bend (`SBEND`) with a positive bend angle α

12.4.3 SBend (*OPAL-t*)

An `SBEND` is a sector bending magnet. An `SBEND` can have independent entrance and exit edge angles. Figure 17 shows an `SBEND` with a positive bend angle, a positive entrance edge angle, and a positive exit edge angle.

L Chord length of the bend reference arc in meters (see Figure 17), given by: $L = 2R\sin\left(\frac{\alpha}{2}\right)$

GAP Full vertical gap of the magnet (meters).

HAPERT Non-bend plane aperture of the magnet (meters). (Defaults to one half the bend radius.)

ANGLE Bend angle (radians). Field amplitude of the bend will be adjusted to achieve this angle. (Note that practically speaking, bend angles greater than $\frac{3\pi}{2}$ (270 degrees) can be problematic. Beyond this, the fringe fields from the entrance and exit pole faces could start to interfere, so be careful when setting up bend angles greater than this. An angle greater than or equal to 2π (360°) is not allowed.)

K0 Field amplitude in y direction (Tesla). If the `ANGLE` attribute is set, `K0` is ignored.

K0S Field amplitude in x direction (Tesla). If the `ANGLE` attribute is set, `K0S` is ignored.

K1 Field gradient index of the magnet, $K_1 = -\frac{R}{B_y}\frac{\partial B_y}{\partial x}$, where R is the bend radius as defined in Figure 17. Not supported in *OPAL-t* any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (rad). Figure 17 shows the definition of a positive entrance edge angle.

E2 Exit edge angle (rad). Figure 17 shows the definition of a positive exit edge angle.

DESIGNENERGY Energy of the bend reference particle (MeV). The reference particle travels approximately the path shown in Figure 17.

FMAPFN Name of the field map for the magnet. Currently maps of type 1DProfile1 can be used. The default option for this attribute is `FMAPN` = `1DPROFILE1-DEFAULT` (see Section 12.4.6). The field map is used to describe the fringe fields of the magnet (see 1DProfile1).

12.4.4 RBend and SBend Examples (*OPAL-t*)

Describing an RBEND or an SBEND in an *OPAL-t* simulation requires effectively identical commands. There are only slight differences between the two. The L attribute has a different definition for the two types of bends (see Section 12.4.1 and Section 12.4.3), and an SBEND has an additional attribute E2 that has no effect on an RBEND (see Section 12.4.3). Therefore, in this section, we will give several examples of how to implement a bend, using the RBEND and SBEND commands interchangeably. The understanding is that the command formats are essentially the same.

When implementing an RBEND or SBEND in an *OPAL-t* simulation, it is important to note the following:

1. Internally *OPAL-t* treats all bends as positive, as defined by Figure 16 and Figure 17. Bends in other directions within the x/y plane are accomplished by rotating a positive bend about its z axis.
2. If the ANGLE attribute is set to a non-zero value, the K0 and K0S attributes will be ignored.
3. When using the ANGLE attribute to define a bend, the actual beam will be bent through a different angle if its mean kinetic energy doesn't correspond to the DESIGNENERGY.
4. Internally the bend geometry is setup based on the ideal reference trajectory, as shown in Figure 16 and Figure 17.
5. If the default field map, 1DPROFILE-DEFAULT (see Section 12.4.6), is used, the fringe fields will be adjusted so that the effective length of the real, soft edge magnet matches the ideal, hard edge bend that is defined by the reference trajectory.

For the rest of this section, we will give several examples of how to input bends in an *OPAL-t* simulation. We will start with a simple example using the ANGLE attribute to set the bend strength and using the default field map (see Section 12.4.6) for describing the magnet fringe fields (see 1DProfile1):

```
Bend: RBEND, ANGLE = 30.0 * Pi / 180.0,
      FMAPFN = "1DPROFILE1-DEFAULT",
      ELEMEDGE = 0.25,
      DESIGNENERGY = 10.0,
      L = 0.5, GAP = 0.02;
```

This is a definition of a simple RBEND that bends the beam in a positive direction 30 degrees (towards the negative x axis as if Figure 16). It has a design energy of 10 MeV, a length of 0.5 m, a vertical gap of 2 cm and a 0° entrance edge angle. (Therefore the exit edge angle is 30°.) We are using the default, internal field map "1DPROFILE1-DEFAULT" see Section 12.4.6 which describes the magnet fringe fields see 1DProfile1. When *OPAL* is run, you will get the following output (assuming an electron beam) for this RBEND definition:

```
RBend > Reference Trajectory Properties
RBend > ===============================
RBend >
RBend > Bend angle magnitude:    0.523599 rad (30 degrees)
RBend > Entrance edge angle:     0 rad (0 degrees)
RBend > Exit edge angle:         0.523599 rad (30 degrees)
RBend > Bend design radius:      1 m
RBend > Bend design energy:      1e+07 eV
RBend >
RBend > Bend Field and Rotation Properties
RBend > ==================================
RBend >
RBend > Field amplitude:         -0.0350195 T
RBend > Field index (gradient):  0 m^-1
RBend > Rotation about x axis:   0 rad (0 degrees)
RBend > Rotation about y axis:   0 rad (0 degrees)
RBend > Rotation about z axis:   0 rad (0 degrees)
RBend >
RBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
RBend > ======================================================================
RBend >
RBend > Reference particle is bent: 0.523599 rad (30 degrees) in x plane
RBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

The first section of this output gives the properties of the reference trajectory like that described in Figure 16. From the value of `ANGLE` and the length, `L`, of the magnet, *OPAL* calculates the 10 MeV reference particle trajectory radius, `R`. From the bend geometry and the entrance angle (0° in this case), the exit angle is calculated.

The second section gives the field amplitude of the bend and its gradient (quadrupole focusing component), given the particle charge ($-e$ in this case so the amplitude is negative to get a positive bend direction). Also listed is the rotation of the magnet about the various axes.

Of course, in the actual simulation the particles will not see a hard edge bend magnet, but rather a soft edge magnet with fringe fields described by the `RBEND` field map file `FMAPFN` (see 1DProfile1). So, once the hard edge bend/reference trajectory is determined, *OPAL* then includes the fringe fields in the calculation. When the user chooses to use the default field map, *OPAL* will automatically adjust the position of the fringe fields appropriately so that the soft edge magnet is equivalent to the hard edge magnet described by the reference trajectory. To check that this was done properly, *OPAL* integrates the reference particle through the final magnet description with the fringe fields included. The result is shown in the final part of the output. In this case we see that the soft edge bend does indeed bend our reference particle through the correct angle.

What is important to note from this first example, is that it is this final part of the bend output that tells you the actual bend angle of the reference particle.

In this next example, we merely rewrite the first example, but use `K0` to set the field strength of the `RBEND`, rather than the `ANGLE` attribute:

```
Bend: RBEND, K0 = -0.0350195,
      FMAPFN = "1DPROFILE1-DEFAULT",
      ELEMEDGE = 0.25,
      DESIGNENERGY = 10.0E6,
      L = 0.5, GAP = 0.02;
```

The output from *OPAL* now reads as follows:

```
RBend > Reference Trajectory Properties
RBend > ===============================
RBend >
RBend > Bend angle magnitude:    0.523599 rad (30 degrees)
RBend > Entrance edge angle:     0 rad (0 degrees)
RBend > Exit edge angle:         0.523599 rad (30 degrees)
RBend > Bend design radius:      0.999999 m
RBend > Bend design energy:      1e+07 eV
RBend >
RBend > Bend Field and Rotation Properties
RBend > ==================================
RBend >
RBend > Field amplitude:         -0.0350195 T
RBend > Field index (gradient):  0 m^-1
RBend > Rotation about x axis:   0 rad (0 degrees)
RBend > Rotation about y axis:   0 rad (0 degrees)
RBend > Rotation about z axis:   0 rad (0 degrees)
RBend >
RBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
RBend > ======================================================================
RBend >
RBend > Reference particle is bent: 0.5236 rad (30.0001 degrees) in x plane
RBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

The output is effectively identical, to within a small numerical error.

Now, let us modify this first example so that we bend instead in the negative x direction. There are several ways to do this:

1.

```
Bend: RBEND, ANGLE = -30.0 * Pi / 180.0,
             FMAPFN = "1DPROFILE1-DEFAULT",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.5, GAP = 0.02;
```

2.

```
Bend: RBEND, ANGLE = 30.0 * Pi / 180.0,
             FMAPFN = "1DPROFILE1-DEFAULT",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.5, GAP = 0.02,
             ROTATION = Pi;
```

3.

```
Bend: RBEND, K0 = 0.0350195,
             FMAPFN = "1DPROFILE1-DEFAULT",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.5, GAP = 0.02;
```

4.

```
Bend: RBEND, K0 = -0.0350195,
             FMAPFN = "1DPROFILE1-DEFAULT",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.5, GAP = 0.02,
             ROTATION = Pi;
```

In each of these cases, we get the following output for the bend (to within small numerical errors).

```
RBend > Reference Trajectory Properties
RBend > ===============================
RBend >
RBend > Bend angle magnitude:    0.523599 rad (30 degrees)
RBend > Entrance edge angle:     0 rad (0 degrees)
RBend > Exit edge angle:         0.523599 rad (30 degrees)
RBend > Bend design radius:      1 m
RBend > Bend design energy:      1e+07 eV
RBend >
RBend > Bend Field and Rotation Properties
RBend > ==================================
RBend >
RBend > Field amplitude:         -0.0350195 T
RBend > Field index (gradient):  -0 m^-1
RBend > Rotation about x axis:   0 rad (0 degrees)
RBend > Rotation about y axis:   0 rad (0 degrees)
RBend > Rotation about z axis:   3.14159 rad (180 degrees)
RBend >
RBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
RBend > ======================================================================
RBend >
RBend > Reference particle is bent: -0.523599 rad (-30 degrees) in x plane
RBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

In general, we suggest to always define a bend in the positive x direction (as in Figure 16) and then use the `ROTATION` attribute to bend in other directions in the x/y plane (as in examples 2 and 4 above).

As a final `RBEND` example, here is a suggested format for the four bend definitions if one where implementing a four dipole chicane:

```
Bend1: RBEND, ANGLE = 20.0 * Pi / 180.0,
              E1 = 0.0,
              FMAPFN = "1DPROFILE1-DEFAULT",
              ELEMEDGE = 0.25,
              DESIGNENERGY = 10.0E6,
              L = 0.25,
              GAP = 0.02,
              ROTATION = Pi;

Bend2: RBEND, ANGLE = 20.0 * Pi / 180.0,
              E1 = 20.0 * Pi / 180.0,
              FMAPFN = "1DPROFILE1-DEFAULT",
              ELEMEDGE = 1.0,
              DESIGNENERGY = 10.0E6,
              L = 0.25,
              GAP = 0.02,
              ROTATION = 0.0;

Bend3: RBEND, ANGLE = 20.0 * Pi / 180.0,
              E1 = 0.0,
              FMAPFN = "1DPROFILE1-DEFAULT",
              ELEMEDGE = 1.5,
              DESIGNENERGY = 10.0E6,
              L = 0.25,
              GAP = 0.02,
              ROTATION = 0.0;

Bend4: RBEND, ANGLE = 20.0 * Pi / 180.0,
              E1 = 20.0 * Pi / 180.0,
              FMAPFN = "1DPROFILE1-DEFAULT",
              ELEMEDGE = 2.25,
              DESIGNENERGY = 10.0E6,
              L = 0.25,
              GAP = 0.02,
              ROTATION = Pi;
```

Up to now, we have only given examples of `RBEND` definitions. If we replaced "RBend" in the above examples with "SBend", we would still be defining valid *OPAL-t* bends. In fact, by adjusting the `L` attribute according to Section 12.4.1 and Section 12.4.3, and by adding the appropriate definitions of the `E2` attribute, we could even get identical results using `SBEND`s instead of `RBEND`s. (As we said, the two bends are very similar in command format.)

Up till now, we have only used the default field map. Custom field maps can also be used. There are two different options in this case see 1DProfile1:

1. Field map defines fringe fields and magnet length.
2. Field map defines fringe fields only.

The first case describes how field maps were used in previous versions of *OPAL* (and can still be used in the current version). The second option is new to *OPAL OPAL*version 1.2.00 and it has a couple of advantages:

1. Because only the fringe fields are described, the length of the magnet must be set using the `L` attribute. In turn, this means that the same field map can be used by many bend magnets with different lengths (assuming they have equivalent fringe fields). By contrast, if the magnet length is set by the field map, one must generate a new field map for each dipole of different length even if the fringe fields are the same.
2. We can adjust the position of the fringe field origin relative to the entrance and exit points of the magnet (see 1DProfile1). This gives us another degree of freedom for describing the fringe fields, allowing us to adjust the effective length of the magnet.

We will now give examples of how to use a custom field map, starting with the first case where the field map describes the fringe fields and the magnet length. Assume we have the following `1DProfile1` field map:

```
1DProfile1 1 1 2.0
 -10.0  0.0  10.0 1
  15.0  25.0 35.0 1
  0.00000E+00
  2.00000E+00
  0.00000E+00
  2.00000E+00
```

We can use this field map to define the following bend (note we are now using the SBEND command):

```
Bend: SBEND, ANGLE = 60.0 * Pi / 180.0,
             E1 = -10.0 * Pi / 180.0,
             E2 = 20.0  Pi / 180.0,
             FMAPFN = "TEST-MAP.T7",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             GAP = 0.02;
```

Notice that we do not set the magnet length using the L attribute. (In fact, we don't even include it. If we did and set it to a non-zero value, the exit fringe fields of the magnet would not be correct.) This input gives the following output:

```
SBend > Reference Trajectory Properties
SBend > ===============================
SBend >
SBend > Bend angle magnitude:    1.0472 rad (60 degrees)
SBend > Entrance edge angle:     -0.174533 rad (-10 degrees)
SBend > Exit edge angle:         0.349066 rad (20 degrees)
SBend > Bend design radius:      0.25 m
SBend > Bend design energy:      1e+07 eV
SBend >
SBend > Bend Field and Rotation Properties
SBend > ==================================
SBend >
SBend > Field amplitude:         -0.140385 T
SBend > Field index (gradient):  0 m^-1
SBend > Rotation about x axis:   0 rad (0 degrees)
SBend > Rotation about y axis:   0 rad (0 degrees)
SBend > Rotation about z axis:   0 rad (0 degrees)
SBend >
SBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
SBend > ======================================================================
SBend >
SBend > Reference particle is bent: 1.0472 rad (60 degrees) in x plane
SBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

Because we set the bend strength using the ANGLE attribute, the magnet field strength is automatically adjusted so that the reference particle is bent exactly ANGLE radians when the fringe fields are included. (Lower output.)

Now we will illustrate the case where the magnet length is set by the L attribute and only the fringe fields are described by the field map. We change the *TEST-MAP.T7* file to:

```
1DProfile1 1 1 2.0
 -10.0  0.0  10.0 1
 -10.0  0.0  10.0 1
  0.00000E+00
  2.00000E+00
  0.00000E+00
  2.00000E+00
```

and change the bend input to:

```
Bend: SBEND, ANGLE = 60.0 * Pi / 180.0,
             E1 = -10.0 * Pi / 180.0,
             E2 = 20.0  Pi / 180.0,
             FMAPFN = "TEST-MAP.T7",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.25,
             GAP = 0.02;
```

This results in the same output as the previous example, as we expect.

```
SBend > Reference Trajectory Properties
SBend > ===============================
SBend >
SBend > Bend angle magnitude:    1.0472 rad (60 degrees)
SBend > Entrance edge angle:     -0.174533 rad (-10 degrees)
SBend > Exit edge angle:         0.349066 rad (20 degrees)
SBend > Bend design radius:      0.25 m
SBend > Bend design energy:      1e+07 eV
SBend >
SBend > Bend Field and Rotation Properties
SBend > ==================================
SBend >
SBend > Field amplitude:         -0.140385 T
SBend > Field index (gradient):  0 m^-1
SBend > Rotation about x axis:   0 rad (0 degrees)
SBend > Rotation about y axis:   0 rad (0 degrees)
SBend > Rotation about z axis:   0 rad (0 degrees)
SBend >
SBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
SBend > ======================================================================
SBend >
SBend > Reference particle is bent: 1.0472 rad (60 degrees) in x plane
SBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

As a final example, let us now use the previous field map with the following input:

```
Bend: SBEND, K0 = -0.1400778,
             E1 = -10.0 * Pi / 180.0,
             E2 = 20.0  Pi / 180.0,
             FMAPFN = "TEST-MAP.T7",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.25,
             GAP = 0.02;
```

Instead of setting the bend strength using `ANGLE`, we use `K0`. This results in the following output:

```
SBend > Reference Trajectory Properties
SBend > ===============================
SBend >
SBend > Bend angle magnitude:    1.0472 rad (60 degrees)
SBend > Entrance edge angle:     -0.174533 rad (-10 degrees)
SBend > Exit edge angle:         0.349066 rad (20 degrees)
SBend > Bend design radius:      0.25 m
SBend > Bend design energy:      1e+07 eV
SBend >
SBend > Bend Field and Rotation Properties
SBend > ==================================
SBend >
SBend > Field amplitude:         -0.140078 T
SBend > Field index (gradient):  0 m^-1
SBend > Rotation about x axis:   0 rad (0 degrees)
SBend > Rotation about y axis:   0 rad (0 degrees)
SBend > Rotation about z axis:   0 rad (0 degrees)
SBend >
SBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
SBend > ======================================================================
SBend >
SBend > Reference particle is bent: 1.04491 rad (59.8688 degrees) in x plane
SBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

In this case, the bend angle for the reference trajectory in the first section of the output no longer matches the reference trajectory bend angle from the lower section (although the difference is small). The reason is that the path of the reference particle through the real magnet (with fringe fields) no longer matches the ideal trajectory. (The effective length of the real magnet is not quite the same as the hard edged magnet for the reference trajectory.)

We can compensate for this by changing the field map file *TEST-MAP.T7* file to:

```
1DProfile1 1 1 2.0
 -10.0  -0.03026  10.0 1
 -10.0  0.03026  10.0 1
  0.00000E+00
  2.00000E+00
  0.00000E+00
  2.00000E+00
```

We have moved the Enge function origins (see 1DProfile1) outward from the entrance and exit faces of the magnet by 0.3026 mm. This has the effect of making the effective length of the soft edge magnet longer. When we do this, the same input:

```
Bend: SBEND, K0 = -0.1400778,
             E1 = -10.0 * Pi / 180.0,
             E2 = 20.0  Pi / 180.0,
             FMAPFN = "TEST-MAP.T7",
             ELEMEDGE = 0.25,
             DESIGNENERGY = 10.0E6,
             L = 0.25,
             GAP = 0.02;
```

produces

```
SBend > Reference Trajectory Properties
SBend > ===============================
SBend >
SBend > Bend angle magnitude:    1.0472 rad (60 degrees)
SBend > Entrance edge angle:     -0.174533 rad (-10 degrees)
SBend > Exit edge angle:         0.349066 rad (20 degrees)
SBend > Bend design radius:      0.25 m
SBend > Bend design energy:      1e+07 eV
SBend >
SBend > Bend Field and Rotation Properties
SBend > ==================================
SBend >
SBend > Field amplitude:         -0.140078 T
SBend > Field index (gradient):  0 m^-1
SBend > Rotation about x axis:   0 rad (0 degrees)
SBend > Rotation about y axis:   0 rad (0 degrees)
SBend > Rotation about z axis:   0 rad (0 degrees)
SBend >
SBend > Reference Trajectory Properties Through Bend Magnet with Fringe Fields
SBend > ======================================================================
SBend >
SBend > Reference particle is bent: 1.0472 rad (60 degrees) in x plane
SBend > Reference particle is bent: 0 rad (0 degrees) in y plane
```

Now we see that the bend angle for the ideal, hard edge magnet, matches the bend angle of the reference particle through the soft edge magnet. In other words, the effective length of the soft edge, real magnet is the same as the hard edge magnet described by the reference trajectory.

12.4.5 Bend Fields from 1D Field Maps (*OPAL-t*)

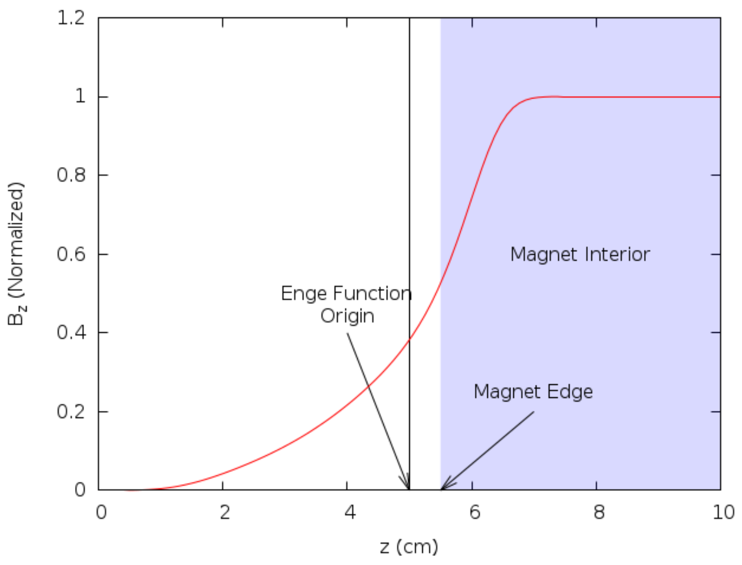

Figure 18: Plot of the entrance fringe field of a dipole magnet along the mid-plane, perpendicular to its entrance face. The field is normalized to 1.0. In this case, the fringe field is described by an Enge function see Equation 12.1 with the parameters from the default `1DProfile1` field map described in Section 12.4.6. The exit fringe field of this magnet is the mirror image.

So far we have described how to setup an `RBEND` or `SBEND` element, but have not explained how *OPAL-t* uses this information to calculate the magnetic field. The field of both types of magnets is divided into three regions:

1. Entrance fringe field.
2. Central field.
3. Exit fringe field.

This can be seen clearly in Figure 45.

The purpose of the `1DProfile1` field map (see 1DProfile1) associated with the element is to define the Enge functions (Equation 12.1) that model the entrance and exit fringe fields. To model a particular bend magnet, one must fit the field profile along the mid-plane of the magnet perpendicular to its face for the entrance and exit fringe fields to the Enge function:

$$F(z) = \frac{1}{1 + e^{\sum_{n=0}^{N_{order}} c_n (z/D)^n}}$$

EQUATION 12.1: Enge function

where D is the full gap of the magnet, N_{order} is the Enge function order and z is the distance from the origin of the Enge function perpendicular to the edge of the dipole. The origin of the Enge function, the order of the Enge function, N_{order}, and the constants c_0 to $c_{N_{order}}$ are free parameters that are chosen so that the function closely approximates the fringe region of the magnet being modeled. An example of the entrance fringe field is shown in Figure 18.

Let us assume we have a correctly defined positive `RBEND` or `SBEND` element as illustrated in Figure 16 and Figure 17. (As already stated, any bend can be described by a rotated positive bend.) *OPAL-t* then has the following information:

$$\begin{aligned}
B_0 &= \text{Field amplitude (T)}\\
R &= \text{Bend radius (m)}\\
n &= -\frac{R}{B_y}\frac{\partial B_y}{\partial x} \text{ (Field index, set using the parameter K1)}\\
F(z) &= \begin{cases} F_{entrance}(z_{entrance}) \\ F_{center}(z_{center}) = 1 \\ F_{exit}(z_{exit}) \end{cases}
\end{aligned}$$

Here, we have defined an overall Enge function, $F(z)$, with three parts: entrance, center and exit. The exit and entrance fringe field regions have the form of Equation 12.1 with parameters defined by the `1DProfile1` field map file given by the element parameter `FMAPFN`. Defining the coordinates:

$$\begin{aligned}
y &\equiv \text{Vertical distance from magnet mid-plane}\\
\Delta_x &\equiv \text{Perpendicular distance to reference trajectory (see Figures)}\\
\Delta_z &\equiv \begin{cases} \text{Distance from entrance Enge function origin perpendicular to magnet entrance face.} \\ \text{Not defined, Enge function is always 1 in this region.} \\ \text{Distance from exit Enge function origin perpendicular to magnet exit face.} \end{cases}
\end{aligned}$$

using the conditions

$$\begin{aligned}
\nabla \cdot \vec{B} &= 0\\
\nabla \times \vec{B} &= 0
\end{aligned}$$

and making the definitions:

$$\begin{aligned}
F'(z) &\equiv \frac{\mathrm{d}F(z)}{\mathrm{d}z}\\
F''(z) &\equiv \frac{\mathrm{d}^2F(z)}{\mathrm{d}z^2}\\
F'''(z) &\equiv \frac{\mathrm{d}^3F(z)}{\mathrm{d}z^3}
\end{aligned}$$

we can expand the field off axis, with the result:

$$B_x(\Delta_x, y, \Delta_z) = -\frac{B_0\frac{n}{R}}{\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z}}}e^{-\frac{n}{R}\Delta_x}\sin\left[\left(\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right)y\right]F(\Delta_z)$$

$$B_y(\Delta_x, y, \Delta_z) = B_0 e^{-\frac{n}{R}\Delta_x}\cos\left[\left(\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right)y\right]F(\Delta_z)$$

$$\begin{aligned}
B_z(\Delta_x, y, \Delta_z) = B_0 e^{-\frac{n}{R}\Delta_x}\Bigg\{&\frac{F'(\Delta_z)}{\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}}\sin\left[\left(\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right)y\right]\\
&-\frac{1}{2\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}}\left(F'''(\Delta_z)-\frac{F'(\Delta_z)F''(\Delta_z)}{F(\Delta_z)}\right)\left[\frac{\sin\left[\left(\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right)y\right]}{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right.\\
&\left.-\,y\frac{\cos\left[\left(\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}\right)y\right]}{\sqrt{\frac{n^2}{R^2}+\frac{F''(\Delta_z)}{F(\Delta_z)}}}\right]\Bigg\}
\end{aligned}$$

These expression are not well suited for numerical calculation, so, we expand them about y to $O(y^2)$ to obtain:

- In fringe field regions:

$$\begin{aligned}
B_x(\Delta_x, y, \Delta_z) &\approx -B_0 \frac{n}{R} e^{-\frac{n}{R}\Delta_x} y \\
B_y(\Delta_x, y, \Delta_z) &\approx B_0 e^{-\frac{n}{R}\Delta_x} \left[F(\Delta_z) - \left(\frac{n^2}{R^2} F(\Delta_z) + F''(\Delta_z) \right) \frac{y^2}{2} \right] \\
B_z(\Delta_x, y, \Delta_z) &\approx B_0 e^{-\frac{n}{R}\Delta_x} y F'(\Delta_z)
\end{aligned}$$

- In central region:

$$\begin{aligned}
B_x(\Delta_x, y, \Delta_z) &\approx -B_0 \frac{n}{R} e^{-\frac{n}{R}\Delta_x} y \\
B_y(\Delta_x, y, \Delta_z) &\approx B_0 e^{-\frac{n}{R}\Delta_x} \left[1 - \frac{n^2}{R^2} \frac{y^2}{2} \right] \\
B_z(\Delta_x, y, \Delta_z) &\approx 0
\end{aligned}$$

These are the expressions *OPAL-t* uses to calculate the field inside an `RBEND` or `SBEND`. First, a particle's position inside the bend is determined (entrance region, center region, or exit region). Depending on the region, *OPAL-t* then determines the values of Δ_x, y and Δ_z, and then calculates the field values using the above expressions.

12.4.6 Default Field Map (*OPAL-t*)

Rather than force users to calculate the field of a dipole and then fit that field to find Enge coefficients for the dipoles in their simulation, we have a default set of values we use from [24] that are set when the default field map, `1DPROFILE1-DEFAULT` is used:

$$\begin{aligned}
c_0 &= 0.478959 \\
c_1 &= 1.911289 \\
c_2 &= -1.185953 \\
c_3 &= 1.630554 \\
c_4 &= -1.082657 \\
c_5 &= 0.318111
\end{aligned}$$

The same values are used for both the entrance and exit regions of the magnet. In general they will give good results. (Of course, at some point as a beam line design becomes more advanced, one will want to find Enge coefficients that fit the actual magnets that will be used in a given design.)

The default field map is the equivalent of the following custom `1DProfile1` (see 1DProfile1 for an explanation of the field map format) map:

```
1DProfile1 5 5 2.0
 -10.0 0.0 10.0 1
 -10.0 0.0 10.0 1
  0.478959
  1.911289
 -1.185953
  1.630554
 -1.082657
  0.318111
  0.478959
  1.911289
 -1.185953
  1.630554
 -1.082657
  0.318111
```

As one can see, the default magnet gap for `1DPROFILE1-DEFAULT` is set to 2.0 cm. This value can be overridden by the `GAP` attribute of the magnet (see Section 12.4.1 and Section 12.4.3).

12.4.7 SBend3D (*OPAL-cycl*)

The `SBEND3D` element enables definition of a bend from 3D field maps. This can be used in conjunction with the `RINGDEFINITION` element to make a ring for tracking through *OPAL-cycl*.

```
label: SBEND3D, FMAPFN=string, LENGTH_UNITS=real, FIELD_UNITS=real;
```

FMAPFN The field map file name.

LENGTH_UNITS Units for length (set to 1.0 for units in mm, 10.0 for units in cm, etc).

FIELD_UNITS Units for field (set to 1.0 for units in T, 0.001 for units in mT, etc).

Field maps are defined using Cartesian coordinates but in a polar geometry. The following conventions have to be fulfilled:

1. 3D Field maps have to be generated in the vertical direction (z coordinate in *OPAL-cycl*) from z = 0 upwards. Maps cannot be generated symmetrically about z = 0 towards negative z values.
2. The field map file must be in the form with columns ordered as follows: $[x, z, y, B_x, B_z, B_y]$.
3. Grid points of the position and field strength have to be written on a grid in (r, z, θ) with the primary direction corresponding to the azimuthal direction, secondary to the vertical direction and tertiary to the radial direction.

`SBEND3D` assumes a dipole symmetry. In a dipole symmetry, fields below the symmetry plane Z=0 have the same field in the direction perpendicular to the symmetry plane, B_z, but field components parallel to the symmetry plane have the opposite direction (sign).

Below are two examples of a `SBEND3D` which loads a field map file named “90degree_Dipole_Magnet.out” defining a hard edge model of 90° dipole magnet with homogenous magnetic field. The first 8 lines are presumed to be header material and are ignored. Positions have units of m and fields units of Tesla. The corresponding 3D magnetic field map is shown in the following figure in the Cartesian coordinate system (x, y, z). A horizontal cross section of the 3D magnetic field map when z = 0 is also shown.

```
Dipole: SBEND3D, FMAPFN="90degree_Dipole_Magnet.out", LENGTH_UNITS=1000.0, FIELD_UNITS ←
    =-10.0;
```

The first few lines of the field map file are as follows:

```
  4550000 4550000 4550000 1
X [LENGTH_UNITS]
Z [LENGTH_UNITS]
Y [LENGTH_UNITS]
BX [FIELD_UNITS]
BZ [FIELD_UNITS]
BY [FIELD_UNITS]
0
4.3586435e-01   5.0000000e-02   1.2803431e+00   0.0000000e+00   1.6214000e+00   0.0000000e ←
    +00
4.2691532e-01   5.0000000e-02   1.2833548e+00   0.0000000e+00   1.6214000e+00   0.0000000e ←
    +00
4.1794548e-01   5.0000000e-02   1.2863039e+00   0.0000000e+00   1.6214000e+00   0.0000000e ←
    +00
```

This is a restricted feature for *OPAL-cycl*.

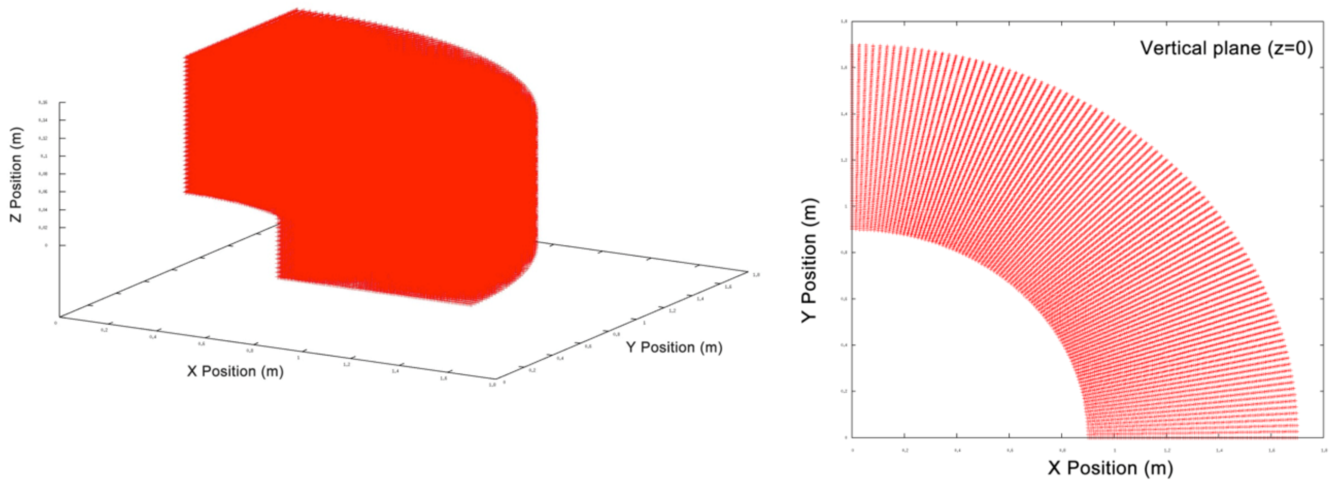

Figure 19: A hard edge model of 90° dipole magnet with homogeneous magnetic field. The right figure is showing the horizontal cross section of the 3D magnetic field map when $z = 0$

12.5 Quadrupole

```
label:QUADRUPOLE, TYPE=string, APERTURE=real-vector,
      L=real, K1=real, K1S=real;
```

The reference system for a quadrupole is a Cartesian coordinate system This is a restricted feature for *OPAL-t*.

A `QUADRUPOLE` has the following real attributes:

K1 The normal quadrupole component $K_1 = \frac{\partial B_y}{\partial x}$. The default is 0 Tm^{-1}. The component is positive, if B_y is positive on the positive x-axis. This implies horizontal focusing of positively charged particles which travel in positive s-direction.

K1S The skew quadrupole component. $K_{1s} = -\frac{\partial B_x}{\partial x}$. The default is 0 Tm^{-1}. The component is negative, if B_x is positive on the positive x-axis.

DK1 The normalised quadrupole coefficient error.

DK1S The normalised skew quadrupole coefficient error.

Example:

```
QP1: QUADRUPOLE, L=1.20, ELEMEDGE=-0.5265, K1=0.11;
```

12.6 Sextupole

```
label: SEXTUPOLE, TYPE=string, APERTURE=real-vector,
       L=real, K2=real, K2S=real;
```

A `SEXTUPOLE` has the following real attributes:

K2 The normal sextupole component $K_2 = \frac{\partial^2 B_y}{\partial x^2}$. The default is 0 Tm^{-2}. The component is positive, if B_y is positive on the x-axis.

K2S The skew sextupole component $K_{2s} = -\frac{\partial^2 B_x}{\partial x^2}$. The default is 0 Tm^{-2}. The component is negative, if B_x is positive on the x-axis.

DK2 The normalised sextupole coefficient error.

DK2S The normalised skew sextupole coefficient error.

Example:

```
S: SEXTUPOLE, L=0.4, K2=0.00134;
```

The reference system for a sextupole is a Cartesian coordinate system

12.7 Octupole

```
label: OCTUPOLE, TYPE=string, APERTURE=real-vector,
      L=real, K3=real, K3S=real;
```

An `OCTUPOLE` has the following real attributes:

K3 The normal octupole component $K_3 = \frac{\partial^3 B_y}{\partial x^3}$. The default is 0 Tm^{-3}. The component is positive, if B_y is positive on the positive x-axis.

K3S The skew octupole component $K_{3s} = -\frac{\partial^3 B_x}{\partial x^3}$. The default is 0 Tm^{-3}. The component is negative, if B_x is positive on the positive x-axis.

DK3 The normalised octupole coefficient error.

DK3S The normalised skew octupole coefficient error.

Example:

```
O3: OCTUPOLE, L=0.3, K3=0.543;
```

The reference system for an octupole is a Cartesian coordinate system

12.8 General Multipole

The `MULTIPOLE` element defines a thick multipole. If the length is non-zero, the strengths are per unit length. If the length is zero, the strengths are the values integrated over the length. With zero length no synchrotron radiation can be calculated.

A `MULTIPOLE` in *OPAL-t* is of arbitrary order.

```
label: MULTIPOLE, TYPE=string, APERTURE=real-vector,
      L=real, KN=real-vector, KS=real-vector;
```

KN A real vector (see Arrays), containing the normal multipole coefficients, $K_n = \frac{\partial^n B_y}{\partial x^n}$. (default is 0 Tm$^{-\mathrm{n}}$). A component is positive, if B_y is positive on the positive x-axis.

KS A real vector (see Arrays), containing the skew multipole coefficients, $K_{n\ s} = -\frac{\partial^n B_x}{\partial x^n}$. (default is 0 Tm$^{-\mathrm{n}}$). A component is negative, if B_x is positive on the positive x-axis.

DKN A real vector (see Arrays), containing the normal normalised multipole strength errors (default is 0 Tm$^{-\mathrm{n}}$).

DKS A real vector (see Arrays), containing the skew normalised multipole strength errors (default is 0 Tm$^{-\mathrm{n}}$).

The number of poles of each component is $(2n+2)$.

Superposition of many multipole components is permitted. The reference system for a multipole is a Cartesian coordinate system

The following example is equivalent to the quadruple example in Section 12.5.

```
M27: MULTIPOLE, L=1, ELEMEDGE=3.8, KN={0.0,0.11};
```

A multipole has no effect on the reference orbit, i.e. the reference system at its exit is the same as at its entrance. Use the dipole component only to model a defective multipole.

12.9 General Multipole With Fringe Field Model

A `MULTIPOLET` is in *OPAL-cycl* a general multipole with extended features. It can represent a straight or curved magnet. In the curved case, the user may choose between constant or variable radius. This model includes fringe fields. The detailed description can be found at: https://gitlab.psi.ch/OPAL/src/uploads/0d3fc561b57e8962ed79a57cd6115e37/8FBB32A4-7FA1-4084-A4A7-CDDB1F949CD3_psi.ch.pdf.

```
label: MULTIPOLET, L=real, TP=real-vector, LFRINGE=real, RFRINGE=real, VAPERT=real, HAPERT= ↩
    real,
       MAXFORDER=real, ROTATION=real, EANGLE=real, BBLENGTH=real, ANGLE=real, MAXXORDER= ↩
           real,
       VARRADIUS=bool, ENTRYOFFSET=real;
```

L Physical length of the magnet (meters). The measurement is between the ends of the field if there were no fringe fields. This also corresponds to the center points of the fringe field curves. (Default: 1 m)

TP A real vector (see Arrays), containing the multipole coefficients of the field expansion on the mid-plane in the body of the magnet: the transverse profile $T(x) = B_0 + B_1 x + B_2 x^2 + \ldots$ is set by TP=B_0, B_1, B_2 (units: $T \cdot m^{-n}$). The order of highest multipole component is arbitrary, but all components up to the maximum must be given, even if they are zero.

VAPERT Vertical (non-bend plane) aperture of the magnet (meters). (Default: 0.5 m)

HAPERT Horizontal (bend plane) aperture of the magnet (meters). (Default: 0.5 m)

LFRINGE Length of the left fringe field (meters). (Default: 0.0 m)

RFRINGE Length of the right fringe field (meters). (Default: 0.0 m)

MAXFORDER The order of the maximum function f_n used in the field expansion (default: 4). See the scalar magnetic potential below. This sets, for example, the maximum power of z in the field expansion of vertical component B_z to $2 \cdot$MAXFORDER.

EANGLE Entrance edge angle (radians). (Default: 0.0 rad)

ROTATION Rotation of the magnet about its central axis (radians, counterclockwise). This enables to obtain skew fields. Only valid for straight magnets with ANGLE set to 0. (Default 0.0 rad)

BBLENGTH The length of the bounding box inside which the field is calculated (meters). Outside the bounding box, this element contributes nothing to the field. The bounding box length is measured along magnet center path in the same way as L. (Default: 0.0 m)

ANGLE Physical angle of the magnet (radians) through which the beam will be bent. If not specified, the magnet is considered to be straight (ANGLE=0.0). This is not the total bending angle since the end fields cause additional bending. The radius of the magnet is set from the LENGTH and ANGLE attributes.

MAXXORDER The number of terms used in the polynomial expansion of the fringe fields. (Default: 20)

VARRADIUS This is to be set TRUE if the magnet has variable radius. More precisely, at each point along the magnet, its radius is computed such that the reference trajectory always remains in the centre of the magnet. In the body of the magnet the radius is set from the LENGTH and ANGLE attributes. It is then continuously changed to be proportional to the dipole field on the reference trajectory while entering the end fields. Only valid for non-straight magnets (ANGLE not zero) and when a non-zero dipole field is specified. (Default: FALSE)

ENTRYOFFSET Normally, the reference point for the magnet's local coordinate system and from where the length (L) attribute is measured from is the start of the magnetic field if there were no fringe fields. The entry fringe complicates things a little as this reference point becomes the center of the fringe field function. When using non-straight magnet in variable radius mode (VARRADIUS is set to true) the internal coordinate system origin can be moved to any point on the magnet center line by setting the EXTRYOFFSET attribute, in meters. Typically, the only useful value is +L/2 (half the L attribute value) which will then place the origin in the center of the magnet. This allows the magnet to be positioned using its center point rather than its entry point. (Default: 0.0 m)

Superposition of many multipole components is permitted. The reference system for a multipole is a Cartesian coordinate system for straight geometry and a (x,s,z) Frenet-Serret coordinate system for curved geometry. In the latter case, the axis $\hat{s}$ is the central axis of the magnet.

The following example shows a combined function magnet with a dipole component of 2 Tesla and a quadrupole gradient of 0.1 Tesla/m.

```
M30: MULTIPOLET, L=1, RFRINGE=0.3, LFRINGE=0.2, ANGLE=PI/6, TP={2.0, 0.1},
VARRADIUS=TRUE, BBLENGTH=2;
```

The field expansion used in this model is based on the following scalar potential:

$$V = zf_0(x,s) + \frac{z^3}{3!}f_1(x,s) + \frac{z^5}{5!}f_2(x,s) + \dots$$

Mid-plane symmetry is assumed and the vertical component of the field on the mid-plane is given by the user under the form of the transverse profile $T(x)$. The full expression for the vertical component is then

$$B_z = f_0 = T(x) \cdot S(s)$$

where $S(s)$ is the fringe field. This element uses the Tanh model for the end fields, having only three parameters (the centre length s_0 and the fringe field lengths λ_{left}, λ_{right}):

$$S(s) = \frac{1}{2}\left[\tanh\left(\frac{s+s_0}{\lambda_{left}}\right) - \tanh\left(\frac{s-s_0}{\lambda_{right}}\right)\right]$$

Starting from Maxwell's laws, the functions f_n are computed recursively and finally each component of the magnetic field is obtained from V using the corresponding geometries.

12.10 Solenoid

```
label: SOLENOID, TYPE=string, APERTURE=real-vector,
      L=real, KS=real;
```

A `SOLENOID` has two real attributes:

KS The solenoid strength $K_s = \frac{\partial B_s}{\partial s}$, default is 0 Tm^{-1}. For positive `KS` and positive particle charge, the solenoid field points in the direction of increasing s.

The reference system for a solenoid is a Cartesian coordinate system Using a solenoid in *OPAL-t* mode, the following additional parameters are defined:

FMAPFN Field maps must be specified.

Example:

```
SP1: SOLENOID, L=1.20, ELEMEDGE=-0.5265, KS=0.11,
     FMAPFN="1T1.T7";
```

12.11 Cyclotron

```
label: CYCLOTRON, TYPE=string, CYHARMON=int,
       PHIINIT=real, PRINIT=real, RINIT=real,
       SYMMETRY=real, RFFREQ=real, FMAPFN=string;
```

A `CYCLOTRON` object includes the main characteristics of a cyclotron, the magnetic field, and also the initial condition of the injected reference particle, and it has currently the following attributes:

TYPE The data format of field map. Currently the following formats are implemented: `RING` (PSI format), `CARBONCYCL`, `CYCIAE`, `AVFEQ`, `FFA` and `BANDRF`. For the details of their data format, please read Field Maps.

CYHARMON The harmonic number of the cyclotron h.

RFFREQ The RF system [MHz], f_{rf}. The particle revolution frequency is given by: f_{rev} = f_{rf} / h.

FMAPFN File name for the magnetic field map. BSCALE: Scale factor for the magnetic field map.

SYMMETRY Defines symmetrical fold number of the B field map data.

GEOMETRY Defines the boundary geometry in order to use it for particle termination (see Chapter Geometry). The particles hitting on the `GEOMETRY` will be deleted, and they are recorded in the HDF5 file *<GEOM>.h5* (or ASCII if ASCIIDUMP is true).

FMLOWE Minimal energy [GeV] the fieldmap can accept. Used in `GAUSSMATCHED` distribution.

FMHIGHE Maximal energy [GeV] the fieldmap can accept. Used in `GAUSSMATCHED` distribution.

RINIT The initial radius [mm] of the reference particle (default: 0).

PHIINIT The initial azimuth [deg] of the reference particle (default: 0).

ZINIT The initial axial position [mm] of the reference particle (default: 0).

PRINIT Initial radial momentum of the reference particle $P_r = \beta_r \gamma$ (default: 0).

PZINIT Initial axial momentum of the reference particle $P_z = \beta_z \gamma$ (default: 0).

MINZ The minimal vertical extent of the machine [mm] (default: -10000.0).

MAXZ The maximal vertical extent of the machine [mm] (default: 10000.0).

MINR Minimal radial extent of the machine [mm] (default: 0.0).

MAXR Minimal radial extent of the machine [mm] (default: 10000.0).

During the tracking, the particle (r, z, θ) will be deleted if `MINZ` $< z <$ `MAXZ` or `MINR` $< r <$ `MAXR`, and it will be recorded in the HDF5 file *OUTFN.h5* or ASCII if ASCIIDUMP is true (see Common Attributes). Example:

```
ring: CYCLOTRON, TYPE=RING, CYHARMON=6, PHIINIT=0.0,
      PRINIT=-0.000240, RINIT=2131.4, SYMMETRY=8.0,
      RFFREQ=50.650, FMAPFN="s03av.nar",
      MAXZ=10, MINZ=-10, MINR=0, MAXR=2500;
```

If `TYPE` is set to `BANDRF`, the 3D electric field map of RF cavity will be read from external H5Hut file (see Read 3D RF field-map). The following extra arguments need to specified:

RFMAPFN The file name(s) for the electric field map(s) in H5Hut binary format.

RFPHI The initial phase(s) [rad] of the electric field map(s).

RFFREQ The frequencies of the electric field maps [MHz]. `RFFREQ=0` indicates a constant field.

ESCALE The scale factor(s) for the electric field map(s).

SUPERPOSE An option whether the electric field map(s) is superposed (see also below).

Example for single electric field map:

```
COMET: CYCLOTRON, TYPE="BANDRF", CYHARMON=2, PHIINIT=-71.0,
       PRINIT=pr0, RINIT=r0, SYMMETRY=1.0, FMAPFN="Tosca_map.txt",
       RFPHI=Pi, RFFREQ=72.0, RFMAPFN="efield.h5part",
       ESCALE=1.06E-6;
```

We can have more than one RF field maps. Example for multiple RF field maps:

```
COMET: CYCLOTRON, TYPE="BANDRF", CYHARMON=2, PHIINIT=-71.0,
       PRINIT=pr0, RINIT=r0, SYMMETRY=1.0, FMAPFN="Tosca_map.txt",
       RFPHI={Pi, 0, Pi, 0}, RFFREQ={72.0, 72.0, 72.0, 72.0},
       RFMAPFN={"e1.h5part", "e2.h5part", "e3.h5part", "e4.h5part"},
       ESCALE={1.06E-6, 3.96E-6, 1.3E-6, 1.E-6}, SUPERPOSE={true, false, false, true};
```

If `SUPERPOSE` is set to true and if a particle is located in the field region, the field is always applied. If `SUPERPOSE` is set to false, then only one field map with `SUPERPOSE` false is applied, the one which has highest priority, is used to do interpolation for the particle tracking. The priority ranking is decided by their sequence in the list of `RFMAPFN` argument, i.e., "e1.h5part" has the highest priority and "e4.h5part" has the lowest priority.

Another method to model an RF cavity is to read the RF voltage profile in the `RFCAVITY` element (see Section 12.15) and make a momentum kick when a particle crosses the RF gap. In the center region of the compact cyclotron, the electric field shape is complicated and may make a significant impact on transverse beam dynamics. Hence a simple momentum kick is not enough and we need to read 3D field map to do precise simulation.

In addition, a trim-coil field model is also implemented to do fine tuning on the magnetic field. The trimcoils can be added with:

TRIMCOIL Array of the trim coil names

TRIMCOILTHRESHOLD Minimum magnetic absolute value of main field [T] for which trim coils are applied (default: 0.0).

A `TRIMCOIL` object can be defined in two ways:

TYPE Type specifies PSI-BFIELD, PSI-PHASE or PSI-BFIELD-MIRRORED trim coil descriptions. The general PSI-BFIELD and PSI-PHASE descriptions are based on rational functions with polynomials in the nominator and the denominator. The function describes the magnetic field [T] resp. the phase shift as function of the radius [mm]. Separate functions can be given for the radial and azimuthal direction. These functions are multiplied together for the function. If a function in a direction is not specified it is the identity 1. The PSI-BFIELD and PSI-PHASE types are described in https://journals.aps.org/prab/pdf/10.1103/PhysRevAccelBeams.22.064602. The PSI-BFIELD-MIRRORED type is described in http://accelconf.web.cern.ch/AccelConf/ipac2017/papers/thpab077.pdf.

RMIN Inner radius of the trim coil [mm]

RMAX Outer radius of the trim coil [mm]

PHIMIN Minimal azimuth [deg] (default $0°$) (not for PSI-BFIELD-MIRRORED)

PHIMAX Maximal azimuth [deg] (default $360°$) (not for PSI-BFIELD-MIRRORED)

BMAX Maximal B field of the trim coils [T]

COEFNUM Coefficients of the numerator for the radial direction, first coefficient is zeroth order. If COEFNUMPHI is not specified, the numerator is 1 (not for PSI-BFIELD-MIRRORED).

COEFDENOM Coefficients of the denominator for the radial direction, first coefficient is zeroth order. If COEFDENOM is not specified, the denominator is 1, and the description will be a normal polynom (not for PSI-BFIELD-MIRRORED).

COEFNUMPHI Coefficients of the numerator for the azimuthal direction, first coefficient is zeroth order. If COEFNUMPHI is not specified, the numerator is 1. (not for PSI-BFIELD-MIRRORED).

COEFDENOMPHI Coefficients of the denominator for the azimuthal direction, first coefficient is zeroth order. If COEFDENOMPHI is not specified, the denominator is 1, and the description will be a normal polynom (not for PSI-BFIELD-MIRRORED).

SLPTC Slopes of the rising edge [1/mm] (for PSI-BFIELD-MIRRORED type only)

Example:

```
tc1:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=2022.09, RMAX=2132.09, BMAX=2.0e-4, SLPTC ↩
    =1;
tc15: TRIMCOIL, TYPE="PSI-BFIELD",          RMIN=3000,    RMAX=4500,    BMAX=13e-4,
      COEFNUM   = {-0.426038643356, 0.311242287271, -0.0484487029431},
      COEFDENOM = {19.3541404562, -22.2057165548, 9.99489842329, -2.00909633025,  ↩
          0.14942099903};

Ring: CYCLOTRON, TYPE=RING, CYHARMON=6, PHIINIT=0.0, PRINIT=0.0,
      RINIT=2131, SYMMETRY=8.0, RFFREQ=50.65, BSCALE=1, FMAPFN="s03av.nar",
      TRIMCOIL={tc1, tc15};
```

This is a restricted feature: *OPAL-cycl*.

12.12 FFA Magnet

OPAL supports two analytical field models that describe FFA magnets. SCALINGFFAMAGNET generates a sector FFA magnet that scales radially. VERTICALFFAMAGNET generates a vertical FFA magnet that scales vertically.

12.12.1 Scaling FFA Magnet

The scaling FFA magnet is a fully scaling field model that includes scaling fringe fields. A scaling FFA magnet has a field profile like

$$B_\phi = \sum_{n=0} f_{2n+1}(\psi)h(r)\left(\frac{z}{r}\right)^{2n+1} \quad B_r = \sum_{n=0}\left[\frac{k-2n}{2n+1}f_{2n} - \tan(\delta)f_{2n+1}\right]h(r)\left(\frac{z}{r}\right)^{2n+1} \quad B_z = \sum_{n=0} f_{2n}(\psi)h(r)\left(\frac{z}{r}\right)^{2n}$$

where r and z are cylindrical polar coordinates, $\psi = \phi - \tan(\delta)\ln(r/r_0)$ is the azimuthal angle in the spiral coordinate system, $delta$, r_0 and k are geometrical constants that define the magnet field dependence and B_0 is the dipole field strength of the magnet at radius r_0. In OPAL, f_0 is a $tanh$ function and higher order terms are chosen so as to satisfy Maxwell's equations.

B0 The nominal dipole field of the magnet [T].

R0 Radial scale [m].

FIELD_INDEX The scaling magnet field index.

TAN_DELTA Tangent of the spiral angle; set to 0 to make a radial sector magnet.

MAX_Y_POWER The maximum power in y that will be considered in the field expansion.

END_LENGTH The end length of the spiral FFA [m].

HEIGHT Full height of the magnet. Particles moving more than height/2. off the midplane (either above or below) are out of the aperture [m].

CENTRE_LENGTH The centre length of the spiral FFA [m].

RADIAL_NEG_EXTENT Particles are considered outside the tracking region if radius is less than R0-RADIAL_NEG_EXTENT [m].

RADIAL_POS_EXTENT Particles are considered outside the tracking region if radius is greater than R0+RADIAL_POS_EXTENT [m].

MAGNET_START Determines the position of the central portion of the magnet field relative to the element start (default is 2*end_length). [m].

MAGNET_END Offset to the end of the magnet, i.e. placement of the next element. Default is centre_length + 4*end_length.

AZIMUTHAL_EXTENT The field will be assumed zero if particles are more than AZIMUTHAL_EXTENT from the magnet centre (psi=0). Default is CENTRE_LENGTH/2.+5.*END_LENGTH [m].

This is a restricted feature: *OPAL-cycl*.

12.12.2 Vertical FFA Magnet

The VERTICALFFAMAGNET is a fully scaling field model that includes scaling fringe fields. A vertical FFA magnet has a field profile like

$$B_x = \sum_n B_0 \exp(mz) \frac{1}{m} \partial_x f_n y^n B_y = \sum_n B_0 \exp(mz) \frac{n+1}{m} f_{n+1} y^n B_z = \sum_n B_0 \exp(mz) f_n y^n$$

where m and B_0 are magnet parameters, f_0 is a $tanh$ function and higher order terms are chosen so as to satisfy Maxwell's equations. The field parameters can be specified in the OPAL input file using the following parameters

B0 The nominal dipole field of the magnet at z = 0, B_0 [T].

FIELD_INDEX The scaling magnet field index, m [m^-1].

MAX_Y_POWER The maximum power in y that will be considered in the field expansion.

END_LENGTH The end length of the VFFA [m].

CENTRE_LENGTH The centre length of the VFFA [m].

WIDTH The full width of the magnet. Particles moving more than WIDTH/2 horizontally, in either direction, are considered out of the tracking region [m].

HEIGHT_NEG_EXTENT Particles are considered outside the tracking region if height is less than HEIGHT_NEG_EXTENT [m].

HEIGHT_POS_EXTENT Particles are considered outside the tracking region if height is greater than HEIGHT_POS_EXTENT [m].

BB_LENGTH The total length of the bounding box. The magnet will be placed symmetrically in the bounding box [m].

VERTICALFFAMAGNET is rectangular; the next element will be placed BB_LENGTH from the start position of the VERTICALFFAMAGNET.

This is a restricted feature: *OPAL-cycl*.

12.13 Ring Definition

```
label: RINGDEFINITION,
       RFFREQ=real, HARMONIC_NUMBER=real, IS_CLOSED=string, SYMMETRY=int,
       LAT_RINIT=real, LAT_PHIINIT=real, LAT_THETAINIT=real,
       BEAM_PHIINIT=real, BEAM_THETAINIT=real, BEAM_PRINIT=real, BEAM_RINIT=real;
```

A `RingDefinition` object contains the main characteristics of a generalized ring. The `RingDefinition` lists characteristics of the entire ring such as harmonic number together with the position of the initial element and the position of the reference trajectory.

The `RingDefinition` can be used in combination with `SBEND3D`, offsets and `VARIABLE_RF_CAVITY` elements to make up a complete ring.

RFFREQ Nominal RF frequency of the ring [MHz].

HARMONIC_NUMBER The harmonic number of the ring - i.e. number of bunches in a single pass.

SYMMETRY Azimuthal symmetry of the ring. Ring elements will be placed repeatedly `SYMMETRY` times.

IS_CLOSED Set to `FALSE` to disable checking for ring closure.

LAT_RINIT Radius of the first element placement in the lattice [m].

LAT_PHIINIT Azimuthal angle of the first element placed in the lattice [degree].

LAT_THETAINIT Angle in the mid-plane relative to the ring tangent for placement of the first element [degree].

BEAM_RINIT Initial radius of the reference trajectory [m].

BEAM_PHIINIT Initial azimuthal angle of the reference trajectory [degree].

BEAM_THETAINIT Additional rotation of the beam direction relative to the ring tangent [degree].

BEAM_PRINIT Transverse momentum $\beta\gamma$ for the reference trajectory.

MIN_R Set the minimum radius for tracking. Particles at lower radius will be assumed to have hit the beam pipe. If set, MAX_R must also be set.

MAX_R Set the maximum radius for tracking. Particles at higher radius will be assumed to have hit the beam pipe. If set, MIN_R must also be set.

In the following example, we define a ring with radius 2.35 m and 4 cells.

```
ringdef: RINGDEFINITION, HARMONIC_NUMBER=6, LAT_RINIT=2350.0, LAT_PHIINIT=0.0,
         LAT_THETAINIT=0.0, BEAM_PHIINIT=0.0, BEAM_PRINIT=0.0,
         BEAM_RINIT=2266.0, SYMMETRY=4.0, RFFREQ=0.2;
```

12.13.1 Local Cartesian Offset

The `LOCAL_CARTESIAN_OFFSET` enables the user to place an object at an arbitrary position in the coordinate system of the preceding element. This enables drift spaces and placement of overlapping elements.

END_POSITION_X x position of the next element start in the coordinate system of the preceding element [m].

END_POSITION_Y y position of the next element start in the coordinate system of the preceding element [m].

END_NORMAL_X x component of the normal vector defining the placement of the next element in the coordinate system of the preceding element [m].

END_NORMAL_Y y component of the normal vector defining the placement of the next element in the coordinate system of the preceding element [m].

12.13.2 Local Cylindrical Offset

The `LOCAL_CYLINDRICAL_OFFSET` enables the user to place an object at an arbitrary position in the coordinate system of the preceding element in cylindrical coordinates. This enables drift spaces and placement of overlapping elements.

THETA_IN Angle between the previous element and the displacement vector [rad].

THETA_OUT Angle between the displacement vector and the next element [rad].

LENGTH Length of the offset [m].

12.14 Source (*OPAL-t*)

Its first purpose is to indicate that the particles are emitted from a gun. This is needed to place the elements in three-dimensional space. Its second purpose is to delete impacting particles that are propagating in reverse direction. This function is optional and can be controlled with the parameter `TRANSPARENT`. The particles hitting on the source are recorded in the `OUTFN` file (see Common Attributes). The `SOURCE` element only works in *OPAL-t*.

TRANSPARENT Boolean to indicate whether impacting particles can propagate further. Its default is `FALSE` such that the particles are deleted.

12.15 RF Cavities (*OPAL-t* and *OPAL-cycl*)

For an `RFCAVITY` the three modes have four real attributes in common:

```
label: RFCAVITY, APERTURE=real-vector, L=real,
       VOLT=real, LAG=real;
```

L The length of the cavity [m] (default: 0 m).

VOLT The peak RF voltage [MV] (default: 0 MV). The effect of the cavity is $\delta E = \mathrm{VOLT} \cdot \sin(2\pi(\mathrm{LAG} - \mathrm{HARMON} \cdot f_0 t))$.

LAG The phase lag [rad] (default: 0). In *OPAL-t* this phase is in general relative to the phase at which the reference particle gains the most energy. This phase is determined using an auto-phasing algorithm (see Appendix Auto-phasing Algorithm). This auto-phasing algorithm can be switched off, see `APVETO`.

DLAG The phase lag error [rad] (default: 0).

12.15.1 *OPAL-t* mode

Using a RF Cavity in *OPAL-t* mode, the following additional parameters are defined:

FMAPFN Field maps in the *T7* format can be specified.

TYPE Type specifies `STANDING` [default] or `SINGLEGAP` structures.

FREQ Defines the frequency of the RF Cavity in units of MHz. A warning is issued when the frequency of the cavity card does not correspond to the frequency defined in the FMAPFN file. The frequency of the cavity card overrides the frequency defined in the FMAPFN file.

APVETO If `TRUE` this cavity will not be auto-phased. Instead the phase of the cavity is equal to `LAG` at the arrival time of the reference particle (arrival at the limit of its field **not** at `ELEMEDGE`).

Example standing wave cavity which mimics a DC gun:

```
gun: RFCAVITY, L=0.018, VOLT=-131/(1.052*2.658),
     FMAPFN="1T3.T7", ELEMEDGE=0.00,
     TYPE=STANDING, FREQ=1.0e-6;
```

Example of a two frequency standing wave cavity:

```
rf1: RFCAVITY, L=0.54, VOLT=19.961, LAG=193.0/360.0,
     FMAPFN="1T3.T7", ELEMEDGE=0.129, TYPE=STANDING,
     FREQ=1498.956;

rf2: RFCavity, L=0.54, VOLT=6.250, LAG=136.0/360.0,
     FMAPFN="1T4.T7", ELEMEDGE=0.129, TYPE=STANDING,
     FREQ=4497.536;
```

12.15.2 *OPAL-cycl* mode

Using a RF Cavity (standing wave) in *OPAL-cycl* mode, the following parameters are defined:

FMAPFN Name of file which stores normalized voltage amplitude curve of cavity gap in ASCII format. (See data format in RF field)

VOLT Peak value of voltage amplitude curve [MV].

TYPE Defines Cavity type, `SINGLEGAP` represents cyclotron type cavity.

FREQ Frequency of the RF Cavity [MHz].

RMIN Radius of the cavity inner edge [mm].

RMAX Radius of the cavity outer edge [mm].

ANGLE Azimuthal position of the cavity in global frame in degree.

PDIS Perpendicular distance (impact parameter) of cavity from center of cyclotron [mm]. If its value is positive, the radius increases clockwise (larger radius has smaller azimuthal angle).

GAPWIDTH Set gap width of cavity [mm].

PHI0 Set initial phase of cavity [deg].

Example of a RF cavity of cyclotron:

```
rf0: RFCAVITY, VOLT=0.25796, FMAPFN="Cav1.dat",
     TYPE=SINGLEGAP, FREQ=50.637, RMIN=350.0,
     RMAX=3350.0, ANGLE=35.0,   PDIS=0.0,
     GAPWIDTH=0.0, PHI0=phi01;
```

Figure 20 shows the simplified geometry of a cavity gap and its parameters.

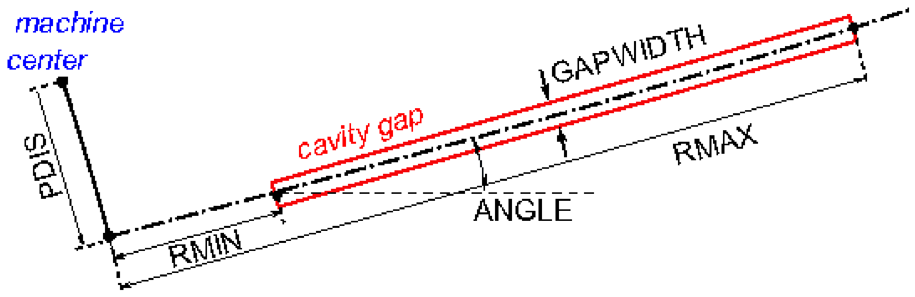

Figure 20: Schematic of the simplified geometry of a cavity gap and parameters

12.16 RF Cavities with Time Dependent Parameters

The `VARIABLE_RF_CAVITY` element can be used to define RF Cavities with Time Dependent Parameters in *OPAL-cycl* mode. Variable RF Cavities must be placed using the `RingDefinition` element.

FREQUENCY_MODEL String naming the time dependence model of the cavity frequency, f [MHz].

AMPLITUDE_MODEL String naming the time dependence model of the cavity amplitude, E_0 [MV/m].

PHASE_MODEL String naming the time dependence model of the cavity phase offset, ϕ [rad].

WIDTH Full width of the cavity [m].

HEIGHT Full height of the cavity [m].

L Full length of the cavity [m].

The field inside the cavity is given by

$$\mathbf{E} = \big(0, 0, E_0(t)\sin[2\pi f(t)t + \phi(t)]\big)$$

with no field outside the cavity boundary. There is no magnetic field or transverse dependence on electric field.

12.16.1 Time Dependence

12.16.1.1 Polynomial Time Dependence

The `POLYNOMIAL_TIME_DEPENDENCE` element is used to define time dependent parameters in RF cavities in terms of a third order polynomial.

P0 Constant term in the polynomial expansion.

P1 First order term in the polynomial expansion [ns^{-1}].

P2 Second order term in the polynomial expansion [ns^{-2}].

P3 Third order term in the polynomial expansion [ns^{-3}].

The polynomial is evaluated as

$$g(t) = p_0 + p_1 t + p_2 t^2 + p_3 t^3.$$

An example of a Variable Frequency RF cavity of cyclotron with polynomial time dependence of parameters is given below:

12.16.1.2 Spline Time Dependence

The `SPLINE_TIME_DEPENDENCE` element is used to define time dependent parameters in RF cavities in terms of a first or third order spline fit.

ORDER Order of the lookup - either 1 for linear interpolation, or 3 for cubic interpolation with quadratic smoothing. Other values make an error.

TIMES Array of real times in ns. There must be at least `ORDER`+1 elements in the array and they must be strictly monotonically increasing.

VALUES Array of real values. The length of `VALUES` must be the same as the length of `TIMES`.

12.16.2 Fringe Field

It is possible to model a soft-edged RF cavity with time dependent parameters using the `VARIABLE_RF_CAVITY_FRINGE_FIELD` element. This will place a full cavity including the field body and fringe fields. `VARIABLE_RF_CAVITY_FRINGE_FIELD` must be placed using the `RingDefinition` element.

FREQUENCY_MODEL String naming the time dependence model of the cavity frequency, f [MHz].

AMPLITUDE_MODEL String naming the time dependence model of the cavity amplitude, E_0 [MV/m].

PHASE_MODEL String naming the time dependence model of the cavity phase offset, ϕ [rad].

WIDTH Full width of the cavity [m].

HEIGHT Full height of the cavity [m].

L Full length of the cavity bounding box [m].

CENTRE_LENGTH Length of the cavity field flat top [m].

END_LENGTH E-fold Length of the cavity field ends [m].

CAVITY_CENTRE Position of the centre of the cavity relative to the start [m].

MAX_ORDER Maximum power in vertical coordinate z to which the field will be evaluated.

```
REAL phi=2.*PI*0.25;

REAL rf_p0=0.00158279;
REAL rf_p1=9.02542e-10;
REAL rf_p2=-1.96663e-16;
REAL rf_p3=2.45909e-23;

RF_FREQUENCY: POLYNOMIAL_TIME_DEPENDENCE, P0=rf_p0, P1=rf_p1,   P2=rf_p2, P3=rf_p3;
RF_AMPLITUDE: POLYNOMIAL_TIME_DEPENDENCE, P0=1.0;
RF_PHASE: POLYNOMIAL_TIME_DEPENDENCE, P0=phi;

HARD_RF_CAVITY: VARIABLE_RF_CAVITY,
            PHASE_MODEL="RF_PHASE", AMPLITUDE_MODEL="RF_AMPLITUDE",
            FREQUENCY_MODEL="RF_FREQUENCY", L=0.100, HEIGHT=0.200, WIDTH=2.000;

SOFT_RF_CAVITY: VARIABLE_RF_CAVITY_FRINGE_FIELD,
            PHASE_MODEL="RF_PHASE", AMPLITUDE_MODEL="RF_AMPLITUDE",
            FREQUENCY_MODEL="RF_FREQUENCY", L=0.200, HEIGHT=0.200, WIDTH=2.000
            CENTRE_LENGTH=0.1, END_LENGTH=0.01, CAVITY_CENTRE=0.1, MAX_ORDER=4;
```

12.17 Traveling Wave Structure

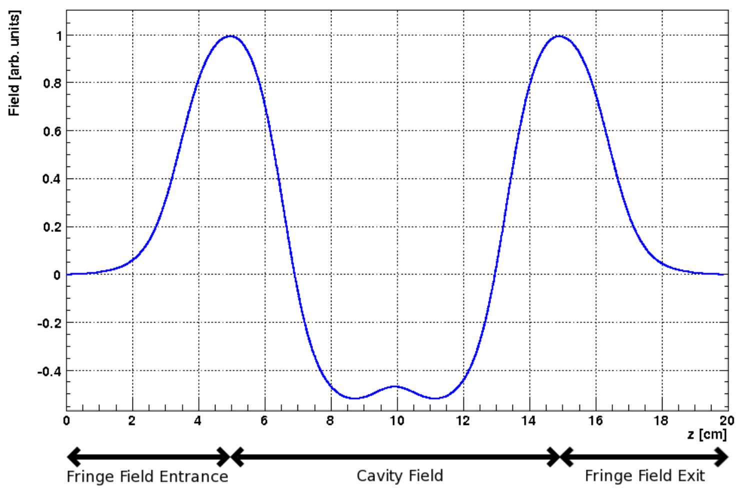

Figure 21: The on-axis field of an S-band (2997.924 MHz) `TRAVELINGWAVE` structure. The field of a single cavity is shown between its entrance and exit fringe fields. The fringe fields extend one half wavelength ($\lambda/2$) to either side.

An example of a 1D `TRAVELINGWAVE` structure field map is shown in Figure 21. This map is a standing wave solution generated by Superfish and shows the field on axis for a single accelerating cavity with the fringe fields of the structure extending to either side. *OPAL-t* reads in this field map and constructs the total field of the `TRAVELINGWAVE` structure in three parts: the entrance fringe field, the structure fields and the exit fringe field.

The fringe fields are treated as standing wave structures and are given by:

$$\mathbf{E_{entrance}}(\mathbf{r},t) = \mathbf{E_{from-map}}(\mathbf{r}) \cdot \mathrm{VOLT} \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \phi_{entrance}\right)$$
$$\mathbf{E_{exit}}(\mathbf{r},t) = \mathbf{E_{from-map}}(\mathbf{r}) \cdot \mathrm{VOLT} \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \phi_{exit}\right)$$

where VOLT and FREQ are the field magnitude and frequency attributes (see below). $\phi_{entrance} = \mathrm{LAG}$, the phase attribute of the element (see below). ϕ_{exit} is dependent upon both LAG and the NUMCELLS attribute (see below) and is calculated internally by *OPAL-t*.

The field of the main accelerating structure is reconstructed from the center section of the standing wave solution shown in Figure 21 using

$$\begin{aligned}\mathbf{E}(\mathbf{r},t) = {} & \frac{\mathrm{VOLT}}{\sin(2\pi \cdot \mathrm{MODE})} \\ & \times \left\{ \mathbf{E_{from-map}}(x,y,z) \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \mathrm{LAG} + \frac{\pi}{2} \cdot \mathrm{MODE}\right) + \right. \\ & \left. \mathbf{E_{from-map}}(x,y,z+d) \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \mathrm{LAG} + \frac{3\pi}{2} \cdot \mathrm{MODE}\right) \right\}\end{aligned}$$

where d is the cell length and is defined as $\mathrm{d} = \lambda \cdot \mathrm{MODE}$. MODE is an attribute of the element (see below). When calculating the field from the map ($\mathbf{E_{from-map}}(x,y,z)$), the longitudinal position is referenced to the start of the cavity fields at $\frac{\lambda}{2}$ (In this case starting at $z = 5.0cm$). If the longitudinal position advances past the end of the cavity map ($\frac{3\lambda}{2} = 15.0cm$ in this example), an integer number of cavity wavelengths is subtracted from the position until it is back within the map's longitudinal range.

A `TRAVELINGWAVE` structure has seven real attributes, one integer attribute, one string attribute and one Boolean attribute:

```
label: TRAVELINGWAVE, APERTURE=real-vector, L=real,
       VOLT=real, LAG=real, FMAPFN=string,
       ELEMEDGE=real, FREQ=real, NUMCELLS=integer,
       MODE=real;
```

L The length of the cavity (default: 0 m). In *OPAL-t* this attribute is ignored, the length is defined by the field map and the number of cells.

VOLT The peak RF voltage (default: 0 MV). The effect of the cavity is $\delta E = \mathrm{VOLT} \cdot \sin(\mathrm{LAG} - 2\pi \cdot \mathrm{FREQ} \cdot t)$.

LAG The phase lag [rad] (default: 0). In *OPAL-t* this phase is in general relative to the phase at which the reference particle gains the most energy. This phase is determined using an auto-phasing algorithm (see Appendix Auto-phasing Algorithm). This auto-phasing algorithm can be switched off, see `APVETO`.

DLAG The phase lag error [rad] (default: 0).

FMAPFN Field maps in the *T7* format can be specified.

FREQ Defines the frequency of the traveling wave structure in units of MHz. A warning is issued when the frequency of the cavity card does not correspond to the frequency defined in the FMAPFN file. The frequency defined in the FMAPFN file overrides the frequency defined on the cavity card.

NUMCELLS Defines the number of cells in the tank. (The cell count should not include the entry and exit half cell fringe fields.)

MODE Defines the mode in units of 2π, for example $\frac{1}{3}$ stands for a $\frac{2\pi}{3}$ structure.

FAST If FAST is true and the provided field map is in 1D then a 2D field map is constructed from the 1D on-axis field, see Fieldmaps Types and Format. To track the particles the field values are interpolated from this map instead of using an FFT based algorithm for each particle and each step. (default: FALSE)

APVETO If `TRUE` this cavity will not be auto-phased. Instead the phase of the cavity is equal to `LAG` at the arrival time of the reference particle (arrival at the limit of its field **not** at `ELEMEDGE`).

Use of a traveling wave requires the particle momentum P and the particle charge CHARGE to be set on the relevant optics command before any calculations are performed.

Example of a L-Band traveling wave structure:

```
lrf0: TRAVELINGWAVE, L=0.0253, VOLT=14.750,
      NUMCELLS=40, ELEMEDGE=2.73066,
      FMAPFN="INLB-02-RAC.Ez", MODE=1/3,
      FREQ=1498.956, LAG=248.0/360.0;
```

12.18 Monitor

A MONITOR detects all particles passing it and writes the position, the momentum and the time when they hit it into an H5hut file. Furthermore the exact position of the monitor is stored. It has always a length of 1 cm consisting of 0.5 cm drift, the monitor of zero length and another 0.5 cm drift. This is to prevent *OPAL-t* from missing any particle. The positions of the particles on the monitor are interpolated from the current position and momentum one step before they would passe the monitor.

The attribute OUTFN defines the file into which the monitor should write the collected data (see Common Attributes). The file is an H5hut file.

If the attribute TYPE is set to TEMPORAL then the data of all particles are written to the H5hut file when the reference particle hits the monitor.

This is a restricted feature for *OPAL-t*.

12.19 Collimators

Four types of collimators are defined:

ECOLLIMATOR Elliptic aperture.

RCOLLIMATOR Rectangular aperture.

FLEXIBLECOLLIMATOR Description of shape and location of holes can be provided.

CCOLLIMATOR Radial rectangular collimator in cyclotrons.

```
label: ECOLLIMATOR, TYPE=string, APERTURE=real-vector,
       L=real, XSIZE=real, YSIZE=real;

label: RCOLLIMATOR,TYPE=string, APERTURE=real-vector,
       L=real, XSIZE=real, YSIZE=real;

label: FLEXIBLECOLLIMATOR, APERTURE=real-vector,
       L=real, DESCRIPTION=string, FNAME=string, OUTFN=string;
```

Each type has the following general attributes (available for both *OPAL-t* and *OPAL-cycl* collimators):

OUTFN The file name into which the collimator should write the collected data. If this attribute is empty, the file will be named as the element label. The file is an H5hut file (or ASCII if ASCIIDUMP is true).

PARTICLEMATTERINTERACTION PARTICLEMATTERINTERACTION is an attribute of the element (see Chapter Particle Matter Interaction). TYPE=SCATTERING must be selected to include scattering interactions and energy loss calculation through the MATERIAL definition (see Available Materials in OPAL). If this is not set, the particle-matter interaction module will not be activated. Then, the particle hitting the collimator will be recorded and directly deleted from the simulation.

The reference system for a collimator is a Cartesian coordinate system.

12.19.1 *OPAL-t* mode

Optically a collimator behaves like a drift space, but during tracking, it also introduces an aperture limit. The aperture is checked at the entrance. If the length is not zero, the aperture is also checked at the exit and at every timestep. Lost particles are saved in an H5hut file defined by `OUTFN`. The `ELEMEDGE` defines the location of the collimator and `L` the length.

`` ECOLLIMATOR`s and `RCOLLIMATOR`s detect all particles which are outside the aperture defin `` `` by `XSIZE `` and `YSIZE`. The `CCOLLIMATOR` isn't supported.

XSIZE The horizontal half-aperture [m] (default: unlimited).

YSIZE The vertical half-aperture [m] (default: unlimited).

For elliptic apertures, `XSIZE` and `YSIZE` denote the half-axes respectively, for rectangular apertures they denote the half-width of the rectangle.

Example:

```
Col: ECOLLIMATOR, L=1.0E-3, ELEMEDGE=3.0E-3, XSIZE=5.0E-4,
     YSIZE=5.0E-4, OUTFN="Coll.h5";
```

The `FLEXIBLECOLLIMATOR` can be used to model both simple, rectangular or elliptic collimators and more complex devices like pepper-pots. The configuration of holes can be described with a special language. This language knows the following commands

rectangle(width, height) A rectangle that is centered at the origin of the 2D coordinate system. The arguments width and heigth can be mathematical expressions.

ellipse(width, height) An ellipse that is centered at the origin of the 2D coordinate system. The arguments width and heigth can be mathematical expressions.

polygon(x_0, y_0; x_1, y_1; x_2, y_2[; x_3, y_3[;… x_N, y_N]]) A polygon with with vertices (x_0, y_0), (x_1, y_1), (x_2, y_2), …, (x_N, y_N). The first vertex doens't have to be repeated, instead (x_N, y_N) is connected with (x_0, y_0). The polygon is then triangulized for a fast detection of stopped particles. In order for the triangulization to work the edges of the polygon may not cross each other. All arguments of the command polygon can be mathematical expressions.

mask('filename.pbm', width, height) A black and white bitmap file (Portable Bitmap format) can be provided to describe the collimator. White pixels stop particles. The first argument is the path to the pixmap file, the second and third are the width and height of the mask in meters. The arguments width and height can be mathematical expressions.

translate(command, shiftx, shifty) Translates the holes that are define by the command by shiftx in the x-direction and shifty in the y-direction. The arguments shiftx and shifty can be mathematical expressions.

rotate(command, angle) Rotates the holes that are defined by the command about the origin of the 2D coordinate system. The argument angle can be a mathematical expression.

union(command1, command2 [, command3 [, command4 […]]]) Collects the holes that are defined the by the commands.

difference(command1, command2) All particles that pass command1 and not command2 pass the difference.

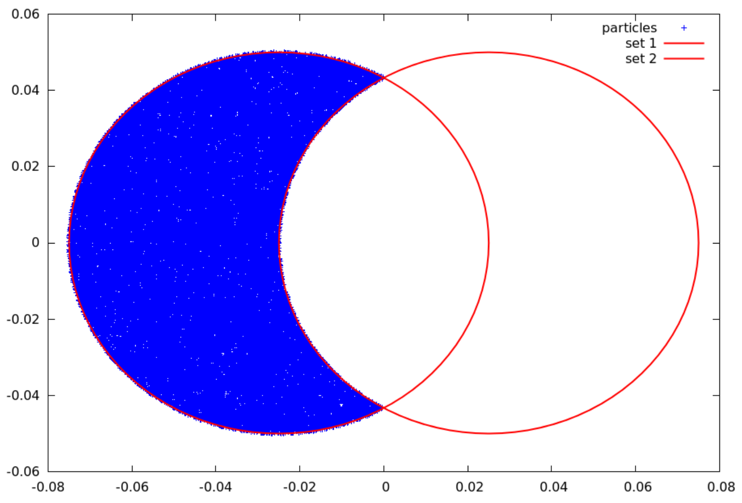

Figure 22: Illustration of a difference between to circles

symmetric_difference(command1, command2) All particles that pass either command but not both at the same time.

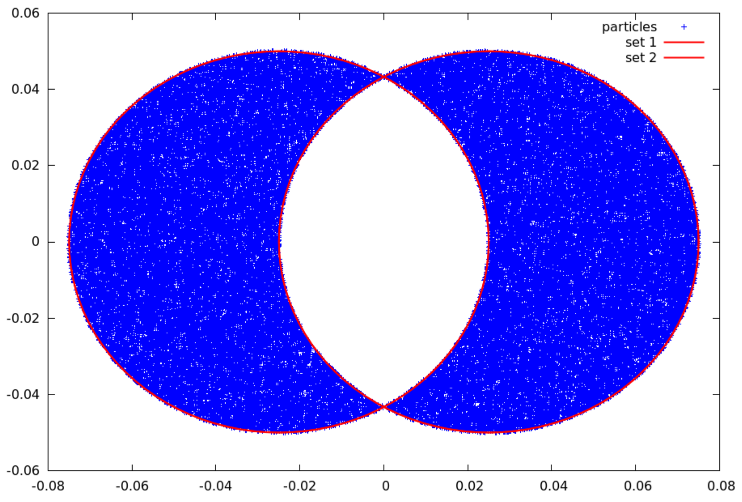

Figure 23: Illustration of a symmetric difference between to circles

intersection(command1, command2) All particles that pass both commands at the same time.

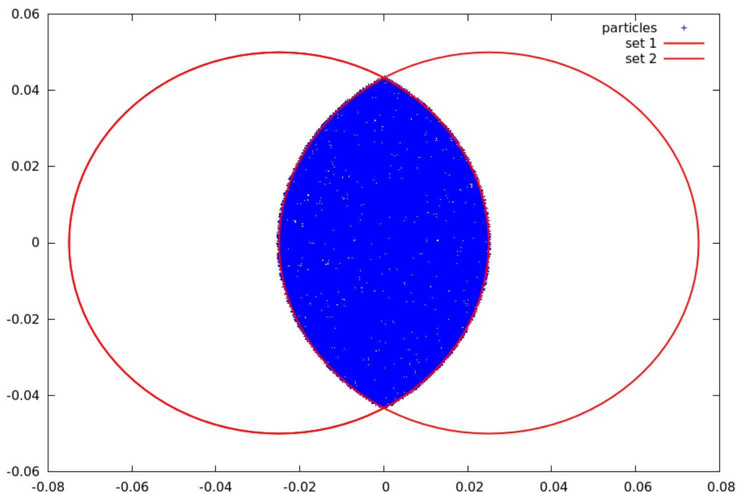

Figure 24: Illustration of a intersection between to circles

repeat(command, N, shiftx, shifty) Repeats the holes that are defined by the command translating each copy successively by shiftx in x-direction and shifty in y-direction. The arguments shiftx and shifty can be mathematical expressions.

repeat(command, N, angle) Repeats the holes that are defined by the command rotating each copy successively. The argument angle can be a mathematical expression.

The supported mathematical constants and functions are listed in the following table.

e	pi	abs(x)	acos(x)
acosh(x)	asin(x)	asinh(x)	atan(x)
atanh(x)	cbrt(x)	ceil(x)	cos(x)
cosh(x)	deg2rad(x)	erf(x)	erfc(x)
exp(x)	exp2(x)	floor(x)	isinf(x)
isnan(x)	log(x)	log2(x)	log10(x)
rad2deg(x)	round(x)	sgn(x)	sin(x)
sinh(x)	sqrt(x)	tan(x)	tanh(x)
tgamma(x)	atan2(y,x)	max(x,y)	min(x,y)

Table 22: Mathematical constants and functions

A simple elliptic collimator with major and minor axis of 4 cm and 3 cm respectively can be defined using

```
ellipse(0.04, 0.03)
```

A regular pepper-pot with rectangular holes can be define like this

```
repeat( // repeat it in y-direction
       repeat( // repeat it in x-direction
              translate(
                        rotate(
                               rectangle(
                                         0.002,
                                         0.002
                                        ),
                               0.78539
                              ),
                        -0.028,
                        -0.028
                      ),
            16,
            0.004,
            0.0
          ),
      16,
      0.0,
      0.004
    )
```

The latter example will produce a holes as in the following picture

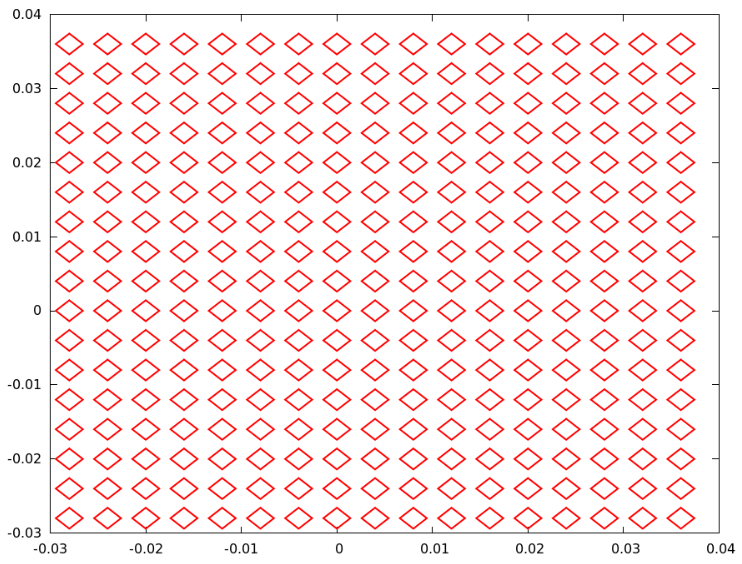

Figure 25: Pepper-pot with rectangle holes

In the `FLEXIBLECOLLIMATOR` command the description of the holes can be provided as a string (using `DESCRIPTION`; the string may not contain comments and newlines) or in a separate file (using `FNAME`; comments and newlines are allowed).

12.19.2 *OPAL-cycl* mode

Only `CCOLLIMATOR` is available for *OPAL-cycl*. This element is radial rectangular collimator which can be used to collimate the radial tail particles. When a particle hits this collimator, it will be absorbed or scattered. The algorithm is based on the Monte Carlo method. Please note when a particle is scattered, it will not be recorded as the lost particle. If this particle leaves the bunch, it will be removed during the integration afterwards, so as to maintain the accuracy of space charge solving. In addition to the general attributes of a collimator (`OUTFN` and `PARTICLEMATTERINTERACTION`), the parameters for describing a `CCOLLIMATOR` are the following:

XSTART The x coordinate of the start point [mm].

XEND The x coordinate of the end point [mm].

YSTART The y coordinate of the start point [mm].

YEND The y coordinate of the end point [mm].

ZSTART The minimum vertical coordinate [mm] (default: -100mm).

ZEND The maximum vertical coordinate [mm] (default: 100mm).

WIDTH The width of the collimator [mm].

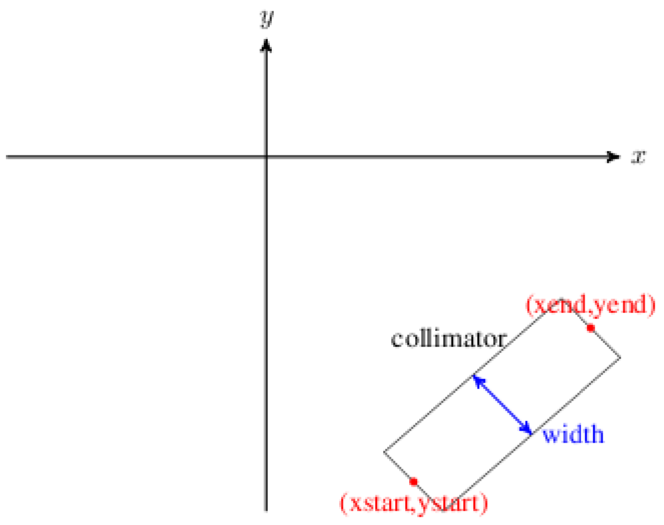

Figure 26: Collimator

Example:

```
REAL y1=-0.0;
REAL y2=0.0;
REAL y3=200.0;
REAL y4=205.0;
REAL x1=-215.0;
REAL x2=-220.0;
REAL x3=0.0;
REAL x4=0.0;

cmphys: PARTICLEMATTERINTERACTION, TYPE=SCATTERING, MATERIAL=COPPER;

cma1: CCOLLIMATOR, XSTART=x1, XEND=x2, YSTART=y1, YEND=y2,
      ZSTART=2, ZEND=100, WIDTH=10.0, PARTICLEMATTERINTERACTION=cmphys ;

cma2: CCOLLIMATOR, XSTART=x3, XEND=x4, YSTART=y3, YEND=y4,
      ZSTART=2, ZEND=100, WIDTH=10.0, PARTICLEMATTERINTERACTION=cmphys;
```

The particles lost on the `CCOLLIMATOR` are recorded in the HDF5 file *OUTFN.h5* (or ASCII if ASCIIDUMP is true).

12.20 Septum (*OPAL-cycl*)

This is a restricted feature for *OPAL-cycl*. The particles hitting on the septum are removed from the bunch and recorded in the `OUTFN` file. There are 5 parameters to describe a `SEPTUM`.

XSTART The x coordinate of the start point [mm].

XEND The x coordinate of the end point [mm].

YSTART The y coordinate of the start point [mm].

YEND The y coordinate of the end point [mm].

WIDTH The width of the septum [mm].

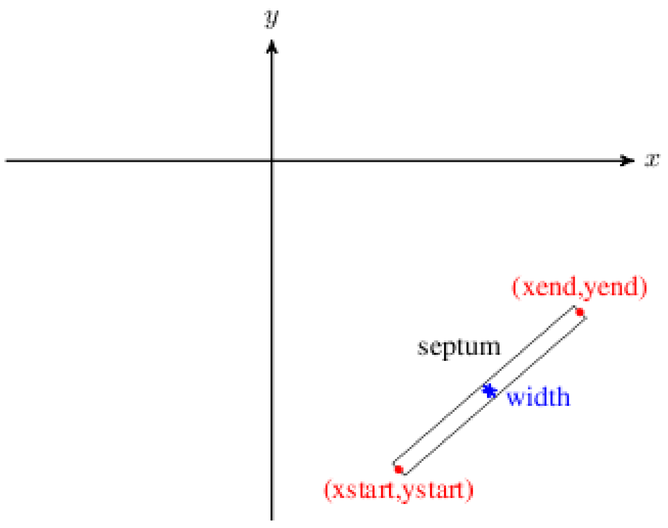

Figure 27: Septum

Example:

```
eec2: SEPTUM, XSTART=4100.0, XEND=4300.0,
              YSTART=-1200.0, YEND=-150.0,
              WIDTH=0.05;
```

The particles lost on the SEPTUM are recorded in the HDF5 file *OUTFN.h5* (or ASCII if ASCIIDUMP is true).

12.21 Probe (*OPAL-cycl*)

The particles hitting on the probe are recorded in the `OUTFN` file (see Common Attributes). There are 5 parameters to describe a probe.

XSTART The x coordinate of the start point [mm].

XEND The x coordinate of the end point [mm].

YSTART The y coordinate of the start point [mm].

YEND The y coordinate of the end point [mm].

STEP The step size of the probe [mm] (for histogram and peak finder output) (default: 1mm).

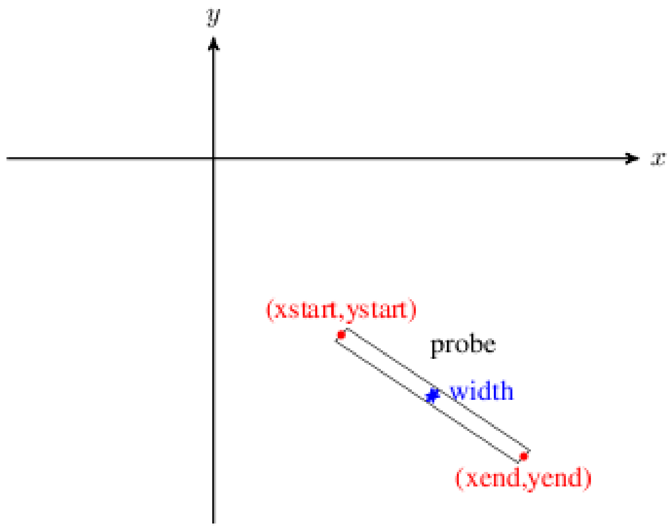

Figure 28: Probe

Example:

```
prob1: PROBE, XSTART=4166.16, XEND=4250.0,
              YSTART=-1226.85, YEND=-1241.3;
```

The particles probed on the PROBE are recorded in the HDF5 file *OUTFN.h5* (or ASCII if ASCIIDUMP is true). Please note that these particles are not deleted in the simulation, however, they are recorded in the "loss" file.

The radius of the particles recorded in the PROBE is recorded in the histogram ".hist" and peak ".peaks" file. The histogram file contains data as recorded in actual probe measurements. The corresponding peaks file contains the peaks found in the probe histogram by the same peak finder used for the PSI measurements. Note that for probes in multiple quadrants the histogram and peaks file is often not meaningful since the absolute radius is stored.

12.22 Output Plane (*OPAL-cycl*)

The output plane element is similar to the Probe element. Information about particles that pass through the plane is recorded in the file specified by the ’OUTFN’ attribute. (see Common Attributes). The location of the plane can be specified in one of two ways indicated by the ’PLACEMENT_STYLE’ attribute. The style ’PROBE’ defines the plane with horizontal extent from ’XSTART’ to ’XEND’ and vertical extent from ’YSTART’ to ’YEND’ in the same manner as the Probe element. The style ’CENTRE_NORMAL’ uses the ’CENTRE’ point and the ’NORMAL’ to define the location and orientation of the plane while ’WIDTH’, ’HEIGHT’ and ’RADIUS’ specify its extent. If any of ’WIDTH’, ’HEIGHT’ or ’RADIUS’ are zero, then that attribute is ignored, making it possible to define circular, rectangular and infinite planes. The plane then adjusts itself the first time the reference particle passes through it so that it is centred on that particle’s crossing and its normal points in that particle’s trajectory direction.

These attributes describe the output plane.

XSTART The x coordinate of the start point for PROBE style placement [m].

XEND The x coordinate of the end point for PROBE style placement [m].

YSTART The y coordinate of the start point for PROBE style placement [m].

YEND The y coordinate of the end point for probe PROBE placement [m].

CENTRE 3-vector position of the plane centre for CENTER_NORMAL style placement [m].

NORMAL 3-vector normal to the plane.

REFERENCE_ALIGNMENT_PARTICLE Set to a particle number (usually 0, the reference particle). The first time that the particle crosses the reference plane, then the plane will be moved to centre on that particle and point in the direction S of the particle.

TOLERANCE Tolerance on position of track intercept [m].

RADIUS Maximum distance from centre of plane for crossings [m].

ALGORITHM The algorithm used to step from the track point to the plane, one of "INTERPOLATION", "RK4".

PLACEMENT_STYLE Set to PROBE to define the plane using XSTART, XEND, YSTART, YEND or CENTRE_NORMAL to define the plane using centre and normal.

VERBOSE Set to 0 for minimal output up to 4 to output diagnostics on every track step. Output is sent to the OPAL console."

Example:

```
outplane1: OUTPUTPLANE, PLACEMENT_STYLE=CENTRE_NORMAL, CENTRE={10, 13.5, 0},
           NORMAL={1,0,0}, WIDTH=1.5, HEIGHT=0.8, RADIUS=1, ALGORITHM=RK4,
           VERBOSE=1, REFERENCE_ALIGNMENT_PARTICLE=0, OUTFN="FileName.txt";
```

12.23 Stripper (*OPAL-cycl*)

A stripper element strip the electron(s) from a particle. The particle hitting the stripper is recorded in the `OUTFN` file (see Common Attributes), which contains the time, coordinates and momentum of the particle at the moment it hit the stripper. The charge and mass are changed. It has the same geometry as the PROBE element. Please note that the stripping physics is not included yet.

There are 9 parameters to describe a stripper.

XSTART The x coordinate of the start point. [mm]

XEND The x coordinate of the end point. [mm]

YSTART The y coordinate of the start point. [mm]

YEND The y coordinate of the end point. [mm]

OPCHARGE Charge number of the outcoming particle. Negative value represents negative charge.

OPMASS Mass of the outcoming particles. [GeV/c^2]

OPYIELD Yield of the outcoming particle (the number of outcoming particles per incoming particle), the default value is 1.

STOP If STOP is true, the particle is stopped and deleted from the simulation; Otherwise, the outcoming particle continues to be tracked along the extraction path.

Example: H_2^+ particle stripping

```
prob1: STRIPPER, XSTARTt=4166.16, XEND=4250.0,
                 YSTART=-1226.85, YEND=-1241.3,
                 OPCHARGE=1, OPMASS=PMASS,
                 OPYIELD=2, STOP=false;
```

No matter what the value of `STOP` is, the particles hitting on the `STRIPPER` are recorded in the HDF5 file *OUTFN.h5* (or ASCII if ASCIIDUMP is true).

12.24 Degrader (*OPAL-t*)

Elliptical degrader with an overall length `L`. The particles lost on a degrader are recorded in the `OUTFN` file (see Common Attributes).

XSIZE Horizontal axis of the transverse elliptical shape [m] (default: 1e6).

YSIZE Vertical axis of the transverse elliptical shape [m] (default: 1e6).

PARTICLEMATTERINTERACTION `PARTICLEMATTERINTERACTION` is an attribute of the element (see Chapter Particle Matter Interaction). `TYPE=SCATTERING` must be selected to include scattering interactions and energy loss calculation through the `MATERIAL` definition (see Available Materials in OPAL). If this is not set, the particle-matter interaction module will not be activated. The particle hitting degrader will be recorded and directly deleted from the simulation.

Example: Graphite degrader of 15 cm thickness.

```
DEGPHYS: PARTICLEMATTERINTERACTION, TYPE=SCATTERING, MATERIAL=GRAPHITE;

DEG1: DEGRADER, L=0.15, ELEMEDGE=0.02, PARTICLEMATTERINTERACTION=DEGPHYS;
```

12.25 Correctors (*OPAL-t*)

Three types of correctors are available:

HKICKER A corrector for the horizontal plane.

VKICKER A corrector for the vertical plane.

KICKER A corrector for both planes.

They act as

```
label:HKICKER, TYPE=string, APERTURE=real-vector,
      L=real, KICK=real;
label:VKICKER, TYPE=string, APERTURE=real-vector,
      L=real, KICK=real;
label:KICKER, TYPE=string, APERTURE=real-vector,
      L=real, HKICK=real, VKICK=real;
```

They have the following attributes:

L The length of the closed orbit corrector (default: 0 m).

KICK The kick angle in rad for either horizontal or vertical correctors (default: 0 rad).

HKICK The horizontal kick angle in rad for a corrector in both planes (default: 0 rad).

VKICK The vertical kick angle in rad for a corrector in both planes (default: 0 rad).

DESIGNENERGY Fix the magnitude of the magnetic field using the given `DESIGNENERGY` and the angle (`KICK`, `HKICK` or `VKICK`). If the design energy isn't set then the actual energy of the reference particle at the position of the corrector is used. The `DESIGNENERGY` is expected in MeV.

A positive kick increases p_x or p_y respectively. Use `KICK` for an `HKICKER` or `VKICKER` and `HKICK` and `VKICK` for a `KICKER`. Instead of using a `KICKER` or a `VKICKER` one could use an `HKICKER` and rotate it appropriately using `PSI`.

Correctors don't change the reference trajectory. Otherwise they are implemented as `RBEND` with $\mathrm{E1} = 0$ and without fringe fields (hard edge model). They can be used to model earth's magnetic field which is neglected in the design trajectory but which has a noticeable effect on the trajectory of a bunch at low energies.

Examples:

```
HK1: HKICKER, KICK=0.001;
VK3: VKICKER, KICK=0.0005;
KHV: KICKER,  HKICK=0.001, VKICK=0.0005;
```

The reference system for an orbit corrector is a Cartesian coordinate system.

12.26 Vacuum

Vacuum element represents the conditions and parameters to consider interactions with the residual gas and the magnetic field. When the particle interacts, it is recorded in the file, which contains the time, coordinates and momentum of the particle at this moment. The particle could produce a new particle, changing the charge and mass.

In *OPAL-cycl* the vacuum region is defined according to the cyclotron boundaries (`MINZ`, `MAXZ`, `MINR` and `MAXR`, see CYCLOTRON element), whereas in *OPAL-t* is described by `L` and `ELEMEDGE` parameters (see Common Attributes).

There are 7 specific parameters to describe the vacuum space.

PRESSURE The average pressure of the residual gas [mbar].

TEMPERATURE Temperature of residual gas [K].

PMAPFN File name of the mid-plane pressure map. This feature is only available for *OPAL-cycl*. The pressure data is stored in a sequence shown in 2D field map on the median plane with primary direction corresponding to the azimuthal direction, secondary direction to the radial direction (same file structure as `Cyclotron TYPE=CARBONCYCL`). If `PMAPFN` is specified, `PRESSURE` parameter is taken as default value for regions in the accelerator out of the limits of the pressure map.

PSCALE Scale factor for the pressure field map (default: 1.0). Only available for *OPAL-cycl*.

GAS Type of gas for residual vacuum: `H2` or `AIR`

STOP If STOP is true, the particle is stopped and deleted from the simulation. Otherwise, the outcoming particle (according to the cross section evaluation) continues to be tracked as `SECONDARY` particle (default: true).

PARTICLEMATTERINTERACTION `PARTICLEMATTERINTERACTION` is an attribute of the element (see Chapter Particle Matter Interaction). `TYPE=BEAMSTRIPPING` must be selected to include stripping interactions with the residual gas and Lorentz stripping.

Example: Vacuum representation with H_2 residual gas.

```
bstp_phys: PARTICLEMATTERINTERACTION, TYPE=BEAMSTRIPPING;

vac: VACUUM, PRESSURE=1E-8, TEMPERATURE=300,
     GAS=H2, STOP=true, PARTICLEMATTERINTERACTION=bstp_phys;
```

No matter what the value of STOP is, the particles stripped are recorded in the HDF5 file (or ASCII if ASCIIDUMP is true).

12.27 Undulator (*OPAL-t*)

OPAL's undulator element comes with its own Finite-Difference Time-Domain full-wave solver, which accounts for space-charge and radiation effects in 3D. It was implemented by means of the MITHRA library, developed by Arya Fallahi.

To use the undulator element and its solver, one needs to compile *OPAL* in the following way:

1. install the MITHRA 2.0 library,
2. set the environment variable `MITHRA_PREFIX=directory/where/you/store/mithra`

3. compile *OPAL* with the option `cmake -DENABLE_OPAL_FEL=yes ..`

When the head of the bunch crosses the start of an undulator in the beamline (defined by `ELEMEDGE`), the solver changes automatically from Poisson to full-wave, and changes back to Poisson once the bunch has passed through the whole undulator and its fringe fields.

The length of the undulator is defined as

$$L = N\lambda + 2\,\mathrm{fringe},$$
$$\mathrm{fringe} = 2\lambda,$$

where λ is the undulator period and N its number of periods. Since the element's length is entirely defined by the undulator periods, there is no `LENGTH` parameter to be specified for the undulator element.

The magnetic field is that of a planar undulator with flat pole faces:

$$B_x = B_0 \cosh(kr)\sin(kz)\cos(\alpha),$$
$$B_y = B_0 \cosh(kr)\sin(kz)\sin(\alpha),$$
$$B_z = B_0 \sinh(kr)\cos(kz),$$

where $r = x\cos(\alpha) + y\sin(\alpha)$ is the radial distance from the undulator axis, $k = 2\pi/\lambda$ the wave-number, α the angle between the magnetic field polarisation and the x-axis, and B_0 the maximum magnetic field value.

The fringe fields are defined as:

$$B_x = B_0 \cosh(kr)kze^{-(kz)^2/2}\cos(\alpha),$$
$$B_y = B_0 \cosh(kr)kze^{-(kz)^2/2}\sin(\alpha),$$
$$B_z = B_0 \sinh(kr)e^{-(kz)^2/2}.$$

The parameters that describe the undulator element and its associated full-wave solver are as follows:

K The undulator strength parameter.

LAMBDA The undulator period λ [m].

NUMPERIODS Number of periods N.

ANGLE Angle α between the magnetic field polarisation and the x-axis [rad] (default: 0).

MESHLENGTH Size in three dimensions (L_x, L_y, L_z) of the computational grid [m], which is in a frame of reference moving at the average speed of the bunch. It should be large enough to contain the whole bunch, as particles outside of it will not perceive any fields. As a rule of thumb, the grid should be 3 times longer than the bunch, since the bunch will slightly shift longitudinally when entering and exiting the undulator, and 10 times wider than the bunch, to avoid spurious radiation reflections, since the Absorbing Boundary Conditions (ABCs) cannot correctly absorb obliquely incident waves.

MESHRESOLUTION Grid-spacing $(\Delta_x, \Delta_y, \Delta_z)$ of the computational domain [m].

DTBUNCH Time-step for the particle update [s]. By default it is equal to the field update time-step, which is automatically chosen by the algorithm in order to satisfy the stability conditon. `DTBUNCH` needs to be equal to or smaller than the field time-step.

TRUNORDER Truncation order of the ABCs. Can be 1 or 2 (default: 2).

TOTALTIME Total time to simulate using the full-wave solver [s]. By default this is set such that the whole passage through the undulator is simulated.

FNAME File specifying which output the full-wave solver should provide. It is equivalent to the job-file in MITHRA, without the parameters `MESH`, `bunch-initialization`, and `UNDULATOR`. This file is optional.

Example of the wiggler element used in the AWA beamline:

```
UND: UNDULATOR, ELEMEDGE = 44.0e-2, K = 10.81, LAMBDA = 8.5e-2, NUMPERIODS = 10, ANGLE = PI ↩
    /2,
     MESHLENGTH = { 12e-3, 12e-3, 4e-3 }, MESHRESOLUTION = { 1e-5, 1e-5, 8e-6},
     FNAME = "wiggler_sims_July_2020/mithra_output.job";
```

12.28 References

[23] *Tait-bryan angles*.

[24] J. E. Spencer and H. A. Enge, *Split-pole magnetic spectrograph for precision nuclear spectroscopy*, Nucl. Instrum. Methods 49, 181 (1967).

Chapter 13

Field Output

There are two routines that can be used to write out the external field used in *OPAL-cycl*.

DUMPFIELDS Write out static magnetic field map on a Cartesian grid

DUMPEMFIELDS Write out electromagnetic field map on a 4D grid in space-time. Cartesian and cylindrical grids are supported. `DUMPEMFIELDS` is an extension of `DUMPFIELDS`.

13.1 DUMPFIELDS Command

The `DUMPFIELDS` statement causes *OPAL-cycl* to write out static magnetic field data on a 3D cartesian grid. The format of field output is:

```
<number of rows>
1 x [m]
2 y [m]
3 z [m]
4 Bx [kGauss]
5 By [kGauss]
6 Bz [kGauss]
0
<x0> <y0> <z0> <Bx0> <By0> <Bz0>
<x1> <y1> <z1> <Bx1> <By1> <Bz1>
...
```

The following attributes are enabled on the `DUMPFIELDS` statement:

FILE_NAME Name of the file to which field data is dumped. It is an error if the location reference by `FILE_NAME` cannot be opened. Any existing file is overwritten.

X_START Start point in the grid in x [m].

DX Grid step size in x [m].

X_STEPS Number of steps in x. It is an error if `X_STEPS` is non-integer or less than 1.

Y_START Start point in the grid in y [m].

DY Grid step size in y [m].

Y_STEPS Number of steps in y. It is an error if `Y_STEPS` is non-integer or less than 1.

Z_START Start point in the grid in z [m].

DZ Grid step size in z [m].

Z_STEPS Number of steps in z. It is an error if `Z_STEPS` is non-integer or less than 1.

This example makes a field map in the midplane (x-y plane) only, starting at $(x,y) = (0,0)$ m, with 101 steps in each direction and a stride of 0.1m. z is always 0.

```
DUMPFIELDS, X_START=0., X_STEPS=101, DX=0.100,
            Y_START=0., Y_STEPS=101, DY=0.100,
            Z_START=0., Z_STEPS=1, DZ=0.100,
            FILE_NAME="FieldMapXY.dat";
```

13.2 DUMPEMFIELDS Command

The `DUMPEMFIELDS` statement causes *OPAL-cycl* to write out electromagnetic field data on a 4D grid. Grids in a Cartesian coordinate system (x,y,z,t) and a cylindrical coordinate system about the z-axis in (r,ϕ,z,t) are supported.

13.2.1 Cartesian Mode

In Cartesian mode the format of the field output is:

```
<number of rows>
1  x [m]
2  y [m]
3  z [m]
4  t [ns]
5  Bx [kGauss]
6  By [kGauss]
7  Bz [kGauss]
8  Ex [MV/m]
9  Ey [MV/m]
10 Ez [MV/m]
0
<x0> <y0> <z0> <t0> <Bx0> <By0> <Bz0> <Ex0> <Ey0> <Ez0>
<x1> <y1> <z1> <t1> <Bx1> <By1> <Bz1> <Ex1> <Ey1> <Ez1>
...
```

The following attributes are enabled on the `DUMPEMFIELDS` statement when operating in Cartesian mode:

FILE_NAME Name of the file to which field data is dumped. It is an error if the location referenced by `FILE_NAME` cannot be opened. Any existing file is overwritten.

COORDINATE_SYSTEM ’CARTESIAN’ must be set. The string is not case sensitive. It is an error if the string is not one of ’CARTESIAN’ or ’CYLINDRICAL’.

X_START Start point in the grid in x [m].

DX Grid step size in x [m].

X_STEPS Number of steps in x. It is an error if `X_STEPS` is non-integer or less than 1.

Y_START Start point in the grid in y [m].

DY Grid step size in y [m].

Y_STEPS Number of steps in y. It is an error if `Y_STEPS` is non-integer or less than 1.

Z_START Start point in the grid in z [m].

DZ Grid step size in z [m].

Z_STEPS Number of steps in z. It is an error if `Z_STEPS` is non-integer or less than 1.

T_START Start point in the grid in time [ns].

DT Grid step size in time [ns].

T_STEPS Number of steps in time. It is an error if `T_STEPS` is non-integer or less than 1.

13.2.2 Cylindrical Mode

In Cylindrical mode the format of the field output is:

```
<number of rows>
1 r [m]
2 phi [deg]
3 z [m]
4 t [ns]
5 Br   [kGauss]
6 Bphi [kGauss]
7 Bz   [kGauss]
8 Er   [MV/m]
9 Ephi [MV/m]
10 Ez  [MV/m]
0
<r0> <phi0> <z0> <t0> <Br0> <Bphi0> <Bz0> <Er0> <Ephi0> <Ez0>
<r1> <phi1> <z1> <t1> <Br1> <Bphi1> <Bz1> <Er1> <Ephi1> <Ez1>
...
```

The following attributes are enabled on the `DUMPEMFIELDS` statement when operating in Cylindrical mode:

FILE_NAME Name of the file to which field data is dumped. It is an error if the location referenced by `FILE_NAME` cannot be opened. Any existing file is overwritten.

COORDINATE_SYSTEM ’CYLINDRICAL’ must be set. The string is not case sensitive. It is an error if the string is not one of ’CARTESIAN’ or ’CYLINDRICAL’.

R_START Start point in the grid in r [m].

DR Grid step size in r [m].

R_STEPS Number of steps in r. It is an error if `R_STEPS` is non-integer or less than 1.

PHI_START Start point in the grid in phi [rad].

DPHI Grid step size in phi [rad].

PHI_STEPS Number of steps in phi. It is an error if `PHI_STEPS` is non-integer or less than 1.

Z_START Start point in the grid in z [m].

DZ Grid step size in z [m].

Z_STEPS Number of steps in z. It is an error if `Z_STEPS` is non-integer or less than 1.

T_START Start point in the grid in time [ns].

DT Grid step size in time [ns].

T_STEPS Number of steps in time. It is an error if `T_STEPS` is non-integer or less than 1.

Chapter 14

Beam Lines

The accelerator to be studied is known to *OPAL* as a sequence of physical elements called a **beam line**. A beam line is built from simpler beam lines whose definitions can be nested to any level. A powerful syntax allows to repeat or to reflect pieces of beam lines. Formally a beam line is defined by a `LINE` command:

```
label:LINE=(member,...,member);
```

label gives a name to the beam line for later reference.

Each `member` may be one of the following:

- An element label,
- A beam line label,
- A sub-line, enclosed in parentheses,

Beam lines can be nested to any level.

14.1 Simple Beam Lines

The simplest beam line consists of single elements:

```
label:LINE=(member,...,member);
```

Example:

```
L:LINE=(A,B,C,D,A,D);
```

ORIGIN Position vector of the origin of the line. All elements in this line that are placed using `ELEMEDGE` use this position as reference.

ORIENTATION Vector of Tait-Bryan angles [bib.tait-bryan] of the orientation of the line at the origin.

14.2 Sub-lines

Instead of referring to an element, a beam line member can refer to another beam line defined in a separate command. This provides a shorthand notation for sub-lines which occur several times in a beam line. Lines and sub-lines can be entered in any order, but when a line is used, all its sub-lines must be known.

Example:

```
L:LINE=(A,B,S,B,A,S,A,B);
S:LINE=(C,D,E);
```

This example produces the following expansion steps:

1. Replace sub-line `S`:

   ```
   (A,B,(C,D,E),B,A,(C,D,E),A,B)
   ```

2. Omit parentheses:

   ```
   A,B,C,D,E,B,A,C,D,E,A,B
   ```

evaluated to constants immediately.

Chapter 15

Beam Command

All *OPAL* commands working on a beam require the setting of various quantities related to this beam. These are entered by a `BEAM` command:

```
label:BEAM, PARTICLE=name, MASS=real, CHARGE=real,
      ENERGY=real, PC=real, GAMMA=real, BCURRENT=real,
      NPART=real, BFREQ=real;
```

The `label` is optional, it defaults to `UNNAMED_BEAM`.

15.1 Particle Definition

The beam particle is defined by `PARTICLE` attribute, which includes a direct assignment of the particle mass and charge, as indicated below. The mass values are taken from Atomic Mass Data Center [25] and Kinetic Database [26]. In the case of heavy ion beams, it is important to note that a specific type of fully ionized isotope are considered. The mass of the ions is calculated by subtracting the mass of the electrons and the binding energy [27] from the atomic mass. For other type of particle beams, this attribute must not be used. Instead, the particle beam is defined by means of `MASS` and `CHARGE` attributes specified by the user.

PARTICLE The name of particles in the machine.

OPAL knows the mass (see Predefined Symbolic Constants) and the charge for the following particles:

ELECTRON The particles are electrons (`MASS` = m_e, `CHARGE` = -1).

POSITRON The particles are positrons (`MASS` = m_e, `CHARGE` = +1).

MUON The particles are of type muon (`MASS` = m_μ, `CHARGE` = -1).

PROTON The particles are protons (`MASS` = m_p, `CHARGE` = +1).

ANTIPROTON The particles are anti-protons (`MASS` = m_p, `CHARGE` = -1).

DEUTERON The particles are of type deuteron (`MASS` = m_d, `CHARGE` = +1).

HMINUS The particles are negative hydrogen ions (H^-) (`MASS` = m_{hm}, `CHARGE` = -1).

H2P The particles are molecular hydrogen ions (H_2^+) (`MASS` = m_{h2p}, `CHARGE` = +1).

ALPHA The particles are of alpha particles (`MASS` = m_α, `CHARGE` = +2).

CARBON The particles are fully-stripped carbon-12 ions (`MASS` = m_c, `CHARGE` = +6).

XENON The particles are fully-stripped xenon-129 ions (`MASS` = m_{xe}, `CHARGE` = +54).

URANIUM The particles are fully-stripped uranium-238 ions (`MASS` = m_u, `CHARGE` = +92).

For other particle types one may enter:

MASS The particle mass in GeV.

CHARGE The particle charge expressed in elementary charges.

15.2 Beam Energy

To specify the energy there are three attributes (in order of priority):

GAMMA The particle energy divided by its mass.

ENERGY The particle energy in GeV.

PC The particle momentum in GeV/c.

15.3 Other Attributes

The other attributes are:

BFREQ The bunch frequency in MHz.

BCURRENT The bunch current in A. BCURRENT $= Q \times$ BFREQ with Q the total charge.

NPART The number of macro particles for the simulations

NSLICE The number of slices per bunch

MOMENTUMTOLERANCE Fractional tolerance to deviations in the distribution compared to the reference momentum at initialisation. If `MOMENTUMTOLERANCE` $<=0$, no tolerance checking is done (default=1e-2).

15.4 References

[25] M. Wang et al., *The AME 2020 atomic mass evaluation (II). Tables, graphs and references*, Chinese Phys. C, 45, 030003 (2021). Atomic Mass Data Center, *Atomic Mass Evaluation - AME2020*.

[26] *Kinetic Database for Astrochemistry*.

[27] *NIST Atomic Spectra Database Ionization Energies Form*, Atomic Spectra Database, NIST Standard Reference Database 78 (Version 5.9).

Chapter 16

Distribution Command

Distribution Type	Description
FROMFILE	Initial distribution read in from text file provided by user.
GAUSS	Initial distribution generated using Gaussian distribution(s).
FLATTOP	Initial distribution generated using flattop distribution(s).
BINOMIAL	Initial distribution generated using binomial distribution(s).
GAUSSMATCHED	Initial distribution generated using matched Gaussian distribution(s).
GUNGAUSSFLATTOPTH	Legacy. Special case of `FLATTOP` distribution.
ASTRAFLATTOPTH	Legacy. Special case of `FLATTOP` distribution.

Table 23: Possible distribution types.

The distribution command is used to introduce particles into an *OPAL* simulation. Like other *OPAL* commands (see Chapter Command Format), the distribution command is of the form:

```
Name:DISTRIBUTION, TYPE = DISTRIBUTION_TYPE,
                   ATTRIBUTE #1 =,
                   ATTRIBUTE #2 =,
                   .
                   .
                   .
                   ATTRIBUTE #N =;
```

The distribution is given a name (which is used to reference the distribution in the *OPAL* input file), a distribution type, and a list of attributes. The types of distributions that are supported are listed in Table 23. The attributes that follow the distribution type further define the particle distribution. Some attributes are universal, while others are specific to the distribution type. In the following sections we will define the distribution attributes, starting with the general, or universal attributes. (Note that, in general, if a distribution type does not support a particular attribute, defining a value for it does no harm. That attribute just gets ignored.)

16.1 Units

The internal units used by *OPAL-t* and *OPAL-cycl* are described in OPAL-t variables and OPAL-cycl variables. When defining a distribution, both *OPAL-t* and *OPAL-cycl* use meters for length and seconds for time. However, there are different options for the units used to input the momentum. This is controlled with the INPUTMOUNITS attribute.

Attribute Name	Value	Description
INPUTMOUNITS	NONE (default for *OPAL-t*)	Use no units for the input momentum (p_x, p_y, p_z). Momentum is given as $\beta_x\gamma$, $\beta_y\gamma$ and $\beta_z\gamma$, as in OPAL-t variables.
INPUTMOUNITS	EVOVERC (default for *OPAL-cycl*)	Use the units eV/c for the input momentum (p_x, p_y, p_z).

Table 24: Definition of INPUTMOUNITS attribute.

16.1.1 Unit conversion of momentum in *OPAL-t* and *OPAL-cycl*

Convert $\beta_x\gamma$ [dimensionless] to [mrad],

$$(\beta\gamma)_{\text{ref}} = \frac{P}{m_0 c} = \frac{Pc}{m_0 c^2}$$

$$P_x[mrad] = 1000 \times \frac{(\beta_x\gamma)}{(\beta\gamma)_{\text{ref}}}$$

Convert from [eV/c] to $\beta_x\gamma$ [dimensionless],

$$(\beta_x\gamma) = \frac{P_x[eV/c]}{m_0 c} = \frac{P_x[eV/c]c}{m_0 c^2}$$

This may be deduced by analogy for the y and z directions.

16.2 General Distribution Attributes

Once the distribution type is chosen, the next attribute to specify is the EMITTED attribute. The EMITTED attribute controls whether a distribution is *injected* or *emitted*. An *injected* distribution is placed in its entirety into the simulation space at the start of the simulation. An *emitted* beam is emitted into the simulation over time as the simulation progresses (e.g. from a cathode in a photoinjector simulation). Currently, only *OPAL-t* supports *emitted* distributions. The default is an *injected* distribution.

Attribute Name	Value	Description
EMITTED	FALSE (default)	The distribution is injected into the simulation in its entirety at the start of the simulation. The particle coordinates for an injected distribution are defined as in OPAL-t variables and OPAL-cycl variables. Note that in *OPAL-t* the entire distribution will automatically be shifted to ensure that the z coordinate will be greater than zero for all particles.
EMITTED	TRUE	The distribution is emitted into the simulation over time as the simulation progresses. Currently only *OPAL-t* supports this type of distribution. In this case, the longitudinal coordinate, as defined by OPAL-t variables, is given in seconds instead of meters. Early times are emitted first.

Table 25: Definition of EMITTED attribute.

Depending on the EMITTED attribute, we can specify several other attributes that do not depend on the distribution type. These are defined in Universal Attributes, Injected Distribution Attributes and Emitted Distribution Attributes.

16.2.1 Universal Attributes

Attribute Name	**Default Value**	**Units**	**Description**
`WRITETOFILE`	`FALSE`	None	Echo initial distribution to text file *data/<basename >* DIST.dat_.
`SCALABLE`	`FALSE`	None	Makes the generation scalable with respect of number of particles. The result depends on the number of cores used.
`WEIGHT`	1.0	None	Weight of distribution when used in a distribution list (see Section 16.5).
`NBIN`	0	None	The distribution (beam) will be broken up into `NBIN` energy bins. This has consequences for the space charge solver (see Energy Bins).
`SBIN`	100	None	Number of sample bins to use per energy bin.
`XMULT`	1.0	None	Value used to scale the x positions of the distribution particles. Applied after the distribution is generated (or read in).
`YMULT`	1.0	None	Value used to scale the y positions of the distribution particles. Applied after the distribution is generated (or read in).
`PXMULT`	1.0	None	Value used to scale the x momentum, p_x, of the distribution particles. Applied after the distribution is generated (or read in).
`PYMULT`	1.0	None	Value used to scale the y momentum, p_y, of the distribution particles. Applied after the distribution is generated (or read in).
`PZMULT`	1.0	None	Value use to scale the z momentum, p_z, of the distribution particles. Applied after the distribution is generated (or read in).
`OFFSETX`	0.0	m	Distribution is shifted in x by this amount after the distribution is generated (or read in). Same as the average x position, $\bar{x}$.
`OFFSETY`	0.0	m	Distribution is shifted in y by this amount after the distribution is generated (or read in). Same as the average y position, $\bar{y}$.
`OFFSETPX`	0.0	Section 16.1	Distribution is shifted in p_x by this amount after the distribution is generated (or read in). Same as the average p_x value, $\bar{p}_x$.
`OFFSETPY`	0.0	Section 16.1	Distribution is shifted in p_y by this amount after the distribution is generated (or read in). Same as the average p_y value, $\bar{p}_y$.
`OFFSETPZ`	0.0	Section 16.1	Distribution is shifted in p_z by this amount after the distribution is generated (or read in). Same as the average p_z value, $\bar{p}_z$.
`ID1`	{0.0, 0.0, 0.0, 0.0, 0.0, 0.0}	Section 16.1	Tracer particle which is written also into *data/track_orbit.dat*. Expects an array with 6 items, x, y, z, p_x, p_y, p_z. Not supported in *OPAL-t*.
`ID2`	{0.0, 0.0, 0.0, 0.0, 0.0, 0.0}	Section 16.1	Tracer particle which is written also into *data/track_orbit.dat*. Expects an array with 6 items, x, y, z, p_x, p_y, p_z. Not supported in *OPAL-t*.

Table 26: Definition of universal distribution attributes. Any distribution type can use these and they are the same whether the beam is *injected* or *emitted*.

16.2.2 Injected Distribution Attributes

Attribute Name	**Default Value**	**Units**	**Description**
`ZMULT`	1.0	None	Value used to scale the z positions of the distribution particles. Applied after the distribution is generated (or read in).
`OFFSETZ`	0.0	m	Distribution is shifted in z by this amount relative to the reference particle. Same as the average z position, $\bar{z}$. To shift the position where the particles are injected please use `ZSTART` in the track command.

Table 27: Definition of distribution attributes that only affect *injected* beams.

16.2.3 Emitted Distribution Attributes

Attribute Name	**Default Value**	**Units**	**Description**
`TMULT`	1.0	None	Value used to scale the t values of the distribution particles. Applied after the distribution is generated (or read in).
`OFFSETT`	0.0	s	Distribution is emitted later by this amount relative to the reference particle.
`EMISSIONSTEPS`	1	None	Number of time steps to take during emission. The simulation time step will be adjusted during emission to ensure that this many time steps will be required to emit the entire distribution.
`EMISSIONMODEL`	None	None	Emission model to use when emitting particles from cathode (see Section 16.4).

Table 28: Definition of distribution attributes that only affect *emitted* beams.

16.3 Distribution Types

16.3.1 `FROMFILE` Distribution Type

The most versatile distribution type is to use a user generated text file as input to *OPAL*. This allows the user to generate their own distribution, if the built in options in *OPAL* are insufficient, and have it either *injected* or *emitted* into the simulation. In Table 29 we list the single attribute specific to this type of distribution type.

Attribute Name	**Default Value**	**Units**	**Description**
`FNAME`	None	None	File name for text file containing distribution particle coordinates.

Table 29: Definition of distribution attributes for a `FROMFILE` distribution type.

An example of an *injected* `FROMFILE` distribution definition is:

```
Name:DISTRIBUTION, TYPE=FROMFILE,
                   FNAME="text file name";
```

an example of an *emitted* `FROMFILE` distribution definition is:

```
Name:DISTRIBUTION, TYPE=FROMFILE,
                   FNAME="text file name",
                   EMITTED=TRUE,
                   EMISSIONMODEL=None;
```

The text input file for the `FROMFILE` distribution type has a slightly different format, depending on whether the distribution is to be *injected* or *emitted*. The *injected* file format is defined in Table 30. The particle coordinates are defined in OPAL-t variables and OPAL-cycl variables. The *emitted* file format is defined in Table 31. The particle coordinates are defined in OPAL-t variables except that z, in meters, is replaced by t in seconds.

N					
x_1	p_{x1}	y_1	p_{y1}	z_1	p_{z1}
x_2	p_{x2}	y_2	p_{y2}	z_2	p_{z2}
.					
.					
x_N	p_{xN}	y_N	p_{yN}	z_N	p_{zN}

Table 30: File format for *injected* `FROMFILE` distribution type. N is the number of particles in the file.

N					
x_1	p_{x1}	y_1	p_{y1}	t_1	p_{z1}
x_2	p_{x2}	y_2	p_{y2}	t_2	p_{z2}
.					
.					
x_N	p_{xN}	y_N	p_{yN}	t_N	p_{zN}

Table 31: File format for *emitted* `FROMFILE` distribution type. N is the number of particles in the file.

Note that for an *emitted* `FROMFILE` distribution, all of the particle's time, t, coordinates will be shifted to negative time (if they are not there already). The simulation clock will then start at $t = 0$ and distribution particles will be emitted into the simulation as the simulation progresses. Also note that, as the particles are emitted, they will be modified according to the type of emission model used. This is defined by the attribute `EMISSIONMODEL`, which is described in Section 16.4. A choice of `NONE` for the `EMISSIONMODEL` (which is the default) can be defined so as not to affect the distribution coordinates at all.

To maintain consistency, N and `NPART` from the `BEAM` command (see Chapter Beam Command) must be equal. In the same way, when using a `FROMFILE` type distribution, the average momentum of the distribution must coincide with the momentum specified in the `BEAM` command by means of `GAMMA`, `ENERGY` or `PC` attributes (see Section Beam Energy), according to the parameter `MOMENTUMTOLERANCE`. In *OPAL-t*, the given momentum in the `BEAM` command must coincide with the z-component of the momentum of the particle distribution in the file. On the other hand, in *OPAL-cycl* the given momentum must coincide with the total momentum of the particle distribution, taking into account that the initial distribution in *OPAL-cycl* is always specified in the local reference frame.

16.3.2 `GAUSS` Distribution Type

As the name implies, the `GAUSS` distribution type can generate distributions with a general Gaussian shape (here we show a one-dimensional example):

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-\bar{x})^2}{2\sigma_x^2}}$$

where $\bar{x}$ is the average value of x. However, the `GAUSS` distribution can also be used to generate an emitted beam with a flat top time profile. We will go over the various options for the `GAUSS` distribution type in this section.

16.3.2.1 Simple GAUSS Distribution Type

We will begin by describing how to create a simple GAUSS distribution type. That is, a simple 6-dimensional distribution with a Gaussian distribution in all dimensions.

Attribute Name	**Default Value**	**Units**	**Description**
SIGMAX	0.0	m	RMS width, σ_x, in transverse x direction.
SIGMAY	0.0	m	RMS width, σ_y, in transverse y direction.
SIGMAR	0.0	m	RMS radius, σ_r, in radial direction. If nonzero SIGMAR overrides SIGMAX and SIGMAY.
SIGMAZ	0.0	m or s	RMS length, σ_z, of the Gaussian in longitudinal (z) direction. SIGMAZ overrides SIGMAT. Use seconds for an emitted bunch, and meters for an injected one.
SIGMAT	0.0	m or s	RMS length, σ_t, of the Gaussian in longitudinal (z) direction. SIGMAZ overrides SIGMAT. Use seconds for an emitted bunch, and meters for an injected one.
SIGMAPX	0.0	Section 16.1	Parameter σ_{px} for defining distribution.
SIGMAPY	0.0	Section 16.1	Parameter σ_{py} for defining distribution.
SIGMAPZ	0.0	Section 16.1	Parameter σ_{pz} for defining distribution.
CUTOFFX	3.0	None	Defines transverse distribution cutoff in the x direction in units of σ_x. If CUTOFFX $= 0$ then actual cutoff in x is set to infinity.
CUTOFFY	3.0	None	Defines transverse distribution cutoff in the y direction in units of σ_y. If CUTOFFY $= 0$ then actual cutoff in y is set to infinity.
CUTOFFR	3.0	None	Defines transverse distribution cutoff in the r direction in units of σ_r. If CUTOFFR $= 0$ then actual cutoff in r is set to infinity. CUTOFFR is only used if SIGMAR > 0.
CUTOFFLONG	3.0	None	Defines longitudinal distribution cutoff in the z or t direction (*injected* or *emitted*) in units of σ_z or σ_t. CUTOFFLONG is different from other dimensions in that a value of 0.0 does not imply a cutoff value of infinity.
CUTOFFPX	3.0	None	Defines cutoff in p_x dimension in units of σ_{px}. If CUTOFFPX $= 0$ then actual cutoff in p_x is set to infinity.
CUTOFFPY	3.0	None	Defines cutoff in p_y dimension in units of σ_{py}. If CUTOFFPY $= 0$ then actual cutoff in p_y is set to infinity.
CUTOFFPZ	3.0	None	Defines cutoff in p_z dimension in units of σ_{pz}. If CUTOFFPZ $= 0$ then actual cutoff is p_z is set to infinity.

Table 32: Definition of the basic distribution attributes for a GAUSS distribution type.

In Table 32 we list the basic attributes available for a GAUSS distribution. We can use these to create a very simple GAUSS distribution:

```
Name:DISTRIBUTION, TYPE       = GAUSS,
                   SIGMAX     = 0.001,
                   SIGMAY     = 0.003,
                   SIGMAZ     = 0.002,
                   SIGMAPX    = 0.0,
                   SIGMAPY    = 0.0,
                   SIGMAPZ    = 0.0,
                   CUTOFFX    = 2.0,
                   CUTOFFY    = 2.0,
                   CUTOFFLONG = 4.0,
                   OFFSETX    = 0.001,
                   OFFSETY    = -0.002,
                   OFFSETZ     = 0.01,
                   OFFSETPZ    = 1200.0;
```

This creates a Gaussian shaped distribution with zero transverse emittance, zero energy spread, $\sigma_x = 1.0\text{mm}$, $\sigma_y = 3.0\text{mm}$, $\sigma_z = 2.0\text{mm}$ and an average energy of:

$$W = 1.2\text{MeV}$$

In the x direction, the Gaussian distribution is cutoff at $x = 2.0 \times \sigma_x = 2.0\text{mm}$. In the y direction it is cutoff at $y = 2.0 \times \sigma_y = 6.0\text{mm}$. This distribution is *injected* into the simulation at an average position of $(\bar{x}, \bar{y}, \bar{z}) = (1.0\text{mm}, -2.0\text{mm}, 10.0\text{mm})$.

16.3.2.2 GAUSS Distribution for Photoinjector

Attribute Name	Default Value	Units	Description
TPULSEFWHM	0.0	s	Flat top time (see Figure 29).
TRISE	0.0	s	Rise time (see Figure 29). If defined will override SIGMAT.
TFALL	0.0	s	Fall time (see Figure 29). If defined will override SIGMAT.
FTOSCAMPLITUDE	0	None	Sinusoidal oscillations can imposed on the flat top in Figure 29. This defines the amplitude of those oscillations in percent of the average flat top amplitude.
FTOSCPERIODS	0	None	Defines the number of oscillation periods imposed on the flat top, t_{flattop}, in Figure 29.

Table 33: Definition of additional distribution attributes for an *emitted* GAUSS distribution type. These are used to generate a distribution with a time profile as illustrated in Figure 29.

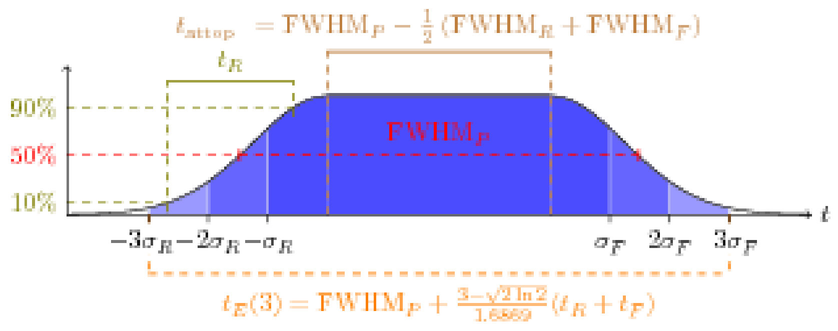

Figure 29: *OPAL* emitted GAUSS distribution with flat top.

A useful feature of the GAUSS distribution type is the ability to mimic the initial distribution from a photoinjector. For this purpose we have the distribution attributes listed in Table 33. Using them, we can create a distribution with the time structure shown in Figure 29. This is a half Gaussian rise plus a uniform flat-top plus a half Gaussian fall. To make it more convenient to mimic measured laser profiles, TRISE and TFALL from Table 33 do not define RMS quantities, but instead are given by (See also Figure 29):

$$\mathrm{TRISE} = t_R = \left(\sqrt{2\ln(10)} - \sqrt{2\ln\left(\frac{10}{9}\right)}\right)\sigma_R$$
$$= 1.6869\sigma_R$$
$$\mathrm{TFALL} = t_F = \left(\sqrt{2\ln(10)} - \sqrt{2\ln\left(\frac{10}{9}\right)}\right)\sigma_F$$
$$= 1.6869\sigma_F$$

where σ_R and σ_F are the Gaussian, RMS rise and fall times respectively. The flat-top portion of the profile, `TPULSEFWHM`, is defined as (See also Figure 29):

$$\mathrm{TPULSEFWHM} = \mathrm{FWHM}_P = t_{\mathrm{flattop}} + \sqrt{2\ln 2}\,(\sigma_R + \sigma_F)$$

Total emission time, t_E, of this distribution, is a function of the longitudinal cutoff, `CUTOFFLONG` (see Table 32), and is given by:

$$t_E(\mathrm{CUTOFFLONG}) = \mathrm{FWHM}_P - \frac{1}{2}(\mathrm{FWHM}_R + \mathrm{FWHM}_F) + \mathrm{CUTOFFLONG}(\sigma_R + \sigma_F)$$
$$= \mathrm{FWHM}_P + \frac{\mathrm{CUTOFFLONG} - \sqrt{2\ln 2}}{1.6869}(\mathrm{TRISE} + \mathrm{TFALL})$$

Finally, we can also impose oscillations over the flat-top portion of the laser pulse in Figure 29, t_{flattop}. This is defined by the attributes `FTOSCAMPLITUDE` and `FTOSCPERIODS` from Table 33. `FTOSCPERIODS` defines how many oscillation periods will be present during the t_{flattop} portion of the pulse. `FTOSCAMPLITUDE` defines the amplitude of those oscillations in percentage of the average profile amplitude during t_{flattop}. So, for example, if we set FTOSCAMPLITUDE $= 5$, and the amplitude of the profile is equal to 1.0 during t_{flattop}, the amplitude of the oscillation will be 0.05.

16.3.2.3 Correlations for GAUSS Distribution (Experimental)

Attribute Name	Default Value	Units	Description
R			All 15 correlations in a single array $(R_{12}, R_{13}, .., R_{56})$.
CORRX	0.0	Section 16.1	x, p_x correlation. (R_{12} in transport notation.)
CORRY	0.0	Section 16.1	y, p_y correlation. (R_{34} in transport notation.)
CORRZ	0.0	Section 16.1	z, p_z correlation. (R_{56} in transport notation.)
CORRT	0.0	Section 16.1	same as and overwritten by `CORRZ`.
R51	0.0	Section 16.1	x, z correlation. (R_{51} in transport notation.)
R52	0.0	Section 16.1	p_x, z correlation. (R_{52} in transport notation.)
R61	0.0	Section 16.1	x, p_z correlation. (R_{61} in transport notation.)
R62	0.0	Section 16.1	p_x, p_z correlation. (R_{62} in transport notation.)

Table 34: Definition of additional distribution attributes for a `GAUSS` distribution type for generating correlations in the beam.

To generate Gaussian initial distribution with dispersion, first we generate the uncorrelated Gaussian inputs matrix $R = (R_1, ..., R_n)$. The mean of R_i is 0 and the standard deviation squared is 1. Then we correlate R. The correlation coefficient matrix σ in x, p_x, z, p_z phase space reads:

$$\sigma = \begin{bmatrix} 1 & c_x & R51 & R61 \\ c_x & 1 & R52 & R62 \\ R51 & R52 & 1 & c_t \\ R61 & R62 & c_t & 1 \end{bmatrix}$$

The Cholesky decomposition of the symmetric positive-definite matrix σ is $\sigma = C^{\mathbf{T}}C$, then the correlated distribution is $C^{\mathbf{T}}R$.

Note: Correlations work for the moment only with the Gaussian distribution and are experimental, so there are no guarantees as to its efficacy or accuracy. Also, these correlations will work, in principle, for an *emitted* beam. However, recall that in this case, z in meters is replaced by t in seconds, so take care.

As an example of defining a correlated beam, let the initial correlation coefficient matrix be:

$$\sigma = \begin{bmatrix} 1 & 0.756 & 0.023 & 0.496 \\ 0.756 & 1 & 0.385 & -0.042 \\ 0.023 & 0.385 & 1 & -0.834 \\ 0.496 & -0.042 & -0.834 & 1 \end{bmatrix}$$

then the corresponding distribution command will read:

```
Dist:DISTRIBUTION, TYPE      = GAUSS,
                   SIGMAX    = 4.796e-03,
                   SIGMAPX   = 231.0585,
                   CORRX     = 0.756,
                   SIGMAY    = 23.821e-03,
                   SIGMAPY   = 1.6592e+03,
                   CORRY     = -0.999,
                   SIGMAZ    = 0.466e-02,
                   SIGMAPZ   = 74.7,
                   CORRZ     = -0.834,
                   OFFSETZ   = 0.466e-02,
                   OFFSETPZ  = 72e6,
                   R61       = 0.496,
                   R62       = -0.042,
                   R51       = 0.023,
                   R52       = 0.385;
```

16.3.3 `FLATTOP` Distribution Type

The `FLATTOP` distribution type is used to define hard edge beam distributions. Hard edge, in this case, means a more or less uniformly filled cylinder of charge, although as we will see this is not always the case. The main purpose of the `FLATTOP` is to mimic laser pulses in photoinjectors, and so we usually will make this an *emitted* distribution. However it can be *injected* as well.

16.3.3.1 Injected `FLATTOP`

The attributes for an *injected* `FLATTOP` distribution are defined in Table 35 and Table 26. At the moment, we cannot define a spread in the beam momentum, so an *injected* `FLATTOP` distribution will currently have zero emittance. An *injected* `FLATTOP` will be a uniformly filled ellipse transversely with a uniform distribution in z. (Basically a cylinder with an elliptical cross section.)

Attribute Name	**Default Value**	**Units**	**Description**
`SIGMAX`	0.0	m	Hard edge width in x direction.
`SIGMAY`	0.0	m	Hard edge width in y direction.
`SIGMAR`	0.0	m	Hard edge radius. If nonzero `SIGMAR` overrides `SIGMAX` and `SIGMAY`.
`SIGMAZ`	0.0	m	Hard edge length in z direction.

Table 35: Definition of the basic distribution attributes for an *injected* `FLATTOP` distribution type.

16.3.3.2 Emitted `FLATTOP`

Attribute Name	Default Value	Units	Description
`SIGMAX`	0.0	m	Hard edge width in x direction.
`SIGMAY`	0.0	m	Hard edge width in y direction.
`SIGMAR`	0.0	m	Hard edge radius. If nonzero `SIGMAR` overrides `SIGMAX` and `SIGMAY`.
`SIGMAT`	0.0	s	RMS rise and fall of half Gaussian in flat top defined in in Figure 29.
`TPULSEFWHM`	0.0	s	Flat top time (see Figure 29).
`TRISE`	0.0	s	Rise time (see Figure 29). If defined will override `SIGMAT`.
`TFALL`	0.0	s	Fall time (see Figure 29). If defined will override `SIGMAT`.
`FTOSCAMPLITUDE`	0	None	Sinusoidal oscillations can imposed on the flat top in Figure 29. This defines the amplitude of those oscillations in percent of the average flat top amplitude.
`FTOSCPERIODS`	0	None	Defines the number of oscillation periods imposed on the flat top, t_{flattop}, in Figure 29.
`LASERPROFFN`		None	File name containing measured laser image.
`IMAGENAME`		None	Used for h5 files. Name of the groups containing the laser image, see regression test.
`INTENSITYCUT`	0.0	None	Parameter defining floor of the background to be subtracted from the laser image in percent of the maximum intensity.
`FLIPX`	`FALSE`		Flip the laser profile in horizontal direction.
`FLIPY`	`FALSE`		Flip the laser profile in vertical direction.
`ROTATE90`	`FALSE`		Rotate the laser profile 90° in counterclockwise direction.
`ROTATE180`	`FALSE`		Rotate the laser profile 180°.
`ROTATE270`	`FALSE`		Rotate the laser profile 270° in counterclockwise direction.

Table 36: Definition of the basic distribution attributes for an *emitted* `FLATTOP` distribution type.

The attributes of an *emitted* `FLATTOP` distribution are defined in Table 36 and Table 26. The `FLATTOP` distribution was really intended for this mode of operation in order to mimic common laser pulses in photoinjectors. The basic characteristic of a `FLATTOP` is a uniform, elliptical transverse distribution and a longitudinal (time) distribution with a Gaussian rise and fall time as described in Section 16.3.2.2. Below we show an example of a `FLATTOP` distribution command with an elliptical cross section of 1 mm by 2 mm and a flat top, in time, 10 ps long with a 0.5 ps rise and fall time as defined in Figure 29.

```
Dist:DISTRIBUTION, TYPE = FLATTOP,
                   SIGMAX = 0.001,
                   SIGMAY = 0.002,
                   TRISE = 0.5e-12,
                   TFALL = 0.5e-12,
                   TPULSEFWHM = 10.0e-12,
                   CUTOFFLONG = 4.0,
                   NBIN = 5,
                   EMISSIONSTEPS = 100,
                   EMISSIONMODEL = ASTRA,
                   EKIN = 0.5,
                   EMITTED = TRUE;
```

16.3.3.3 Transverse Distribution from Laser Profile (Under Development)

An alternative to using a uniform, elliptical transverse profile is to define the `LASERPROFFN`, `IMAGENAME` and `INTENSITYCUT` attributes from Table 36. Then, *OPAL-t* will use the laser image as the basis to sample the transverse distribution.

This distribution option is not yet available.

16.3.3.4 `GUNGAUSSFLATTOPTH` Distribution Type

This is a legacy distribution type. A `GUNGAUSSFLATTOPTH` is the equivalent of a `FLATTOP` distribution, except that the `EMITTED` attribute will set to `TRUE` automatically and the `EMISSIONMODEL` will be automatically set to `ASTRA`.

16.3.3.5 `ASTRAFLATTOPTH` Distribution Type

This is a legacy distribution type. A `ASTRAFLATTOPTH` is the equivalent of a `FLATTOP` distribution, except that the `EMITTED` attribute will set to `TRUE` automatically and the `EMISSIONMODEL` will be automatically set to `ASTRA`. There are a few other differences with how the longitudinal time profile of the distribution is generated.

16.3.4 `BINOMIAL` Distribution Type

The `BINOMIAL` type of distribution is based on [28]. The shape of the binomial distribution is governed by one parameter m. By varying this single parameter one obtains the most commonly used distributions for our type of simulations, as listed in Table 37 and shown in Figure 30.

m	**Distribution**	**Density**	**Profile**
0.0	Hollow shell	$\frac{1}{\pi}\delta(1-r^2)$	$\frac{1}{\pi}(1-x^2)^{-0.5}$
0.5	Flat profile	$\frac{1}{2\pi}(1-r^2)^{-0.5}$	$\frac{1}{2}$
1.0	Uniform	$\frac{1}{\pi}$	$\frac{2}{\pi}(1-x^2)^{0.5}$
1.5	Elliptical	$\frac{3}{2\pi}(1-r^2)^{0.5}$	$\frac{1}{4}(1-x^2)$
2.0	Parabolic	$\frac{2}{\pi}(1-r^2)$	$\frac{3}{8\pi}(1-x^2)^{1.5}$
$\rightarrow\infty(>$ 10000)	Gaussian	$\frac{1}{2\pi\sigma_x\sigma_y}exp(-\frac{x^2}{2\sigma_x^2}-\frac{y^2}{2\sigma_y^2})$	$\frac{1}{\sqrt{2\pi}\sigma_x}exp(-\frac{x^2}{2\sigma_x^2})$

Table 37: Different distributions specified by a single parameter m

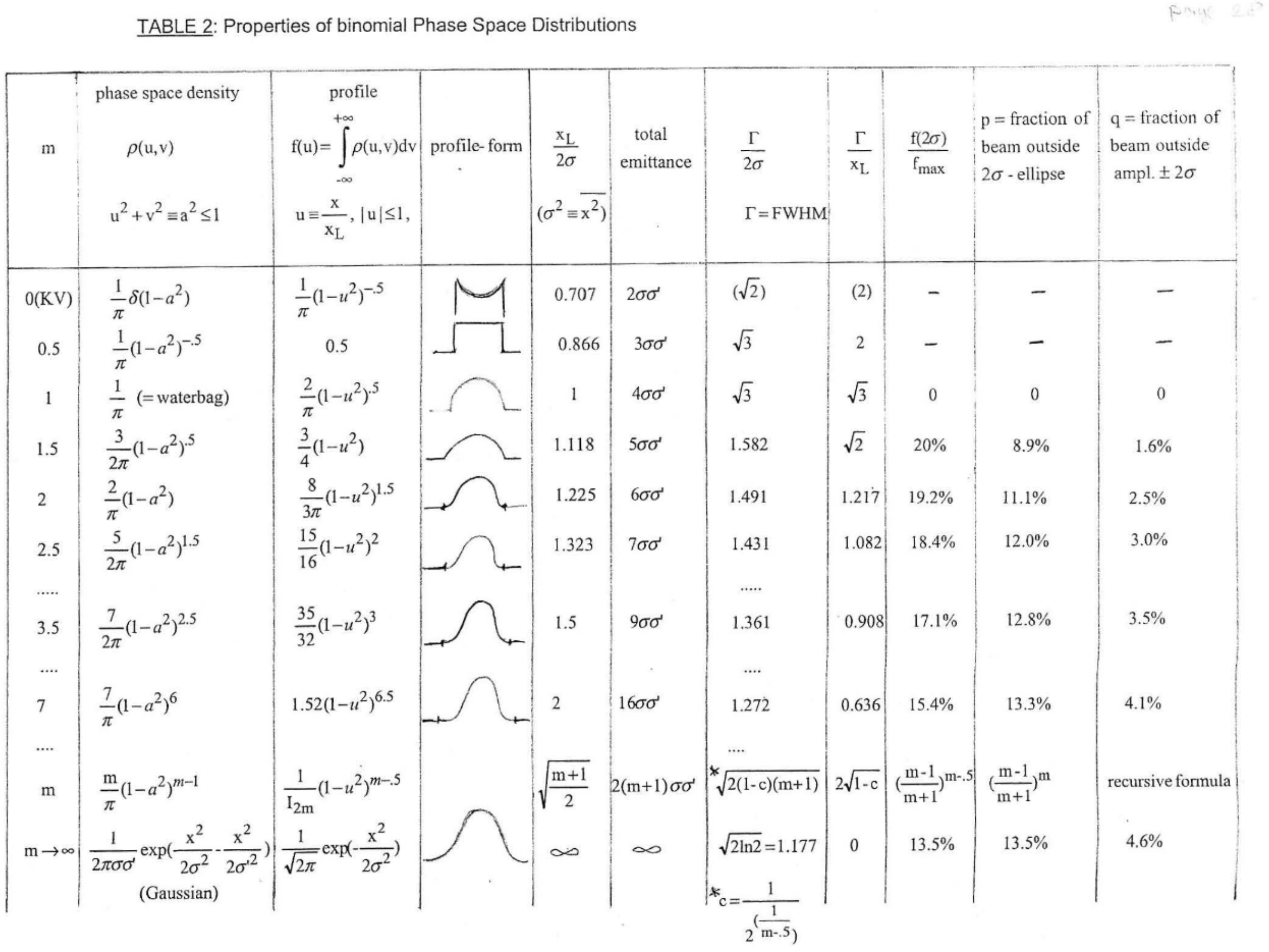

TABLE 2: Properties of binomial Phase Space Distributions

m	phase space density $\rho(u,v)$ $u^2+v^2 \equiv a^2 \le 1$	profile $f(u)=\int_{-\infty}^{+\infty}\rho(u,v)dv$ $u \equiv \frac{x}{x_L}$, $\lvert u\rvert \le 1$,	profile- form	$\frac{x_L}{2\sigma}$ $(\sigma^2 \equiv \overline{x^2})$	total emittance	$\frac{\Gamma}{2\sigma}$ $\Gamma = \mathrm{FWHM}$	$\frac{\Gamma}{x_L}$	$\frac{f(2\sigma)}{f_{max}}$	p = fraction of beam outside 2σ - ellipse	q = fraction of beam outside ampl. $\pm 2\sigma$
0(KV)	$\frac{1}{\pi}\delta(1-a^2)$	$\frac{1}{\pi}(1-u^2)^{-.5}$		0.707	$2\sigma\sigma'$	$(\sqrt{2})$	(2)	–	–	–
0.5	$\frac{1}{\pi}(1-a^2)^{-.5}$	0.5		0.866	$3\sigma\sigma'$	$\sqrt{3}$	2	–	–	–
1	$\frac{1}{\pi}$ (=waterbag)	$\frac{2}{\pi}(1-u^2)^{.5}$		1	$4\sigma\sigma'$	$\sqrt{3}$	$\sqrt{3}$	0	0	0
1.5	$\frac{3}{2\pi}(1-a^2)^{.5}$	$\frac{3}{4}(1-u^2)$		1.118	$5\sigma\sigma'$	1.582	$\sqrt{2}$	20%	8.9%	1.6%
2	$\frac{2}{\pi}(1-a^2)$	$\frac{8}{3\pi}(1-u^2)^{1.5}$		1.225	$6\sigma\sigma'$	1.491	1.217	19.2%	11.1%	2.5%
2.5	$\frac{5}{2\pi}(1-a^2)^{1.5}$	$\frac{15}{16}(1-u^2)^2$		1.323	$7\sigma\sigma'$	1.431	1.082	18.4%	12.0%	3.0%
.....						.....				
3.5	$\frac{7}{2\pi}(1-a^2)^{2.5}$	$\frac{35}{32}(1-u^2)^3$		1.5	$9\sigma\sigma'$	1.361	0.908	17.1%	12.8%	3.5%
....						....				
7	$\frac{7}{\pi}(1-a^2)^6$	$1.52(1-u^2)^{6.5}$		2	$16\sigma\sigma'$	1.272	0.636	15.4%	13.3%	4.1%
....						....				
m	$\frac{m}{\pi}(1-a^2)^{m-1}$	$\frac{1}{I_{2m}}(1-u^2)^{m-.5}$		$\sqrt{\frac{m+1}{2}}$	$2(m+1)\sigma\sigma'$	$^*\sqrt{2(1-c)(m+1)}$	$2\sqrt{1-c}$	$(\frac{m-1}{m+1})^{m-.5}$	$(\frac{m-1}{m+1})^{m}$	recursive formula
$m \to \infty$	$\frac{1}{2\pi\sigma\sigma'}\exp(-\frac{x^2}{2\sigma^2}-\frac{x'^2}{2\sigma'^2})$ (Gaussian)	$\frac{1}{\sqrt{2\pi}}\exp(-\frac{x^2}{2\sigma^2})$		∞	∞	$\sqrt{2\ln 2}=1.177$	0	13.5%	13.5%	4.6%
						$^*c=\frac{1}{2^{(\frac{1}{m-.5})}}$				

Figure 30: Properties of binomial Phase Space Distributions (taken from [28]).

The attributes of a BINOMIAL distribution are defined in Table 38.

Attribute Name	Default Value	Units	Description
MX	10001		Defines parameter *m* for the binomial distribution in *x*
MY	10001		Defines parameter *m* for the binomial distribution in *y*
MT	10001		Defines parameter *m* for the binomial distribution in *z*
MZ	10001		Same as and overwritten by MT.

Table 38: Definition of the basic distribution attributes for a BINOMIAL distribution type.

The width and the (x, p_x) phase space is given by the usual SIGMAX (σ_x), SIGMAXP (σ_{xp}) and CORRX (σ_{12}) and defined as follows (similarly for the other dimensions):

$$\varepsilon_x = \sigma_x\sigma_{xp}\cos\left(\arcsin\left(\sigma_{12}\right)\right)$$

$$\beta_x = \frac{\sigma_x^2}{\varepsilon_x}$$

$$\gamma_x = \frac{\sigma_{xp}^2}{\varepsilon_x}$$

$$\alpha_x = -\sigma_{12}\sqrt{(\beta_x\gamma_x)}$$

Example:

```
Dist:DISTRIBUTION, TYPE    = BINOMIAL,
                   SIGMAX  = 2.15e-03,
                   SIGMAPX = 1E-6,
                   CORRX   = 0.0,
                   MX      = 0.01,
                   SIGMAY  = 0.50*23.e-03,
                   SIGMAPY = 28.0,
                   CORRY   = 0.5,
                   MY      = 990.0,
                   SIGMAT  = 1.0e-1,
                   SIGMAPT = 11.96,
                   CORRT   = -0.5,
                   MT      = 2.0,
```

16.3.5 `GAUSSMATCHED` Matched Gauss Distribution Type

The attributes of a `GAUSSMATCHED` distribution are defined in Table 39. `Limitation:` Does not consider Trimcoil field maps!

Attribute Name	**Default Value**	**Units**	**Description**
`DENERGY`	1E-3	GeV	Energy step size for closed orbit finder
`EX`	1E-6	m rad	Projected normalized emittance in x
`EY`	1E-6	m rad	Projected normalized emittance in y
`ET`	1E-6	m rad	Projected normalized emittance in t
`NSTEPS`	720		Number of integration steps of closed orbit finder
`NSECTORS`	1		Number of sectors to average field for closed orbit finder
`SECTOR`	TRUE		Match using single sector (true) or all sectors (false)
`ORDERMAPS`	7		Order used in the field expansion
`RGUESS`	-1		Guess value of radius (m) for closed orbit finder
`RESIDUUM`	1E-8		Residuum for the closed orbit finder and sigma matrix generator
`MAXSTEPSCO`	100		Maximum steps used to find closed orbit
`MAXSTEPSSI`	500		Maximum steps used to find matched distribution

Table 39: Definition of the basic distribution attributes for a `GAUSSMATCHED` distribution type.

16.3.6 `MULTIGAUSS` Distribution type

The purpose of this distribution is to mimic photoinjectors in which the laser beam consists of a train of Gaussian pulses [29]. Therefore this distribution has a uniform elliptical transverse distribution, and a train of equally spaced normal distributions along the z or t axis.

This distribution can be emitted or injected. When emitted, each particle acquires momentum according to the emission model. When injected, the momentum follows a normal distribution, and the user can specify $(\sigma_{px}, \sigma_{py}, \sigma_{pz})$.

Attribute Name	**Default Value**	**Units**	**Description**
`SIGMAX`	0.0	m	Laser radius in transverse x direction.
`SIGMAY`	0.0	m	Laser radius in transverse y direction.
`SIGMAR`	0.0	m	Laser radius, σ_r, in radial direction. If nonzero `SIGMAR` overrides `SIGMAX` and `SIGMAY`.
`SIGMAZ`	0.0	m or s	RMS length of each Gaussian pulse in longitudinal (z) direction. `SIGMAZ` overrides `SIGMAT`. Use seconds for an emitted bunch, and meters for an injected one.
`SIGMAT`	0.0	m or s	RMS length of each Gaussian pulse in longitudinal (z) direction. `SIGMAZ` overrides `SIGMAT`. Use seconds for an emitted bunch, and meters for an injected one.
`SEPPEAKS`	0.0	m or s	Peak-to-peak distance between the Gaussian pulses in longitudinal (z) direction. Use seconds for an emitted bunch, and meters for an injected one.
`NPEAKS`	1	None	Number of pulses along the longitudinal (z) direction.
`CUTOFFLONG`	3.0	None	Cutoff distance from the center of the first and last Gaussian pulses in the z or t direction (*injected* or *emitted*) in units of σ_z or σ_t. `CUTOFFLONG` is different from other dimensions in that a value of 0.0 does not imply a cutoff value of infinity.
`SIGMAPX`	0.0	Section 16.1	Parameter σ_{px} for the normal distribution of the momentum. This parameter is ignored for an emitted bunch.
`SIGMAPY`	0.0	Section 16.1	Parameter σ_{py} for the normal distribution of the momentum. This parameter is ignored for an emitted bunch.
`SIGMAPZ`	0.0	Section 16.1	Parameter σ_{pz} for the normal distribution of the momentum. This parameter is ignored for an emitted bunch.
`CUTOFFPX`	3.0	None	Defines cutoff in p_x dimension in units of σ_{px}. If `CUTOFFPX` $= 0$ then actual cutoff in p_x is set to infinity. This parameter is ignored for an emitted bunch.
`CUTOFFPY`	3.0	None	Defines cutoff in p_y dimension in units of σ_{py}. If `CUTOFFPY` $= 0$ then actual cutoff in p_y is set to infinity. This parameter is ignored for an emitted bunch.
`CUTOFFPZ`	3.0	None	Defines cutoff in p_z dimension in units of σ_{pz}. If `CUTOFFPZ` $= 0$ then actual cutoff is p_z is set to infinity. This parameter is ignored for an emitted bunch.

Table 40: Definition of the basic distribution attributes for a `MULTIGAUSS` distribution type.

In Table 40 the basic attributes available for a `MULTIGAUSS` distribution are listed.

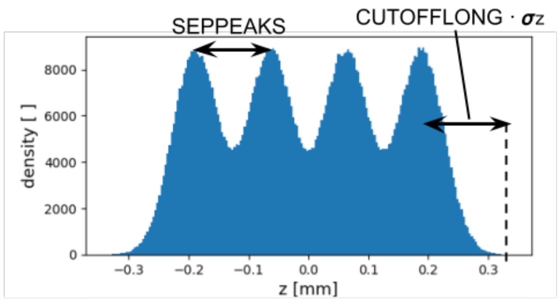

Figure 31: Example of an injected `MULTIGAUSS` distribution.

An example (Figure 31) of a `MULTIGAUSS` injected bunch could be:

```
Dist: DISTRIBUTION, TYPE = MULTIGAUSS,
                    SIGMAPX = 1e-2, SIGMAPY = 1e-2, SIGMAPZ = 1e-2,  // In units of  ↩
                        betaGamma
                    CUTOFFPX = 4.0, CUTOFFPY = 4.0, CUTOFFPZ = 4.0,  // In units of SIGMAP
                    SIGMAR = 340e-6,
                    SIGMAZ = 90e-6 / 2.355, // FWHM  = 2.355 * sigma
                    CUTOFFLONG = 4.0,  // In units of SIGMAZ
                    SEPPEAKS = 126e-6,
                    NPEAKS = 4,
                    EMITTED = FALSE;
```

16.4 Emission Models

When emitting a distribution from a cathode, there are several ways in which we can model the emission process in order to calculate the thermal emittance of the beam. In this section we discuss the various options available.

16.4.1 Emission Model: `NONE` (default)

The emission model `NONE` is the default emission model used in *OPAL-t*. It has a single attribute, listed in Table 41. The `NONE` emission model is very simplistic. It merely adds the amount of energy defined by the attribute `EKIN` to the longitudinal momentum, p_z, for each particle in the distribution as it leaves the cathode.

Attribute Name	**Default Value**	**Units**	**Description**
`EKIN`	1.0	eV	Thermal energy added to beam during emission.

Table 41: Attributes for the `NONE` and `ASTRA` emission models.

An example of using the `NONE` emission model is given below. This option allows us to emit transversely cold (zero x and y emittance) beams into our simulation. We must add some z momentum to ensure that the particles drift into the simulation space. If in this example one were to specify `EKIN = 0`, then you would likely get strange results as the particles would not move off the cathode, causing all of the emitted charge to pile up at $z = 0$ in the first half time step before the beam space charge is calculated.

```
Dist:DISTRIBUTION, TYPE = FLATTOP,
                   SIGMAX = 0.001,
                   SIGMAY = 0.002,
                   TRISE = 0.5e-12,
                   TFALL = 0.5e-12,
                   TPULSEFWHM = 10.0e-12,
                   CUTOFFLONG = 4.0,
                   NBIN = 5,
                   EMISSIONSTEPS = 100,
                   EMISSIONMODEL = NONE,
                   EKIN = 0.5,
                   EMITTED = TRUE;
```

One thing to note, it may be that if you are emitting your own distribution using the `TYPE = FROMFILE` option, you may want to set `EKIN = 0` if you have already added some amount of momentum, p_z, to the particles.

16.4.2 Emission Model: ASTRA

The `ASTRA` emittance model uses the same single parameter as the `NONE` option as listed in Table 41. However, in this case, the energy defined by the `EKIN` attribute is added to each emitted particle's momentum in a random way:

$$p_{total} = \sqrt{\left(\frac{\text{EKIN}}{mc^2}+1\right)^2 - 1}$$
$$p_x = p_{\text{total}} \sin(\theta)\cos(\phi)$$
$$p_y = p_{\text{total}} \sin(\theta)\sin(\phi)$$
$$p_z = p_{\text{total}} |\cos(\theta)|$$

where θ is a random angle between 0 and π, and ϕ is given by

$$\phi = 2.0 \arccos\left(\sqrt{x}\right)$$

with x a random number between 0 and 1.

16.4.3 Emission Model: NONEQUIL

The `NONEQUIL` emission model is based on an actual physical model of particle emission as described in [30], [31], [32]. The attributes needed by this emission model are listed in Table 42.

Attribute Name	Default Value	Units	Description
`ELASER`	4.86	eV	Photoinjector drive laser energy. (Default is 255nm light.)
`W`	4.31	eV	Photocathode work function. (Default is atomically clean copper.)
`FE`	7.0	eV	Fermi energy of photocathode. (Default is atomically clean copper.)
`CATHTEMP`	300.0	K	Operating temperature of photocathode.

Table 42: Attributes for the `NONEQUIL` emission models.

An example of using the `NONEQUIL` emission model is given below. This model is relevant for metal cathodes and cathodes such as `CsTe`.

```
Dist:DISTRIBUTION, TYPE = GAUSS,
                   SIGMAX = 0.001,
                   SIGMAY = 0.002,
                   TRISE = 1.0e-12,
                   TFALL = 1.0e-12,
                   TPULSEFWHM = 15.0e-12,
                   CUTOFFLONG = 3.0,
                   NBIN = 10,
                   EMISSIONSTEPS = 100,
                   EMISSIONMODEL = NONEQUIL,
                   ELASER = 6.48,
                   W = 4.1,
                   FE = 7.0,
                   CATHTEMP = 325,
                   EMITTED = TRUE;
```

16.5 Distribution List

It is possible to use multiple distributions in the same simulation. We do this be using a distribution list in the RUN command (see Chapter Tracking). Assume we have defined several distributions: DIST1, DIST2 and DIST3. If we want to use just one of these distributions in a simulation, we would use the following RUN command to start the simulation:

```
RUN, METHOD = "PARALLEL-T",
     BEAM = beam_name,
     FIELDSOLVER = field_solver_name,
     DISTRIBUTION = DIST1;
```

If we want to use all the distributions at the same time, then the command would instead be:

```
RUN, METHOD = "PARALLEL-T",
     BEAM = beam_name,
     FIELDSOLVER = field_solver_name,
     DISTRIBUTION = {DIST1, DIST2, DIST3};
```

In this second case, the first distribution (DIST1) is the master distribution. The main consequence of this is that all distributions in the list will be forced to the same EMITTED condition as DIST1. So, if DIST1 is to be *emitted*, then all other distributions in the list will be forced to this same condition. If DIST1 is to be *injected*, then all other distribution is the list will also be *injected*.

The number of particles in the simulation is defined in the BEAM command see Chapter Beam Command. The number of particles in each distribution in a distribution list is determined by this number and the WEIGHT attribute of each distribution (Table 26). If all distributions have the same WEIGHT value, then the number of particles will be divided up evenly among them. If, however we have a distribution list consisting of two distributions, and one has twice the WEIGHT of the other, then it will have twice the particles as its partner. The exception here is any FROMFILE distribution type. In this case, the WEIGHT attribute and the number of particles in the BEAM command are ignored. The number of particles in any FROMFILE distribution type is defined by the text file containing the distribution particle coordinates. (Section 16.3.1).

16.6 References

[28] W. Joho, *Representation of beam ellipses for transport calculations*, PSI Internal Report TM-11-14, Paul Scherrer Institute (1980).

[29] J. G. Power and C. Jing, *Temporal Laser Pulse Shaping for RF Photocathode Guns: The Cheap and Easy way using UV Birefringent Crystals*, AIP Conf. Proc. 1086, 689 (2009).

[30] K. Flöttmann, *Note on the thermal emittance of electrons emitted by Cesium Telluride photo cathodes*, Tech. Rep. DESY-TESLA-FEL-97-01, Deutsches Elektronen-Synchrotron (1997).

[31] J. E. Clendenin et al., *Reduction of thermal emittance of RF guns*, Nucl. Instrum. Methods A 455, 198 (2000).

[32] D. H. Dowell and J. F. Schmerge, *Quantum efficiency and thermal emittance of metal photocathodes*, Phys. Rev. ST Accel. Beams 12, 074201 (2009).

Chapter 17

Field Solver

Space charge effects are included in the simulation by specifying a field solver described in this chapter and attaching it to the track command as described in Chapter Tracking. By default, the code does not assume any symmetry i.e. full 3D. In the near future it is planed to implement also a slice (2D) model. This will allow the use of less numbers of macro-particles in the simulation which reduces the computational time significantly.

The space charge forces are calculated by solving the 3D Poisson equation with open boundary conditions using a standard or integrated Green function method. The image charge effects of the conducting cathode are also included using a shifted Green function method. If more than one Lorentz frame is defined, the total space charge forces are then the summation of contributions from all Lorentz frames. More details will be given in Version 2.0.0.

17.1 FFT Based Particle-Mesh (PM) Solver

The Particle-Mesh (PM) solver is one of the oldest improvements over the PP solver. Still one of the best references is the book by R.W. Hockney & J.W. Eastwood [33]. The PM solver introduces a discretization of space. The rectangular computation domain $\Omega := [-L_x, L_x] \times [-L_y, L_y] \times [-L_t, L_t]$, just big enough to include all particles, is segmented into a regular mesh of $M = M_x \times M_y \times M_t$ grid points. For the discussion below we assume $N = M_x = M_y = M_t$.

The solution of Poisson's equation is an essential component of any self-consistent electrostatic beam dynamics code that models the transport of intense charged particle beams in accelerators. If the bunch is small compared to the transverse size of the beam pipe, the conducting walls are usually neglected. In such cases the Hockney method may be employed [33], [34] and [35]. In that method, rather than computing N_p^2 point-to-point interactions (where N_p is the number of macro-particles), the potential is instead calculated on a grid of size $(2N)^d$, where N is the number of grid points in each dimension of the physical mesh containing the charge, and where d is the dimension of the problem. Using the Hockney method, the calculation is performed using Fast Fourier Transform (FFT) techniques, with the computational effort scaling as $(2N)^d (log_2 2N)^d$.

When the beam bunch fills a substantial portion of the beam pipe transversely, or when the bunch length is long compared with the pipe transverse size, the conducting boundaries cannot be ignored. Poisson solvers have been developed previously to treat a bunch of charge in an open-ended pipe with various geometries [36], [37].

The solution of the Poisson equation,

$$\nabla^2 \phi = -\rho/\varepsilon_0,$$

for the scalar potential, ϕ, due to a charge density, ρ, and appropriate boundary conditions, can be expressed as,

$$\phi(x,y,z) = \int\int\int \mathrm{d}x' \, \mathrm{d}y' \, \mathrm{d}z' \rho(x',y',z') G(x,x',y,y',z,z'),$$

where $G(x,x',y,y',z,z')$ is the Green function, subject to the appropriate boundary conditions, describing the contribution of a source charge at location (x',y',z') to the potential at an observation location (x,y,z).

For an isolated distribution of charge this reduces to

$$\phi(x,y,z) = \int\int\int \mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}z'\rho(x',y',z')G(x-x',y-y',z-z'),$$

EQUATION 17.1: Convolution solution

where

$$G(u,v,w) = \frac{1}{\sqrt{u^2+v^2+w^2}}.$$

A simple discretization of Equation 17.1 on a Cartesian grid with cell size (h_x,h_y,h_z) leads to,

$$\phi_{i,j,k} = h_x h_y h_z \sum_{i'=1}^{M_x}\sum_{j'=1}^{M_y}\sum_{k'=1}^{M_t} \rho_{i',j',k'} G_{i-i',j-j',k-k'},$$

EQUATION 17.2: Open brute force convolution

where $\rho_{i,j,k}$ and $G_{i-i',j-j',k-k'}$ denote the values of the charge density and the Green function, respectively, defined on the grid M.

17.1.1 FFT-based Convolutions and Zero Padding

FFTs can be used to compute convolutions by appropriate zero-padding of the sequences. Discrete convolutions arise in solving the Poisson equation, and one is typically interested in the following,

$$\bar{\phi}_j = \sum_{k=0}^{K-1} \bar{\rho}_k \bar{G}_{j-k} \quad , \quad \begin{array}{l} j = 0,\dots,J-1 \\ k = 0,\dots,K-1 \\ j-k = -(K-1),\dots,J-1 \end{array}$$

EQUATION 17.3: Brute force convolution

where $\bar{G}$ corresponds to the free space Green function, $\bar{\rho}$ corresponds to the charge density, and $\bar{\phi}$ corresponds to the scalar potential. The sequence $\{\bar{\phi}_j\}$ has J elements, $\{\bar{\rho}_k\}$ has K elements, and $\{\bar{G}_m\}$ has $M = J+K-1$ elements.

One can zero-pad the sequences to a length $N \geq M$ and use FFT's to efficiently obtain the $\{\bar{\phi}_j\}$ in the unpadded region. This defines a zero-padded charge density, ρ,

$$\rho_k = \begin{cases} \bar{\rho}_k & \text{if } k = 0,\dots,K-1 \\ 0 & \text{if } k = K,\dots,N-1. \end{cases}$$

Define a periodic Green function, G_m, as follows,

$$G_m = \begin{cases} \bar{G}_m & \text{if } m = -(K-1),\dots,J-1 \\ 0 & \text{if } m = J,\dots,N-K, \\ G_{m+iN} = G_m & \text{for } i \text{ integer }. \end{cases}$$

EQUATION 17.4: Periodic Green function

Now consider the sum

$$\phi_j = \frac{1}{N}\sum_{k=0}^{N-1} W^{-jk}\left(\sum_{n=0}^{N-1}\rho_n W^{nk}\right)\left(\sum_{m=0}^{N-1} G_m W^{mk}\right), \qquad 0 \leq j \leq N-1,$$

EQUATION 17.5: FFT convolution

where $W = e^{-2\pi i/N}$. This is just the FFT-based convolution of $\{\rho_k\}$ with $\{G_m\}$. Then,

$$\phi_j = \sum_{n=0}^{K-1} \sum_{m=0}^{N-1} \bar{\rho}_n G_m \frac{1}{N} \sum_{k=0}^{N-1} W^{(m+n-j)k} \qquad 0 \le j \le N-1.$$

Now use the relation

$$\sum_{k=0}^{N-1} W^{(m+n-j)k} = N\delta_{m+n-j,iN} \qquad (i \text{ an integer}).$$

It follows that

$$\phi_j = \sum_{n=0}^{K-1} \bar{\rho}_n G_{j-n+iN} \qquad 0 \le j \le N-1.$$

But G is periodic with period N. Hence,

$$\phi_j = \sum_{n=0}^{K-1} \bar{\rho}_n G_{j-n} \qquad 0 \le j \le N-1.$$

EQUATION 17.6: Final equation

In the physical (unpadded) region, $j \in [0, J-1]$, so the quantity $j-n$ in Equation 17.6 satisfies $-(K-1) \le j-n \le J-1$. In other words the values of G_{j-n} are identical to $\bar{G}_{j-n}$. Hence, in the physical region the FFT-based convolution, Equation 17.5, matches the convolution in Equation 17.3.

As stated above, the zero-padded sequences need to have a length $N \ge M$, where M is the number of elements in the Green function sequence $\{x_m\}$. In particular, one can choose $N = M$, in which case the Green function sequence is not padded at all, and only the charge density sequence, $\{r_k\}$, is zero-padded, with $k = 0, \ldots, K-1$ corresponding to the physical region and $k = K, \ldots, M-1$ corresponding to the zero-padded region.

The above FFT-based approach – zero-padding the charge density array, and circular-shifting the Green function in accordance with Equation 17.4 – will work in general. In addition, if the Green function is a symmetric function of its arguments, the value at the end of the Green function array (at grid point $J-1$) can be dropped, since it will be recovered implicitly through the symmetry of Equation 17.4. In that case the approach is identical to the Hockney method [33], [34] and [35]. Lastly, note that the above proof that the convolution, Equation 17.5, is identical to Equation 17.3 in the unpadded region, works even when W^{-jk} and W^{mk} are replaced by W^{jk} and W^{-mk}, respectively, in Equation 17.5. In other words, the FFT-based approach can be used to compute

$$\bar{\phi}_j = \sum_{k=0}^{K-1} \bar{\rho}_k \bar{G}_{j+k} \quad , \quad \begin{array}{l} j = 0, \ldots, J-1 \\ k = 0, \ldots, K-1 \\ j-k = -(K-1), \ldots, J-1 \end{array}$$

EQUATION 17.7: Brute force correlation

simply by changing the direction of the Fourier transform of the Green function and changing the direction of the final Fourier transform.

17.1.2 Algorithm used in *OPAL*

As a result, the solution of Equation 17.2 is then given by

$$\phi_{i,j,k} = h_x h_y h_z \mathrm{FFT}^{-1}\{(\mathrm{FFT}\{\rho_{i,j,k}\})(\mathrm{FFT}\{G_{i,j,k}\})\}$$

EQUATION 17.8: Solution of brute force convolution

where the notation has been introduced that $\mathrm{FFT}\{.\}$ denotes a forward FFT in all 3 dimensions, and $\mathrm{FFT}^{-1}\{.\}$ denotes a backward FFT in all 3 dimensions.

17.1.3 Interpolation Schemes

More details will be given in Version 2.0.0.

17.2 Particle-Particle-Particle-Mesh (P^3M) Solver

The P^3M solver of Hockney and Eastwood [35] takes into account collisions between particles in an electrostatic one-one PIC simulation (every simulation particle is a real particle) in an efficient manner compared to PIC with excessive mesh refinement or a direct N-body summation. The main idea behind this approach is a splitting of the total force F into two components

$$F = F_{sr} + F_{lr}$$

where F_{sr} is the short-range component which can be computed efficiently in the real-space with a small cut-off radius by direct summation, whereas F_{lr} is the long-range component and this can be calculated efficiently in the Fourier space with a few Fourier modes due to its rapid spectral decay. Consequently, we split the Green's function G also into two components as

$$G(r) = \psi(r) + \phi(r) = \frac{1-f(r)}{r} + \frac{f(r)}{r}$$

where $\psi(r)$ is the short-range or the particle-particle Green's function and $\phi(r)$ is the long range or the particle-mesh Green's function. Apart from certain smoothness conditions there is a lot of flexibility in the choice of $f(r)$ and this leads to different screening shapes for the particles. The standard choice from the Ewald summation corresponds to [55], [54]

$$f(r) = erf(\alpha r)$$

where α is the interaction splitting parameter which determines the relative significance of the particle-particle part to the particle-mesh part. It is usually chosen as $\alpha = C/r_c$, where r_c is the cut-off or interaction radius and C is a postive constant. This choice of Green's function corresponds to Gaussian shaped screening charges. In OPAL, the `P3M` solver uses this Green's function when the option is specifed as `STANDARD`.

Another popular choice for $f(r)$ corresponds to truncated polynomials of different orders as given in Table I of appendix B in [54]. The lowest order function in the table corresponds to

$$f(r) = \frac{\xi(3-\xi^2)}{2}$$

where $\xi = r/r_c$. We use the integrated version of this Green's function when we specify the option for Green's function as `INTEGRATED` in the `P3M` solver in OPAL. The reason to use this one instead of the integrated version of the standard Green's function described before is the availability of a closed form expression when performing the integration.

17.2.1 Use of P^3M solver

At the moment, the `P3M` solver is only available in *OPAL-T* when emission is not active. It uses `OPEN` boundary conditions. The interaction splitting parameter α is used only for the `STANDARD` Green's function option. We can specify the solver in the input file as follows

```
REAL inter_rad = 3.125e-5;

FS_P3M: Fieldsolver, FSTYPE = "P3M", MX = 64, MY = 64, MT = 64, PARFFTX = decx,
        PARFFTY = decy, PARFFTT = decz, RC=inter_rad, GREENSF = INTEGRATED;
```

17.3 Iterative Space Charge Solver

This is a scalable parallel solver for the Poisson equation within a Particle-In-Cell (PIC) code for the simulation of electron beams in particle accelerators of irregular shape. The problem is discretized by Finite Differences. Depending on the treatment of the

Dirichlet boundary the resulting system of equations is symmetric or `mildly' non-symmetric positive definite. In all cases, the system is solved by the preconditioned conjugate gradient algorithm with smoothed aggregation (SA) based algebraic multigrid (AMG) preconditioning. More details are given in [38].

This solver is enabled with `ENABLE_SAAMG_SOLVER=ON` in the *OPAL* compilation. It requires Parmetis and Trilinos to be installed.

17.4 Energy Binning

The beam out of a cathode or in a plasma wake field accelerator can have a large energy spread. In this case, the static approximation using one Lorentz frame might not be sufficient. Multiple Lorentz frames can be used so that within each Lorentz frame the energy spread is small and hence the electrostatic approximation is valid. More details will be given in Version 2.0.0.

17.5 The FIELDSOLVER Command

See Table 43 for a summary of the `FIELDSOLVER` command.

Command	**Purpose**
`FIELDSOLVER`	Specify a fieldsolver
`FSTYPE`	Specify the type of field solver: `FFT`, `FFTPERIODIC`, `SAAMG`, `P3M` and `NONE`. Further arguments are enabled with the AMR solver (cf. Section 17.6).
`PARFFTX`	If `TRUE`, the dimension x is distributed among the processors
`PARFFTY`	If `TRUE`, the dimension y is distributed among the processors
`PARFFTT`	If `TRUE`, the dimension z is distributed among the processors
`MX`	Number of grid points in x specifying rectangular grid
`MY`	Number of grid points in y specifying rectangular grid
`MT`	Number of grid points in z specifying rectangular grid
`BCFFTX`	Boundary condition in x [`OPEN`] (`FFT` + `AMR_MG` only).
`BCFFTY`	Boundary condition in y [`OPEN`] (`FFT` + `AMR_MG` only).
`BCFFTZ`	Boundary condition in z [`OPEN,PERIODIC`] (`FFT` + `AMR_MG` only).
`GREENSF`	Defines the Greens function for the FFT-based solvers (`FFT` + `P3M` only).
`BBOXINCR`	Enlargement of the bounding box in %.
`GEOMETRY`	Geometry to be used as domain boundary (`SAAMG` only).
`ITSOLVER`	Type of iterative solver (`SAAMG` + `AMR_MG` only).
`INTERPL`	Interpolation used for boundary points (`SAAMG` only).
`TOL`	Tolerance for iterative solver (`SAAMG` only).
`MAXITERS`	Maximum number of iterations of iterative solver (`SAAMG` only).
`PRECMODE`	Behavior of the preconditioner (`SAAMG` only).
`RC`	Defines the cut-off radius in the boosted frame for the P3M solver (`P3M` only).
`ALPHA`	Defines the interaction splitting parameter for the P3M solver with standard Green's function (`P3M` + `GREENSF=STANDARD` only).

Table 43: Fieldsolver command attributes

17.5.1 Fieldsolver type

At present `FFT` based solver is the most stable solver. Other solvers include Finite Element solvers and a Multigrid solver with Shortley-Weller boundary conditions for irregular domains.

17.5.2 Domain Decomposition

The dimensions in x, y and z can be parallel (`TRUE`) or serial `FALSE`. The default settings are: parallel in z and serial in x and y.

17.5.3 Number of Grid Points

Number of grid points in x, y and z for a rectangular grid.

17.5.4 Boundary Conditions

Two boundary conditions can be selected independently among x, y namely: `OPEN` and for z `OPEN` & `PERIODIC`. In the case you select for z periodic you are about to model a DC-beam.

17.5.5 Greens Function

Two Greens functions can be selected: `INTEGRATED`, `STANDARD`. The integrated Green's function is described in [39], [40], [41]. Default setting is `INTEGRATED`.

17.5.6 Bounding Box Enlargement

The bounding box defines a minimal rectangular domain including all particles. With `BBOXINCR` the bounding box can be enlarged by a factor given in percent of the minimal rectangular domain. Default value is 2.0.

17.5.7 Geometry

The list of geometries defining the beam line boundary. For further details see Chapter Geometry.

17.5.8 Iterative Solver

The iterative solver (`ITSOLVER`) for solving the preconditioned system: `CG` (default), `BICGSTAB` or `GMRES`.

17.5.9 Interpolation for Boundary Points

The interpolation method (`INTERPL`) for grid points near the boundary: `CONSTANT`, `LINEAR` (default) or `QUADRATIC`.

17.5.10 Tolerance

The tolerance (`TOL`) for the iterative solver used by the `SAAMG` solver. Default value is 1e-8.

17.5.11 Maximal Iterations

The maximal number of iterations the iterative solver performs (`MAXITERS`). Default value is 100.

17.5.12 Preconditioner Behavior

The behavior of the preconditioner (`PRECMODE`) can be: `STD`, `HIERARCHY` or `REUSE`. This argument is only relevant when using the `SAAMG` solver and should **only be set if the consequences to simulation and solver are evident**. A short description is given in Table 44.

Value	**Behavior**
`STD`	The preconditioner is rebuilt in every time step
`HIERARCHY`	The hierarchy (tentative prolongator) is reused (enabled by default)
`REUSE`	The preconditioner is reused

Table 44: Preconditioner behavior command summary

17.5.13 Cut-off Radius

The real space cut-off radius for the `P3M` solver. Within the interaction radius all the collisions are calculated using direct summation. Default value is 0 which corresponds to no particle-particle part.

17.5.14 Interaction splitting parameter

The interaction splitting parameter α determines the relative significance of the particle-particle part to the particle-mesh part in the `P3M` solver. If α is very large then the particle-mesh part is more significant and if it is very small then the particle-particle part is the dominant one. It is usually chosen as $\alpha = C/r_c$ where C is a positive constant usually of $\mathscr{O}(1)$. Default value of α is $1e8$. It is used only for the `STANDARD` Green's function option.

17.5.15 Number of Energy Bins

Suppose dE the energy spread in the particle bunch is to large, the electrostatic approximation is no longer valid. One solution to that problem is to introduce k energy bins and perform k separate field solves in which dE is again small and hence the electrostatic approximation valid. In case of a cyclotron (see Cyclotron) the number of energy bins must be at minimum the number of neighboring bunches (`NNEIGHBB`) i.e. ENBINS $\leq$ NNEIGHBB.

The variable `MINSTEPFORREBIN` defines the number of integration step that have to pass until all energy bins are merged into one.

17.6 Adaptive Mesh Refinement (AMR) Solver

After compiling *OPAL* with `ENABLE_AMR=ON`, the option `AMR=TRUE` enables further commands to be used in the Fieldsolver command (cf. Table 45).

The current AMR interface in *OPAL* is based on *AMReX* [42] which provides the multigrid solvers `FMG` (till release 18.07) and `ML`. We also provide a *Trilinos* based solver which is described in Section 17.6.1.

In order to setup an AMR simulation, the user has to specify the number of AMR levels. The hierarchy is built based on the values of the refinement ratios, blocking factors and maximum grid sizes of the base level. The maximum grid size of the next higher level is given by the division with the refinement ratio. The same is true for the blocking factors. The mesh refinement follows user-dependent rules that are provided by `AMR_TAGGING`. The various mesh refinement methods are provided in Table 46.

Command	**Purpose**
`FSTYPE`	AMR Poisson solvers: `FMG` (*BoxLib*), `ML` (*AMReX*) and `AMR_MG`
`AMR_MAXLEVEL`	Maximum adaptive mesh refinement level (single level if `AMR_MAXLEVEL` is zero).
`AMR_REFX`	Grid cell refinement ratio in x, only `AMR_REFX=2` is tested.
`AMR_REFY`	Grid cell refinement ratio in y, only `AMR_REFY=2` is tested.
`AMR_REFZ`	Grid cell refinement ratio in z, only `AMR_REFZ=2` is tested.
`AMR_MAXGRIDX`	Maximum grid size of base level in x. It has to be smaller than `MX` when running in parallel.
`AMR_MAXGRIDY`	Maximum grid size of base level in y. It has to be smaller than `MY` when running in parallel.
`AMR_MAXGRIDZ`	Maximum grid size of base level in z. It has to be smaller than `MZ` when running in parallel.
`AMR_BFX`	*AMReX* blocking factor in x. `AMR_MAXGRIDX` has to be a multiple.
`AMR_BFY`	*AMReX* blocking factor in y. `AMR_MAXGRIDY` has to be a multiple.
`AMR_BFZ`	*AMReX* blocking factor in z. `AMR_MAXGRIDZ` has to be a multiple.
`AMR_TAGGING`	Mesh-refinement strategy [`CHARGE_DENSITY`, `POTENTIAL`, `EFIELD`, `MOMENTA`, `MAX_NUM_PARTICLES`, `MIN_NUM_PARTICLES`]. Note that this attribute is defined as a string value (see String Attributes), so it must be quoted.
`AMR_DENSITY`	Charge density refinement threshold when `AMR_TAGGING="CHARGE_DENSITY"`. See also Table 46.
`AMR_MAX_NUM_PART`	Refinement threshold for `AMR_TAGGING="MAX_NUM_PARTICLES"`. See also Table 46.
`AMR_MIN_NUM_PART`	Refinement threshold for `AMR_TAGGING="MIN_NUM_PARTICLES"`. See also Table 46.
`AMR_SCALING`	Refinement threshold for `AMR_TAGGING="POTENTIAL"` and `AMR_TAGGING="EFIELD"`. See also Table 46.
`AMR_DOMAIN_RATIO`	Box ratio of the AMR computation domain. It is an array of size 3. The entries define the ratio in (x, y, z) direction. For example, $[1, 0.75, 0.75]$ yields a computation domain of $[-1,1] \times [-0.75, 0.75] \times [-0.75, 0.75]$.

Table 45: AMR extensions to the `FIELDSOLVER` command

Value	**Behavior**
`POTENTIAL`	Mark each cell if $\phi_{cell}^{level} \geq \alpha \max \phi^{level}$, where $\alpha \in [0,1]$ is the scaling factor `AMR_SCALING`
`EFIELD`	Mark each cell if the electric field component of any direction satisfies $E_{d,cell}^{level} \geq \alpha \max E_d^{level}$, where $d = x,y,z$ and $\alpha \in [0,1]$ is the scaling factor `AMR_SCALING`
`MOMENTA`	It performs a loop over all particles of a level and computes the dot product of the momenta. Every cell that contains a particle with $\|\mathbf{p}\| \geq \alpha \max_{level} \|\mathbf{p}\|$ is refined. The scalar $\alpha \in [0,1]$ is a user-defined value `AMR_SCALING`.
`CHARGE_DENSITY`	If the charge density of a cell is greater or equal to the value specified with `AMD_DENSITY` the cell is tagged for refinement
`MIN_NUM_PARTICLES`	Cells with equal or more particles are refined. The bound is specified with `AMR_MIN_NUM_PART`
`MAX_NUM_PARTICLES`	Cells with equal or less particles are refined. The bound is specified with `AMR_MAX_NUM_PART`

Table 46: Mesh refinement strategies

17.6.1 Hardware-Architecture Independent AMR Poisson Solver

This solvers is enabled with `ENABLE_AMR_MG_SOLVER=ON` and requires a working *Trilinos* installation with at least the following packages:

- *Tpetra* [43]
- *Ifpack2* [44]
- *Amesos2* and *Belos* [45]
- *MueLu* [46]

Some base level linear solvers may require additional third party libraries. These are SUPERLU [47], UMFPACK [48], PARDISO_MKL [49] [50], MUMPS [51] and LAPACK [52]. A full list of the arguments and linear solvers is given in Table 47. The solver is tested with *Trilinos* version 12.14.1. The corresponding paper is [53].

Command	**Purpose**
AMR_MG_SMOOTHER	The pre- and post-smoother which is either [GS (Gauss-Seidel), JACOBI or SGS (symmetric Gauss-Seidel)]. Default: GS
AMR_MG_NSWEEPS	The number of smoothing steps. Default: 8
AMR_MG_PREC	The preconditioner of the bottom linear solver. Please see [44] for further information. [NONE, ILUT, CHEBYSHEV, RILUK, SA, JACOBI, BLOCK_JACOBI, GS, BLOCK_GS]. Default: NONE
AMR_MG_INTERP	The prolongator of the level solution to next higher level [PC (piecewise constant), TRILINEAR, LAGRANGE (coarse-fine interface only)]. Default: PC
AMR_MG_NORM	The norm of the convergence criterion [L1_NORM, L2_NORM, LINF_NORM]. Default: LINF_NORM
AMR_MG_VERBOSE	Boolean to enable/disable solver output. It writes an SDDS file. Default: FALSE
AMR_MG_REBALANCE	Boolean to rebalance the smoothed aggregation preconditioner or linear solver (if TRUE, it uses subcommunicators to reduce the communication overhead). Default: FALSE
AMR_MG_REUSE	Reuse type of the smoothed aggregation multigrid solver of MueLu. Please see [46] for further information. [NONE, RP, RAP, SYMBOLIC, FULL]. Default: RAP
AMR_MG_TOL	The tolerance of the solver. Default: 10^{-10}
ITSOLVER	The solver of the linear system of equations on the base level. [BICGSTAB, MINRES, PCPG, CG, GMRES, STOCHASTIC_CG, RECYCLING_CG, RECYCLING_GMRES, KLU2, SUPERLU, UMFPACK, PARDISO_MKL, MUMPS, LAPACK, SA]. Please see [45] for further information. Default: CG

Table 47: Extension of the FIELDSOLVER command for the AMR Poisson Solver

17.6.2 Use of AMR

AMR is only available in the multi-bunch mode (cf. Section 8.8) of *OPAL-cycl*. As soon as more than one bunch is in the simulation, the AMR hierarchy is built. Note that *AMReX* handles the MPI parallelism, hence, other Poisson solvers of *OPAL* (cf. FSTYPE in Table 43) are not available.

17.6.3 AMR Example

In the example below we show an AMR simulation setup. It has a $[128]^3$ base grid and creates two AMR levels. The maximum grid size of the base level is 32. Hence, we can have 4 MPI-processes per spatial dimension on level zero.

```
// global options
OPTION, AMR              = TRUE;
OPTION, AMR_REGRID_FREQ  = 10;
OPTION, AMR_YT_DUMP_FREQ = 100000;
...

// initialize kinetic energy etc.
REAL Edes      = .072;
REAL turns     = 8;
REAL nstep     = 360;
REAL frequency = 50.650;
...

// define the cyclotron
ring: CYCLOTRON, ...
rf0: RFCAVITY, ...
rf1: RFCAVITY, ...
```

```
rf2: RFCAVITY, ...
rf3: RFCAVITY, ...
rf4: RFCAVITY, ...
l1: LINE = (ring, rf0, rf1, rf2, rf3, rf4);

// define the distribution
Dist1: DISTRIBUTION, ...

// fieldsolver command
Fs1: FIELDSOLVER, FSTYPE=AMR_MG,
                  MX=128, MY=128, MT=128,
                  PARFFTX=true, PARFFTY=true, PARFFTT=true,
                  BCFFTX=open, BCFFTY=open, BCFFTT=open,
                  BBOXINCR=20, AMR_MAXLEVEL=2,
                  AMR_MAXGRIDX=32, AMR_MAXGRIDY=32, AMR_MAXGRIDZ=32,
                  AMR_BFX=16, AMR_BFY=16, AMR_BFZ=16,
                  AMR_REFX=2, AMR_REFY=2, AMR_REFZ=2,
                  AMR_DOMAIN_RATIO={1.0, 0.75, 0.75},
                  AMR_TAGGING="CHARGE_DENSITY", AMR_DENSITY=1.0e-9,
                  AMR_MG_VERBOSE=true, AMR_MG_REBALANCE=true, AMR_MG_REUSE=FULL,
                  ITSOLVER=SA, AMR_MG_NORM=LINF_NORM, AMR_MG_NSWEEPS=12;

beam1: BEAM, PARTICLE=PROTON, pc=P0, NPART=1e5, BCURRENT=2.0E-3, CHARGE=1.0, BFREQ=  ↩
    frequency;

SELECT, LINE=l1;

TRACK, LINE=l1, BEAM=beam1, MAXSTEPS=nstep*turns, STEPSPERTURN=nstep,TIMEINTEGRATOR=RK4;
RUN, METHOD="CYCLOTRON-T", BEAM=beam1, FIELDSOLVER=Fs1, DISTRIBUTION=Dist1,
    MBMODE=FORCE, TURNS=11, MB_BINNING=GAMMA_BINNING, MB_ETA=0.25;

ENDTRACK;
STOP;
```

17.7 References

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Chapter 18

Tracking

18.1 Track Mode

Before starting to track, a LINE and a BEAM must be selected. The time step (`DT`) and the maximal steps to track (`MAXSTEPS`) or `ZSTOP` should be set. This command causes *OPAL* to enter "tracking mode", in which it accepts only the track commands (see Table 48). In order to perform several tracks, specify arrays of parameter in `DT`, `MAXSTEPS` and `ZSTOP`. This can be used to change the time step manually.

Command	**Purpose**
`TRACK`	Enter tracking mode
`LINE`	Label of `LINE` or `SEQUENCE`
`BEAM`	Label of `BEAM`
`T0`	Initial time [s]
`DT`	Array of time step sizes for tracking [s]
`MAXSTEPS`	Array of maximal number of time steps
`ZSTART`	z-location [m], from where to run simulation
`ZSTOP`	Array of z-location [m], after which the simulation switches to the next set of `DT`, `MAXSTEPS` and `ZSTOP`
`STEPSPERTURN`	Number of time steps per revolution period
`TIMEINTEGRATOR`	Defines the time integrator used in *OPAL-cycl*
`name=expression`	Parameter relation
`RUN`	Run particles for specified number of turns or steps
`ENDTRACK`	Leave tracking mode

Table 48: Commands accepted in Tracking Mode

The attributes of the command are:

LINE The label of a preceding LINE (no default).

BEAM The named `BEAM` command defines the particle mass, charge and reference momentum (default: `UNNAMED_BEAM`).

T0 The initial time [s] of the simulation, its default value is 0.

DT Array of time step sizes for tracking, default length of the array is 1 and its only value is 1 ps.

MAXSTEPS Array of maximal number of time steps, default length of the array is 1 and its only value is 10.

ZSTART Initial position of the reference particle along the reference trajectory, default position is 0.0 m.

ZSTOP Array of z-locations [m], default length of the array is 1 and its only value is $1E6$ [m]. The simulation switches to the next set, $i+1$, of `DT`, `MAXSTEPS` and `ZSTOP` if either it has been tracking with the current set for more than MAXSTEPS_i steps or the mean position has reached a z-position larger than ZSTOP_i. If set i is the last set of the array then the simulation stops.

TIMEINTEGRATOR Define the time integrator. Currently only available in *OPAL-cycl*. The valid options are `RK4`, `LF2` and `MTS`:

- RK4 the fourth-order Runge-Kutta integrator. This is the default integrator for *OPAL-cycl*.
- LF2 the second-order Boris-Buneman (leapfrog-like) integrator. Currently, `LF-2` is only available for multi-particles with/without space charge. For single particle tracking and tune calculations, use the `RK4` for the time being.
- MTS the multiple-time-stepping integrator. Considering that the space charge fields change much slower than the external fields in cyclotrons, the space charge can be calculated less frequently than the external field interpolation, so as to reduce time to solution. The outer step (determined by `STEPSPERTURN`) is used to integrate space charge effects. A constant number of sub-steps per outer step is used to query external fields and to move the particles. The number of sub-steps can be set with the option `MTSSUBSTEPS` and its default value is 1. When using this integrator, the input file has to be rewritten in the units of the outer step. For example, extracts of the input file suited for `LF2` or `RK4` read

```
Option, PSDUMPFREQ=100;
Option, REPARTFREQ=20;
Option, SPTDUMPFREQ=50;
Option, VERSION=10600;
REAL turns=5;
REAL nstep=3000;

TRACK, LINE=l1, BEAM=beam1, MAXSTEPS=nstep*turns, STEPSPERTURN=nstep, TIMEINTEGRATOR= ↩
    LF2
RUN, METHOD="CYCLOTRON-T", BEAM=beam1, FIELDSOLVER=Fs1, DISTRIBUTION=Dist1;

ENDTRACK;
```

and should be transformed to

```
Option, MTSSUBSTEPS=10;
Option, PSDUMPFREQ=10;
Option, REPARTFREQ=2;
Option, SPTDUMPFREQ=5;
Option, VERSION=10600;
REAL turns=5;
REAL nstep=300;
TRACK, LINE=l1, BEAM=beam1, MAXSTEPS=nstep*turns, STEPSPERTURN=nstep,
TIMEINTEGRATOR=MTS;
    RUN, METHOD = "CYCLOTRON-T", BEAM=beam1, FIELDSOLVER=Fs1, DISTRIBUTION=Dist1;
ENDTRACK;
```

In general all step quantities should be divided by `MTSSUBSTEPS`.

In our first experiments on PSI injector II cyclotron, simulations with reduced space charge solving frequency by a factor of 10 lie still very close to the original solution. How large `MTSSUBSTEPS` can be chosen of course depends on the importance of space charge effects.

STEPSPERTURN Number of time steps per revolution period. Only available for *OPAL-cycl*, default value is 720.

In *OPAL-cycl*, instead of setting time step, the time steps per-turn should be set. The command format is:

```
TRACK, LINE=name, BEAM=name, MAXSTEPS=value, STEPSPERTURN=value;
```

Particles are tracked in parallel, i.e. the coordinates of all particles are transformed at each beam element as it is reached.

OPAL leaves **track mode** when it sees the command

```
ENDTRACK;
```

18.2 Track Particles

This command starts or continues the actual tracking:

```
RUN, METHOD=string, FIELDSOLVER=label, DISTRIBUTION=label-vector, BEAM=label,
     TURNS=integer, MBMODE=string, PARAMB=float,
     BOUNDARYGEOMETRY=string, TRACKBACK=logical;
```

The `RUN` command initialises tracking and uses the most recent particle bunch for initial conditions. The particle positions may be the result of previous tracking.

Its attributes are:

METHOD The name (a string, see String Attributes) of the tracking method to be used. For the time being the following methods are known:

- `PARALLEL-T` This method puts *OPAL* in *OPAL-t* mode (see Chapter OPAL-t).
- `CYCLOTRON-T` This method puts *OPAL* in *OPAL-cycl* mode (see Chapter OPAL-cycl).

FIELDSOLVER The field solver to be used (see Chapter Field Solver).

DISTRIBUTION The particle distribution to be used (see Chapter Distribution).

BEAM The particle beam (see Chapter Beam Command) to be used is specified.

TURNS The number of turns (integer) to be tracked (default: 1, namely single bunch).

In *OPAL-cycl*, this parameter represents the number of bunches that will be injected into the cyclotron. In restart mode, the code firstly reads an attribute `NumBunch` from *.h5* file which records how many bunches have already been injected. If `NumBunch` $<$ `TURNS`, the last `TURNS` $-$ `NumBunch` bunches will be injected in sequence by reading the initial distribution from the *.h5* file.

MBMODE This defines which mode of multi-bunch runs. There are two options for it, namely, `AUTO` and `FORCE`. See Multi-bunch Mode for their explanations in detail.

For restarting run with `TURNS` larger than one, if the existing bunches of the read-in step is larger than one, the mode is forcedly set to `FORCE`. Otherwise, it is forcedly set to `AUTO`.

This argument is available for *OPAL-cycl*.

PARAMB This is a control parameter to define when to start to transfer from single bunch to multi-bunches for `AUTO` mode (default: 5.0). This argument is only available for `AUTO` mode multi-bunch run in *OPAL-cycl*.

MB_BINNING Type of energy binning in multi-bunch mode: `GAMMA_BINNING` or `BUNCH_BINNING` (default: `GAMMA_BINNING`). When `BUNCH_BINNING` binning, then all particles of a bunch are in the same energy bin. When `GAMMA_BINNING` binning, then the bin depends on the momentum of the particle. Only available in *OPAL-cycl*.

MB_ETA The scale parameter for binning in multi-bunch mode (default: 0.01). Only used in `MB_BINNING=GAMMA_BINNING`. Only available in *OPAL-cycl*.

BOUNDARYGEOMETRY The boundary geometry specification is used for particle termination (see Chapter Geometry).

TRACKBACK The particles are tracked backward in time if `TRACKBACK=TRUE`. *OPAL* starts at `ZSTART` and tracks the bunch back in time. It changes the size of the time step when it crosses the thresholds given in the `ZSTOP` attribute of the `TRACK` command and stops once it reaches the lowest item of `ZSTOP`. Only available in *OPAL-t*. Default is `FALSE`.

Example:

```
RUN, FILE="table", TURNS=5, MBMODE=AUTO, PARAMB=10.0,
     METHOD="CYCLOTRON-T", BEAM=beam1, FIELDSOLVER=Fs1,
     DISTRIBUTION=Dist1;
```

This command tracks 5 bunches in cyclotron and writes the results on file `table`.

Chapter 19

Wakefields

OPAL-t provides methods to compute CSR and short-range geometric wakefields.

19.1 Geometric Wakefields

Basically there are two different kind of wakefields that can be used. The first one is the wakefield of a round, metallic beam pipe that can be calculated numerically (see Section 19.3). Since this also limits the applications of wakefields we also provide a way to import a discretized wakefield from a file The wakefield of a round, metallic beam pipe with radius a can be calculated by inverse FFT of the beam pipe impedance. There are known models for beam pipes with `DC` and `AC` conductivity. The `DC` conductivity of a metal is given by

$$\sigma_{DC} = \frac{ne^2\tau}{m}$$

EQUATION 19.1: DC conductivity

with n the density of conduction electrons with charge e, τ the relaxation time, and m the electron mass. The `AC` conductivity, a response to applied oscillation fields, is given by

$$\sigma_{AC} = \frac{\sigma_{DC}}{1 - i\omega\tau}$$

EQUATION 19.2: AC conductivity

with ω denoting the frequency of the fields.

The longitudinal impedance with `DC` conductivity is given by

$$Z_{Ldc}(k) = \frac{1}{ca}\frac{2}{\frac{\lambda}{k} - \frac{ika}{2}}$$

EQUATION 19.3: Longitudinal impedance

where

$$\lambda = \sqrt{\frac{2\pi\sigma|k|}{c}}(i + sign(k))$$

with c denoting the speed of light and k the wave number.

The longitudinal wake can be obtained by an inverse Fourier transformation of the impedance. Since $Re(Z_L(k))$ drops at high frequencies faster than $Im(Z_L(k))$ the cosine transformation can be used to calculate the wake. The following equation holds in both, the `DC` and `AC`, case

$$W_L(s) = 10^{-12}\frac{2c}{\pi}Re\left(\int_0^\infty Re(Z_L(k))\cos(ks)dk\right)$$

EQUATION 19.4: Longitudinal wakefield

with $Z_L(k)$ either representing $Z_{L_{DC}}(k)$ or $Z_{L_{AC}}(k)$ depending on the conductivity. With help of the Panofsky-Wenzel theorem

$$Z_L(k) = \frac{k}{c}Z_T(k).$$

we can deduce the transverse wakefield from Equation 19.4:

$$W_T(s) = 10^{-12}\frac{2c}{\pi}Re\left(\int_0^\infty Re(\frac{c}{k}Z_L(k))\cos(ks)dk\right).$$

EQUATION 19.5: Transverse wakefield

To calculate the integrals in Equation 19.4 and Equation 19.5 numerically the Simpson integration schema with equidistant mesh spacing is applied. This leads to an integration with small Δk with a big N which is computational not optimal with respect to efficiency. Since we calculate the wakefield usually just once in the initialization phase the overall performance will not be affected from this.

19.2 CSR Wakefields

The electromagnetic field due to a particle moving on a circle in free space can be calculated exactly with the Liénard-Wiechert potentials. The field has been calculated for all points on the same circle [56] ,[57]. For high particle energies the radiated power is almost exclusively emitted in forward direction, whereas for low energies a fraction is also emitted in transverse and backward direction. For the case of high-energetic particles an impedance in forward direction can be calculated [58]. The procedure is then the same as for a regular wakefield with the important difference that wakes exert forces on trailing particles only. The electromagnetic fields of a particle propagating on the mid-plane between two parallel metallic plates that stretch to infinity [57] and for finite plates [59] can also be calculated. For the infinite plates an impedance can be calculated [58].

All of these approaches for CSR neglect any transient effects due to the finite length of the bend. Instead they describe the steady state case of a bunch circling infinitely long in the field of a dipole magnet. In [60] the four different stages of a bunch passing a bending magnet are treated separately and for each a corresponding wake function is derived. This model is used in *OPAL-t* for `1D-CSR`.

The 1-dimensional approach also neglects any influence of the transverse dimensions and of changes in current density between retarded and current time. On the other hand it gives a good approximation of effects due to CSR in short time.

In addition to the `1D-CSR` model also one that makes use of an integrated Green function [61], `1D-CSR-IGF`.

19.3 The WAKE Command

The general input format for the `WAKE` command is:

```
label: WAKE, TYPE=string, NBIN=real, CONST_LENGTH=bool,
       CONDUCT=string, Z0=real, FORM=string, RADIUS=real,
       SIGMA=real, TAU=real, FILTERS=string-array;
```

The format for a CSR wake is

```
label:WAKE, TYPE=string, NBIN=real, FILTERS=string-array;
```

Command	**Purpose**
`WAKE`	Specify a wakefield
`TYPE`	Specify the wake function [`1D-CSR`, `1D-CSR-IGF`, `LONG-SHORT-RANGE`, `TRANSV-SHORT-RANGE`]
`NBIN`	Number of bins used in the calculation of the line density
`CONST_LENGTH`	`TRUE` if the length of the bunch is considered to be constant
`CONDUCT`	Conductivity [`AC`, `DC`]
`Z0`	Impedance of the beam pipe in [Ω]
`FORM`	The form of the beam pipe [`ROUND`]
`RADIUS`	The radius of the beam pipe in [m]
`SIGMA`	Material constant dependent on the beam pipe material in [$\Omega^{-1}m$]
`TAU`	Material constant dependent on the beam pipe material in [s]
`FNAME`	Specify a file that provides a wake function
`FILTER`	The names of the filters that should be applied

Table 49: Wakefield command summary

WAKE Define the Wakefield to be used. The `WAKE` command defines data for a wake function on an element (see Common Attributes for all Elements).

TYPE Define the wakefield type. A string value (see String Attributes) to specify the wake function, either `1D-CSR`, `1D-CSR-IGF`, `LONG-SHORT-RANGE` or `TRANSV-SHORT-RANGE`.

NBIN The number of bins used in the calculation of the line density.

CONST_LENGTH With the `CONST_LENGTH` flag the bunch length can be set to be constant. This has no effect on CSR wakefunctions.

CONDUCT The conductivity of the bunch which can be set to either `AC` or `DC`. This has no effect on CSR wakefunctions.

Z0 Define the impedance Z_0 of the beam pipe in [Ω]. This has no effect on CSR wakefunctions.

FORM Define the form of the beam pipe can be set to `ROUND`. This has no effect on CSR wakefunctions.

RADIUS Define the radius of the beam pipe [m]. This has no effect on CSR wakefunctions.

SIGMA Define the σ of the beam pipe (material constant), see Equation 19.1. This has no effect on CSR wakefunctions.

TAU The τ defines the relaxation time of the beam pipe and is needed to calculate the impedance of the beam pipe see Equation 19.1. This has no effect on CSR wakefunctions.

FNAME Import a wakefield from a file. Since we only need values of the wake function at several discrete points to calculate the force on the particle it is also possible to specify these in a file.To get required data points of the wakefield not provide in the file we linearly interpolate the available function values. The files are specified in the SDDS format [62], [63]. Whenever a file is specified *OPAL* will use the wakefield found in the file and ignore all other commands related to round beam pipes.

FILTER List of Filters. Array of names of filters to be applied to the longitudinal histogram of the bunch to get rid of the noise and to calculate derivatives. All the filters are applied to the line density in the order they appear in the array. The last filter is also used for calculating the derivatives. The actual filters have to be defined elsewhere.

19.4 The FILTER Command

Filters can be defined which then are applied to the line density of the bunch. The following smoothing filters are implemented: `SAVITZKY-GOLAY`, `STENCIL`, `FIXEDFFTLOWPASS`, `RELATIVEFFTLOWPASS`. The input format for them is

```
label: FILTER, TYPE=string, NFREQ=real, THRESHOLD=real,
       NPOINTS=real, NLEFT=real, NRIGHT=real, POLYORDER=real
```

TYPE The type of filter: `SAVITZKY-GOLAY`, `STENCIL`, `FIXEDFFTLOWPASS`, `RELATIVEFFTLOWPASS`

NFREQ Only used in `FIXEDFFTLOWPASS`: the number of frequencies to keep

THRESHOLD Only used in `RELATIVEFFTLOWPASS`: the minimal strength of frequency compared to the strongest to consider.

NPOINTS Only used in `SAVITZKY-GOLAY`: width of moving window in number of points

NLEFT Only used in `SAVITZKY-GOLAY`: number of points to the left

NRIGHT Only used in `SAVITZKY-GOLAY`: number of points to the right

POLYORDER Only used in `SAVITZKY-GOLAY`: polynomial order to be used in least square approximation

The `SAVITZKY-GOLAY` filter and the ones based on the FFT routine provide a derivative on a natural way. For the `STENCIL` filter a second order stencil is used to calculate the derivative.

An implementation of the `SAVITZKY-GOLAY` filter can be found in the Numerical Recipes. The `STENCIL` filter uses the following two stencil consecutively to smooth the line density:

$$f_i = \frac{7 \cdot f_{i-4} + 24 \cdot f_{i-2} + 34 \cdot f_i + 24 \cdot f_{i+2} + 7 \cdot f_{i+4}}{96}$$

and

$$f_i = \frac{7 \cdot f_{i-2} + 24 \cdot f_{i-1} + 34 \cdot f_i + 24 \cdot f_{i+1} + 7 \cdot f_{i+2}}{96}.$$

For the derivative a standard second order stencil is used:

$$f_i' = \frac{f_{i-2} - 8 \cdot f_{i-1} + 8 \cdot f_{i+1} - f_{i+2}}{h}$$

This filter was designed by Ilya Pogorelov for the ImpactT implementation of the CSR 1D model.

The FFT based smoothers calculate the Fourier coefficients of the line density. Then they set all coefficients corresponding to frequencies above a certain threshold to zero. Finally the back-transformation is calculate using this coefficients. The two filters differ in the way they identify coefficients which should be set to zero. `FIXEDFFTLOWPASS` uses the n lowest frequencies whereas `RELATIVEFFTLOWPASS` searches for the coefficient which has the biggest absolute value. All coefficients which, compared to this value, are below a threshold (measure in percents) are set to zero. For the derivative the coefficients are multiplied with the following function (this is equivalent to a convolution):

$$g_i = \begin{cases} i\frac{2\pi\imath}{N \cdot L} & i < N/2 \\ -i\frac{2\pi\imath}{N \cdot L} & i > N/2 \end{cases}$$

where N is the total number of coefficients/sampling points and L is the length of the bunch.

19.5 References

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Chapter 20

Geometry

At present the GEOMETRY command is still an **experimental feature** which is not to be used by the general user. It can be used to act as a terminator for particles that cross the geometry surface and to specify boundaries conditions for the SAAMG field solver. The command can be used in two modes:

1. specify a H5hut file holding the surface mesh of a complicated boundary geometry
2. use a predefined geometry: ELLIPTIC, RECTANGULAR or BOXCORNER

20.1 Geometry Command

Command	Purpose	Default Value
GEOMETRY	Specify a geometry	
FGEOM	Specifies the geometry file, an H5hut file, containing the surface mesh of the geometry.	
LENGTH	The length of the specified geometry in [m].	1.0
TOPO	The topology of the geometry: ELLIPTIC, RECTANGULAR or BOXCORNER. If FGEOM is selected TOPO is overwritten.	ELLIPTIC
S	The start of the specified geometry in [m].	1.0
A	The semi-major axis of the ellipse or the half aperture of the rectangle (horizontally) in [m].	0.025
B	The semi-minor axis of the ellipse or the half aperture of the rectangle (vertically) in [m].	0.025
C	The height of the corner in [m]. BOXCORNER only.	0.01
L1	The first part of the geometry with height B in [m]. BOXCORNER only.	0.5
L2	The second part of the geometry with height B-C in [m]. BOXCORNER only.	0.2
ZSHIFT	Shift in z direction. Only used with a H5hut geometry.	0.0
XYZSCALE	Multiplicative scaling factor for coordinates. Only used with a H5hut geometry.	1.0
XSCALE	Multiplicative scaling factor for x-coordinates. Only used with a H5hut geometry.	1.0
YSCALE	Multiplicative scaling factor for y-coordinates. Only used with a H5hut geometry.	1.0
ZSCALE	Multiplicative scaling factor for z-coordinates. Only used with a H5hut geometry.	1.0
INSIDEPOINT	A point inside the geometry. Only used with a H5hut geometry.	

Table 50: Geometry command summary

An example of an elliptic geometry:

```
Name: GEOMETRY, TOPO=ELLIPTIC, LENGTH=1.0, A=0.005, B=0.005;
```

The geometry element must later be passed to the FIELDSOLVER command. If only particle termination is desired, any solver can be used and it is not necessary to specify the geometry in the field solver command.

In the RUN command the boundary geometry has always to be specified in order to load it and use it for particle termination.

Chapter 21

Physics Models Used in the Particle Matter Interaction Model

The command to define particle-matter interactons is `PARTICLEMATTERINTERACTION`.

TYPE Specifies the particle-matter interaction handler. Currently, there are the two following implemented methods: `SCATTERING` for physical processes of beam scattering and energy loss by heavy charged particles and `BEAMSTRIPPING` for interactions with residual gas and Lorentz stripping.

MATERIAL The material of the surface (see Available Materials in OPAL).

ENABLERUTHERFORD Switch to disable Rutherford scattering (default: true).

LOWENERGYTHR Low-energy threshold [MeV] for energy loss calculation. Particles with lower energy will be removed (default: 0.01 MeV).

The so defined instance has then to be added to an element using the attribute.

21.1 The Energy Loss

The energy loss is simulated using the Bethe-Bloch equation.

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{Kz^2Z}{A\beta^2}\left[\frac{1}{2}\ln\frac{2m_ec^2\beta^2\gamma^2Tmax}{I^2} - \beta^2\right],$$

where Z is the atomic number of absorber, A is the atomic mass of absorber, m_e is the electron mass, z is the charge number of the incident particle, $K = 4\pi N_A r_e^2 m_e c^2$, r_e is the classical electron radius, N_A is the Avogadro's number, I is the mean excitation energy. β and γ are kinematic variables. T_{max} is the maximum kinetic energy which can be imparted to a free electron in a single collision.

$$T_{max} = \frac{2m_ec^2\beta^2\gamma^2}{1+2\gamma m_e/M+(m_e/M)^2},$$

where M is the incident particle mass.

This expression is valid for energies from 600 keV to 10 GeV for incident beams (see PARTICLE definition) of `PROTON`, `DEUTERON`, `MUON`, `HMINUS` and `H2P`; and also for `ALPHA` particles from 10 MeV to 1 GeV.

The stopping power is compared with PSTAR program of NIST in Figure 32.

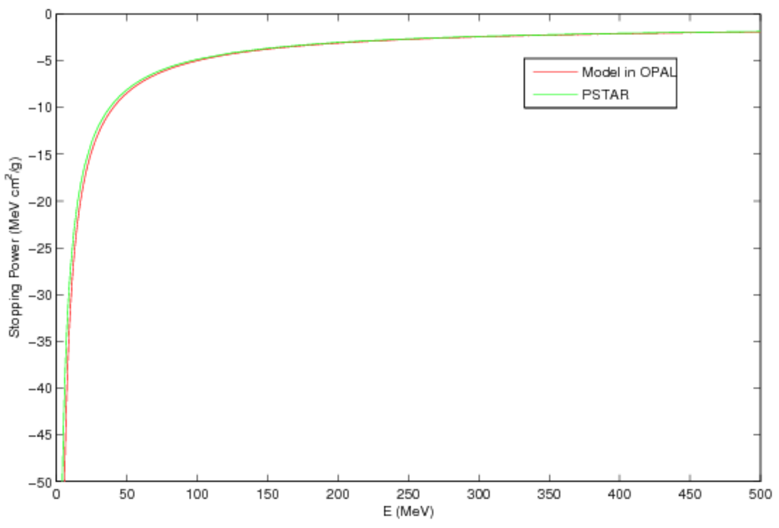

Figure 32: The comparison of stopping power with PSTAR.

The energy loss in the low-energy region is calculated using semi-empirical fitting formulas of Andersen and Ziegler [72].

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = 10^{-21}\frac{N_A}{A}\cdot\varepsilon,$$

where the energy loss is in MeV cmˆ2/g and ε is a fitted function of the stopping cross section.

$$\varepsilon = \frac{\varepsilon_{low}\cdot\varepsilon_{high}}{\varepsilon_{low}+\varepsilon_{high}}$$

In case of incident protons in the material for energies from 10 keV to 600 keV, the fitting functions are given by:

$$\varepsilon_{low} = A2\cdot T_s^{0.45}$$

$$\varepsilon_{high} = \frac{A3}{T_s}\ln\left(1+\frac{A4}{T_s}+A5\cdot T_s\right)$$

where T_s is the kinetic energy (in keV) divided by the proton mass (in amu). For T_s between 1 and 10 keV, the fitted function is given by:

$$\varepsilon = A1\cdot T_s^{0.5}$$

In case of incident alpha particles for energies from 1 keV to 10 MeV, the stopping power functions is expressed as:

$$\varepsilon_{low} = B1\cdot(1000T)^{B2}$$

$$\varepsilon_{high} = \frac{B3}{T}\ln\left(1+\frac{B4}{T}+B5\cdot T\right)$$

where T is the kinetic energy in MeV. The numerical values of coefficients of the empirical formulas are showed in Table 52.

The particles lost due to excessive energy loss (final energy null or lower than `LOWENERGYTHR`) are recorded in a HDF5 file (or ASCII if ASCIIDUMP is true). The loss file name is compound by the associated element name and the `PARTICLEMATTERINTERACT` name.

Energy straggling: For relatively thick absorbers such that the number of collisions is large, the energy loss distribution is shown to be Gaussian in form. For non-relativistic heavy particles the spread σ_0 of the Gaussian distribution is calculated by:

$$\sigma_0^2 = 4\pi N_A r_e^2 (m_e c^2)^2 \rho \frac{Z}{A}\Delta s,$$

where ρ is the density, Δs is the thickness.

21.2 The Coulomb Scattering

The Coulomb scattering is treated as two independent events: the multiple Coulomb scattering and the large angle Rutherford scattering. Using the distribution given in Classical Electrodynamics, by J. D. Jackson [64], the multiple- and single-scattering distributions can be written:

$$P_M(\alpha)\,\mathrm{d}\alpha = \frac{1}{\sqrt{\pi}} e^{-\alpha^2}\,\mathrm{d}\alpha,$$

$$P_S(\alpha)\,\mathrm{d}\alpha = \frac{1}{8\ln(204Z^{-1/3})}\frac{1}{\alpha^3}\,\mathrm{d}\alpha,$$

where $\alpha = \frac{\theta}{<\Theta^2>^{1/2}} = \frac{\theta}{\sqrt{2}\theta_0}$.

The transition point is $\theta = 2.5\sqrt{2}\theta_0 \approx 3.5\theta_0$,

$$\theta_0 = \frac{13.6MeV}{\beta cp} z\sqrt{\Delta s/X_0}[1+0.038\ln(\Delta s/X_0)],$$

where p is the momentum, Δs is the step size, and X_0 is the radiation length.

21.2.1 Multiple Coulomb Scattering

Generate two independent Gaussian random variables with mean zero and variance one: z_1 and z_2. If $z_2\theta_0 > 3.5\theta_0$, start over. Otherwise,

$$x = x + \Delta s p_x + z_1\Delta s\theta_0/\sqrt{12} + z_2\Delta s\theta_0/2,$$

$$p_x = p_x + z_2\theta_0.$$

Generate two independent Gaussian random variables with mean zero and variance one: z_3 and z_4. If $z_4\theta_0 > 3.5\theta_0$, start over. Otherwise,

$$y = y + \Delta s p_y + z_3\Delta s\theta_0/\sqrt{12} + z_4\Delta s\theta_0/2,$$

$$p_y = p_y + z_4\theta_0.$$

21.2.2 Large Angle Rutherford Scattering

Generate a random number ξ_1, *if* $\xi_1 < \frac{\int_{2.5}^{\infty} P_S(\alpha)d\alpha}{\int_0^{2.5} P_M(\alpha)\,\mathrm{d}\alpha + \int_{2.5}^{\infty} P_S(\alpha)\,\mathrm{d}\alpha} = 0.0047$, sampling the large angle Rutherford scattering.

The cumulative distribution function of the large angle Rutherford scattering is

$$F(\alpha) = \frac{\int_{2.5}^{\alpha} P_S(\alpha)\,\mathrm{d}\alpha}{\int_{2.5}^{\infty} P_S(\alpha)\,\mathrm{d}\alpha} = \xi,$$

where ξ is a random variable. So

$$\alpha = \pm 2.5\sqrt{\frac{1}{1-\xi}} = \pm 2.5\sqrt{\frac{1}{\xi}}.$$

Generate a random variable P_3, *if* $P_3 > 0.5$

$$\theta_{Ru} = 2.5\sqrt{\frac{1}{\xi}}\sqrt{2}\theta_0,$$

else

$$\theta_{Ru} = -2.5\sqrt{\frac{1}{\xi}}\sqrt{2}\theta_0.$$

The angle distribution after Coulomb scattering is shown in Figure 33. The line is from Jackson's formula, and the points are simulations with Matlab. For a thickness of $\Delta s = 1e-4\ m$, $\theta = 0.5349\alpha$ (in degree).

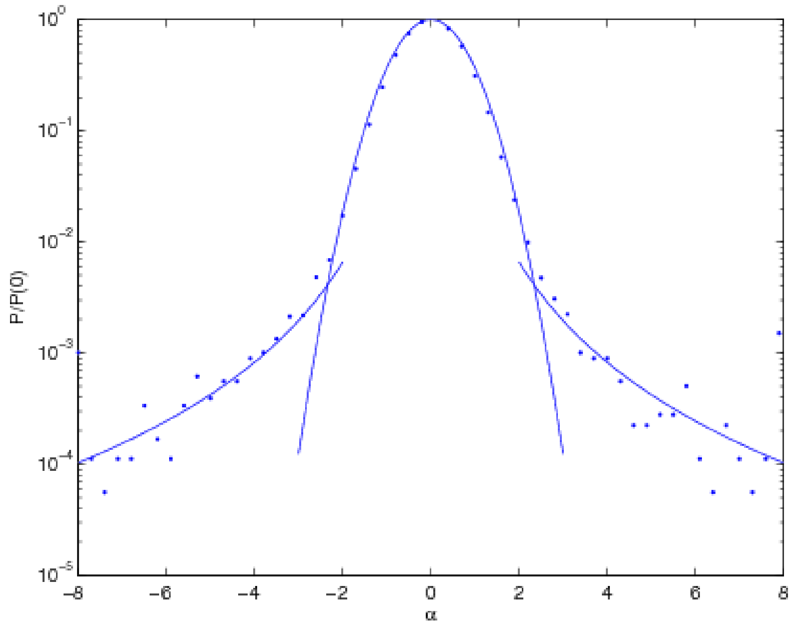

Figure 33: The comparison of Coulomb scattering with Jackson's book.

21.3 Beam Stripping physics

Beam stripping physics takes into account two different physical processes: interaction with residual gas and electromagnetic stripping (also called Lorentz stripping). Given the stochastic nature of such interactions, the processes are modeled as a Monte Carlo method.

Both processes are described in the same way: Assuming that particles are normally incident on a homogeneous medium and that they are subjected to a process with a mean free path λ between interactions, the probability of suffering an interaction before reaching a path length x is:

$$P(x) = 1 - e^{-x/\lambda}$$

where $P(x)$ is the statistic cumulative interaction probability of the process.

Figure 34 summarizes the iterative steps evaluated by the algorithm.

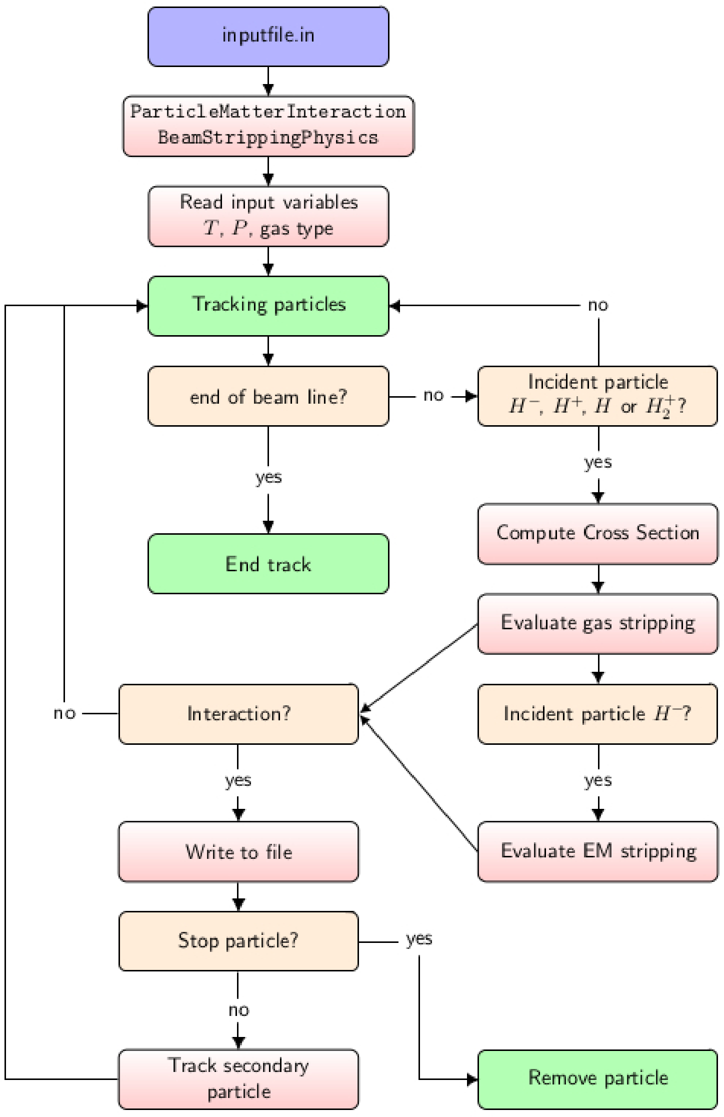

Figure 34: The diagram of BeamStrippingPhysics in *OPAL*.

21.3.1 Residual gas interaction

The mean free path of the interaction is related with the density of interaction centers and the cross section: $\lambda = 1/N\sigma$. Assuming a beam flux incident in an ideal gas with density N (number of gas molecules per unit volume under the vacuum condition), the number of particles interacting depends on the gas composition and the different reactions to be considered. Thus, in agreement with Dalton's law of partial pressures:

$$\frac{1}{\lambda_{total}} = \sum \frac{1}{\lambda_k} = N_{total} \cdot \sigma_{total} = \sum_j N_j \, \sigma^j_{total} = \sum_j \left(\sum_i N_j \, \sigma^j_i \right)$$

where the first summation is over all gas components and the second summation is over all processes for each component.

The fraction loss of the beam for unit of travelled length is: $f_g = 1 - e^{-\delta_s/\lambda_{total}}$. For a individual particle, f_g represents the interaction probability and it is evaluated through an independent random variable each step δ_s.

Gas stripping could be applied for four different types of incoming particles: negative hydrogen ions (HMINUS), protons (PROTON), neutral hydrogen atoms (HYDROGEN), hydrogen molecule ions (H2P) and deuterons (DEUTERON). Single / Double - electron detachment or capture reactions are considered for each of them.

Cross sections are calculated according to energy of the particle employing analytic expressions fitted to cross section experimental data. The suitable function is selected in each case according to the type of incident particle and the residual gas under consideration. There are different fitting expressions:

- Nakai function [65]

$$\sigma_{qq'} = \sigma_0\,[f(E_1)+a_7\cdot f(E_1/a_8)]$$
$$f(E) = \frac{a_1\cdot\left(\frac{E}{E_R}\right)^{a_2}}{1+\left(\frac{E}{a_3}\right)^{a_2+a_4}+\left(\frac{E}{a_5}\right)^{a_2+a_6}}$$
$$E_R = hcR_\infty\cdot\frac{m_H}{m_e}$$
$$E_1 = E_0 - E_{th}$$

where σ_0 is a convenient cross section unit ($\sigma_0 = 1\cdot 10^{-16}\,\mathrm{cm}^2$), E_0 is the incident projectile energy in keV, E_{th} is the threshold energy of reaction in keV, and the symbols a_i denote adjustable parameters.

- Tabata function [66]: A linear combination of the Nakai function, $f(E)$, improved and fitted with a greater number of experimental data and considering more setting parameters. The enhancement of the function makes it possible to extrapolate the cross section data to some extent.
- Barnett function [67]:

$$\ln[\sigma(E)] = \frac{1}{2}a_0 + \sum_{i=1}^{k} a_i\cdot T_i(X)$$
$$X = \frac{(\ln E - \ln E_{min}) - (\ln E_{max} - \ln E)}{\ln E_{max} - \ln E_{min}}$$

where T_i are the Chebyshev orthogonal polynomials.

- Bohr function [68]:

$$\sigma = \begin{cases} 4\pi a_0^2\frac{z_t+z_t^2}{z_i}\left(\frac{v_0}{v}\right)^2 & z_t < 15 \\ \pi a_0^2\frac{z_t^{2/3}}{z_i}\left(\frac{v_0}{v}\right) & z_t > 15 \end{cases}$$

where z_i and z_t are the charge of the incident particle and the charge of the target nuclei, a_0 is the Bohr radius, $v_0 = e^2/4\pi\varepsilon_0\hbar$ is the characteristic Bohr velocity and v is the incident particle velocity.

21.3.2 Electromagnetic stripping

In case of `HMINUS` particles, the second electron is slightly bounded, so it is relevant to consider the detachement by the magnetic field. The orthogonal component of the magnetic field to the median plane (read from `CYCLOTRON` element), produces an electric field according to Lorentz transformation, $E=\gamma\beta cB$. The fraction of particles dissociated by the electromagnetic field during a time step δ_t is:

$$f_{em} = 1 - e^{-\delta_t/\gamma\tau}$$

where τ is the particle lifetime in the rest frame, determined theoretically [69]:

$$\tau = \frac{4mz_T}{S_0N^2\hbar(1+p)^2\left(1-\frac{1}{2k_0z_t}\right)}\cdot\exp\left(\frac{4k_0z_T}{3}\right)$$

where $z_T = -\varepsilon_0/eE$ is the outer classical turning radius, ε_0 is the binding energy, p is a polarization factor of the ionic wave function, $k_0^2 = 2m(-\varepsilon_0)/\hbar^2$, S_0 is a spectroscopy coefficient, and the normalization constant is $N = (2k_0(k_0+\alpha)(2k_0+\alpha))^{1/2}/\alpha$, where α is a parameter for the ionic potential function.

The electromagnetic stripping calculation is restricted to *OPAL-cycl*.

21.4 The *ScatteringPhysics* Substeps

Small step is needed in the routine of ScatteringPhysics.

If a large step is given in the main input file, in the file *ScatteringPhysics.cpp*, it is divided by a integer number *n* to make the step size using for the calculation of scattering physics less than 1.01e-12 s. As shown by Figure 35 and Figure 36 in the following subsection, first we track one step for the particles already in the element and the newcomers, then another (n-1) steps to make sure the particles in the element experience the same time as the ones in the main bunch.

Now, if the particle leave the element during the (n-1) steps, we track it as in a drift and put it back to the main bunch when finishing (n-1) steps.

21.4.1 The Flow Diagram of *ScatteringPhysics* Class in OPAL

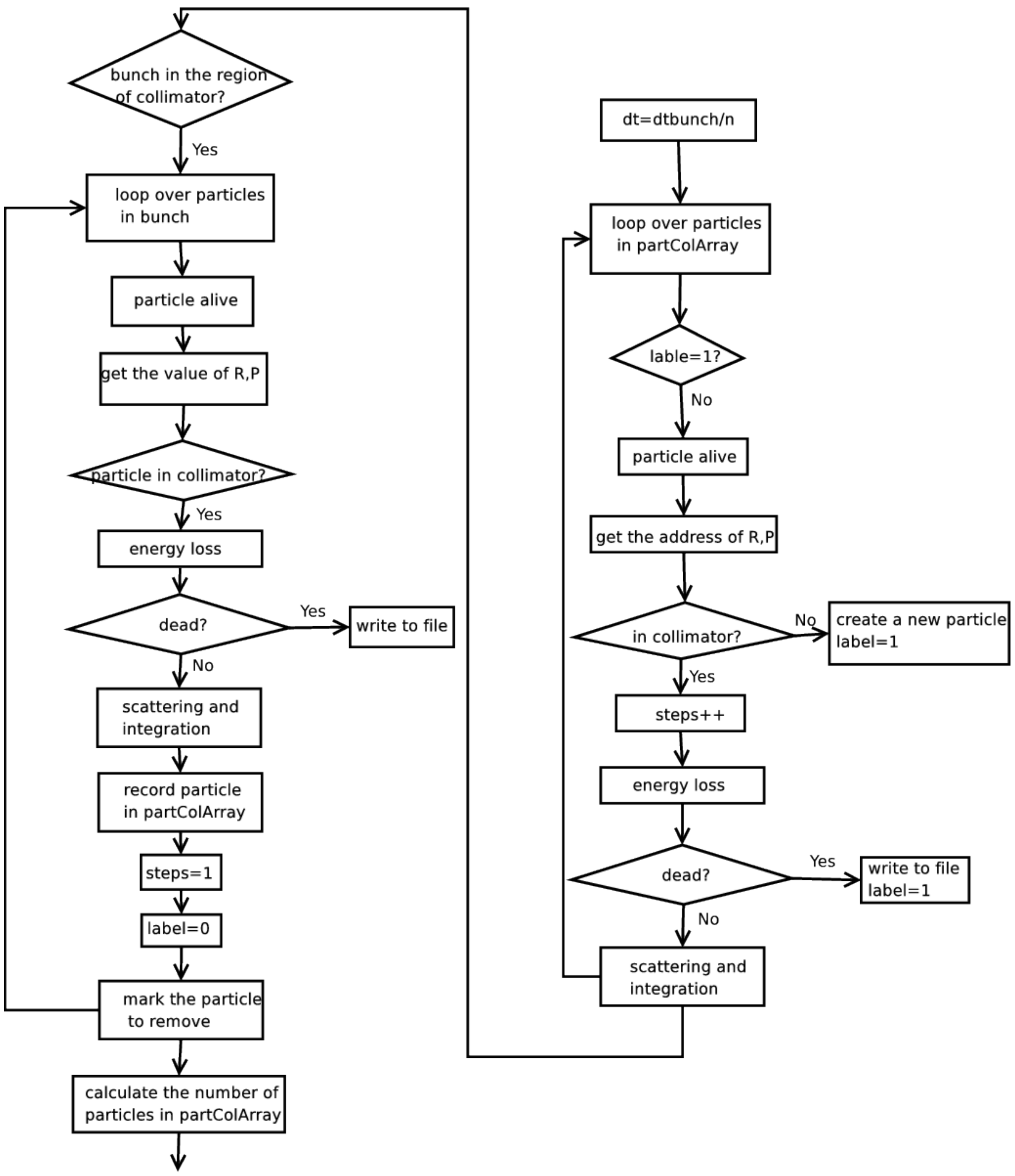
bunch in the region of collimator?
Yes
loop over particles in bunch
particle alive
get the value of R,P
particle in collimator?
Yes
energy loss
dead?
Yes
write to file
No
scattering and integration
record particle in partColArray
steps=1
label=0
mark the particle to remove
calculate the number of particles in partColArray
dt=dtbunch/n
loop over particles in partColArray
lable=1?
No
particle alive
get the address of R,P
in collimator?
No
create a new particle label=1
Yes
steps++
energy loss
dead?
Yes
write to file label=1
No
scattering and integration

Figure 35: The diagram of ScatteringPhysics in *OPAL*.

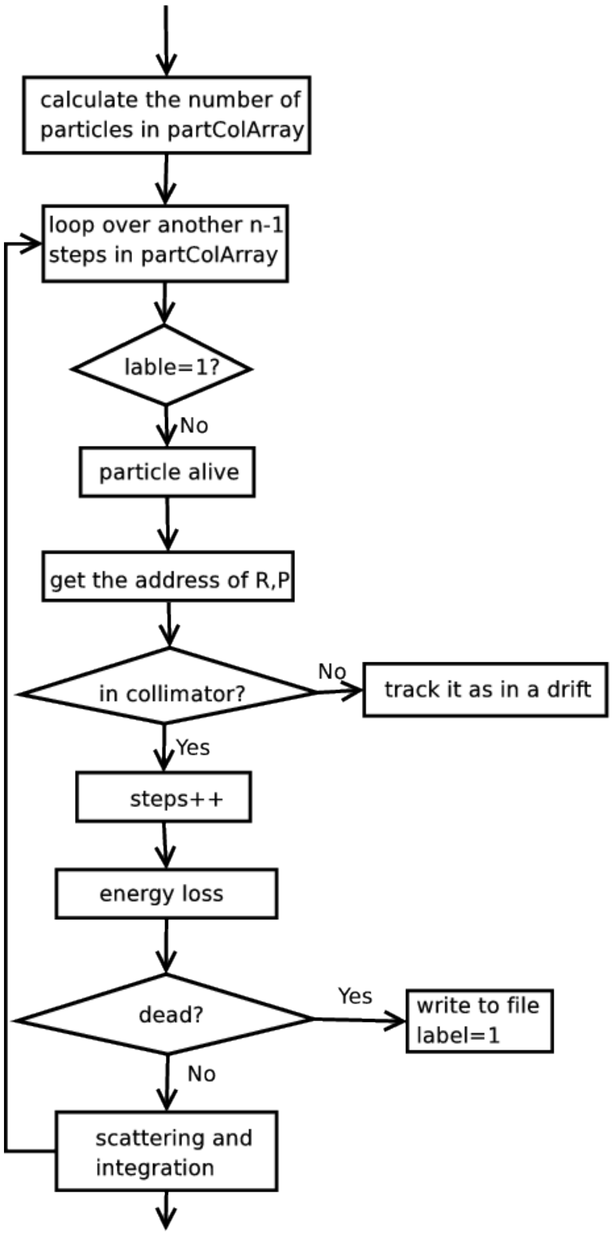

Figure 36: The diagram of ScatteringPhysics in *OPAL* (continued).

21.5 Available Materials in *OPAL*

Different materials have been implemented in *OPAL* for scattering interactions and energy loss calculation. The materials that are supported are listed in Table 51, including the atomic number, Z, the atomic weight, A, the mass density, ρ, the radiation lenght, $X0$, and the mean excitation energy, I. In addition, the coefficients of the Andersen-Ziegler empirical formulas for the stopping power in the low-energy region are illustrated in Table 52.

Material (*OPAL* Name)	**Z**	**A**	ρ [g/cm^3]	**X0** [g/cm^2]	**I** [eV]
`Air`	7	14	1.205E-3	36.62	85.7
`Aluminum`	13	26.9815384	2.699	24.01	166.0
`AluminaAl2O3`	50	101.9600768	3.97	27.94	145.2
`Beryllium`	4	9.0121831	1.848	65.19	63.7
`BoronCarbide`	26	55.251	2.52	50.13	84.7
`Copper`	29	63.546	8.96	12.86	322.0
`Gold`	79	196.966570	19.32	6.46	790.0
`Graphite`	6	12.0172	2.210	42.7	78.0
`GraphiteR6710`	6	12.0172	1.88	42.7	78.0
`Kapton`	6	12	1.420	40.58	79.6
`Molybdenum`	42	95.95	10.22	9.80	424.0
`Mylar`	6.702	12.88	1.400	39.95	78.7
`Titanium`	22	47.867	4.540	16.16	233.0
`Water`	10	18.0152	1	36.08	75.0

Table 51: List of materials with their atomic and nuclear properties [70] [71].

Material (*OPAL* Name)	**A1**	**A2**	**A3**	**A4**	**A5**	**B1**	**B2**	**B3**	**B4**	**B5**
`Air`	2.954	3.350	1.683e3	1.900e3	2.513e-2	1.9259	0.5550	27.15125	26.0665	6.2768
`Aluminum`	4.154	4.739	2.766e3	1.645e2	2.023e-2	2.5	0.625	45.7	0.1	4.359
`AluminaAl2O3`	1.187e1	1.343e1	1.069e4	7.723e2	2.153e-2	5.4	0.53	103.1	3.931	7.767
`Beryllium`	2.248	2.590	9.660e2	1.538e2	3.475e-2	2.1895	0.47183	7.2362	134.30	197.96
`BoronCarbide`	3.519	3.963	6065.0	1243.0	7.782e-3	5.013	0.4707	85.8	16.55	3.211
`Copper`	3.969	4.194	4.649e3	8.113e1	2.242e-2	3.114	0.5236	76.67	7.62	6.385
`Gold`	4.844	5.458	7.852e3	9.758e2	2.077e-2	3.223	0.5883	232.7	2.954	1.05
`Graphite`	0.0	2.601	1.701e3	1.279e3	1.638e-2	3.80133	0.41590	12.9966	117.83	242.28
`GraphiteR6710`	0.0	2.601	1.701e3	1.279e3	1.638e-2	3.80133	0.41590	12.9966	117.83	242.28
`Kapton`	0.0	2.601	1.701e3	1.279e3	1.638e-2	3.83523	0.42993	12.6125	227.41	188.97
`Molybdenum`	6.424	7.248	9.545e3	4.802e2	5.376e-3	9.276	0.418	157.1	8.038	1.29
`Mylar`	2.954	3.350	1683	1900	2.513e-02	1.9259	0.5550	27.15125	26.0665	6.2768
`Titanium`	4.858	5.489	5.260e3	6.511e2	8.930e-3	4.71	0.5087	65.28	8.806	5.948
`Water`	4.015	4.542	3.955e3	4.847e2	7.904e-3	2.9590	0.53255	34.247	60.655	15.153

Table 52: List of materials with the coefficients of the Andersen-Ziegler empirical formulas for the stopping power in the low-energy region [72].

21.6 Example of an Input File

particlematterinteraction.in

FX5 is a slit in x direction, the APERTURE is **POSITIVE**, the first value in APERTURE is the left part, the second value is the right part. FX16 is a slit in y direction, the APERTURE is **NEGATIVE**, the first value in APERTURE is the down part, the second value is the up part.

21.7 A Simple Test

A cold Gaussian beam with $\sigma_x = \sigma_y = 5$ mm. The position of the collimator is from 0.01 m to 0.1 m, the half aperture in y direction is 3 mm. Figure 37 shows the trajectory of particles which are either absorbed or deflected by a copper slit. As a benchmark of the collimator model in *OPAL*, Figure 38 shows the energy spectrum and angle deviation at z=0.1 m after an elliptic collimator.

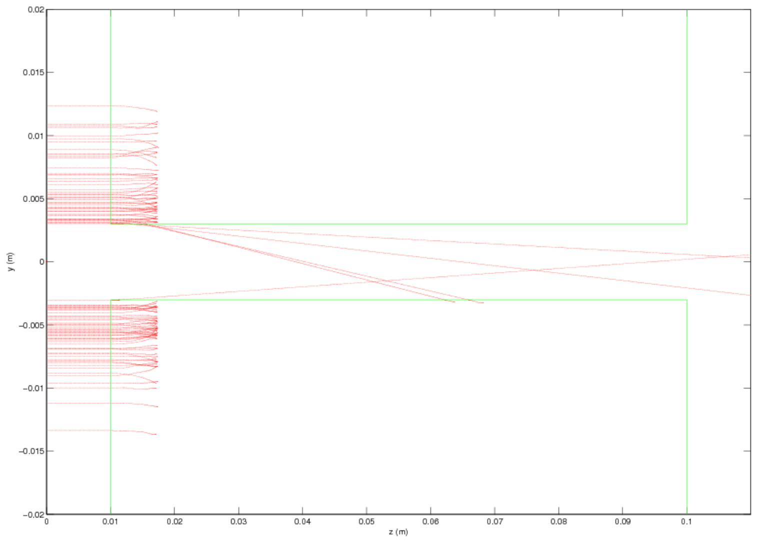

Figure 37: The passage of protons through the collimator.

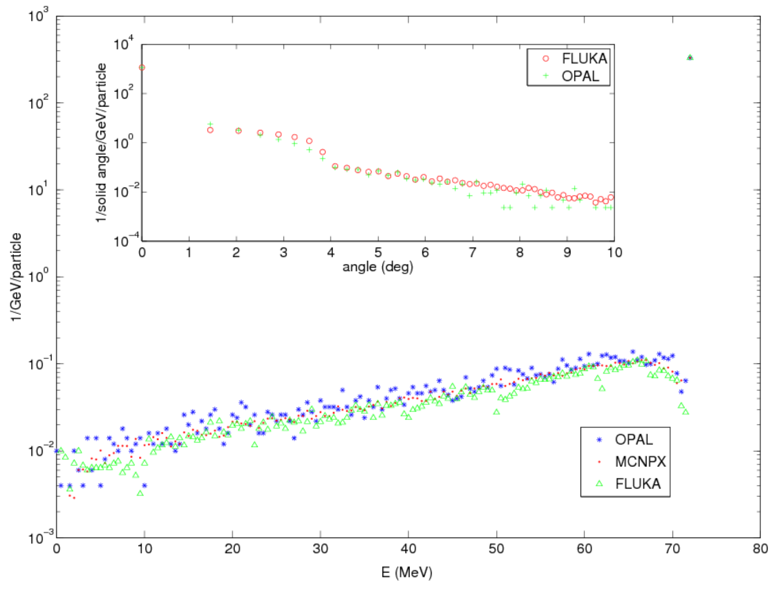

Figure 38: The energy spectrum and scattering angle at z=0.1 m

21.8 References

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Chapter 22

Multi Objective Optimization

Optimization methods deal with finding a feasible set of solutions corresponding to extreme values of some specific criteria. Problems consisting of more than one criterion are called *multi-objective optimization problems*. Multiple objectives arise naturally in many real world optimization problems, such as portfolio optimization, design, planning and many more [73], [74], [75], [76], [77]. It is important to stress that multi-objective problems are in general harder and more expensive to solve than single-objective optimization problems.

In this chapter we introduce multi-objective optimization problems and discuss techniques for their solution with an emphasis on evolutionary algorithms.

Note
For multi-objective optimization *OPAL* uses `opt-pilot` developed by Y. Ineichen. `opt-pilot` has been fully integrated into *OPAL*. Instructions can be found on the `opt-pilot` wiki page.

22.1 Definition

As with single-objective optimization problems, multi-object optimization problems consist of a solution vector and optionally a number of equality and inequality constraints. Formally, a general multi-objective optimization problem has the form

$$\begin{array}{rll} \min & f_m(\mathbf{x}), & m = \{1,\ldots,M\} \\ \text{subject to} & g_j(\mathbf{x}) \geq 0, & j = \{1,\ldots,J\} \\ & -\infty \leq x_i^L \leq \mathbf{x} = x_i \leq x_i^U \leq \infty, & i = \{0,\ldots,n\}. \end{array}$$

The M objectives are minimized, subject to J inequality constraints. An n-vector contains all the design variables with appropriate lower and upper bounds, constraining the design space.

In contrast to single-objective optimization the objective functions span a multi-dimensional space in addition to the design variable space – for each point in design space there exists a point in objective space. The mapping from the n dimensional design space to the M dimensional objective space visualized in Figure 39 is often non-linear. This impedes the search for optimal solutions and increases the computational cost as a result of expensive objective function evaluation. Additionally, depending in which of the two spaces the algorithm uses to determine the next step, it can be difficult to assure an even sampling of both spaces simultaneously.

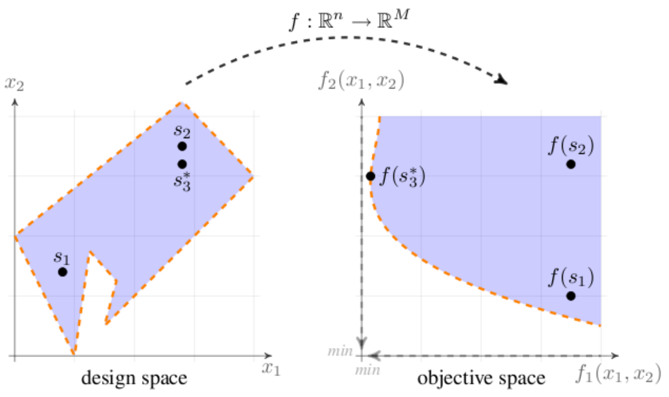

Figure 39: The (often non-linear) mapping $f : \mathbb{R}^n \rightarrow \mathbb{R}^M$ from design to objective space. The dashed lines represent the constraints in design space and the set of solutions (Pareto front) in objective space.

A special subset of multi-objective optimization problems where all objectives and constraints are linear, called *Multi-objective linear programs*, exhibit formidable theoretical properties that facilitate convergence proofs. In this thesis we strive to address arbitrary multi-objective optimization problems with non-linear constraints and objectives. No general convergence proofs are readily available for these cases.

22.2 Pareto Optimality

In most multi-objective optimization problems we have to deal with conflicting objectives. Two objectives are conflicting if they possess different minima. If all the mimima of all objectives coincide the multi-objective optimization problem has only one solution. To facilitate comparing solutions we define a partial ordering relation on candidate solutions based on the concept of dominance. A solution is said to dominate another solution if it is no worse than the other solution in all objectives and if it is strictly better in at least one objective. A more formal description of the dominance relation is given in [78].

The properties of the dominance relation include transitivity

$$x_1 \preceq x_2 \wedge x_2 \preceq x_3 \Rightarrow x_1 \preceq x_3,$$

and asymmetricity, which is necessary for an unambiguous order relation

$$x_1 \preceq x_2 \Rightarrow x_2 \npreceq x_1.$$

Using the concept of dominance, the sought-after set of Pareto optimal solution points can be approximated iteratively as the set of non-dominated solutions.

The problem of deciding if a point truly belongs to the Pareto set is NP-hard. As shown in Figure 40 there exist "weaker" formulations of Pareto optimality. Of special interest is the result shown in [79], where the authors present a polynomial (in the input size of the problem and $1/\varepsilon$) algorithm for finding an approximation, with accuracy ε, of the Pareto set for database queries.

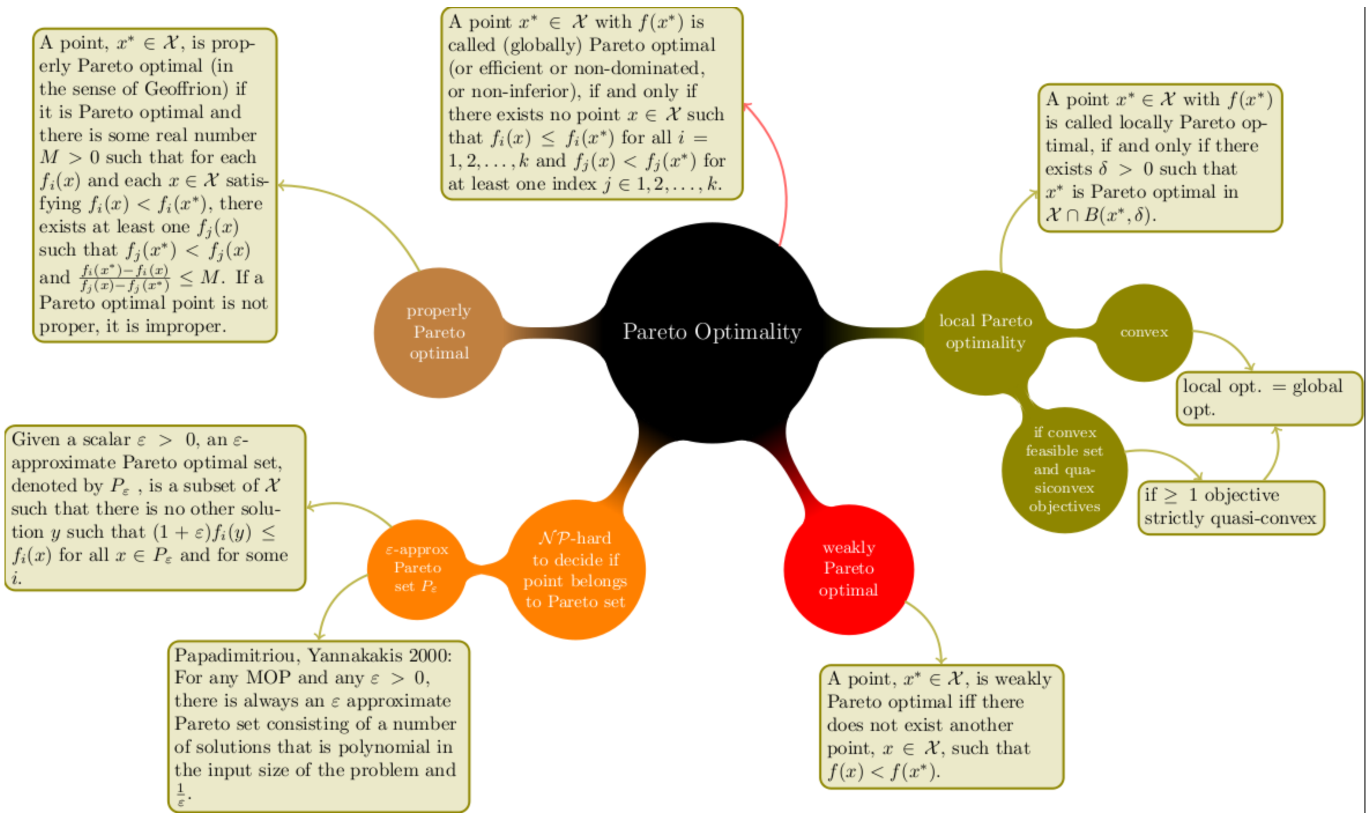
A point $x^* \in \mathcal{X}$ with $f(x^*)$ is called (globally) Pareto optimal (or efficient or non-dominated, or non-inferior), if and only if there exists no point $x \in \mathcal{X}$ such that $f_i(x) \leq f_i(x^*)$ for all $i = 1, 2, \ldots, k$ and $f_j(x) < f_j(x^*)$ for at least one index $j \in 1, 2, \ldots, k$.
A point, $x^* \in \mathcal{X}$, is properly Pareto optimal (in the sense of Geoffrion) if it is Pareto optimal and there is some real number $M > 0$ such that for each $f_i(x)$ and each $x \in \mathcal{X}$ satisfying $f_i(x) < f_i(x^*)$, there exists at least one $f_j(x)$ such that $f_j(x^*) < f_j(x)$ and $\frac{f_i(x^*)-f_i(x)}{f_j(x)-f_j(x^*)} \leq M$. If a Pareto optimal point is not proper, it is improper.
A point $x^* \in \mathcal{X}$ with $f(x^*)$ is called locally Pareto optimal, if and only if there exists $\delta > 0$ such that x^* is Pareto optimal in $\mathcal{X} \cap B(x^*, \delta)$.
properly Pareto optimal
Pareto Optimality
local Pareto optimality
convex
local opt. = global opt.
if convex feasible set and quasiconvex objectives
if ≥ 1 objective strictly quasi-convex
Given a scalar $\varepsilon > 0$, an ε-approximate Pareto optimal set, denoted by P_ε , is a subset of $\mathcal{X}$ such that there is no other solution y such that $(1+\varepsilon)f_i(y) \leq f_i(x)$ for all $x \in P_\varepsilon$ and for some i.
ε-approx Pareto set P_ε
$\mathcal{NP}$-hard to decide if point belongs to Pareto set
weakly Pareto optimal
Papadimitriou, Yannakakis 2000: For any MOP and any $\varepsilon > 0$, there is always an ε approximate Pareto set consisting of a number of solutions that is polynomial in the input size of the problem and $\frac{1}{\varepsilon}$.
A point, $x^* \in \mathcal{X}$, is weakly Pareto optimal iff there does not exist another point, $x \in \mathcal{X}$, such that $f(x) < f(x^*)$.

Figure 40: Various definitions regarding Pareto optimality.

22.3 MOGA Theory

Some links to "What is the tradeoff between population size and the number of generations in genetic algorithms":

1. https://cstheory.stackexchange.com/questions/5156/what-is-the-tradeoff-between-population-size-and-the-number-of-generations in-ge
2. https://www.researchgate.net/post/What_is_the_optimal_recommended_population_size_for_differential_evolution2
3. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=1688360

22.4 Optimiser OPAL Commands

22.4.1 Basic Syntax

One needs to define the design variables, objectives and constraints one by one:

```
d1: DVAR, VARIABLE="x1", LOWERBOUND=-1.0, UPPERBOUND=1.0;
d2: DVAR, VARIABLE="x2", LOWERBOUND=-1.0, UPPERBOUND=1.0;
d3: DVAR, VARIABLE="x3", LOWERBOUND=-1.0, UPPERBOUND=1.0;
```

This defines three design variables named `d1`, `d2` and `d3`. For every variable name e.g. `x1` a corresponding variable with underscores `_x1_` has to exist in the template input file, see also the example input file.

Bounds for design variables should always be given.

```
obj1: OBJECTIVE, EXPR="-statVariableAt('energy', 1.0)";
obj2: OBJECTIVE, EXPR="statVariableAt('emit_x', 1.0)";
```

This defines two objectives named `obj1` and `obj2` maximizing the energy and minimizing the emittance in x-direction. The function `statVariableAt` accecpts as first argument the name of a variable form the `.stat` output file. As second argument it accepts the location where the variable should be evaluated in s-coordinates. The optimiser knows several mathematical functions and methods to access output files (see below).

Note that objectives are always minimised, so in this case a solution where the final energy is maximal and the final horizontal emittance is minimal is looked for.

```
con1: CONSTRAINT, EXPR="statVariableAt('rms_x', 1.0) < 1.0";
con2: CONSTRAINT, EXPR="statVariableAt('numParticles', 1.0) > 1000";
```

This defines two constraints. The syntax is similar to the `OBJECTIVE` syntax.

The first constraint consists of only design variables and will be evaluated before the simulation. The second constraint will be evaluated after the simulation.

22.4.2 OPTIMIZE Command

The `OPTIMIZE` command initiates optimization.

Attribute	**Description**
INPUT	Path to input file.
OUTPUT	Name used in output file generation.
OUTDIR	Name of directory used to store generation output files.
OBJECTIVES	List of objectives to be used.
DVARS	List of optimization variables to be used.
CONSTRAINTS	List of constraints to be used.
INITIALPOPULATION	Size of the initial population.
STARTPOPULATION	A generation file (JSON format) to be started from (optional). In case the number of individuals of the provided file is lower than INITIALPOPULATION, it creates the remaining individuals randomly within the bounds of the DVARS. In case the number of individuals is greater it takes the first INITIALPOPULATION individuals.
NUM_MASTERS	Number of master nodes.
NUM_COWORKERS	Number processors per worker.
DUMP_DAT	Dump old generation data format with frequency, default: false.
DUMP_FREQ	Dump generation data format with frequency, default: 1
DUMP_OFFSPRING	Dump offspring (instead of parent population), default: true.
NUM_IND_GEN	Number of individuals in a generation.
MAXGENERATIONS	Number of generations to run.
EPSILON	Tolerance of hypervolume criteria, default: 0.001.
EXPECTED_HYPERVOL	The reference hypervolume, default: 0.
HYPERVOLREFERENCE	The reference point (real array) for the hypervolume, default: origin.
CONV_HVOL_PROG	Converge if change in hypervolume is smaller, default: 0.
ONE_PILOT_CONVERGE	default: false
SOL_SYNCH	Solution exchange frequency, default: 0.
INITIAL_OPTIMIZATION	Optimize speed of first generation creation (useful when number of infeasible solutions large), default: false
BIRTH_CONTROL	Enforce strict population sizes, default: false. If true, population sizes and generations are strictly as defined by INITIALPOPULATION, NUM_IND_GEN and the classic genetic algorithm. If false, optimisation is done to keep all workers busy at all times. This means that population sizes can be larger (in case INITIAL_OPTIMIZATION is true) and individuals might have been created in a previous generation.
MUTATION_PROBABILITY	Mutation probability of individual, default: 0.5.
MUTATION	Mutation type of an individual (ONEBIT (single gene), INDEPENDENTBIT (default, multiple genes)).
GENE_MUTATION_PROBABILITY	Mutation probability of single gene (used in INDEPENDENTBIT mutation only), default: 0.5.
RECOMBINATION_PROBABILITY	Probability for individuals to combine (crossover), default: 0.5.
CROSSOVER	Method of child generation based on two individuals (BLEND (default), NAIVEONEPOINT, NAIVEUNIFORM or SIMULATEDBINARY)
SIMBIN_CROSSOVER_NU	Simulated binary crossover parameter ν, default: 2.0.
SIMTMPDIR	Directory where simulations are run.
TEMPLATEDIR	Directory where templates are stored.
FIELDMAPDIR	Directory where field maps are stored.
DISTDIR	Directory where distributions are stored (optional).
RESTART_FILE	H5 file to restart the *OPAL* simulations from (optional). Each individual copies the H5 to its simulation directory in order to avoid overwriting of the original file. This attributes is used together with RESTART_STEP.
RESTART_STEP	Restart from given H5 step (optional). Used together with RESTART_FILE.

Table 53: Attributes for the OPTIMIZE command.

22.4.3 DVAR Command

The `DVAR` command defines a variable for optimization.

Attribute	**Description**
`VARIABLE`	Variable name that should be varied during optimization.
`LOWERBOUND`	Lower limit of the range of values that the variable should assume.
`UPPERBOUND`	Upper limit of the range of values that the variable should assume.

Table 54: Attributes for the command `DVAR`.

22.4.4 OBJECTIVE Command

The `OBJECTIVE` command defines an objective for optimization.

Attribute	**Description**
`EXPR`	Expression to minimize during optimization.

Table 55: Attributes for the command `OBJECTIVE`.

22.4.5 CONSTRAINT Command

The `CONSTRAINT` command defines a constraint for optimization.

Attribute	**Description**
`EXPR`	Expression that should be fulfilled during optimization.

Table 56: Attributes for the command `CONSTRAINT`.

22.4.6 Available Expressions

The following expressions are available:

The `EXPR` The optimiser parser knows the following mathematical functions (which are mapped directly to the STL <cmath> functions with the same name):

- `sqrt(x)` : square root of x
- `pow(x,k)` : x to the power k
- `exp(x)` : *e* to the power x
- `log(x)` : natural logarithm of x
- `ceil(x)` : round x upward to the smallest integral value that is not less than x
- `floor(x)` : round x downward to smallest integral value that is not greater than x
- `fabs(x)` : absolute value of x
- `fmod(x,y)`: floating point remainder of x/y
- `sin(x)` : sine of angle x (in radians)
- `asin(x)` : the arcsin of x (return value in radians)

- `cos(x)` : cosine of angle x (in radians)
- `acos(x)` : the arc cosine of x (return value in radians)
- `tan(x)` : tangent of angle x (in radians)
- `atan(x)` : the arc tangent of x (return value in radians)

In addition the optimiser parser has one non-STL function:

- `sq(x)` : square of x

There are several methods to access output data:

Function	Description
fromFile(<file>)	Simple functor that reads vector data from a file. If the file contains more than one value the sum is returned.

sddsVariableAt(<var>, <refpos>, <sdds_file>)
sddsVariableAt(<var>, <refvar>, <refpos>, <sdds_file>)
	A simple expression to get SDDS value near a specific position <refpos> of <refvar> (default: spos) for a variable <var>. If another <refvar> is provided, the values should be monotonically increasing.

statVariableAt(<var>, <refpos>)
statVariableAt(<var>, <refvar>, <refpos>)
	The same as `sddsVariableAt`, uses OPALs statistics file.

sumErrSq(<meas_file>, <var_name>, <sdds_file>)	A simple expression computing the sum of all measurement errors (given as first and third argument) for a variable (second argument) according to $result = \frac{1}{n} * \sqrt{\sum_{i=0}^{n}(measurement_i - value_i)^2}$
radialPeak(<file>, <turn>)	A simple expression to get the n-th peak of a radial probe file..
sumErrSqRadialPeak(<meas_file>, <sim_file>, <begin>, <end>)	A simple expression computing the sum of all peak errors (given as first and second argument) for a range of peaks (third argument and fourth argument) $result = \frac{1}{n} * \sqrt{\sum_{i=start}^{end}(measurement_i - value_i)^2}$
probVariableWithID(<var>, <id>, <probe_file>)	Returns the value of the variable (first argument) with a certain ID (second argument) from probe loss file (third argument).
septum(<probe>)	Returns the minimum bin count between the last and second last turn at the given probe. It uses the *<probe>.hist* and *<probe>.peaks* file (cf. Probe element).

Table 57: Available functions for the `EXPR` attributes for `OBJECTIVE` and `CONSTRAINT`.

22.4.7 Example Input File

Example input file 05-DL_QN3.in for the optimization using the template file tmpl/05-DL_QN3.tmpl:

```
OPTION, ECHO=FALSE;
OPTION, INFO=TRUE;

TITLE, STRING="OPAL Test MAB, 2016-10-13";

REAL up = 0.0000977;
REAL loc = 2.0;

dv0: DVAR, VARIABLE="QDX1_K1", LOWERBOUND=0, UPPERBOUND=35;
dv1: DVAR, VARIABLE="QDX2_K1", LOWERBOUND=0, UPPERBOUND=34;
dv2: DVAR, VARIABLE="QFX1_K1", LOWERBOUND=-35, UPPERBOUND=0;

drmsx:   OBJECTIVE, EXPR="fabs(statVariableAt('rms_x', ${loc}) - ${up})";
drmsy:   OBJECTIVE, EXPR="fabs(statVariableAt('rms_y', ${loc}) - 0.0001833)";
goalfun: OBJECTIVE, EXPR="statVariableAt('rms_x', 2.00)";
```

```
OPTIMIZE, INPUT="tmpl/05-DL_QN3.tmpl", OBJECTIVES = {drmsx, drmsy, goalfun},
          DVARS = {dv0, dv1, dv2}, INITIALPOPULATION=5, MAXGENERATIONS=3,
          NUM_IND_GEN=3, MUTATION_PROBABILITY=0.43,
          NUM_MASTERS=1, NUM_COWORKERS=1, SIMTMPDIR="simtmpdir",
          TEMPLATEDIR="tmpl", FIELDMAPDIR="fieldmaps", OUTPUT="optLinac",
          OUTDIR="results";

QUIT;
```

Template file tmpl/05-DL_QN3.tmpl. Note that the design variables start and end with underscores:

```
OPTION, ECHO=FALSE;
OPTION, INFO=FALSE;
OPTION, PSDUMPFREQ=1000000;
OPTION, STATDUMPFREQ=20;
OPTION, CZERO=TRUE;
OPTION, IDEALIZED=TRUE;
OPTION, VERSION=10900;

TITLE, STRING="OPAL Test MAB, 2016-10-13";

//////////////////////////////
// Begin Content
//////////////////////////////

REAL SOL  = 2.9979246E8;
REAL Pcen = 100.0E6;
REAL BRho = Pcen/SOL;
REAL QK1  = 6.2519;
REAL QSTR = QK1*BRho/2.0;

QDX1: QUADRUPOLE, ELEMEDGE=0.0,  L=0.10, APERTURE="circle(0.1)",
                 K1=_QDX1_K1_ * BRho / 2;
QFX1: QUADRUPOLE, ELEMEDGE=0.91, L=0.20, APERTURE="circle(0.1)",
                 K1=_QFX1_K1_ * BRho / 2;
QDX2: QUADRUPOLE, ELEMEDGE=1.92, L=0.10, APERTURE="circle(0.1)",
                 K1=_QDX2_K1_ * BRho / 2;

FODO: LINE = (QDX1, QFX1, QDX2);

//////////////////////////////
// Begin Summary
//////////////////////////////

FODO_Full: LINE = (FODO), ORIGIN={0,0,0}, ORIENTATION={0.0, 0.0, 0.0};

//////////////////////////////
// End Summary
//////////////////////////////

// SC calculations on:
Fs1:FIELDSOLVER, FSTYPE = FFT, MX = 16, MY = 16, MT = 16,
                  PARFFTX = true, PARFFTY = true, PARFFTT = true,
                  BCFFTX = open, BCFFTY = open, BCFFTT = open,
                  BBOXINCR = 1, GREENSF = INTEGRATED;
Fs2:FIELDSOLVER, FSTYPE = NONE, MX = 16, MY = 16, MT = 16,
                 PARFFTX = true, PARFFTY = true, PARFFTT = true,
                 BCFFTX = open, BCFFTY = open, BCFFTT = open,
                 BBOXINCR = 1, GREENSF = INTEGRATED;
```

```
Dist2: DISTRIBUTION, TYPE="FROMFILE", FNAME="fodo_opal.in";


REAL MINSTEPFORREBIN = 500;

REAL qb=77.0e-12;
REAL bfreq=1300.0E6;
REAL bcurrent=qb*bfreq;

beam1: BEAM, PARTICLE = ELECTRON, pc = P0, NPART = 5000, BFREQ = bfreq,
             BCURRENT = bcurrent, CHARGE = -1;

SELECT, LINE=FODO_Full;

TRACK, LINE=FODO_Full, BEAM=beam1, MAXSTEPS={6e5}, DT={1e-12}, ZSTOP={2.02};

RUN, METHOD = "PARALLEL-T", BEAM = beam1, FIELDSOLVER = Fs2, DISTRIBUTION = Dist2;

ENDTRACK;

QUIT;
```

Run *OPAL* with:

```
mpirun /path/to/opal --info 5 05-DL_QN3.in
```

22.4.8 Output

The solutions for each generation will be saved in either a plain ASCII (if `DUMP_DAT` true) and JSON format. The Pareto front of all individuals is in a JSON file, `ParetoFront_.json`. There are three log files `opt.trace.0`, `opt-progress.0` and `pilot.trace.0` that log the job management. E.g. to count the total number of dispatched simulations:

```
cat opt.trace.0 | grep dispatched | wc -l
```

or to count all invalid simulations:

```
cat opt.trace.0 | grep invalid | wc -l
```

22.5 References

[73] A. Persson et al., *Simulation-based multi-objective optimization of a real-world scheduling problem*, in Proceedings of the 38th conference on Winter Simulation Conference (WSC'06), pp. 1757–1764 (Monterey, CA, USA, 2006).

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[78] K. Deb, *Multi-Objective Optimization Using Evolutionary Algorithms*, Wiley (2009).

[79] C. Papadimitriou and M. Yannakakis, *Multiobjective query optimization*, in Proceedings of the twentieth ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems, pp. 52–59 (Santa Barbara, CA, USA, 2001).

Chapter 23

Sampler

This is a modification of the optimiser. Instead of performing a multi-objective optimisation, it creates samples of the design variables and runs those simulations. This feature can be used for example as training / validation of neural networks or uncertainty quantification (UQ).

23.1 Sampler OPAL Commands

It uses almost the same syntax as the optimiser (see Optimiser OPAL commands).

23.1.1 Basic Syntax

One needs to define the design variables and their sampling method. The syntax for design variables is described in the section DVAR Command.

23.1.2 SAMPLE Command

It allows **random** (`RASTER=FALSE`) and **raster** mode.

Attribute	Description
RASTER	Boolean to choose how the sample spaces for the DVARS are combined, see below, (default: true).
INPUT	Path to input file.
OUTPUT	Name used for the output of the result.
OUTDIR	Name of directory where the simulations are run and the result file is stored.
DVARS	List of design variables to be used.
OBJECTIVES	List of objectives which are evaluated for each simulation. The results are stored to the result file.
SAMPLINGS	List of sample methods to be used.
NUM_MASTERS	Number of master nodes.
NUM_COWORKERS	Number processors per worker.
TEMPLATEDIR	Directory where templates are stored.
FIELDMAPDIR	Directory where field maps are stored.
DISTDIR	Directory where distributions are stored (optional).
KEEP	List of file extensions (e.g. STAT, H5) that shouldn't be deleted. If nothing is specified, all files are kept. If objectives are defined and list is empty all files are deleted.
RESTART_FILE	H5 file to restart the OPAL simulations from (optional). Each individual copies the H5 to its simulation directory in order to avoid overwriting of the original file. This attributes is used together with RESTART_STEP.
RESTART_STEP	Restart from given H5 step (optional). Used together with RESTART_FILE.
JSON_DUMP_FREQ	Defines how often new individuals are appended to the final JSON file i.e. every time JSON_DUMP_FREQ samples finished they are written (default: All individuals are written at the end).

Table 58: Attributes for the command SAMPLE.

The difference between RASTER=TRUE and RASTER=FALSE can be depicted in the following figure.

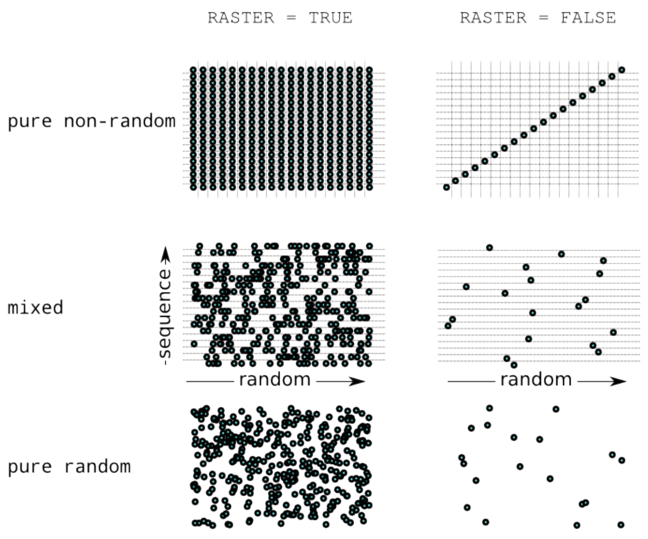


Figure 41: Sampling methods

The two sampling methods differ in the number of samples since with RASTER=TRUE every combination of individual sampling is computed. Thus the total number is $N = N_1 \times N_2 \times \ldots \times N_n$ where n is the number of DVARS. If for some DVAR a random sampling is chosen then for every sampling point a new random number is computed. With RASTER=FALSE the number of sampling points is $N = \min(N_1, N_2, \ldots, N_n)$, each item of a sequence is used only once.

23.1.3 SAMPLING Command

Attribute	Description
VARIABLE	Name of the design variable.
TYPE	Sampling method (see Section 23.1.4).
RANDOM	Boolean to control whether sampling mode is random or sequential. Default is sequential.
SEED	Seed for random sampling (default: 42).
STEP	Increment for randomized sequences (default: 1).
FNAME	File to read the samples from.
N	Number of samples per this design variable. In case of random mode, the minimum value over all design variables is used.

Table 59: Attributes for the command SAMPLING.

23.1.4 Available Sampling Methods

Method	Description
FROMFILE	The samples are provided by a file. A column represents the values of a design variable. The first line is the header reading the variable name. Not all variables need to be provided in the file. This allows also reading variables from different files.
UNIFORM	In sequence mode: Generates an equidistant sequence taking the lower and upper bound of the design variable command as limits. In random mode: Uniform random sampling of floats. It takes the lower and upper bound of the design variable command as limits.
UNIFORM_INT	In sequence mode: Generates an equidistant sequence of integers taking the lower and upper bound of the design variable command as limits. In random mode: Uniform random sampling of integers. It takes the lower and upper bound of the design variable command.
GAUSSIAN	In sequence mode: Generates a sequence with a gaussian distribution taking the difference between upper and lower bound of the design variable as 10 σ. In random mode: Gaussian random sampling of floats. The upper and lower bound are the $\pm 5\,\sigma$ limits of the distribution.
LATIN_HYPERCUBE	In random mode only. Each dimension is discretized into N (i.e. number of samples) equally distant bins. In order to sample a bin in every dimension is randomly selected where the same bin in a dimension occurs only once (exclusive sampling).
RANDOM_SEQUENCE_UNIFORM_INT	In random mode only. Similar to UNIFORM_INT in sequence mode but the values are returned randomly and a value may occur several times or never. Together with the STEP attribute.
RANDOM_SEQUENCE_UNIFORM	In random mode only. Similar to UNIFORM in sequence mode but the values are returned randomly and a value may occur several times or never. Together with the STEP attribute.

Table 60: Available sampling methods.

23.2 Example Input File

```
OPTION, INFO=TRUE;
```

```
// Design variables
nstep:  DVAR, VARIABLE="nstep", LOWERBOUND=10,     UPPERBOUND=40;
MX:     DVAR, VARIABLE="MX",    LOWERBOUND=16,     UPPERBOUND=32;

// Sampling methods
SM1: SAMPLING, VARIABLE="nstep", TYPE="FROMFILE",    FNAME="samples.dat";
SM2: SAMPLING, VARIABLE="MX",    TYPE="UNIFORM_INT", SEED=122, N = 6;

SAMPLE,
    RASTER          = false,
    DVARS           = {nstep, MX},
    SAMPLINGS       = {SM1, SM2},
    INPUT           = "Ring.tmpl",
    OUTPUT          = "RingSample",
    OUTDIR          = "RingSample",
    TEMPLATEDIR     = "template",
    FIELDMAPDIR     = "Fieldmaps",
    NUM_MASTERS     = 1,
    NUM_COWORKERS   = 1;
QUIT;
```

The samples of `nstep` are provided by `samples.dat` that could look like this:

```
MX    nstep
16    10
17    11
18    12
19    13
20    14
21    15
22    16
23    17
24    18
25    19
```

Although the file contains samples for `MX`, too, they are not considered. The corresponding template file `Ring.tmpl` reads:

```
OPTION, ECHO=FALSE;
OPTION, PSDUMPFREQ=100000;
OPTION, SPTDUMPFREQ = 10;
OPTION, PSDUMPEACHTURN=false;
OPTION, REPARTFREQ=20;
OPTION, ECHO=FALSE;
OPTION, STATDUMPFREQ=1;
OPTION, CZERO=FALSE;
OPTION, MEMORYDUMP=TRUE;
OPTION, TELL=TRUE;
OPTION, VERSION=10900;

Title,string="OPAL-cycl: the first turn acceleration in PSI 590MeV Ring";

REAL Edes=.072;
REAL gamma=(Edes+PMASS)/PMASS;
REAL beta=sqrt(1-(1/gamma^2));
REAL gambet=gamma*beta;
REAL P0 = gamma*beta*PMASS;
REAL brho = (PMASS*1.0e9*gambet) / CLIGHT;

//value,{gamma,brho,Edes,beta,gambet};

REAL phi01=139.4281;
REAL phi02=phi01+180.0;
REAL phi04=phi01;
REAL phi05=phi01+180.0;
REAL phi03=phi01+10.0;

REAL volt1st=0.9;
REAL volt3rd=0.9*4.0*0.112;

REAL turns = 1;
REAL nstep=_nstep_;

REAL frequency=50.650;
REAL frequency3=3.0*frequency;

ring: CYCLOTRON, TYPE=RING, CYHARMON=6, PHIINIT=0.0,
  PRINIT=-0.000174, RINIT=2130.0, SYMMETRY=8.0, RFFREQ=frequency,
  FMAPFN="s03av.nar";

rf0: RFCAVITY, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE=SINGLEGAP,
  FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=35.0,  PDIS = 416.0,
  GAPWIDTH = 220.0, PHI0=phi01;

rf1: RFCAVITY, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE=SINGLEGAP,
  FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=125.0, PDIS = 416.0,
  GAPWIDTH = 220.0, PHI0=phi02;

rf2: RFCAVITY, VOLT=volt3rd, FMAPFN="Cav3.dat", TYPE=SINGLEGAP,
  FREQ=frequency3,RMIN = 1900.0, RMAX = 4500.0, ANGLE=170.0, PDIS = 452.0,
  GAPWIDTH = 250.0, PHI0=phi03;

rf3: RFCAVITY, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE=SINGLEGAP,
  FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=215.0, PDIS = 416.0,
  GAPWIDTH = 220.0, PHI0=phi04;

rf4: RFCAVITY, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE=SINGLEGAP,
  FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=305.0, PDIS = 416.0,
  GAPWIDTH = 220.0, PHI0=phi05;

l1: LINE = (ring,rf0,rf1,rf2,rf3,rf4);

Dist1: DISTRIBUTION, TYPE=gauss,
  sigmax = 2.0e-03,
  sigmapx = 1.0e-7,
  corrx = 0.0,
  sigmay = 2.0e-03,
  sigmapy = 1.0e-7,
  corry = 0.0,
  sigmat = 2.0e-03,
  sigmapt = 3.394e-4,
  corrt=0.0;

Fs1: FIELDSOLVER, FSTYPE=FFT, MX=_MX_, MY=16, MT=16,
   PARFFTX=true, PARFFTY=true, PARFFTT=true,
   BCFFTX=open, BCFFTY=open, BCFFTT=open, BBOXINCR=2;

beam1: BEAM, PARTICLE=PROTON, PC=P0, NPART=8192, BCURRENT=1.0E-3, CHARGE=1.0,
             BFREQ= frequency;

SELECT, LINE=l1;

TRACK, LINE=l1, BEAM=beam1, MAXSTEPS=nstep*turns, STEPSPERTURN=360, TIMEINTEGRATOR=RK4;
RUN, METHOD="CYCLOTRON-T", BEAM=beam1, FIELDSOLVER=Fs1, DISTRIBUTION=Dist1;
```

```
ENDTRACK;
STOP;
```

Appendix A

OPAL Language Syntax

Words in *italic font* are syntactic entities, and characters in `monospaced font` must be entered as shown. Comments are given in **bold font**.

A.1 Statements

comment	:	`//` *anything-except-newline*
	|	`/*` *anything-except* `*/` `*/`
identifier	:	`[a-zA-Z][a-zA-Z0-9-]`
integer	:	`[0-9]+`
string	:	`'` *anything-except-single-quote* `'`
	|	`"` anything-except-double-quote `"`
command	:	*keyword attribute-list*
	|	*label* `:` *keyword attribute-list*
keyword	:	*identifier*
label	:	*identifier*
attribute-list	:	*empty*
	|	*attribute-list* `,` *attribute*
attribute	:	*attribute-name* **// only for logical attribute**
	|	*attribute-name* `=` *attribute-value* **// expression evaluated**
	|	*attribute-name* `:=` *attribute-value* **// expression retained**
attribute-name	:	*identifier*
attribute-value	:	*string-expression*
	|	*logical-expression*
	|	*real-expression*
	|	*array-expression*
	|	*constraint*
	|	*variable-reference*
	|	*place*
	|	*range*
	|	*token-list*
	|	*token-list-array*
	|	*regular-expression*

A.2 Real expressions

real-expression	:	*real-term*
	|	+ *real-term*
	|	− *real-term*
	|	*real-expression* + *real-term*
	|	*real-expression* − *real-term*
real-term	:	*real-factor*
	|	*real-term* * *real-factor*
	|	*real-term* / *real-factor*
real-factor	:	*real-primary*
	|	*real-factor* ^ *real-primary*
real-primary	:	*real-literal*
	|	*symbolic-constant*
	|	#
	|	*real-name*
	|	*array* [*index*]
	|	*object-name* → *real-attribute*
	|	*object-name* → *array-attribute* [*index*]
	|	*table-reference*
	|	*real-function* ()
	|	*real-function* (*real-expression*)
	|	*real-function* (*real-expression* , *real-expression*)
	|	*function-of-array* (*array-expression*)
	|	(*real-expression*)
real-function	:	`RANF`
	|	`GAUSS`
	|	`ABS`
	|	`TRUNC`
	|	`ROUND`
	|	`FLOOR`
	|	`CEIL`
	|	`SIGN`
	|	`SQRT`
	|	`LOG`
	|	`EXP`
	|	`SIN`
	|	`COS`
	|	`ABS`
	|	`TAN`
	|	`ASIN`
	|	`ACOS`
	|	`ATAN`
	|	`ATAN2`
	|	`MAX`
	|	`MIN`
	|	`MOD`
	|	`POW`
function-of-array	:	`VMIN`
	|	`VMAX`
	|	`VRMS`
	|	`VABSMAX`

A.3 Real variables and constants:

real-prefix	:	empty
	|	`REAL`

	|	REAL CONST
	|	CONST
real-definition	:	*real-prefix real-name = real-expression*
		// expression evaluated
	|	*real-prefix real-name* := *real-expression*
		// expression retained
symbolic-constant	:	PI
	|	TWOPI
	|	DEGRAD
	|	RADDEG
	|	E
	|	EMASS
	|	PMASS
	|	HMMASS
	|	UMASS
	|	CMASS
	|	MMASS
	|	DMASS
	|	XEMASS
	|	CLIGHT
	|	*real-name*
real-name	:	*identifier*
object-name	:	*identifier*
table-name	:	*identifier*
column-name	:	*identifier*

A.4 Logical expressions:

logical-expression	:	*and-expression*
	|	*logical-expression* || *and-expression*
and-expression	:	*relation*
	|	*and-expression* && *relation*
relation	:	*logical-name*
	|	TRUE
	|	FALSE
	|	*real-expression relation-operator real-expression*
logical-name	:	*identifier*
relation-operator	:	==
	|	!=
	|	<
	|	>
	|	>=
	|	⇐

A.5 Logical variables:

logical-prefix	:	BOOL
	|	BOOL CONST
logical-definition	:	*logical-prefix logical-name = logical-expression*
		// expression evaluated
	|	*logical-prefix logical-name* `:=` *logical-expression*
		// expression retained

A.6 String expressions:

string-expression	:	*string*
	|	*identifier* **// taken as a string**
	|	*string-expression* & *string*

A.7 String constants:

string-prefix	:	`STRING`
string-definition	:	*string-prefix string-name* = *string-expression* **// expression evaluated**
	|	*string-prefix string-name* := *string-expression* **// expression retained**

A.8 Real array expressions:

array-expression	:	*array-term*
	|	+ *array-term*
	|	− *array-term*
	|	*array-expression* + *array-term*
	|	*array-expression* − *array-term*
array-term	:	*array-factor*
	|	*array-term* ⋆ *array-factor*
	|	*array-term* / *array-factor*
array-factor	:	*array-primary*
	|	*array-factor* ^ *array-primary*
array-primary	:	{ *array-literal* }
	|	*array-reference*
	|	*real-function* (*array-expression*)
	|	(*array-expression*)
array-literal	:	*real-expression*
	|	*array-literal* , *real expression*
array-reference	:	*array-name*
	|	*object-name* → *array-attribute*
array-name	:	*identifier*

A.9 Real array definitions:

array-prefix	:	`REAL VECTOR`
array-definition	:	*array-prefix array-name* = *array-expression*
	|	*array-prefix array-name* := *array-expression*

A.10 Constraints:

constraint	:	*array-expression constraint-operator array-expression*
constraint-operator	:	==
	|	<
	|	>

A.11 Variable references:

variable-reference	:	*real-name*
	|	*object-name* → *attribute-name*

A.12 Token lists:

token-list	:	*anything-except-comma*
token-list-array	:	*token-list*
	|	*token-list-array* `,` *token-list*

A.13 Regular expressions:

regular-expression	:	"*`UNIX-regular-expression`*"

Appendix B

OPAL-t Field Maps

B.1 Introduction

In this chapter details of the different types of field maps in *OPAL-t* are presented. *OPAL-t* can use many different types of field maps input in several different file formats. What types of maps are supported and in what format has tended to be a function mostly of what developers have needed, and to a lesser extent what users have asked for. The list below shows all field maps that are currently supported and also field maps that are not yet supported, but on the list of things to do when we get a chance.

B.2 Comments in Field Maps

The possibility to add comments (almost) everywhere in field map files is common to all field maps. Comments are initiated by a # and contain the rest of a line. Comments are accepted at the beginning of the file, between the lines and at the end of a line. If in the following sections two values are shown on one line then they have to be on the same line. They should not be separated by a comment and, consequently, be on different lines. Three examples of valid comments:

```
# This is valid a comment
1DMagnetoStatic 40 # This is another valid comment
-60.0 60.0 9999
  # and this is also a valid comment
0.0 2.0 199
```

The following examples will break the parsing of the field maps:

```
1DMagnetoStatic # This is an invalid comment
40
-60.0 60.0 # This is another invalid comment # 9999
0.0 2.0 199
```

B.3 Normalization

All field maps that are in ASCII are normalized with the maximum absolute value of the longitudinal field on the axis. The only exceptions is the type 1DProfile1. This behavior can be disabled by adding `FALSE` at the end of the first line of the field map.

B.4 Field Map Warnings and Errors

If *OPAL-t* encounters an error while parsing a field map it disables the corresponding element, outputs a warning message and continues the simulation. The following messages may be output:

```
************ W A R N I N G ***********************************
THERE SEEMS TO BE SOMETHING WRONG WITH YOUR FIELD MAP file.t7.
There are only 10003 lines in the file, expecting more.
Please check the section about field maps in the user manual.
**************************************************************
```

In this example there is something wrong with the number of grid spacings provided in the header of the file. Make sure that you provide the number of grid **spacings** and not the number of grid **points**! The two numbers always differ by 1.

```
************ W A R N I N G ***********************************
THERE SEEMS TO BE SOMETHING WRONG WITH YOUR FIELD MAP file.t7.
There are too many lines in the file, expecting only 10003 lines.
Please check the section about field maps in the user manual.
**************************************************************
```

Again there seems to be something wrong with the number of grid spacings provided in the header. In this example *OPAL-t* found more lines than it expected. Note that comments and empty lines at the end of a file are ignored such that **they don't cause** this warning.

```
************ W A R N I N G ***********************************
THERE SEEMS TO BE SOMETHING WRONG WITH YOUR FIELD MAP file.t7.
_error_msg_
expecting: '_expecting_' on line 3,
found instead: '_found_'.
**************************************************************
```

Where "*error_msg*" is either

`Didn't find enough values!`	If *OPAL-t* expects more values on this line.
`Found more values than expected!`	If *OPAL-t* expects less values on this line.
`Found wrong type of values!`	If *OPAL-t* found e.g. characters instead of an integer number.

"*expecting*" is replaced by the types of values *OPAL-t* expects on the line. E.g. it could be replaced by `double double int`. Finally "*found*" is replaced by the actual content of the line without any comment possibly following the values. If line 3 of a file consists of `-60.0 60.0 # This is an other invalid comment # 9999` *OPAL-t* will output `-60.0 60.0`.

```
************** W A R N I N G *********************************
DISABLING FIELD MAP file.t7 SINCE FILE COULDN'T BE FOUND!
**************************************************************
```

This warning could be issued if the file name is mistyped or otherwise if the file couldn't be read.

```
************ W A R N I N G **********************************
THERE SEEMS TO BE SOMETHING WRONG WITH YOUR FIELDMAP file.t7.
Could not determine the file type.
Please check the section about field maps in the user manual.
*************************************************************
```

In this case *OPAL-t* didn't recognize the string of characters which identify the type of field map stored in the file.

For one-dimensional field maps an other warning may be issued:

```
* ************ W A R N I N G ***************************************************
* IT SEEMS THAT YOU USE TOO FEW FOURIER COMPONENTS TO SUFFICIENTLY WELL        *
* RESOLVE THE FIELD MAP 'file.T7'.                                             *
* PLEASE INCREASE THE NUMBER OF FOURIER COMPONENTS!                            *
* The ratio (f_i - F_i)^2 / F_i^2 is 0.019685 and                              *
* the ratio (max_i(|f_i - F_i|) / max_i(|F_i|) is 0.019023.                    *
* Here F_i is the field as in the field map and f_i is the reconstructed       *
* field.                                                                       *
* The lower limit for the two ratios is 1e-2                                   *
* ******************************************************************************
```

This warning is issued when the low pass filter that is applied to the field sampling uses too few Fourier coefficients. In this case increase the number of Fourier coefficients, see the next section for details. The relevant criteria are that

$$\frac{\sum_{i=1}^{N}(F_{z,i}-\tilde{F}_{z,i})^2}{\sum_{i=1}^{N}F_{z,i}^2} \leq 0.01,$$

and

$$\frac{\max_i |F_{z,i}-\tilde{F}_{z,i}|}{\max_i |F_{z,i}|} \leq 0.01,$$

where F_{z_i} is the field sampling as in the file and $\tilde{F}_{z,i}$ is the one-dimensional field reconstructed from the result received after applying the low pass filter.

B.5 Types and Format

Field maps in *OPAL-t* come in three basic types:

1. 2D or 3D field map. For this type of map, a field is specified on a grid and linear interpolation is used to find field values at intermediate points.
2. 1D on axis field map. For this type of map, one on-axis field profile is specified. *OPAL-t* calculates a Fourier series from this profile and then uses the first, second and third derivatives of the series to compute the off-axis field values. (This type of field is very smooth numerically, but can be inaccurate far from the field axis.) Only a few (user specified) terms from the Fourier series are used.
3. Enge function [80] field map. This type of field map uses Enge functions to describe the fringe fields of a magnet. Currently, this is only used for `RBEND` and `SBEND` elements see RBend (OPAL-t) and SBend (OPAL-t).

It is important to note that in all cases, the input field map will be normalized so that the peak field magnitude value on axis is equal to either 1 MV/m in the case of electric field maps (static or dynamic), or 1 T in the case of magnetic field maps. (The sign of the values from the field map are preserved.) Therefore, the field multiplier for the map in your simulation will be the peak field value on axis in those respective units.

Depending on the field map type, *OPAL-t* uses different length units (either cm or meters). This is due to the origin programs of the field maps used (e.g. Poisson/Superfish [81] uses cm). So be careful.

There are no required field extensions for any *OPAL-t* field map (e.g. .T7, .dat etc.). *OPAL-t* determines the type of field map by a string descriptor which is the first element on the first line of the file. Below we list the possible descriptors. (Note that we list all of the descriptors/field map types that we plan to eventually implement. Not all of them are, which is indicated in the description.)

1DElectroStatic 1D electrostatic field map. 1D field maps are described by the on-axis field. ***Not implemented yet***. A work around is to use a 1DDynamic field map with a very low frequency.

1DMagnetoStatic 1D magnetostatic field map. See Section B.8.

AstraMagnetoStatic 1D magnetostatic field map with possibly non-equidistant sampling. This file type is compatible with ASTRA field maps with small changes. See Section B.9.

1DDynamic 1D dynamic electromagnetic field map. See Section B.10.

AstraDynamic 1D dynamic electromagnetic field map with possibly non-equidistant sampling. This file type is compatible with ASTRA field maps with small changes. See Section B.11.

1DProfile1 This type of field map specifies the Enge functions (see [80]) for the entrance and exit fringe fields of a magnet. Currently this type of field map is only used by `RBEND` and `SBEND` elements see RBend (OPAL-t) and SBend (OPAL-t). See Section B.12.

2DElectroStatic 2D electrostatic field map. 2D field maps are described by the electromagnetic field in one half-plane. See Section B.13.

2DMagnetoStatic 2D magnetostatic field map. Other than this descriptor at the head of the file, the format for this field map type is identical to the T7 file format as produced by Poisson [81]. See Section B.14.

2DDynamic 2D dynamic electromagnetic field map. Other than this descriptor at the head of the file, the format for this field map type is identical to the T7 field format as produced by Superfish [81]. See Section B.15.

3DElectroStatic 3D electrostatic field map. ***Not implemented yet***.

3DMagnetoStatic 3D magnetostatic field map, see Section B.16.

3DMagnetoStatic_Extended 2D magnetostatic field map of field on mid-plane that *OPAL* extends to 3D.

3DDynamic 3D dynamic electromagnetic field map. See Section B.18.

We will give examples and descriptions of each of the implemented field map types in the sections below.

B.6 Field Map Orientation

In the case of 2D and 3D field maps an additional string has to be provided describing the orientation of the field map.

For 2D field maps this can either be

XZ if the primary direction is in z direction and the secondary in r direction.

ZX if the primary direction is in r direction and the secondary in z direction.

For 3D field maps this can be

XYZ if the primary direction is in z direction, the secondary in y direction and the tertiary in x direction

Each line after the header corresponds to a grid point of the field map. This point can be referred to by two indices in the case of a 2D field map and three indices in the case of a 3D field map, respectively. Each column describes either E_z, E_r, B_z, B_r or H_ϕ in the 2D case and E_x ,E_y ,E_z, B_x, B_y, B_z in the 3D case.

By primary, secondary and tertiary direction is meant the following (see also Figure 42):

- The index of the primary direction increases the fastest, the index of the tertiary direction the slowest.
- The order of the columns is accordingly: if the z direction in an 2D electrostatic field map is the primary direction then E_z is on the first column, E_r on the second. For all other cases it's analogous.
- For the 2D dynamic case in XZ orientation there are four columns: E_z, E_r, $|E|$ (unused) and H_ϕ in that order. In the other orientations the first and the second columns are interchanged ,but the third and fourth columns are unchanged.

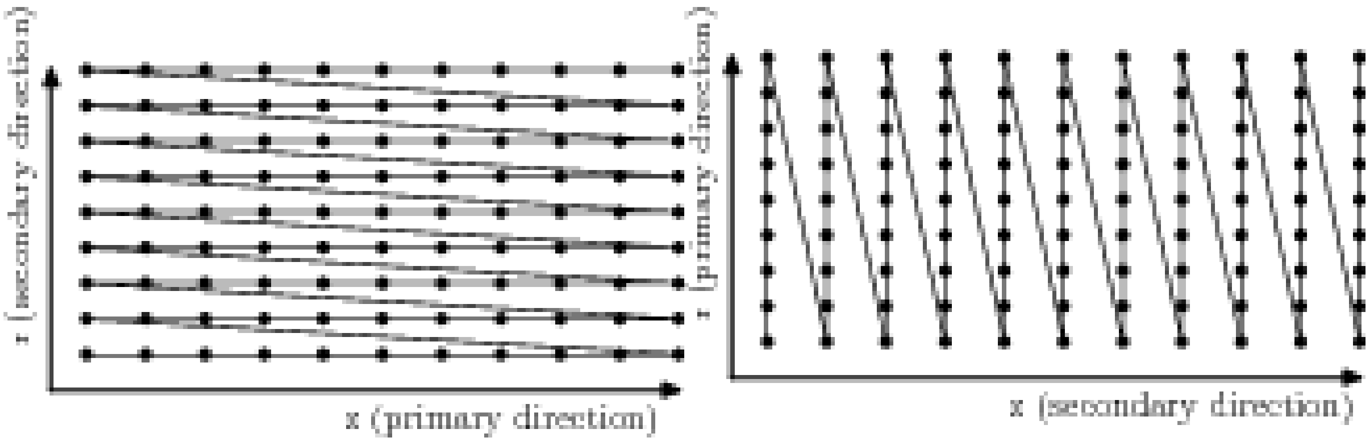


Figure 42: Ordering of points for 2D field maps in T7 files (left XZ orientation, right ZX orientation)

B.7 FAST Attribute for 1D Field Maps

For some 1D field maps, there exists a Boolean attribute, `FAST`, which can be used to speed up the calculation. When set to true (`FAST = TRUE`), *OPAL-t* will generate a 2D internal field map and then use bi-linear interpolation to calculate field values during the simulation, rather than the generally slower Fourier coefficient technique. The caution here is that this can introduce unwanted numerical noise if you set the grid spacing too coarse for the 2D map.

As a general warning: be wise when you choose the type of field map to be used! Figure 43 shows three pictures of the longitudinal phase space after three gun simulations using different types of field maps. In the first picture we used a 1DDynamic field map see Section B.10 resulting in a smooth longitudinal distribution. In the middle picture we set the `FAST` attribute to true, resulting in some fine structure in the phase space due to the bi-linear interpolation of the internally generated 2D field map. Finally, in the last figure, we generated directly a 2D field map from Superfish [81]. Here we could observe two different structures: first the fine structure, stemming from the bi-linear interpolation, and secondly a much stronger structure of unknown origin, but presumably due to errors in the Superfish [81] interpolation algorithm.

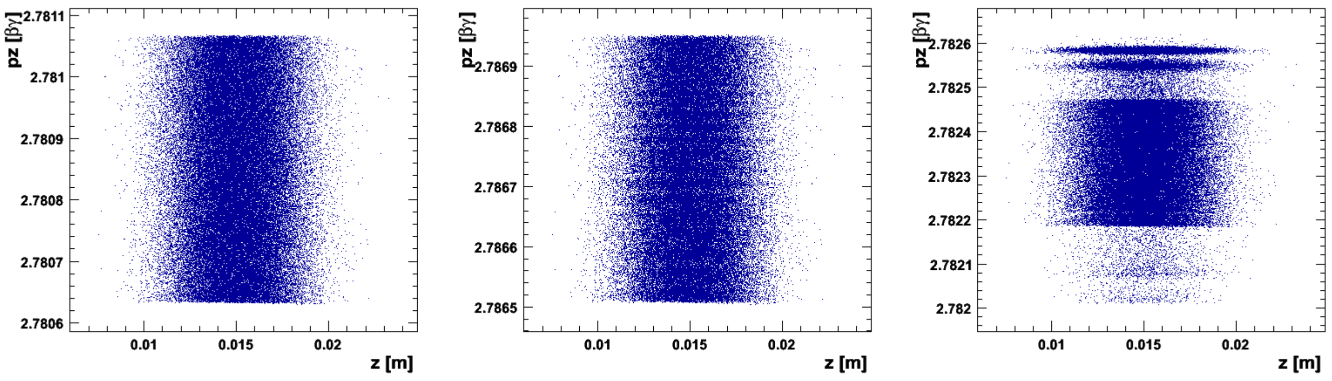


Figure 43: The longitudinal phase space after a gun simulation using a 1D field map (on-axis field) of the gun, a 1D field map (on-axis field) of the gun in combination with the `FAST` switch, and a 2D field map of the gun generated by Superfish.

B.8 1DMagnetoStatic

```
1DMagnetoStatic 40
-60.0 60.0 9999
  0.0  2.0 199
  0.00000e+00
  4.36222e-06
  8.83270e-06
  + 9'994 lines
  1.32490e-05
  1.73710e-05
  2.18598e-05
```

A 1D field map describing a magnetostatic field using 10000 grid points (9999 grid spacings) in the longitudinal direction. The field is non-negligible from -60.0 cm to +60.0 cm relative to `ELEMEDGE` in the longitudinal direction. From the 10000 field values, 5000 complex Fourier coefficients are calculated. However, only 40 are kept when calculating field values during a simulation. *OPAL-t* normalizes the field values internally such that $\max(|B_{\text{on axis}}|) = 1.0\text{T}$. If the `FAST` attribute is set to true in the input deck, a 2D field map is generated internally with 200 values in the radial direction, from 0 cm to 2 cm, for each longitudinal grid point.

1DMagnetoStatic	$N_{Fourier}$	TRUE | FALSE (optional)
z_{start} (in cm)	z_{end} (in cm)	N_z
r_{start} (in cm)	r_{end} (in cm)	N_r
$B_{z,1}$ (T)		
$B_{z,2}$ (T)		
.		
.		
.		
B_{z,N_z+1} (T)		

Table 61: Layout of a `1DMagnetoStatic` field map file.

A `1DMagnetoStatic` field map has the general form shown in Table 61. The first three lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`1DMagnetoStatic`) and how many Fourier coefficients to keep ($N_{Fourier}$) when doing field calculations.

Line 2 This tells gives the extent of the field map (from z_{start} to z_{end}) relative to the `ELEMEDGE` of the field map, and how many grid spacings there are in the field map.

Line 3 If one sets `FAST = TRUE` for the field map, this tells *OPAL-t* the radial extent of the internally generated 2D field map. Otherwise this line is ignored. (Although it must always be present.)

The lines following the header give the 1D field map grid values from 1 to $N_z + 1$. From these, $N_z/2$ complex Fourier coefficients are calculated, of which only $N_{Fourier}$ are used when finding field values during the simulation.

B.9 AstraMagnetostatic

```
AstraMagnetostatic 40
  -3.0000000e-01   0.0000000e+00
  -2.9800000e-01   2.9075045e-05
  -2.9600000e-01   5.9367702e-05
  -2.9400000e-01   9.0866460e-05
  -2.9200000e-01   1.2374798e-04
  -2.9000000e-01   1.5799850e-04
...
```

```
  2.9000000e-01   1.5799850e-04
  2.9200000e-01   1.2374798e-04
  2.9400000e-01   9.0866460e-05
  2.9600000e-01   5.9367702e-05
  2.9800000e-01   2.9075045e-05
  3.0000000e-01   0.0000000e+00
```

A 1D field map describing a magnetostatic field using N non-equidistant grid points in the longitudinal direction. From these values N equidistant field values are computed from which in turn $N/2$ complex Fourier coefficients are calculated. In this example only 40 Fourier coefficients are kept when calculating field values during a simulation. The z-position of each field sampling is in the first column (in meters), the corresponding longitudinal on-axis magnetic field amplitude is in the second column. As with the 1DMagnetoStatic see Section B.8 field maps, *OPAL-t* normalizes the field values to $\max(|B_{\text{on axis}}|) = 1.0$T. In the header only the first line is needed since the information on the longitudinal dimension is contained in the first column of the data. (*OPAL-t* does not provide a `FAST` version of this map type.)

AstraDynamic	$N_{Fourier}$	TRUE | FALSE (optional)
z_1 (in meters)	$B_{z,1}$ (T)	
z_2 (in meters)	$B_{z,s}$ (T)	
.		
.		
.		
z_N (in meters)	$B_{z,N}$ (T)	

Table 62: Layout of an `AstraMagnetoStatic` field map file.

An `AstraMagnetoStatic` field map has the general form shown in Table 62. The first line forms the file header and tells *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`AstraMagnetoStatic`) and how many Fourier coefficients to keep ($N_{Fourier}$) when doing field calculations.

The lines following the header gives N non-equidistant field values and their corresponding z positions (relative to `ELEMEDGE`). From these, *OPAL-t* will use cubic spline interpolation to find N equidistant field values within the range defined by the z positions. From these equidistant field values, $N/2$ complex Fourier coefficients are calculated, of which only $N_{Fourier}$ are used when finding field values during the simulation.

B.10 1DDynamic

```
1DDynamic 40
-3.0 57.0 4999
1498.953425154
0.0 2.0 199
  0.00000e+00
  4.36222e-06
  8.83270e-06
  + 4'994 lines
  1.32490e-05
  1.73710e-05
  2.18598e-05
```

A 1D field map describing a dynamic field using 5000 grid points (4999 grid spacings) in the longitudinal direction. The field is non-negligible from -3.0 cm to 57.0 cm relative to `ELEMEDGE` in the longitudinal direction. The field frequency is 1498.953425154MHz. From the 5000 field values, 2500 complex Fourier coefficients are calculated. However, only 40 are kept when calculating field values during the simulation. *OPAL-t* normalizes the field values internally such that $\max(|E_{onaxis}|) =$

$1\mathrm{MV/m}$. If the FAST switch is set to true in the input deck, a 2D field map is generated internally with 200 values in the radial direction, from 0.0 cm to 2.0 cm, for each longitudinal grid point.

1DDynamic	$N_{Fourier}$	TRUE | FALSE (optional)
z_{start} (in cm)	z_{end} (in cm)	N_z
$Frequency$ (in MHz)		
r_{start} (in cm)	r_{end} (in cm)	N_r
$E_{z,1}$ (MV/m)		
$E_{z,2}$ (MV/m)		
.		
.		
.		
E_{z,N_z+1} (MV/m)		

Table 63: Layout of a 1DDynamic field map file.

A 1DDynamic field map has the general form shown in Table 63. The first four lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (1DDynamic) and how many Fourier coefficients to keep ($N_{Fourier}$) when doing field calculations.

Line 2 This tells gives the extent of the field map (from z_{start} to z_{end}) relative to the ELEMEDGE of the field map, and how many grid spacings there are in the field map.

Line 3 Field frequency.

Line 4 If one sets FAST = TRUE for the field map, this tells *OPAL-t* the radial extent of the internally generated 2D field map. Otherwise this line is ignored. (Although it must always be present.)

The lines following the header give the 1D field map grid values from 1 to $N_z + 1$. From these, $N_z/2$ complex Fourier coefficients are calculated, of which only $N_{Fourier}$ are used when finding field values during the simulation.

B.11 AstraDynamic

```
AstraDynamic 40
2997.924
   0.0000000e+00   0.0000000e+00
   5.0007941e-04   2.8090000e-04
   9.9991114e-04   5.6553000e-04
   1.4996762e-03   8.4103000e-04
   ...
   1.9741957e-01   1.4295000e-03
   1.9792448e-01   1.1306000e-03
   1.9841987e-01   8.4103000e-04
   1.9891525e-01   5.6553000e-04
   1.9942016e-01   2.8090000e-04
   1.9991554e-01   0.0000000e+00
```

A 1D field map describing a dynamic field using N non-equidistant grid points in longitudinal direction. From these N non-equidistant field values N equidistant field values are computed from which in turn $N/2$ complex Fourier coefficients are calculated. In this example only 40 Fourier coefficients are kept when calculating field values during the simulation. The z-position of each sampling is in the first column (in meters), the corresponding longitudinal on-axis electric field amplitude is in the second column. *OPAL-t* normalizes the field values such that $\max(|E_{\text{on axis}}|) = 1\mathrm{MV/m}$. The frequency of this field is 2997.924MHz. (*OPAL-t* does not provide a FAST version of this map type.)

AstraMagnetoStatic	$N_{Fourier}$	TRUE | FALSE (optional)
Frequency (in MHz)		
z_1 (in meters)	$E_{z,1}$ (MV/m)	
z_2 (in meters)	$E_{z,s}$ (MV/m)	
.		
.		
.		
z_N (in meters)	$E_{z,N}$ (MV/m)	

Table 64: Layout of an `AstraDynamic` field map file.

An `AstraDynamic` field map has the general form shown in Table 64. The first line forms the file header and tells *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`AstraDynamic`) and how many Fourier coefficients to keep ($N_{Fourier}$) when doing field calculations.

Line 2 Field frequency.

The lines following the header gives N non-equidistant field values and their corresponding z positions (relative to `ELEMEDGE`). From these, *OPAL-t* will use cubic spline interpolation to find N equidistant field values within the range defined by the z positions. From these equidistant field values, $N/2$ complex Fourier coefficients are calculated, of which only $N_{Fourier}$ are used when finding field values during the simulation.

B.12 1DProfile1

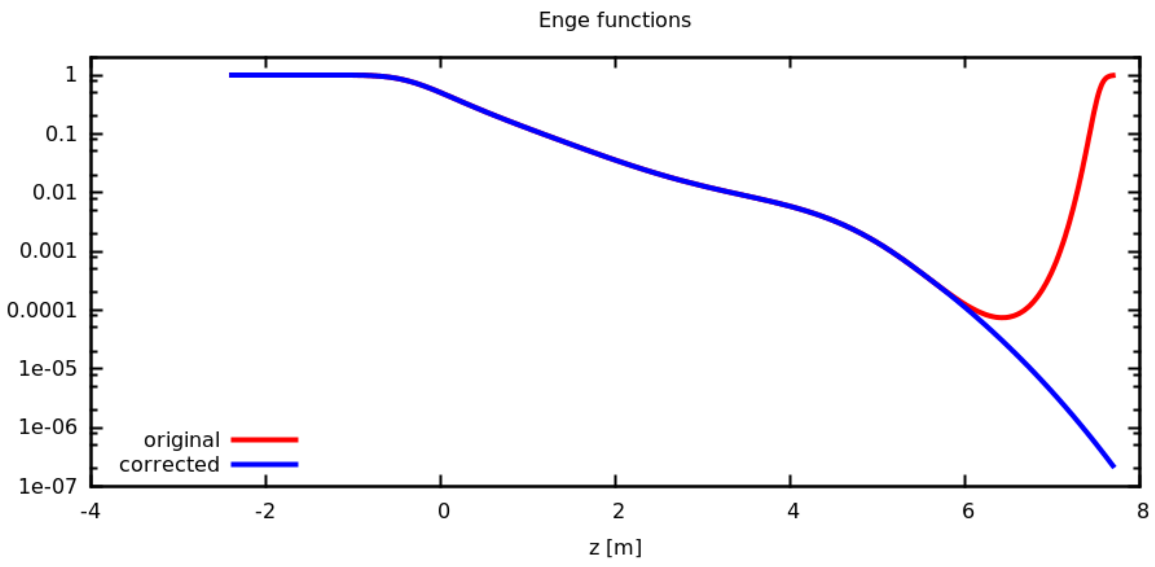
A `1DProfile1` field map is used to define Enge functions [80] that describe the fringe fields for the entrance and exit of a magnet:

$$F(z) = \frac{1}{1 + e^{\sum_{n=0}^{N_{order}} c_n (z/D)^n}}$$

where D is the full gap of the magnet, N_{order} is the Enge function order and z is the distance from the Enge function origin perpendicular to the edge of the magnet. The constants, c_n, and the Enge function origin are fitted parameters chosen to best represent the fringe field of the magnet being modeled.

A `1DProfile1` field map describes two Enge functions: one for the magnet entrance and one for the magnet exit. An illustration of this is shown in Figure 45. In the top part of the figure we see a plot of the relative magnet field strength along the mid-plane for a rectangular dipole magnet. To describe this field with a `1DProfile1` field map, an Enge function is fit to the entrance fringe field between *zbegin_entry* and *zend_entry* in the figure, using the indicated entrance origin. Likewise, an Enge function is fit to the exit fringe field between *zbegin_exit* and *zend_exit* using the indicated exit origin. The parameters for these two Enge functions are subsequently entered into a `1DProfile1` field map, as described below.

When selecting the Enge coefficients, care must be taken to ensure that the polynomial degree is odd and that the coefficient for the highest degree is positive. This ensures that the value of the function inside the dipole is 1 and converges to 0 far outside the dipole. If these two conditions are not met, then the value of the function increases again from some point onwards. In the Figure Figure 44 the effect of a negative coefficient for the highest degree in the original data is shown. To improve the fieldmap it was chosen some point from which on the polynomial was replaced by a polynomial of the same degree but all coefficients except for the highest order and the constant value are zero. The two remaining coefficients were chosen such that the values of the two polynomials and their derivatives are equal at the connection.



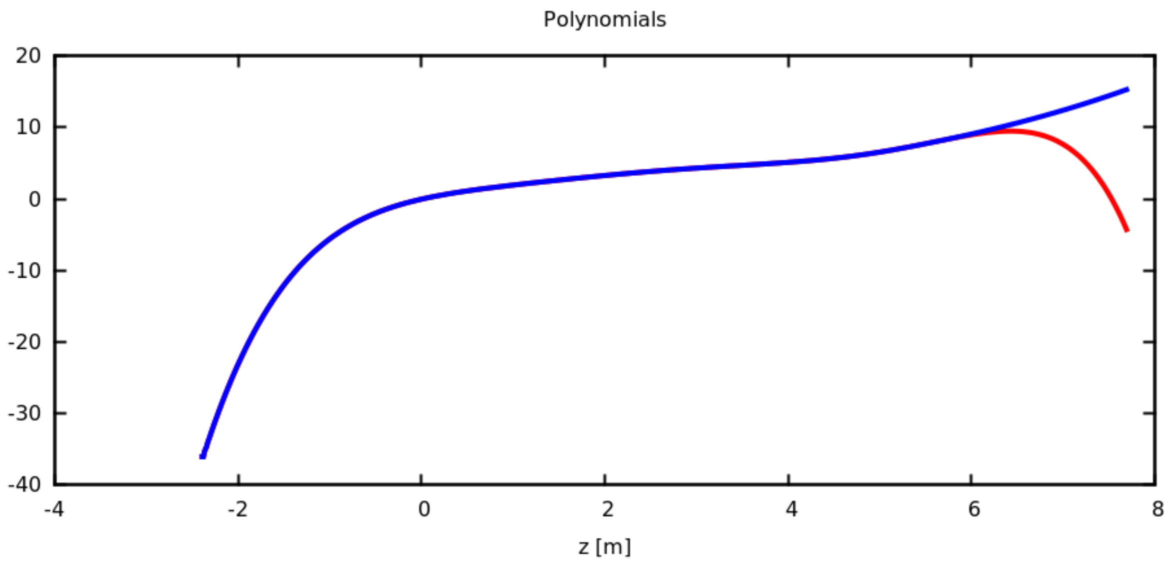


Figure 44: Effect of a negative coefficient for the highest degree in the original data.

Currently, `1DProfile1` field maps are only implemented for `RBEND` and `SBEND` elements sees RBend (OPAL-t), SBend (OPAL-t) and Bend Fields from 1D Field Maps (OPAL-t).

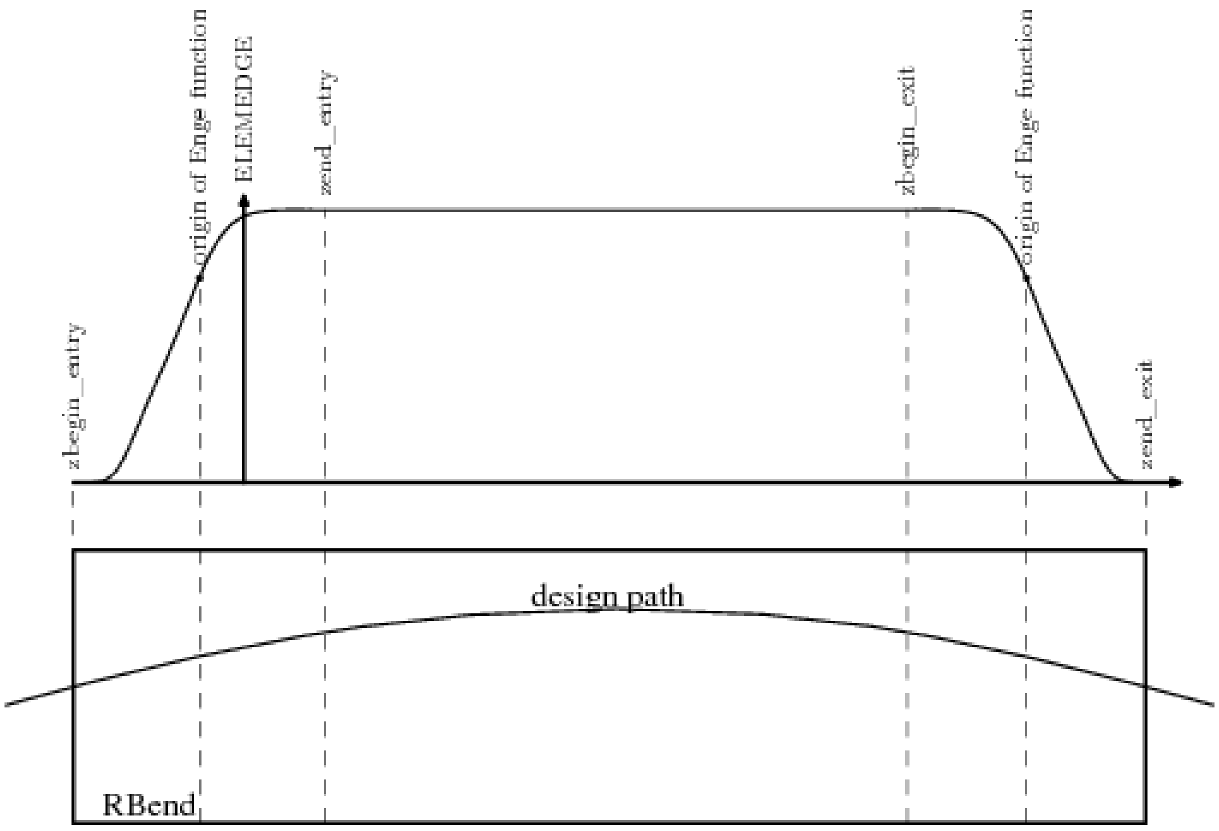


Figure 45: Example of Enge functions describing the entrance and exit fringe fields of a rectangular bend magnet. The top part of the figure shows the relative field strength on the mid-plane. The bottom part of the figure shows an example of a particle trajectory through the magnet. Note that the magnet field is naturally divided into three regions: entrance fringe field, central field, and exit fringe field.

A `1DProfile1` field map has the general form shown in Table 65. The first three lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`1DProfile1`), the Enge coefficient order for the entrance fringe fields ($N_{Enge Entrance}$), the Enge coefficient order for the exit fringe fields ($N_{Enge Exit}$), and the gap of the magnet.

Line 2 The first three values on the second line are used to define the extent of the fringe fields for the entrance region of the magnet. This can be done two different ways as will be described below see Section B.12.1 and Section B.12.2. The fourth value on line 2 is not currently used (but must still be present).

Line 3 The first three values on the third line are used to define the extent of the fringe fields for the exit region of the magnet. This can be done two different ways as will be described below see Section B.12.1 and Section B.12.2. The fourth value on line 3 is not currently used (but must still be present).

The lines following the three header lines give the entrance region Enge coefficients from c_0 to $c_{N_{Enge Entrance}}$, followed by the exit region Enge coefficients from c_0 to $c_{N_{Enge Exit}}$.

There are two types of `1DProfile1` field map files: `1DProfile Type 1` and `1DProfile1 Type 2`. The difference between the two is a small change in how the entrance and exit fringe field regions are described. This will be explained in Section B.12.1 and Section B.12.2.

1DProfile1	$N_{Enge Entrance}$	$N_{Enge Exit}$	*Gap* (in cm)
Entrance Parameter 1 (in cm)	Entrance Parameter 2 (in cm)	Entrance Parameter 3	Place Holder
Exit Parameter 1 (in cm)	Exit Parameter 2 (in cm)	Exit Parameter 3	Place Holder
$c_{0\,Entrance}$			
$c_{1\,Entrance}$			
.			
.			
.			
$c_{N_{Enge Entrance}}$			
$c_{0\,Exit}$			
$c_{1\,Exit}$			
.			
.			
.			
$c_{N_{Enge Exit}}$			

Table 65: Layout of a `1DProfile1` field map file.

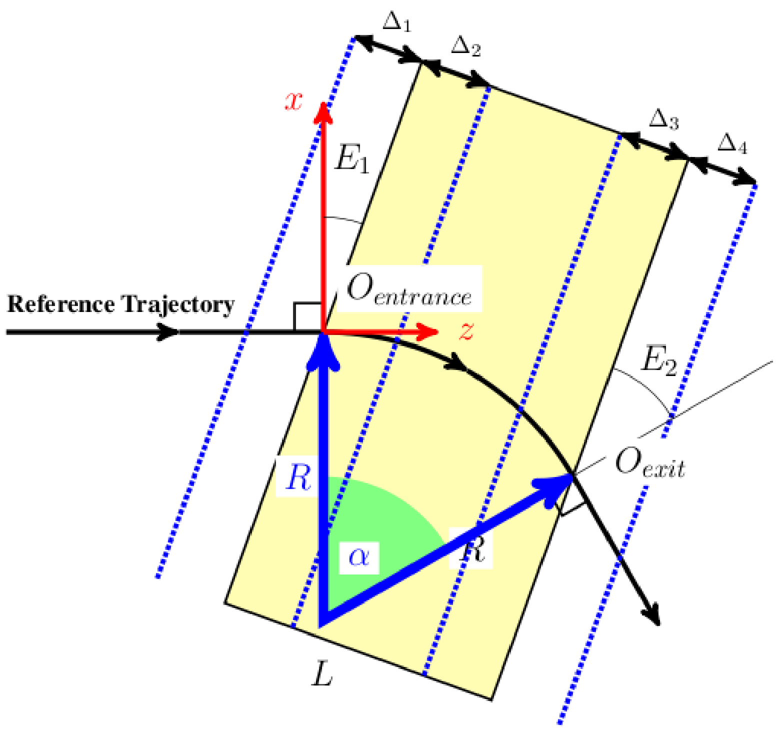


Figure 46: Illustration of a rectangular bend (`RBEND`, see RBend (OPAL-t) showing the entrance and exit fringe field regions. Δ_1 is the perpendicular distance in front of the entrance edge of the magnet where the magnet fringe fields are non-negligible. Δ_2 is the perpendicular distance behind the entrance edge of the magnet where the entrance Enge function stops being used to calculate the magnet field. The reference trajectory entrance point is indicated by $O_{entrance}$. Δ_3 is the perpendicular distance in front of the exit edge of the magnet where the exit Enge function starts being used to calculate the magnet field. (In the region between Δ_2 and Δ_3 the field of the magnet is a constant value.) Δ_4 is the perpendicular distance after the exit edge of the magnet where the magnet fringe fields are non-negligible. The reference trajectory exit point is indicated by O_{exit}

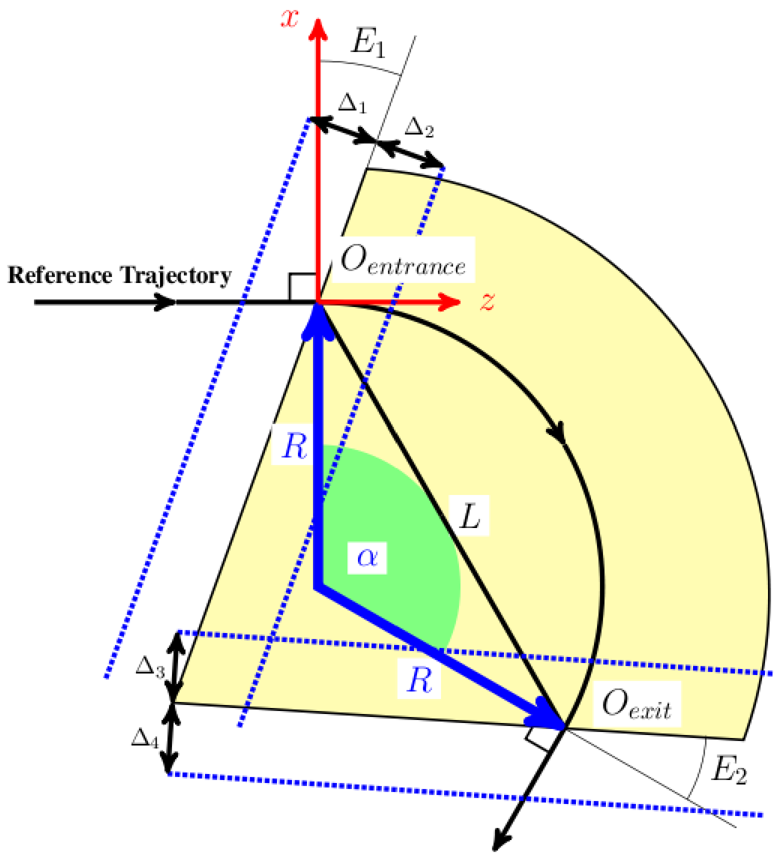


Figure 47: Illustration of a sector bend (`SBEND`, see SBend (OPAL-t)) showing the entrance and exit fringe field regions. Δ_1 is the perpendicular distance in front of the entrance edge of the magnet where the magnet fringe fields are non-negligible. Δ_2 is the perpendicular distance behind the entrance edge of the magnet where the entrance Enge function stops being used to calculate the magnet field. The reference trajectory entrance point is indicated by $O_{entrance}$. Δ_3 is the perpendicular distance in front of the exit edge of the magnet where the exit Enge function starts being used to calculate the magnet field. (In the region between Δ_2 and Δ_3 the field of the magnet is a constant value.) Δ_4 is the perpendicular distance after the exit edge of the magnet where the magnet fringe fields are non-negligible. The reference trajectory exit point is indicated by O_{exit}.

B.12.1 1DProfile1 Type 1 for Bend Magnet

A `1DProfile1 Type 1` field map is the same `1DProfile1` field map found in versions of *OPAL* previous to *OPAL* *OPAL*version1.2.0 . Figure 46 and Figure 47 illustrate the fringe field regions for an `RBEND` and an `SBEND` element. Referring to the general field map file shown in Table 65, the values on lines 2 and 3 are given by:

$$
\begin{aligned}
Entrance\,Parameter\,1 &= Entrance\,Parameter\,2 - \Delta_1 \\
Entrance\,Parameter\,3 &= Entrance\,Parameter\,2 + \Delta_2 \\
Exit\,Parameter\,2 &= L - Entrance\,Parameter\,2 \\
Exit\,Parameter\,1 &= Exit\,Parameter\,2 - \Delta_3 \\
Exit\,Parameter\,3 &= Exit\,Parameter\,2 + \Delta_4
\end{aligned}
$$

The value of $Entrance\,Parameter\,2$ can be any value. *OPAL* only cares about the relative differences between parameters. Also note that, internally, the origins of the entrance and exit Enge functions correspond to the reference trajectory entrance and exit points see Figure 46 and Figure 47.

Internally, *OPAL* reads in a `1DProfile Type 1` map and uses the provided parameters to calculate the values of:

$$L = Exit\,Parameter\,2 - Entrance\,Parameter\,2$$
$$\Delta_1 = Entrance\,Parameter\,2 - Entrance\,Parameter\,1$$
$$\Delta_2 = Entrance\,Parameter\,3 - Entrance\,Parameter\,2$$
$$\Delta_3 = Exit\,Parameter\,2 - Exit\,Parameter\,1$$
$$\Delta_4 = Exit\,Parameter\,3 - Exit\,Parameter\,2$$

These values, combined with the entrance fringe field Enge coefficients c_0 through $c_{N_{Enge_Entrance}}$ and exit fringe field Enge coefficients c_0 through $c_{N_{Enge_Exit}}$, allow *OPAL* to find field values anywhere within the magnet. (Again, note that a `1DProfile Type 1` map always places the entrance Enge function origin at the entrance point of the reference trajectory and the exit Enge function origin at the exit point of the reference trajectory.)

```
1DProfile1 6 7 3.0
-6.0 -2.0 2.0  1000
24.0 28.0 32.0 0
  0.00000e+00
  4.36222e-06
  8.83270e-06
  + 9 lines
  1.32490e-05
  1.73710e-05
  2.18598e-05
```

A 1D field map describing the fringe field of an element using 7 Enge coefficients for the entrance fringe field and 8 Enge coefficients for the exit fringe field (polynomial order 6 and 7 respectively). The element has a gap height of 3.0 cm, and a length of 30.0 cm. The entrance fringe field is non-negligible from 4.0 cm in front of the magnet's entrance edge and reaches the core strength at 4.0 cm behind the entrance edge of the magnet. (The entrance edge position is given by the element's `ELEMEDGE` attribute.) The exit fringe field region begins 4.0 cm in front of the exit edge of the magnet and is non-negligible 4.0 cm after the exit edge of the magnet. The value 1000 at the end of line 2 and 0 at the end of line 3 do not have any meaning.

B.12.2 1DProfile1 Type 2 for Bend Magnet

The `1DProfile1 Type 2` field map file format was introduced in *OPAL OPAL*version1.2.0 to allow for more flexibility when defining the Enge functions for the entrance and exit fringe fields. Specifically, a `1DProfile1 Type 2` map does not contain any information about the length of the magnet. Instead, that value is set using the element's `L` attribute. In turn, this allows us the freedom to make slight changes to how the parameters on lines 2 and 3 of the field map file shown in Table 65 are defined. Now

$$Entrance\,Parameter\,2 = \perp \text{ distance of entrance Enge function origin from magnet entrance edge}$$
$$Exit\,Parameter\,2 = \perp \text{ distance of exit Enge function origin from magnet exit edge}$$

The other parameters are defined the same as before:

$$Entrance\,Parameter\,1 = Entrance\,Parameter\,2 - \Delta_1$$
$$Entrance\,Parameter\,3 = Entrance\,Parameter\,2 + \Delta_2$$
$$Exit\,Parameter\,1 = Exit\,Parameter\,2 - \Delta_3$$
$$Exit\,Parameter\,3 = Exit\,Parameter\,2 + \Delta_4$$

As before, internally, *OPAL* reads in a `1DProfile Type 2` map and uses the provided parameters to calculate the values of:

$$\Delta_1 = Entrance\,Parameter\,2 - Entrance\,Parameter\,1$$
$$\Delta_2 = Entrance\,Parameter\,3 - Entrance\,Parameter\,2$$
$$\Delta_3 = Exit\,Parameter\,2 - Exit\,Parameter\,1$$
$$\Delta_4 = Exit\,Parameter\,3 - Exit\,Parameter\,2$$

These values, combined with the length of the magnet, `L` (set by the element attribute) and the entrance fringe field Enge coefficients c_0 through $c_{N_{Enge_Entrance}}$ and exit fringe field Enge coefficients c_0 through $c_{N_{Enge_Exit}}$, allow *OPAL* to find field values anywhere within the magnet.

The `1DProfile1 Type 2` field map file format has two main advantages:

1. The Enge function origins can be adjusted to more accurately model a magnet's fringe fields as they are no longer fixed to the entrance and exit points of the reference trajectory.
2. Two magnets with the same fringe fields, but different lengths, can be modeled with a single `1DProfile Type 2` field map file rather than two separate files.

```
1DProfile1 6 7 3.0
-6.0 -2.0 2.0 0
-2.0  2.0 6.0 0
  0.00000e+00
  4.36222e-06
  8.83270e-06
  + 9 lines
  1.32490e-05
  1.73710e-05
  2.18598e-05
```

A 1D field map describing the fringe field of an element using 7 Enge coefficients for the entrance fringe field and 8 Enge coefficients for the exit fringe field (polynomial order 6 and 7 respectively). The element has a gap height of 3.0 cm. The entrance fringe field is non-negligible from 4.0 cm in front of the magnet's entrance edge and reaches the core strength at 4.0 cm behind the entrance edge of the magnet. The exit fringe field region begins 4.0 cm in front of the exit edge of the magnet and is non-negligible 4.0 cm after the exit edge of the magnet. The value 0 at the end of line 2 and 0 at the end of line 3 do not have any meaning. The entrance Enge function origin is 2.0 cm in front (upstream) of the magnet's entrance edge. The exit Enge function origin is 2.0 cm behind (downstream of) the exit edge of the magnet.

B.13 2DElectroStatic

```
2DElectroStatic XZ
-3.0 51.0 4999
0.0 2.0 199
  0.00000e+00  0.00000e+00
  4.36222e-06  0.00000e+00
  8.83270e-06  0.00000e+00
  + 999994 lines
  1.32490e-05  0.00000e+00
  1.73710e-05  0.00000e+00
  2.18598e-05  0.00000e+00
```

A 2D field map describing an electrostatic field using 5000 grid points in the longitudinal direction times 200 grid points in the radial direction. The field between the grid points is calculated using bi-linear interpolation. The field is non-negligible from -3.0 cm to 51.0 cm relative to `ELEMEDGE` and the 200 grid points in the radial direction span the distance from 0.0 cm to 2.0 cm. The field values are ordered in XZ orientation, so the index in the longitudinal direction changes fastest and therefore E_z values are stored in the first column and E_r values in the second see Section B.6. *OPAL-t* normalizes the field so that $\max(|E_{z,\text{ on axis}}|) = 1\text{MV/m}$.

2DElectroStatic	Orientation (XZ or ZX)	TRUE | FALSE (optional)
z_{start} (or r_{start}) (in cm)	z_{end} (or r_{end}) (in cm)	N_z (or N_r)
r_{start} (or z_{start}) (in cm)	r_{end} (or z_{end}) (in cm)	N_r (or N_z)
$E_{z,1}$ (or $E_{r,1}$) (MV/m)	$E_{r,1}$ (or $E_{z,1}$) (MV/m)	
$E_{z,2}$ (or $E_{r,2}$) (MV/m)	$E_{r,2}$ (or $E_{z,2}$) (MV/m)	
.		
.		
.		
$E_{z,N}$ (or $E_{r,N}$) (MV/m)	$E_{r,N}$ (or $E_{z,N}$) (MV/m)	

Table 66: Layout of a `2DElectroStatic` field map file.

A `2DElectroStatic` field map has the general form shown in Table 66. The first three lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`2DElectroStatic`) and the field orientation see Section B.6.

Line 2 This gives the extent of the field map and how many grid spacings there are in the fastest changing index direction see Section B.6.

Line 3 This gives the extent of the field map and how many grid spacings there are in the slowest changing index direction (see Section B.6.

The lines following the header give the 2D field map grid values from 1 to $N = (N_z + 1) \times (N_r + 1)$. The order of these depend on the field orientation see Section B.6 and can be one of two formats:

If Orientation = XZ E_z (MV/m) E_r (MV/m)

If Orientation = ZX E_r (MV/m) E_z (MV/m)

B.14 2DMagnetoStatic

```
2DMagnetoStatic ZX
0.0 2.0 199
-3.0 51.0 4999
  0.00000e+00  0.00000e+00
  0.00000e+00  4.36222e-06
  0.00000e+00  8.83270e-06
  + 999994 lines
  0.00000e+00  1.32490e-05
  0.00000e+00  1.73710e-05
  0.00000e+00  2.18598e-05
```

A 2D field map describing a magnetostatic field using 5000 grid points in the longitudinal direction times 200 grid points in the radial direction. The field between the grid points is calculated using bi-linear interpolation. The field is non-negligible from -3.0 cm to 51.0 cm relative to `ELEMEDGE` and the 200 grid points in the radial direction span the distance from 0.0 cm to 2.0 cm. The field values are ordered in the ZX orientation, so the index in the radial direction changes fastest and therefore B_r values are stored in the first column and B_z values in the second see Section B.6. *OPAL-t* normalizes the field so that $\max(|B_{z,\text{ on axis}}|) = 1T$.

2DMagnetoStatic	Orientation (XZ or ZX)	TRUE | FALSE (optional)
z_{start} (or r_{start}) (in cm)	z_{end} (or r_{end}) (in cm)	N_z (or N_r)
r_{start} (or z_{start}) (in cm)	r_{end} (or z_{end}) (in cm)	N_r (or N_z)
$B_{z,1}$ (or $B_{r,1}$) (T)	$B_{r,1}$ (or $B_{z,1}$) (T)	
$B_{z,2}$ (or $B_{r,2}$) (T)	$B_{r,2}$ (or $B_{z,2}$) (T)	
.		
.		
.		
$B_{z,N}$ (or $B_{r,N}$) (T)	$B_{r,N}$ (or $B_{z,N}$) (T)	

Table 67: Layout of a `2DMagnetoStatic` field map file.

A `2MagnetoStatic` field map has the general form shown in Table 67. The first three lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`2DMagnetoStatic`) and the field orientation see Section B.6.

Line 2 This gives the extent of the field map and how many grid spacings there are in the fastest changing index direction see Section B.6.

Line 3 This gives the extent of the field map and how many grid spacings there are in the slowest changing index direction (see Section B.6.

The lines following the header give the 2D field map grid values from 1 to $N = (N_z + 1) \times (N_r + 1)$. The order of these depend on the field orientation see Section B.6 and can be one of two formats:

If Orientation = XZ B_z (T) B_r (T)

If Orientation = ZX B_r (T) B_z (T)

B.15 2DDynamic

```
2DDynamic XZ
-3.0 51.0 4121
1498.953425154
0.0 1.0 75
  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00
  4.36222e-06  0.00000e+00  0.00000e+00  4.36222e-06
  8.83270e-06  0.00000e+00  0.00000e+00  8.83270e-06
  + 313266 lines
  1.32490e-05  0.00000e+00  0.00000e+00  1.32490e-05
  1.73710e-05  0.00000e+00  0.00000e+00  1.73710e-05
  2.18598e-05  0.00000e+00  0.00000e+00  2.18598e-05
```

A 2D field map describing a dynamic field oscillating with a frequency of 1498.953425154MHz. The field map provides 4122 grid points in the longitudinal direction times 76 grid points in radial direction. The field between the grid points is calculated with a bi-linear interpolation. The field is non-negligible between -3.0 cm and 51.0 cm relative to `ELEMEDGE` and the 76 grid points in radial direction span the distance from 0.0 cm to 1.0 cm. The field values are ordered in the XZ orientation, so the index in the longitudinal direction changes fastest and therefore E_z values are stored in the first column and E_r values in the second. The third column contains the electric field magnitude, $|E|$, and is not used (but must still be included). The fourth column is H_ϕ in A/m. The third and fourth columns are always the same and do not depend on the field orientation see Section B.6. *OPAL-t* normalizes the field so that $\max(|E_{z,\text{ on axis}}|) = 1\text{MV}/\text{m}$.

2DDynamic	Orientation (XZ or ZX)	TRUE | FALSE (optional)	
z_{start} (or r_{start}) (in cm)	z_{end} (or r_{end}) (in cm)	N_z (or N_r)	
Frequency (in MHz)			
r_{start} (or z_{start}) (in cm)	r_{end} (or z_{end}) (in cm)	N_r (or N_z)	
$E_{z,1}$ (or $E_{r,1}$) (MV/m))	$E_{r,1}$ (or $E_{z,1}$) (MV/m)	$\|E_1\|$ (MV/m)	$H_{\phi,1}$ (A/m)
$E_{z,2}$ (or $E_{r,2}$) (MV/m))	$E_{r,2}$ (or $E_{z,2}$) (MV/m)	$\|E_2\|$ (MV/m)	$H_{\phi,2}$ (A/m)
.			
.			
.			
$E_{z,N}$ (or $E_{r,N}$) (MV/m))	$E_{r,N}$ (or $E_{z,N}$) (MV/m)	latexmath:[$	E_N

Table 68: Layout of a `2DDynamic` field map file.

A `2DDynamic` field map has the general form shown in Table 68. The first four lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`2DDynamic`) and the field orientation see Section B.6.

Line 2 This gives the extent of the field map and how many grid spacings there are in the fastest changing index direction see Section B.6.

Line 3 Field frequency.

Line 4 This gives the extent of the field map and how many grid spacings there are in the slowest changing index direction see Section B.6.

The lines following the header give the 2D field map grid values from 1 to $N = (N_z + 1) \times (N_r + 1)$. The order of these depend on the field orientation see Section B.6 and can be one of two formats:

If Orientation = XZ E_z (MV/m) E_r (MV/m) $|E|$ (MV/m) H_ϕ (A/m)

If Orientation = ZX E_r (MV/m) E_z (MV/m) $|E|$ (MV/m) H_ϕ (A/m)

The third item (the field magnitude) on each data line is not used by *OPAL-t*, but must be there.

B.16 3DMagnetoStatic

```
3DMagnetoStatic
-1.5 1.5 227
-1.0 1.0 151
-3.0 51.0 4121
0.00e+00 0.00e+00 0.00e+00
0.00e+00 4.36e-06 0.00e+00
0.00e+00 8.83e-06 0.00e+00
+ 142'852'026 lines
0.00e+00 1.32e-05 0.00e+00
0.00e+00 1.73e-05 0.00e+00
0.00e+00 2.18e-05 0.00e+00
```

A 3D field map describing a magnetostatic field. The field map provides 4122 grid points in z-direction times 228 grid points in x-direction and 152 grid points in y-direction. The field between the grid points is calculated with a tri-linear interpolation. The field is non-negligible between -3.0 cm to 51.0 cm relative to `ELEMEDGE`, the 228 grid points in x-direction range from -1.5 cm to 1.5 cm and the 152 grid points in y-direction range from -1.0 cm to 1.0 cm relative to the design path. The field values are ordered such that the index in z-direction changes fastest, then the index in y-direction while the index in x-direction changes slowest. The columns correspond to B_x, B_y and B_z.

3DMagnetoStatic	TRUE | FALSE (optional)	
x_{start} (in cm)	x_{end} (in cm)	N_x
y_{start} (in cm)	y_{end} (in cm)	N_y
z_{start} (in cm)	z_{end} (in cm)	N_z
$B_{x,1}$ (A/m)	$B_{y,1}$ (A/m)	$B_{z,1}$ (A/m)
$B_{x,2}$ (A/m)	$B_{y,2}$ (A/m)	$B_{z,2}$ (A/m)
.		
.		
.		
$B_{x,N}$ (A/m)	$B_{y,N}$ (A/m)	$B_{z,N}$ (A/m)

Table 69: Layout of a `3DMagnetoStatic` field map file.

A `3DMagnetoStatic` field map has the general form shown in Table 69. The first five lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`3DMagnetoStatic`).

Line 3 This gives the extent of the field map and how many grid spacings there are in the slowest changing index direction.

Line 4 This gives the extent of the field map and how many grid spacings there are in the next fastest changing index direction.

Line 5 This gives the extent of the field map and how many grid spacings there are in the fastest changing index direction.

The lines following the header give the 3D field map grid values from 1 to $N = (N_z + 1) \times (N_y + 1) \times (N_x + 1)$.

B.17 3DMagnetoStatic_Extended

```
3DMagnetoStatic_Extended
-9.9254 9.9254 133
-2.0 1.0 15
-22.425 47.425 465
 -8.10970000e-05
 -8.38540000e-05
 -8.64960000e-05
+ 62'438 lines
 -8.64960000e-05
 -8.38540000e-05
 -8.10970000e-05
```

A 3D field map describing a magnetostatic field on the mid-plane. The field map provides 466 grid points in z-direction times 134 grid points in x-direction. The field is non-negligible between -22.425 cm to 47.425 cm relative to `ELEMEDGE`, the 134 grid points in x-direction range from -9.9254cm to 9.9254cm. The field should be integrated using Maxwell's equations from the mid-plane to 2.0 cm using 16 grid points. The mid-plane is regarded as a perfect magnetic conductor (PMC) i.e. the magnetic field on the mid-plane has no tangential component. This leads to a symmetry where the perpendicular component is mirrored whereas the tangential component is anti-parallel. Instead of integrating the field from the mid-plane to -2.0 cm and 1.0 cm we only integrate it to +2.0 cm and store only the upper half of the field map. For positions $R(x,\,-y,\,z)$ with $y > 0.0$ the correct field can then be derived from the $R(x,\,y,\,z)$.

	TRUE | FALSE (optional)	
x_{start} (in cm)	x_{end} (in cm)	N_x
y_{start} (in cm)	y_{end} (in cm)	N_y
z_{start} (in cm)	z_{end} (in cm)	N_z
$B_{y,1}$ (T)		
$B_{y,2}$ (T)		
.		
.		
.		
$B_{y,N}$ (T)		

Table 70: Layout of a `3DMagnetoStatic_Extended` field map file.

A `3DMagnetoStatic_Extended` field map has the general form shown in Table 70. The first four lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`3DMagnetoStatic_Extended`).

Line 2 This gives the extent of the field map and how many grid spacings there are in the slowest changing direction.

Line 3 This gives the extent of the field map and how many grid spacings there are in the next fastest changing direction.

Line 4 This gives the extent of the field map and how many grid spacings there are in the fastest changing direction.

The lines following the header give the 3D field map grid values from 1 to $N = (N_z + 1) \times (N_x + 1)$. The order of these depend on the field orientation see Section B.6 and can currently only be the format shown in Table 70.

B.18 3DDynamic

```
3DDynamic
1498.9534
-1.5 1.5 227
```

```
-1.0 1.0 151
-3.0 51.0 4121
0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00 0.00e+00
4.36e-06 0.00e+00 4.36e-06 0.00e+00 4.36e-06 0.00e+00
8.83e-06 0.00e+00 8.83e-06 0.00e+00 8.83e-06 0.00e+00
+ 142'852'026 lines
1.32e-05 0.00e+00 1.32e-05 0.00e+00 1.32e-05 0.00e+00
1.73e-05 0.00e+00 1.73e-05 0.00e+00 1.73e-05 0.00e+00
2.18e-05 0.00e+00 2.18e-05 0.00e+00 2.18e-05 0.00e+00
```

A 3D field map describing a dynamic field oscillating with 1.4989534. The field map provides 4122 grid points in z-direction times 228 grid points in x-direction and 152 grid points in y-direction. The field between the grid points is calculated with a tri-linear interpolation. The field is non-negligible between -3.0 cm to 51.0 cm relative to `ELEMEDGE`, the 228 grid points in x-direction range from -1.5 cm to 1.5 cm and the 152 grid points in y-direction range from -1.0 cm to 1.0 cm relative to the design path. The field values are ordered such that the index in z-direction changes fastest, then the index in y-direction while the index in x-direction changes slowest. The columns correspond to E_x, E_y, E_z, H_x, H_y and H_z. *OPAL-t* normalizes the field so that $\max(|E_{z,\text{ on axis}}|) = 1\text{MV/m}$.

3DDynamic	TRUE | FALSE (optional)				
Frequency (in MHz)					
x_{start} (in cm)	x_{end} (in cm)	N_x			
y_{start} (in cm)	y_{end} (in cm)	N_y			
z_{start} (in cm)	z_{end} (in cm)	N_z			
$E_{x,1}$ (MV/m))	$E_{y,1}$ (MV/m)	$E_{z,1}$ (MV/m)	$H_{x,1}$ (A/m)	$H_{y,1}$ (A/m)	$H_{z,1}$ (A/m)
$E_{x,2}$ (MV/m))	$E_{y,2}$ (MV/m)	$E_{z,2}$ (MV/m)	$H_{x,2}$ (A/m)	$H_{y,2}$ (A/m)	$H_{z,2}$ (A/m)
.					
.					
.					
$E_{x,N}$ (MV/m))	$E_{y,N}$ (MV/m)	$E_{z,N}$ (MV/m)	$H_{x,N}$ (A/m)	$H_{y,N}$ (A/m)	$H_{z,N}$ (A/m)

Table 71: Layout of a `3DDynamic` field map file.

A `3DDynamic` field map has the general form shown in Table 71. The first five lines form the file header and tell *OPAL-t* how the field map data is being presented:

Line 1 This tells *OPAL-t* what type of field file it is (`3DDynamic`).

Line 2 Field frequency.

Line 3 This gives the extent of the field map and how many grid spacings there are in the slowest changing index direction.

Line 4 This gives the extent of the field map and how many grid spacings there are in the next fastest changing index direction.

Line 5 This gives the extent of the field map and how many grid spacings there are in the fastest changing index direction.

The lines following the header give the 3D field map grid values from 1 to $N = (N_z + 1) \times (N_y + 1) \times (N_x + 1)$.

B.19 References

[80] J. E. Spencer and H. A. Enge, *Split-pole magnetic spectrograph for precision nuclear spectroscopy*, Nucl. Instrum. Methods 49, 181 (1967).

[81] J. H. Billen and L. M. Young, *Poisson superfish*, Tech. Rep. LA-UR-96-1834, Los Alamos National Laboratory (2004).

Appendix C

OPAL - MADX Conversion Guide

We note with α,β and γ the Twiss parameters.

$$
\begin{aligned}
\sigma_{beam} = & \begin{pmatrix} \sigma_x & \sigma_{xp_x} \\ \sigma_{xp_x} & \sigma_{p_x} \end{pmatrix} = \begin{pmatrix} \sigma_x & \delta \cdot \sqrt{\sigma_x \sigma_{p_x}} \\ \delta \cdot \sqrt{\sigma_x \sigma_{p_x}} & \sigma_{p_x} \end{pmatrix} = \begin{pmatrix} < x^2 > & < xp_x > \\ < xp_x > & < p_x^2 > \end{pmatrix} \\
= & \begin{pmatrix} \frac{1}{N}\sum_{i=1}^N x_i^2 & \frac{1}{N}\sum_{i=1}^N x_i p_{x_i} \\ \frac{1}{N}\sum_{i=1}^N x_i p_{x_i} & \frac{1}{N}\sum_{i=1}^N p_{x_i}^2 \end{pmatrix} = \varepsilon \cdot \begin{pmatrix} \beta & -\alpha \\ -\alpha & \gamma \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\bar{p}_x = & \sqrt{\frac{1}{N}\sum_{i=1}^N p_{x_i}^2} = \sqrt{\sigma_{p_x}} & \bar{x} = & \sqrt{\frac{1}{N}\sum_{i=1}^N x_i^2} \\
\bar{p}_y = & \sqrt{\frac{1}{N}\sum_{i=1}^N p_{y_i}^2} = \sqrt{\sigma_{p_y}} & \bar{y} = & \sqrt{\frac{1}{N}\sum_{i=1}^N y_i^2}
\end{aligned}
$$

$$
\begin{aligned}
\gamma = & \frac{E_{kin} + m_p}{m_p} & \beta = & \sqrt{1 - \frac{1}{\gamma^2}} = \frac{v}{c} \\
(\beta\gamma) = & \frac{E_{kin} + m_p}{m_p} \cdot \sqrt{1 - \frac{1}{\gamma^2}} = \frac{\beta}{\sqrt{1-\beta^2}} & \mathrm{B}\rho = & \frac{(\beta\gamma) \cdot m_p \cdot 10^9}{c} \text{ [T m]} \\
m_p = & 0.939277[GeV] & c = & 299792458[m/s]
\end{aligned}
$$

Quantity	**MADX**		**Conversion**			***OPAL-Output***	
Momenta	$\bar{p}_x$	[rad]	$\bar{p}_x[\beta\gamma]$	=	$(\bar{p}_x\,[\text{rad}])\cdot(\beta\gamma)$	$\bar{p}_x$	$[\beta\gamma]$
Correlation of $\bar{x}$,$\bar{p}_x$	δ	[1]	δ	=	$(\sigma_{xp_x}\,[\text{m rad}])\,/\,((\bar{p}_x\,[\text{rad}])\cdot(\bar{x}\,[\text{m}]))$	δ	[1]
				=	$(\sigma_{xp_x}\,[\text{m rad}])\,/\sqrt{(\sigma_x\,[\text{m}^2])\cdot\left(\sigma_{p_x}\left[\text{rad}^2\right]\right)}$		
Emittance	ε_x	[m rad]	$\varepsilon_x[\text{m}\,\beta\gamma]$	=	$\sqrt{(\bar{p}_x\,[\beta\gamma])^2\cdot(\bar{x}\,[\text{m}])^2-(\delta\cdot(\bar{x}\,[\text{m}])\cdot(\bar{p}_x\,[\beta\gamma]))^2}$	ε_x	$[\text{m}\,\beta\gamma]$
				=	$\sqrt{\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)\cdot(\sigma_x\,[\text{m}^2])-\left(\delta\cdot\sqrt{(\sigma_x\,[\text{m}^2])\cdot\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)}\right)^2}$		
				=	$\sqrt{\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)\cdot(\sigma_x\,[\text{m}^2])-(\sigma_{xp_x}\,[\text{m}\,\beta\gamma])^2}$		
Twiss Parameter α	α	[1]	$\alpha\,[1]$	=	$-\delta\cdot(\bar{x}\,[\text{m}])\cdot(\bar{p}_x\,[\beta\gamma])\,/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$	α_T	[1]
				=	$-\delta\cdot\sqrt{(\sigma_x\,[\text{m}^2])\cdot\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)}\,/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$		
Twiss Parameter β_T	β_T	[m/rad]	$\beta_T\,[\text{m}/\beta\gamma]$	=	$(\bar{x}\,[\text{m}])^2\,/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$	β_T	$[\text{m}/\beta\gamma]$
				=	$\left(\sigma_x\left[\text{m}^2\right]\right)/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$		
Twiss Parameter γ_T	γ_T	[rad/m]	$\gamma_T\,[\beta\gamma/\text{m}]$	=	$(\bar{p}_x\,[\beta\gamma])^2\,/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$	γ_T	$[\beta\gamma/\text{m}]$
				=	$\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)/\,(\varepsilon_x\,[\text{m}\,\beta\gamma])$		
Focusing strength	k_1	$\left[\text{m}^{-2}\right]$	$k_1\,[\text{T}/\text{m}]$	=	$\left(k_1\left[\text{m}^{-2}\right]\right)\cdot(\text{B}\rho\,[\text{T m}])$	k_1	$[\text{T}/\text{m}]$

Quantity	**MADX**		**Conversion**			**OPAL-Input**	
Element Position	`at :=`	[m]	`ELEMEDGE`	=	(Center of the element) - (Length of the element)/2	`ELEMEDGE` =	[m]
	Center of the element					Begin of the element	

Quantity	`OPAL-Output`		Conversion			`OPAL-Input`	
Momenta	$\bar{p}_x$	$[\beta\gamma]$	$p_x\,[\mathrm{eV}]$	=	$m_p \cdot 10^9 \cdot \left(\sqrt{(\bar{p}_x\,[\beta\gamma])^2+1}-1\right)$	$\bar{p}_x$	[eV]

Appendix D

Auto-phasing Algorithm

D.1 Standing Wave Cavity

In *OPAL-t* the elements are implemented as external fields that are read in from a file. The fields are described by a 1D, 2D or 3D sampling (equidistant or non-equidistant). To get the actual field at any position a linear interpolation multiplied by $\cos(\omega t + \varphi)$, where ω is the frequency and φ is the lag. The energy gain of a particle then is

$$\Delta E(\varphi, r) = q V_0 \int_{z_\text{begin}}^{z_\text{end}} \cos(\omega t(z,\varphi) + \varphi) E_z(z,r) dz.$$

To maximize the energy gain we have to take the derivative with respect to the lag, φ and set the result to zero:

$$\begin{aligned}\frac{\mathrm{d}\Delta E(\varphi, r)}{\mathrm{d}\varphi} &= -\int_{z_\text{begin}}^{z_\text{end}} (1 + \omega \frac{\partial t(z,\varphi)}{\partial \varphi}) \sin(\omega t(z,\varphi) + \varphi) E_z(z,r) \\ &= -\cos(\varphi) \int_{z_\text{begin}}^{z_\text{end}} (1 + \omega \frac{\partial t(z,\varphi)}{\partial \varphi}) \sin(\omega t(z,\varphi)) E_z(z,r) dz \\ &\quad - \sin(\varphi) \int_{z_\text{begin}}^{z_\text{end}} (1 + \omega \frac{\partial t(z,\varphi)}{\partial \varphi}) \cos(\omega t(z,\varphi)) E_z(z,r) dz \equiv 0.\end{aligned}$$

Thus to get the maximum energy the lag has to fulfill

$$\tan(\varphi) = -\frac{\Gamma_1}{\Gamma_2},$$

EQUATION D.1: Lag rule

where

$$\Gamma_1 = \sum_{i=1}^{N-1} (1 + \omega \frac{\partial t}{\partial \varphi}) \int_{z_{i-1}}^{z_i} \sin\left(\omega (t_{i-1} + \Delta t_i \frac{z - z_{i-1}}{\Delta z_i})\right) \left(E_{z,i-1} + \Delta E_{z,i} \frac{z - z_{i-1}}{\Delta z_i}\right) dz$$

EQUATION D.2: Gamma 1

and

$$\Gamma_2 = \sum_{i=1}^{N-1} (1 + \omega \frac{\partial t}{\partial \varphi}) \int_{z_{i-1}}^{z_i} \cos\left(\omega (t_{i-1} + \Delta t_i \frac{z - z_{i-1}}{\Delta z_i})\right) \left(E_{z,i-1} + \Delta E_{z,i} \frac{z - z_{i-1}}{\Delta z_i}\right) dz.$$

EQUATION D.3: Gamma 2

Between two sampling points we assume a linear correlation between the electric field and position respectively between time and position. The products in the integrals between two sampling points can be expanded and solved analytically. We then find

$$\Gamma_1 = \sum_{i=1}^{N-1} (1+\omega\frac{\partial t}{\partial \varphi})\Delta z_i (E_{z,i-1}(\Gamma_{11,i} - \Gamma_{12,i}) + E_{z,i}\Gamma_{12,i})$$

and

$$\Gamma_1 = \sum_{i=1}^{N-1} (1+\omega\frac{\partial t}{\partial \varphi})\Delta z_i (E_{z,i-1}(\Gamma_{21,i} - \Gamma_{22,i}) + E_{z,i}\Gamma_{22,i})$$

where

$$\Gamma_{11,i} = \int_0^1 \sin(\omega(t_{i-1}+\tau\Delta t_i))d\tau = -\frac{\cos(\omega t_i) - \cos(\omega t_{i-1})}{\omega \Delta t_i}$$

$$\Gamma_{12,i} = \int_0^1 \sin(\omega(t_{i-1}+\tau\Delta t_i))\tau d\tau = \frac{-\omega\Delta t_i \cos(\omega t_i) + \sin(\omega t_i) - \sin(\omega t_{i-1})}{\omega^2(\Delta t_i)^2}$$

$$\Gamma_{21,i} = \int_0^1 \cos(\omega(t_{i-1}+\tau\Delta t_i))d\tau = \frac{\sin(\omega t_i) - \sin(\omega t_{i-1})}{\omega \Delta t_i}$$

$$\Gamma_{22,i} = \int_0^1 \cos(\omega(t_{i-1}+\tau\Delta t_i))\tau d\tau = \frac{\omega\Delta t_i \sin(\omega t_i) + \cos(\omega t_i) - \cos(\omega t_{i-1})}{\omega^2(\Delta t_i)^2}$$

It remains to find the progress of time with respect to the position. In *OPAL* this is done iteratively starting with

```
K[i] = K[i-1] + (z[i] - z[0]) * q * V;
b[i] = sqrt(1. - 1. / ((K[i] - K[i-1]) / (2.*m*c^2) + 1)^2);
t[i] = t[0] + (z[i] - z[0]) / (c * b[i])
```

By doing so we assume that the kinetic energy, K, increases linearly and proportional to the maximal voltage. With this model for the progress of time we can calculate φ according to Equation D.1. Next a better model for the kinetic Energy can be calculated using

$\texttt{K[i] = K[i-1] + q } \Delta\texttt{z[i](cos(}\varphi\texttt{)(Ez[i-1](}\Gamma_{21}\texttt{[i] - }\Gamma_{22}\texttt{[i]) + Ez[i]}\Gamma_{22}\texttt{[i])}$

$\texttt{ - sin(}\varphi\texttt{)(Ez[i-1](}\Gamma_{11}\texttt{[i] - }\Gamma_{12}\texttt{[i]) + Ez[i]}\Gamma_{12}\texttt{[i])).}$

With the updated kinetic energy the time model and finally a new φ, that comes closer to the actual maximal kinetic energy, can be obtained. One can iterate a few times through this cycle until the value of φ has converged.

D.2 Traveling Wave Structure

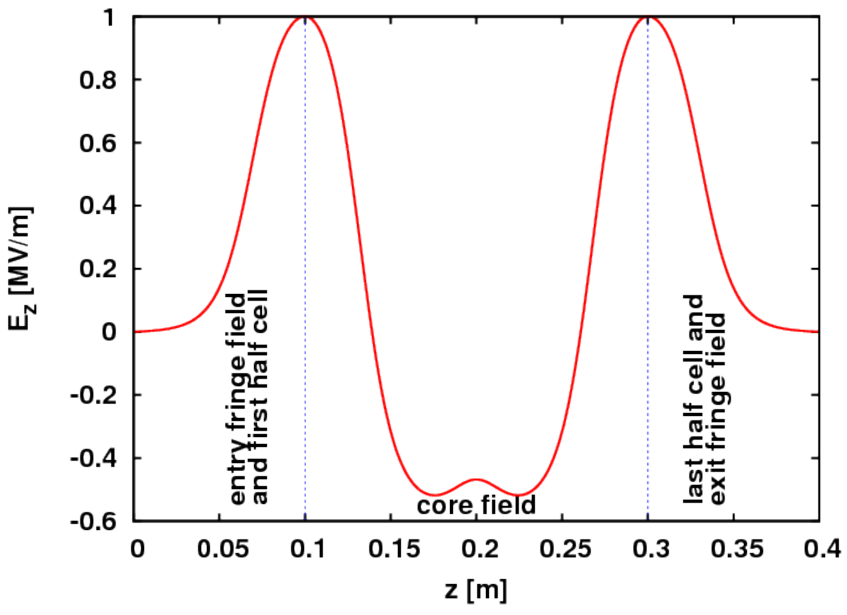


Figure 48: Field map 'FINLB02-RAC.T7' of type 1DDynamic

Auto phasing in a traveling wave structure is just slightly more complicated. The field of this element is composed of a standing wave entry and exit fringe field and two standing waves in between, see Figure 48.

$$\Delta E(\varphi,r) = qV_0 \int_{z_\text{begin}}^{z_\text{beginCore}} \cos(\omega t(z,\varphi)+\varphi)E_z(z,r)dz$$

$$+qV_\text{core} \int_{z_\text{beginCore}}^{z_\text{endCore}} \cos(\omega t(z,\varphi)+\varphi_\text{c1}+\varphi)E_z(z,r)dz$$

$$+qV_\text{core} \int_{z_\text{beginCore}}^{z_\text{endCore}} \cos(\omega t(z,\varphi)+\varphi_\text{c2}+\varphi)E_z(z+s,r)dz$$

$$+qV_0 \int_{z_\text{endCore}}^{z_\text{end}} \cos(\omega t(z,\varphi)+\varphi_\text{ef}+\varphi)E_z(z,r)dz,$$

where s is the cell length. Instead of one sum as in Equation D.2 and Equation D.3 there are four sums with different numbers of summands.

D.2.1 Example

```
FINLB02_RAC: TravelingWave, L=2.80, VOLT=14.750*30/31,
             NUMCELLS=40, FMAPFN="FINLB02-RAC.T7",
             ELEMEDGE=2.67066, MODE=1/3,
             FREQ=1498.956, LAG=FINLB02_RAC_lag;
```

For this example we find

$$\begin{aligned}
V_{\text{core}} &= \frac{V_0}{\sin(2.0/3.0\pi)} = \frac{2V_0}{\sqrt{3.0}}\\
\varphi_{\text{c1}} &= \frac{\pi}{6}\\
\varphi_{\text{c2}} &= \frac{\pi}{2}\\
\varphi_{\text{ef}} &= -2\pi \cdot (\text{NUMCELLS} - 1) \cdot \text{MODE} = 26\pi
\end{aligned}$$

D.2.2 Alternative Approach for Traveling Wave Structures

If β doesn't change much along the traveling wave structure (ultra relativistic case) then $t(z,\varphi)$ can be approximated by $t(z,\varphi) = \frac{\omega}{\beta c} z + t_0$. For the example from above the energy gain is approximately

$$\begin{aligned}
\Delta E(\varphi, r) = q\,V_0 \int_0^{1.5\cdot s} &\cos\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) E_z(z,r)\,dz\\
&+ \frac{2q\,V_0}{\sqrt{3}} \int_{1.5\cdot s}^{40.5\cdot s} \cos\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{\pi}{6}+\varphi\right) E_z(z \quad ,r) dz\\
&+ \frac{2q\,V_0}{\sqrt{3}} \int_{1.5\cdot s}^{40.5\cdot s} \cos\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{\pi}{2}+\varphi\right) E_z(z+s,r) dz\\
&+ q\,V_0 \int_{40.5\cdot s}^{42\cdot s} \cos\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) E_z(z,r)\,dz.
\end{aligned}$$

Here $\beta c = 2.9886774 \cdot 10^8$ m s^{-2}, $\omega = 2\pi \cdot 1.4989534 \cdot 10^9$ Hz and, the cell length, $s = 0.06\bar{6}$ m. To maximize this energy we have to take the derivative with respect to φ and set the result to 0. We split the field up into the core field, $E_z^{(1)}$ and the fringe fields (entry fringe field plus first half cell concatenated with the exit fringe field plus last half cell), $E_z^{(2)}$. The core fringe field is periodic with a period of $3\,s$. We thus find

$$\begin{aligned}
0 \equiv \int_0^{1.5\cdot s} &\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) E_z^{(2)}(z,r)\,dz\\
&+ \frac{2}{\sqrt{3}} \int_0^{39\cdot s} \sin\left(\omega\left(\frac{z+1.5\,s}{\beta c}+t_0\right)+\frac{\pi}{6}+\varphi\right) E_z^{(1)}(z \bmod(3\,s), r)\,dz\\
&+ \frac{2}{\sqrt{3}} \int_0^{39\cdot s} \sin\left(\omega\left(\frac{z+1.5\,s}{\beta c}+t_0\right)+\frac{\pi}{2}+\varphi\right) E_z^{(1)}((z+s) \bmod(3\,s), r)\,dz\\
&+ \int_{1.5\cdot s}^{3\cdot s} \sin\left(\omega\left(\frac{z+39\,s}{\beta c}+t_0\right)+\varphi\right) E_z^{(2)}(z,r)\,dz
\end{aligned}$$

This equation is much simplified if we take into account that $\omega/\beta c \approx 10\pi$. We then get

$$\begin{aligned}
0 \equiv \int_0^{3\cdot s} &\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) E_z^{(2)}(z)\,dz\\
&+ \frac{26}{\sqrt{3}} \int_0^{3\cdot s} \left(\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{7\pi}{6}+\varphi\right) + \sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{5\pi}{6}+\varphi\right)\right) E_z^{(1)}(z)\,dz\\
&= \int_0^{3\cdot s} \sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) \left(E_z^{(2)} - 26 \cdot E_z^{(1)}\right)(z)\,dz
\end{aligned}$$

where we used $(z' = z+s)$

$$\int_0^{3\cdot s} \sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{3\pi}{2}+\varphi\right) E_z^{(1)}((z+s) \bmod(3s), r)dz$$

$$= \int_s^{4\cdot s} \sin\left(\omega\left(\frac{z'-s}{\beta c}+t_0\right)+\frac{3\pi}{2}+\varphi\right) E_z^{(1)}(z' \mathrm{mod}(3s), r)dz'$$

$$= \int_0^{3\cdot s} \sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{5\pi}{6}+\varphi\right) E_z^{(1)}(z, r)\,dz.$$

In the last equal sign we used the fact that both functions, $\sin(\frac{\omega}{\beta c}z)$ and $E_z^{(1)}$ have a periodicity of $3\cdot s$ to shift the boundaries of the integral.

Using the convolution theorem we find

$$0 \equiv \int_0^{3\cdot s} g(\xi - z)(G - 26\cdot H)(z)\,dz = \mathscr{F}^{-1}\left(\mathscr{F}(g)\cdot(\mathscr{F}(G) - 26\cdot\mathscr{F}(H))\right)$$

where

$$g(z) = \begin{cases} -\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)\right) & 0 \le z \le 3\cdot s \\ 0 & \text{otherwise} \end{cases}$$
$$G(z) = \begin{cases} E_z^{(2)}(z) & 0 \le z \le 3\cdot s \\ 0 & \text{otherwise} \end{cases}$$
$$H(z) = \begin{cases} E_z^{(1)}(z) & 0 \le z \le 3\cdot s \\ 0 & \text{otherwise} \end{cases}$$

and

$$-\frac{\omega}{\beta c}\xi = \varphi.$$

Here we also used some trigonometric identities:

$$\begin{aligned} &\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\pi+\frac{\pi}{6}+\varphi\right)+\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\pi-\frac{\pi}{6}+\varphi\right) \\ &= -\left(\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\frac{\pi}{6}+\varphi\right)+\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)-\frac{\pi}{6}+\varphi\right)\right) \\ &= -2\cdot\cos\left(\frac{\pi}{6}\right)\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) \\ &= -\sqrt{3}\sin\left(\omega\left(\frac{z}{\beta c}+t_0\right)+\varphi\right) \end{aligned}$$

Appendix E

Benchmarks

E.1 *OPAL-t* compared with TRANSPORT & TRACE 3D

E.1.1 TRACE 3D

TRACE 3D is an interactive beam dynamics program that calculates the envelopes of a bunched beam, including linear space-change forces [82]. It provides an instantaneous beam profile diagram and delineates the transverse and longitudinal phase plane, where the ellipses are characterized by the Twiss parameters and emittances (total and unnormalized).

E.1.2 TRACE 3D Units

TRACE 3D supports the following internal coordinates and units for the three phase planes:

- **horizontal plane:** x [mm] is the displacement from the center of the beam bunch; x' [mrad] is the beam divergence;
- **vertical plane:** y [mm] is the displacement from the center of the beam bunch; y' [mrad] is the beam divergence;
- **longitudinal plane:** z [mm] is the displacement from the center of the beam bunch; Δp/p [mrad] is the difference between the particle's longitudinal momentum and the reference momentum of the beam bunch.

For input and output, however, z and Δp/p are replaced by $\Delta\phi$ [degree] and ΔW [keV], respectively the displacement in phase and energy. The relationships between these longitudinal coordinates are:

$$z = -\frac{\beta\lambda}{360}\Delta\phi$$

and

$$\frac{\Delta p}{p} = \frac{\gamma}{\gamma+1}\frac{\Delta W}{W}$$

where β and γ are the relativist parameters, λ is the free-space wavelength of the RF and W is the kinetic energy [MeV] at the beam center. This internal conversion can be displayed using the *command W* (see [82] page 42).

E.1.3 TRACE 3D Input beam

In TRACE 3D, the input beam is described by the following set of parameters:

- **ER**: particle rest mass [MeV/c^{2}];
- **Q**: charge state (+1 for protons);

- **W**: beam kinetic energy [MeV]
- **XI**: beam current [mA]
- **BEAMI**: array with initial Twiss parameters in the three phase planes

  BEAMI = $\alpha_x, \beta_x, \alpha_y, \beta_y, \alpha_\phi, \beta_\phi$

  The alphas are dimensionless, β_x and β_y are expressed in m/rad (or mm/mrad) and β_ϕ in deg/keV;
- **EMITI**: initial total and unnormalized emittances in x-x', y-y', and $\Delta\phi$-ΔW planes.

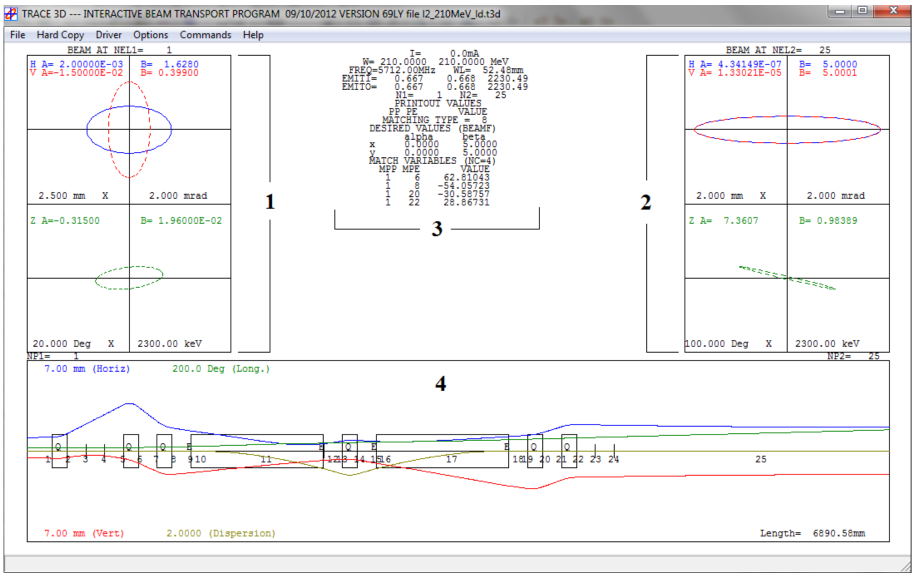
  EMITI = $\varepsilon_x, \varepsilon_y, \varepsilon_\phi$

  The transversal emittances are expressed in π-mm-mrad and in π-deg-keV the longitudinal emittance.

In this beam dynamics code, the total emittance in each phase plane is five times the RMS emittance in that plane and the displayed beam envelopes are $\sqrt{5}$-times their respective RMS values.

E.1.3.1 TRACE 3D Graphic Interface

An example of TRACE 3D graphic interface is shown in Figure 49.



```
         I=       0.0mA
   W= 210.0000  210.0000 MeV
 FREQ=5712.00MHz    WL=  52.48mm
EMITI=    0.667     0.668  2230.49
EMITO=    0.667     0.668  2230.49
        N1=     1   N2=    25
        PRINTOUT VALUES
          PP PE        VALUE
      MATCHING TYPE =  8
   DESIRED VALUES  (BEAMF)
            alpha        beta
   x       0.0000       5.0000
   y       0.0000       5.0000
   MATCH VARIABLES  (NC=4)
     MPP MPE          VALUE
      1    6       62.81043
      1    8      -54.05723
      1   20      -30.58757
      1   22       28.86731
```

Figure 49: TRACE 3D graphic interface where: (1) input beam in transverse plane (above) and longitudinal plane (below); (2) output beam in transverse plane (above) and longitudinal plane (below); (3) summary of beam parameters such as input and output emittances and desired value for matching function; (4) line lattice with different elements and beam envelope. The color legend is: blue line for horizontal plane, red line for vertical plane, green line for longitudinal plane and yellow line for dispersion.

E.1.4 TRANSPORT

TRANSPORT is a computer program for first-order and second-order matrix multiplication, intended for the design of beam transport system [83]. The TRANSPORT version for Windows provides a graphic beam profile diagram, as well as a sigma matrix description of the simulated beam and line [84]. Differently from TRACE 3D, the ellipses are characterized by the sigma-matrix coefficients and the Twiss parameters and emittances (total and unnormalized) are reported as output information.

E.1.5 TRANSPORT Units

At any specified position in the system, an arbitrary charged particle is represented by a vector, whose components are positions, angles and momentum of the particle with respect to the reference trajectory. The standard units and internal coordinates in TRANSPORT are:

- **horizontal plane:** x [cm] is the displacement of the arbitrary ray with respect to the assumed central trajectory; θ [mrad] is the angle the ray makes with respect to the assumed central trajectory;
- **vertical plane:** y [cm] is the displacement of the arbitrary ray with respect to the assumed central trajectory; ϕ [mrad] is the angle the ray makes with respect to the assumed central trajectory;
- **longitudinal plane:** l [cm] is the path length difference between the arbitrary ray and the central trajectory; δ [%] is the fractional momentum deviation of the ray from the assumed central trajectory.

Even if TRANSPORT supports this standard set of units [cm, mrad and %]; however using **card 15**, the users can redefine the units (see page 99 on TRANSPORT documentation [83] for more details).

E.1.6 TRANSPORT Input beam

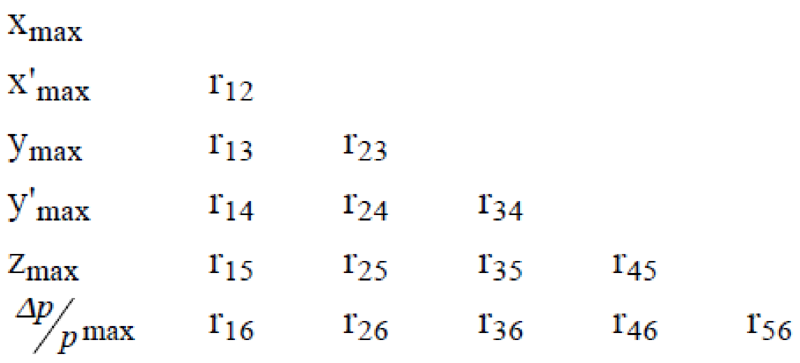
The input beam is described in **card 1** in terms of the semi-axes of a six-dimensional erect ellipsoid beam. In terms of diagonal sigma-matrix elements, the input beam in TRANSPORT is expressed by 7 parameters:

- $\sqrt{\sigma_{ii}}$ [cm] represents one-half of the horizontal (i=1), vertical (i=3) and longitudinal extent (i=5);
- $\sqrt{\sigma_{ii}}$ [mrad] represents one-half of the horizontal (i=2), vertical (i=4) beam divergence;
- $\sqrt{\sigma_{66}}$ [%] represents one-half of the momentum spread;
- p(0) is the momentum of the central trajectory [GeV/c].

If the input beam is tilted (Twiss alphas not zero), **card 12** must be used, inserting the 15 correlations r_{ij} parameters among the 6 beam components. The correlation parameters are defined as following:

$$r_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii} gma_{jj}}}$$

As explained before, with the **card 15**, it is possible to transform the TRANSPORT standard units in TRACE-like units. In this way, the TRACE 3D sigma-matrix for the input beam, printed out by *command Z*, can be directly used as input beam in TRANSPORT. An example of TRACE 3D sigma-matrix structure is shown in Figure 50.



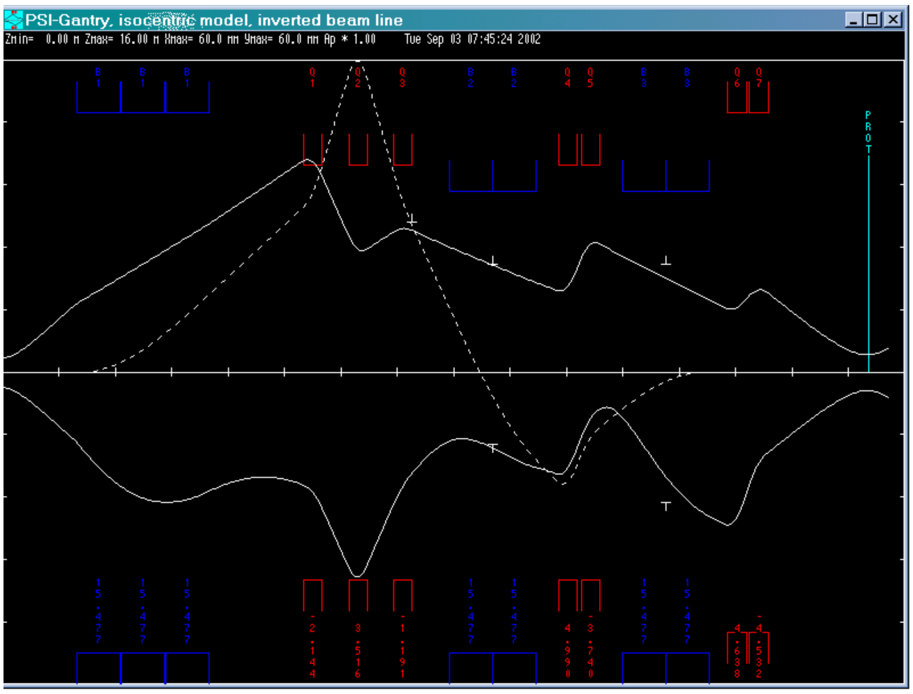
x_{max}					
x'_{max}	r_{12}				
y_{max}	r_{13}	r_{23}			
y'_{max}	r_{14}	r_{24}	r_{34}		
z_{max}	r_{15}	r_{25}	r_{35}	r_{45}	
$\Delta p/p_{max}$	r_{16}	r_{26}	r_{36}	r_{46}	r_{56}

Figure 50: Sigma-matrix structure in TRACE 3D [82]

From the sigma-matrix coefficients, TRANSPORT reports in output the Twiss parameters and the total, unnormalized emittance. Even in this case, a factor 5 is present between the emittances calculated by TRANSPORT and the corresponding RMS values.

E.1.6.1 TRANSPORT Graphic Interface

An improved version of TRANSPORT has been embedded in a new graphic shell written in C++ and is providing GUI type tools, which makes it easier to design new beam lines. A screen shot of a modern GUI Transport interface [84] is shown in Figure 51.



```
Zmin=  0.00 m Zmax= 16.00 m Xmax= 60.0 mm Ymax= 60.0 mm Ap * 1.00     Tue Sep 03 07:45:24 2002
```

Figure 51: GUI TRANSPORT graphic interface [85]. The continuous lines describe the beam envelope in the vertical plane (above) and horizontal plane (below). The dashed line displays the dispersion. The elements in the beam line are drawn as blue and red rectangles

E.1.7 Comparison TRACE 3D and TRANSPORT

This study has been done following the same trend of the Regression Test in *OPAL*, replacing the electron beam with a same energy proton beam. Due to the different beam rigidity, the bending magnet features have been redefined with a new magnetic field.

The simulated beam transport line contains:

- drift space (DRIFT 1): 0.250 m length;
- bending magnet (SBEND or RBEND): 0.250 m radius of curvature;
- drift space (DRIFT 2): 0.250 m length.

Keeping fixed the lattice structure, many similar transport lines have been tested adding entrance and exit edge angles to the bending magnet, changing the bending plane (vertical bending magnet) and direction (right or left). In all the cases, the difficulties arise from the non-achromaticity of the system and an increase in the horizontal and longitudinal emittance is expected. In addition, the coupling between these two planes has to be accurately studied.

In the following paragraph, an example of Sector Bending magnet (SBEND) simulation with entrance and exit edge angles is discussed.

E.1.7.1 Input beam

The starting simulation has been performed with TRACE 3D code. According to Section E.1.3, the simulated input beam is described by the following parameters:

```
ER = 938.27
W = 7
FREQ = 700
BEAMI = 0.0, 4.0,0.0, 4.0, 0.0, 0.0756
EMITI = 0.730, 0.730, 7.56
```

Thanks to the TRACE 3D graphic interface, the input beam can immediately be visualized in the three phase plane as shown in Figure 52.

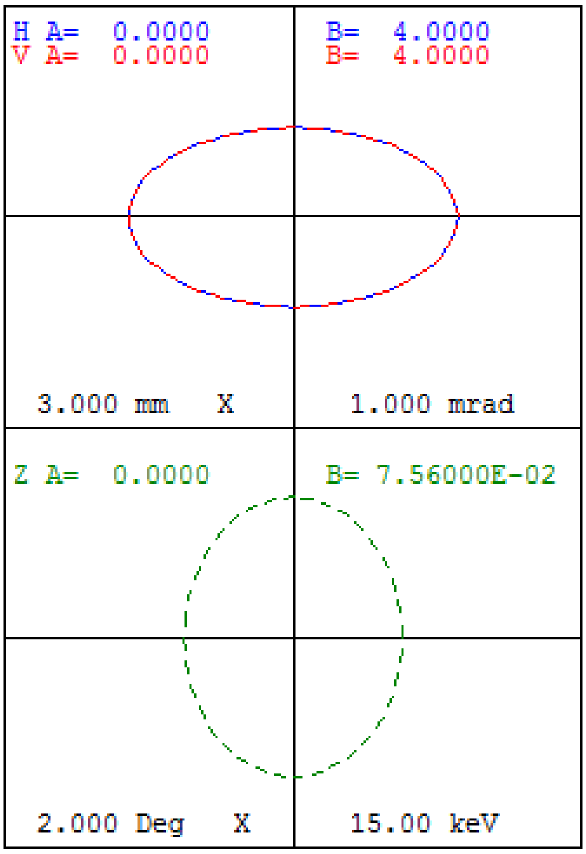
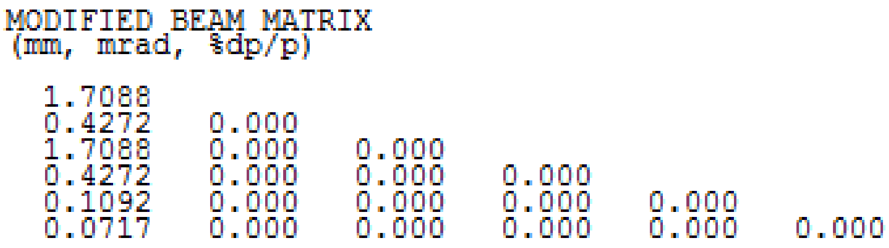


Figure 52: TRACE 3D input beam in the transversal plane (above) and in the longitudinal plane (below)

The corresponding sigma-matrix with the relative units is displayed by command Z:



```
MODIFIED BEAM MATRIX
(mm, mrad, %dp/p)

  1.7088
  0.4272   0.000
  1.7088   0.000   0.000
  0.4272   0.000   0.000   0.000
  0.1092   0.000   0.000   0.000   0.000
  0.0717   0.000   0.000   0.000   0.000   0.000
```

Figure 53: TRACE 3D sigma-matrix for the beam

Before entering the TRACE 3D sigma-matrix coefficients in TRANSPORT, a changing in the units is required using the **card 15** in the following way:

```
15. 1. 'MM' 0.1 ; //express in mm the horizontal and vertical beam size
15. 5. 'MM' 0.1 ; //express in mm the beam length
```

At this point, the TRANSPORT input beam is defined by **card 1**:

```
1.0 1.709 0.427 1.709 0.427 0.11 0.0717 0.1148 /BEAM/ ;
```

using exactly the same sigma-matrix coefficients of Figure 53. Other two cards must be added in order to use exactly the TRACE 3D R-matrix formalism:

```
16. 3. 1863.153; //proton mass, as ratio of electron mass
22. 0.05 0.0 700 0.0 /SPAC/ ; //space charge card
```

E.1.7.2 SBEND in TRACE 3D

The bending magnet definition in TRACE 3D requires:

Parameter	**Value**	**Description**
NT	8	Type code for bending
α [deg]	30	angle of bend in horizontal plane
ρ [mm]	250	radius of curvature of central trajectory
n	0	field-index gradient
vf	0	flag for vertical bending

Table 72: Bending magnet description in TRACE 3D and values used in the simulation

The edge angles are described with another type code and parameters which include also the fringe field. They must be added before and after the bending magnet if entrance and exit edge angles are present and if the fringe field has to be taken into account. In particular for the entrance edge angle:

Parameter	**Value**	**Description**
NT	9	Type code for edge
β [deg]	10	pole-face rotation
ρ [mm]	250	radius of curvature of central trajectory
g [mm]	20	total gap of magnet
K_1	0.36945	fringe-field factor
K_2	0.36945	fringe-field factor

Table 73: Edge angle description in TRACE 3D and values used in the simulation

A same configuration has been used for exit edge angle using $\beta = 5°$. The beam envelopes in the three phase planes for this simulation are shown in Figure 54.

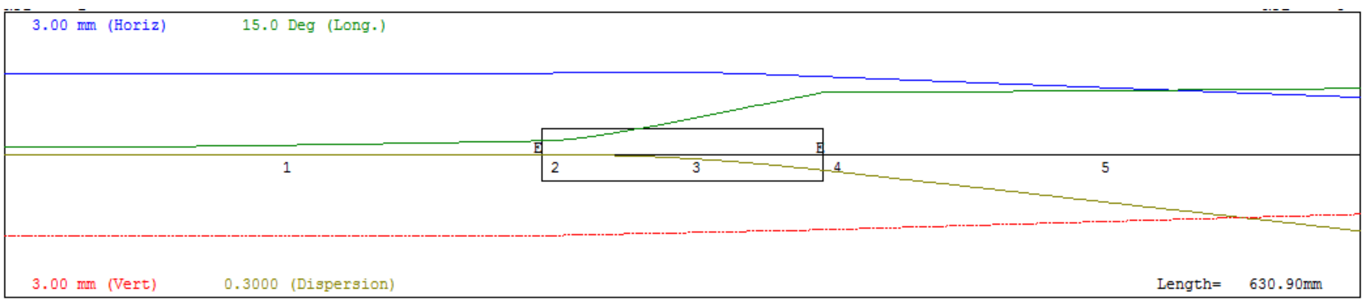


Figure 54: Beam envelopes in TRACE 3D for a SBEND with entrance and exit edge angles. The blue line describes the beam envelope in the horizontal plane, the red line in the vertical plane, the green line in the longitudinal plane. The yellow line displays the dispersion

E.1.7.3 SBEND in TRANSPORT

The bending magnet definition in TRANSPORT requires:

Parameter	**Value**	**Description**
Card	4	Type code for bending
L [m]	30	Effective length of the central trajectory
B_0 [kG]	250	Central field strength
n	0	field-index gradient

Table 74: Bending magnet description in TRANSPORT and values used in the simulation

As for TRACE 3D, the edge angles are described with another card and parameters. In TRANSPORT, however, the fringe field is not automatically included with the edge angle, but it is described by a own card as reported in the Table 75.

Parameter	**Value**	**Description**
Card	2	Type code for edge
β [deg]	10	pole-face rotation
Card	16	Type code for fringe field
g [mm]	10	half-gap of magnet
K_1	0.36945	fringe-field factor
K_2	0.36945	fringe-field factor

Table 75: Edge angle and fringe field description in TRANSPORT and values used in the simulation

Running the Graphic TRANSPORT version, the beam envelopes in the transverse phase planes for this simulation are shown in Figure 55.

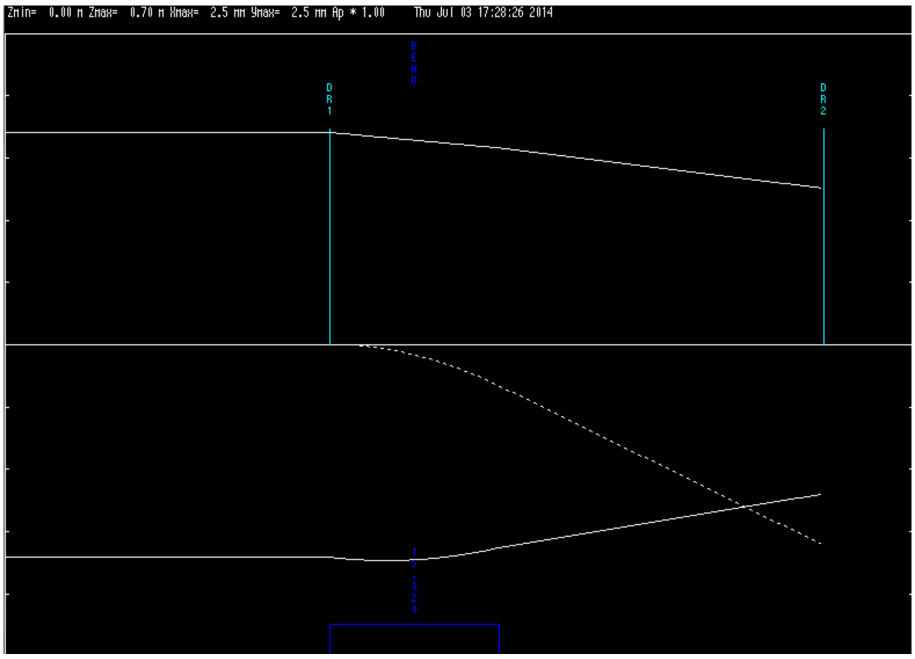


Figure 55: Beam envelopes in TRANSPORT for a SBEND with entrance and exit edge angles. The continuous lines describe the beam envelope in the vertical plane (above) and horizontal plane (below). The dashed line displays the dispersion.

E.1.7.4 Beam size and emittance comparison

In the next table, the results of the comparison between TRACE 3D and TRANSPORT in terms of the transversal beam sizes at the end of each element in the line are summarized.

Position	z (m)	σ_x (mm)	σ_y (mm)	σ_x (mm)	σ_y (mm)
Input	0.000	1.709	1.709	1.709	1.709
Drift 1	0.250	1.712	1.712	1.712	1.712
Edge	0.250	1.712	1.712	1.712	1.712
Bend	0.381	1.638	1.587	1.638	1.587
Edge	0.381	1.638	1.587	1.638	1.587
Drift 2	0.631	1.206	1.264	1.206	1.264

Table 76: Transversal beam size at the end of each element in the line printed out by TRACE 3D and TRANSPORT

The perfect agreement between these two codes arises immediately looking at Figure 56.

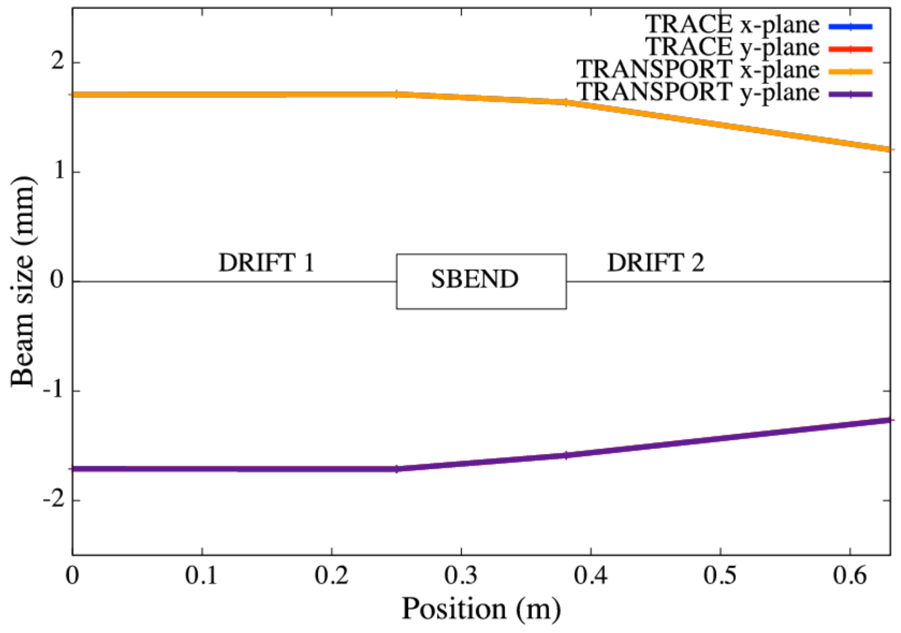


Figure 56: Transversal beam size comparison between TRACE 3D and TRANSPORT

The same comparison has been performed in terms of horizontal and longitudinal emittance, both expressed in π-mm-mrad. While the vertical emittance remains constant and equal to the initial value ($\varepsilon_y = 0.730$ π-mm-mrad) , the horizontal and longitudinal emittances are expected growing after the bending magnet. The results are reported in Table 77 and in Figure 57.

Position	z (m)	ε_x	ε_z	ε_x	ε_z
Input	0	0.730	0.08	0.730	0.08
Drift 1	0.250	0.730	0.08	0.730	0.08
Edge	0.250	0.730	0.08	0.730	0.08
Bend	0.381	0.973	0.65	0.973	0.65
Edge	0.381	0.973	0.65	0.973	0.65
Drift 2	0.631	0.973	0.65	0.973	0.65

Table 77: Horizontal and longitudinal emittance comparison between TRACE 3D and TRANSPORT, both expressed in π-mm-mrad

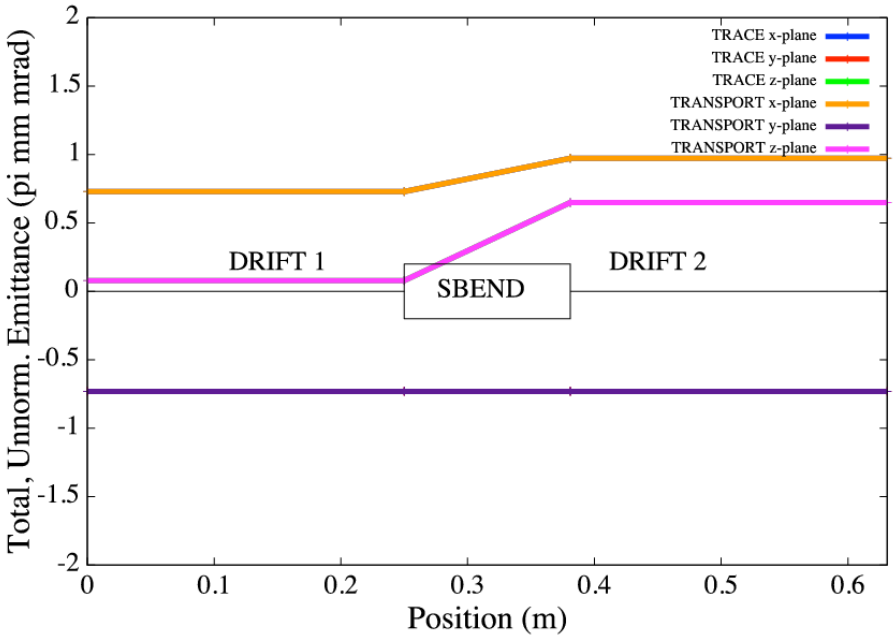


Figure 57: Emittance comparison between TRACE and TRANSPORT

E.1.7.5 From TRACE 3D to TRANSPORT

Parameter	**Trace 3D**	**Transport**
Bend card	8	4
Angle	Input parameter [deg]	Output information [deg]
Magn. field	Calculated. [T]	Input parameter [kG]
Radius of curv.	Input parameter [mm]	Output information [m]
Field-index	Input parameter	Input parameter
Effect. length	Calculated [mm]	Input parameter [m]
Edge card	9	2
Edge angle	Input parameter [deg]	Input parameter [deg]
Vertical gap	9	16.5
Gap	Total [mm]	Half-gap [cm]
Fringe field card	9	16.7 / 16.8
K_1	Default: 0.45	Default: 0.5
K_2	Default: 2.8	Default: 0
Bend direction	Bend angle sign	Coord. rotation
Horiz. right	Angle > 0	Angle > 0
Horiz. left	Angle < 0	Card 20
Vertical bend	Card 8, vf > 0	Card 20

Table 78: Bending magnet features in TRACE 3D and TRANSPORT

E.1.8 Relations to *OPAL-t*

In *OPAL*, the beam dynamics approach (time integration) is hence completely different from the envelope-like supported by TRACE 3D and TRANSPORT. The three codes support different units and require diverse parameters for the input beam. A summary of their main features is reported in Table 79.

Code	**TRACE 3D**	**TRANSPORT**	***OPAL***
Type	Envelope	Envelope	Time integration
Input	Twiss, Emittance	Sigma, Momentum	Sigma, Energy
Units	mm-mrad, deg-keV	cm-rad, cm-%	m-$\beta\gamma$

Table 79: Main features of the three beam dynamics codes: TRACE 3D, TRANSPORT and *OPAL*

E.1.9 *OPAL-t* Units

OPAL-t supports the following internal coordinates and units for the three phase planes:

- **horizontal plane:** X [m] horizontal position of a particle relative to the axis of the element; PX [$\beta_x\gamma$] horizontal canonical momentum;
- **vertical plane:** Y [m] vertical position of a particle relative to the axis of the element; PY [$\beta_y\gamma$] horizontal canonical momentum;
- **longitudinal plane:** Z [m] longitudinal position of a particle in floor-coordinates; PZ [$\beta_z\gamma$] longitudinal canonical momentum;

E.1.10 *OPAL-t* Input beam

For the input beam, a `GAUSS` distribution type has been chosen. For transferring the TRANSPORT (or TRACE 3D) input beam in terms of sigma-matrix coefficients, it necessary to:

- adjust the units: from mm to m;
- correct for the factor $\sqrt{5}$: from total to RMS distribution;
- multiply for the relativistic factor $\beta\gamma = 0.1224$ for 7 MeV protons;

In case of the modified sigma-matrix in Figure 53, the corresponding *OPAL* parameters for the `GAUSS` distributions are:

```
T3D SIGMA                       OPAL -T
-------------------------------------------------------
1.7088 mm             SIGMAX  = 1.7088/sqrt(5)e-3         m
0.4272 mrad           SIGMAPX = 0.4272/sqrt(5)*0.1224e-3
1.7088 mm             SIGMAY  = 1.7088/sqrt(5)e-3        m
0.4272 mrad           SIGMAPY = 0.4272/sqrt(5)*0.1224e-3
0.1092 mm             SIGMAZ  = 0.1092/sqrt(5)e-3        m
0.0717 %              SIGMAPZ = (0.0717*10)/sqrt(5)*0.1224e-3
```

At the end of this calculation, the input beam in *OPAL* is:

```
D1: DISTRIBUTION, TYPE=GAUSS,
SIGMAX = 0.7642e-03,  SIGMAPX= 0.0234e-03,  CORRX= 0.0,
SIGMAY = 0.7642e-03,  SIGMAPY= 0.0234e-03,  CORRY= 0.0,
SIGMAZ = 0.0488e-03,  SIGMAPZ= 0.0392e-03,  CORRZ= 0.0, R61= 0.0,
INPUTMOUNITS=NONE;
```

E.1.11 Comparison TRACE 3D and *OPAL-t*

In this section, the comparison between TRACE 3D and *OPAL-t* is discussed starting from `SBEND` definition in *OPAL-t*. The transport line described in Section E.1.7 has been simulated in *OPAL* using 10.000 particles and 10^{-11} s time step. The bending magnet features of Table 72 and Table 73 have been transformed in *OPAL* language as:

```
Bend: SBEND, ANGLE = 30.0 * Pi/180.0,
             K1=0.0,
             E1=0, E2=0,
             FMAPFN = "1DPROFILE1-DEFAULT",
             ELEMEDGE = 0.250,  // end of first drift
             DESIGNENERGY = 7E+06,  // ref energy eV
             L = 0.1294,
             GAP = 0.02;
```

- **SBEND without edge angles:**

```
// Bending magnet configuration:
K1=0.0,
E1=0, E2=0,
```

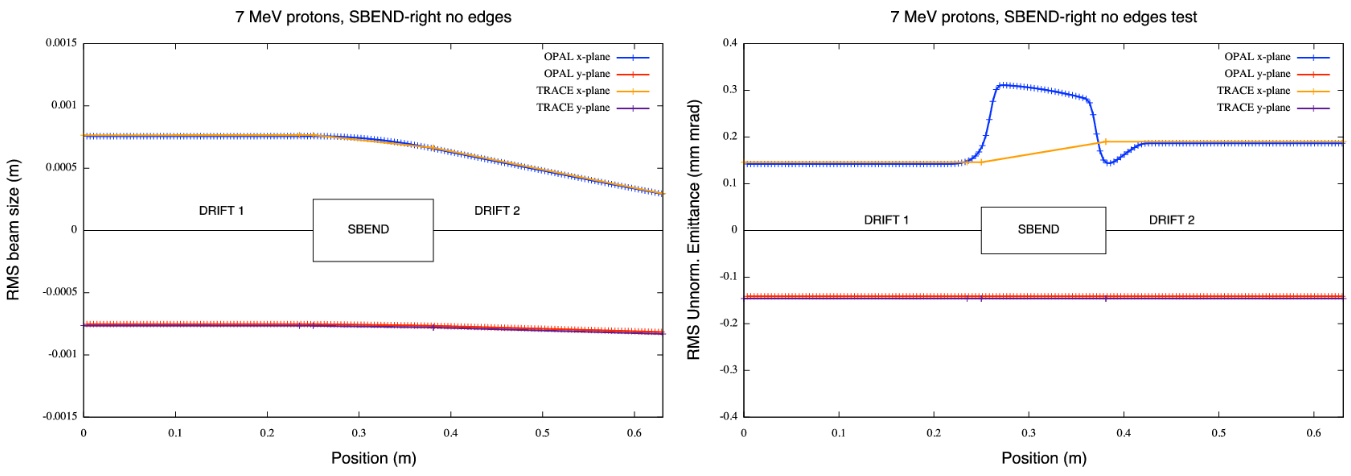


Figure 58: TRACE 3D and *OPAL* comparison: SBEND without edge angles,

A good overall agreement has been found between the two codes in term of beam size and emittance. The different behavior inside the bending magnet for the horizontal emittance is still undergoing study and it's probably due to a diverse coordinate system in the two codes.

- **SBEND with edge angles:**

```
// Bending magnet configuration:
K1=0.0,
E1=10*Pi/180.0, E2=5* Pi/180.0,
```

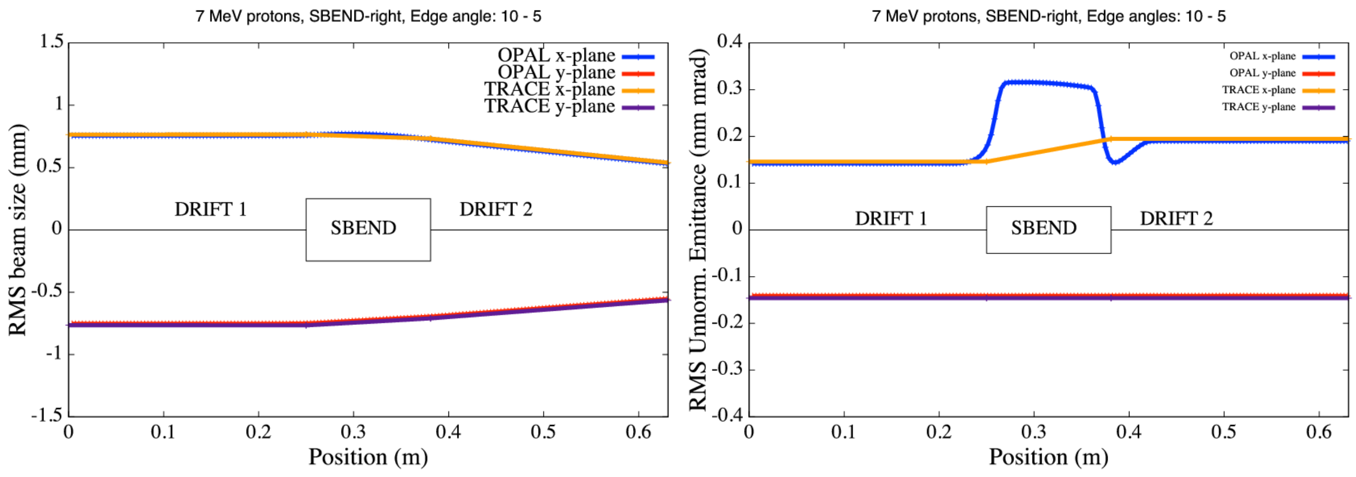


Figure 59: TRACE 3D and *OPAL* comparison: SBEND with edge angles

Even in this case, a good overall agreement has been found between the two codes in term of beam size and emittance.

- **SBEND with field index:**

  The field index parameter K1 is defined as:

$$K1 = \frac{1}{B\rho}\frac{\partial B_y}{\partial x},$$

  RBend (OPAL-t). Instead, in TRACE 3D the field index parameter n is:

$$n = -\frac{\rho}{B_y}\frac{\partial B_y}{\partial x}.$$

  In order to have a significant focusing effect on both transverse planes, the transport line has been simulated in TRACE 3D using $n = 1.5$. Since, a different definition exists between *OPAL* and TRACE 3D on the field index, the n-parameter translation in *OPAL* language has been done with the following tests:

  - TEST 1: K1 $=$ n/ρ^2
  - TEST 2: K1 $=$ n
  - TEST 3: K1 $=$ n/ρ

    Only the TEST 2 reports a reasonable behavior on the beam size and emittance, as shown in Figure 60 using:

```
// Bending magnet configuration:
K1=1.5
E1=0, E2=0,
```

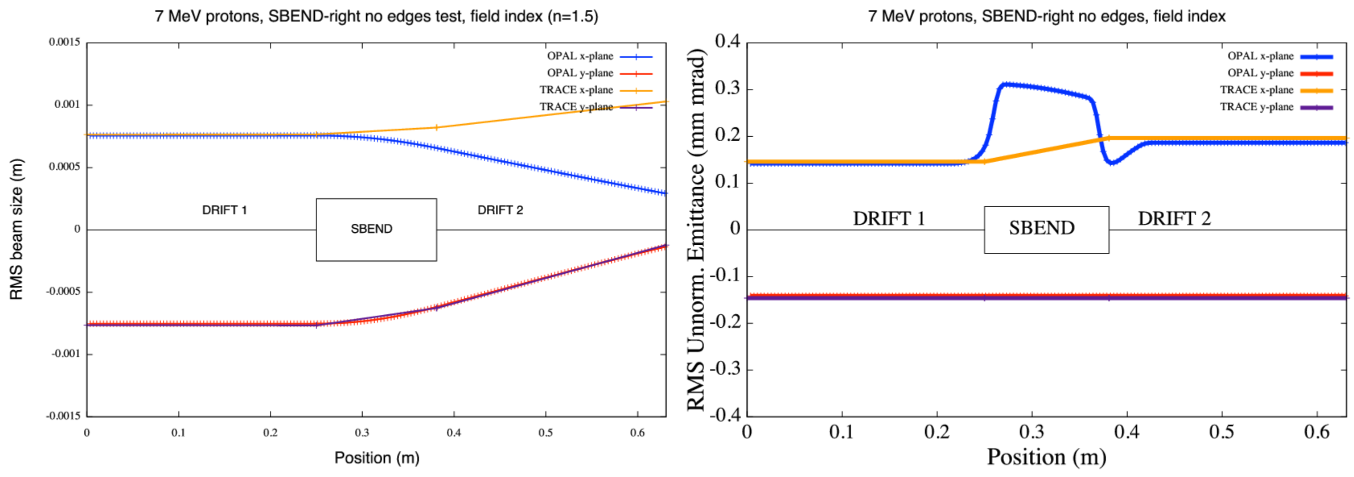


Figure 60: TRACE 3D and *OPAL* comparison: SBEND with field index and default field map

Concerning the emittances and vertical beam size, a perfect agreement has been found, instead a defocusing effect appears in the horizontal plane. These results have been obtained with the default field map provided by *OPAL*. However, a better result, only in the beam size as shown in Figure 61, is achieved using a test field map in which the fringe field extension has been changed in the thin lens approximation.

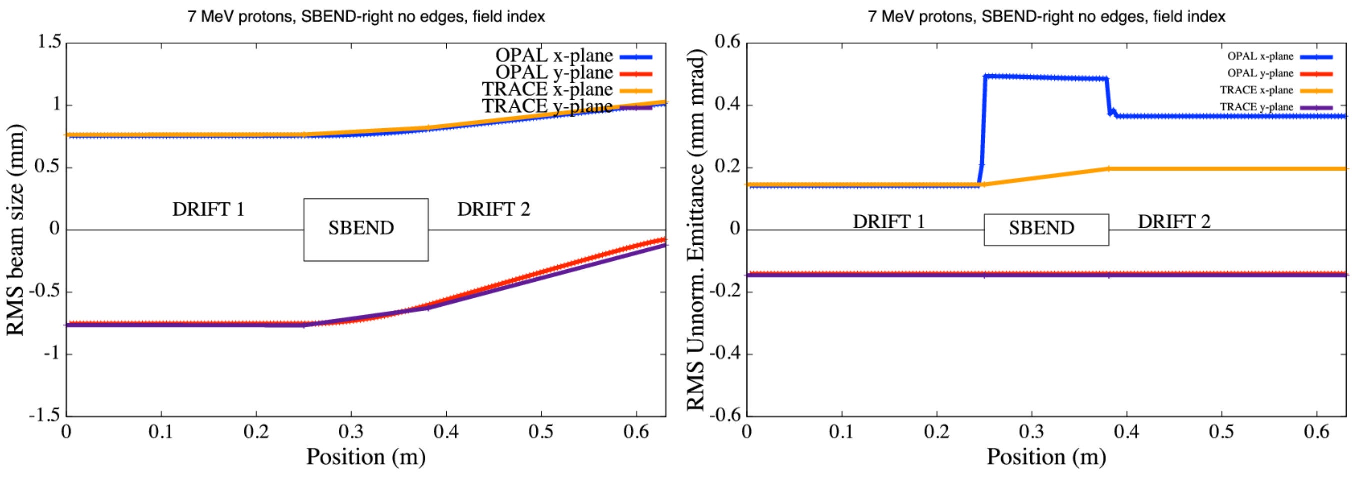


Figure 61: TRACE 3D and *OPAL* comparison: SBEND with field index and test field map

E.1.11.1 From TRACE 3D to *OPAL-t*

Parameter	**Trace 3D**	***OPAL-t***
Bend card	8	`SBEND` or `RBEND`
Angle	Input parameter [deg]	Input/Calc. parameter [rad]
Magn. field	Calculated. [T]	Input/Calc parameter [T]
Radius of curv.	Input parameter [mm]	Output information [m]
Field-index	Input parameter	Input parameter
Length	Calculated [mm]	Input/Calc parameter [m]
Length type	Effective	Straight
Edge card	9	`SBEND` or `RBEND`
Edge angle	Input parameter [deg]	Input parameter [rad]
Vertical gap	9	`SBEND` or `RBEND`
Gap	Total [mm]	Total [m]
Fringe field card	9	FIELD MAP
K_1	Default: 0.45	-
K_2	Default: 2.8	-
Bend direction	Bend angle sign	Coord. rotation
Horiz. right	Angle > 0	Angle > 0
Horiz. left	Angle < 0	Angle < 0
Vertical bend	Card 8, vf > 0	Coord. rotation

Table 80: Bending magnet features in TRACE 3D and *OPAL-t*

E.1.12 Conclusion

- **TRACE 3D and TRANSPORT:**
  - a perfect agreement has been found between these two codes in transversal envelope and emittance;
  - changing the TRANSPORT units, the input beam parameters, in terms of sigma-matrix coefficients, can directly be imported from TRACE 3D file.
- **TRACE 3D and *OPAL-t*:**
  - a good agreement has been found between these two codes in case of sector bending magnet with and without edge angles;
  - the default magnetic field map seems not working properly if the field index is not zero
  - an improvement of the test map used is needed in order to match the TRACE 3D emittance see Figure 61.

E.2 Hard Edge Dipole Comparison with ELEGANT

E.2.1 *OPAL* Dipole

When defining a dipole (`SBEND` or `RBEND`) in *OPAL*, a fringe field map which defines the range of the field and the Enge coefficients is required. If no map is provided, the code uses a default map. Here is a dipole definition using the default map:

```
bend1: SBEND, ANGLE = bend_angle,
E1 = 0, E2 = 0,
FMAPFN = "1DPROFILE1-DEFAULT",
ELEMEDGE = drift_before_bend,
DESIGNENERGY = bend_energy,
L = bend_length,
WAKEF = FS_CSR_WAKE;
```

Please refer to 1DProfile1 for the definition of the field map and the default map `1DPROFILE1-DEFAULT`. It defines a fringe field that extends to 10 cm away from a dipole edge in both directions and it has both B_y and B_z components. This makes the comparison between *OPAL* and other codes which uses a hard edge dipole by default,cumbersome because one needs to carefully integrate thought the fringe field region in *OPAL* in order to come up with the integrated fringe field value (FINT in ELEGANT) that usually used by these codes, e.g. the ELEGANT and the TRACE3D. So we need to find a default map for the hard edge dipole in *OPAL*.

E.2.2 Map for Hard Edge Dipole

The proposed default map for a hard edge dipole can be:

```
1DProfile1  0  0  2
-0.00000001 0.0 0.00000001 3
-0.00000001 0.0 0.00000001 3
-99.9
-99.9
```

On the first line, the two zeros following `1DProfile1` are the orders of the Enge coefficient for the entrance and exit edge of the dipole. $2cm$ is the default dipole gap width. The second line defines the fringe field region of the entrance edge of the dipole which extends from $-0.00000001cm$ to $0.00000001cm$. The third line defines the same fringe field region for the exit edge of the dipole. The 3s on both line don't mean anything, they are just placeholders. On the fourth and fifth line, the zeroth order Enge coefficients for both edges are given. Since they are large negative numbers, the field in the fringe field region has no B_z component and its B_y component is just like the field in the middle of the dipole.

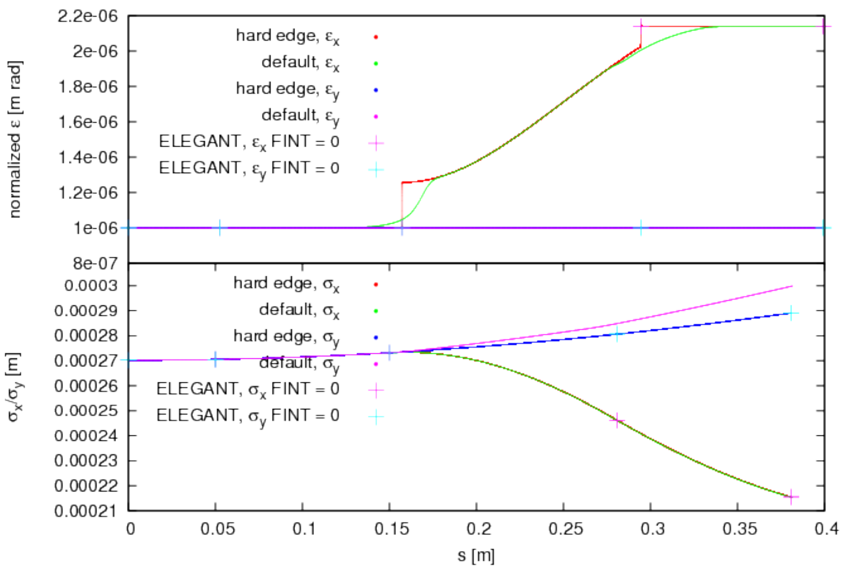


Figure 62: Compare emittances and beam sizes obtained by using the hard edge map (*OPAL*), the default map (*OPAL*), and the ELEGANT

Figure 62 compares the emittances and beam sizes obtained by using the hard edge map, the default map and the ELEGANT. One can see that the results produced by the hard edge map match the ELEGANT results when FINT is set to zero.

E.2.3 Integration Time Step

When the hard edge map is used for a dipole, finer integration time step is needed to ensure the accurate of the calculation. Figure 63 compares the normalized emittances generated using the hard edge map in *OPAL* with varying time steps to those from the

ELEGANT. 0.01ps seems to be a optimal time step for the fringe field region. To speed up the simulations, one can use larger time steps outside the fringe field regions. In Figure 63, one can observe a discontinuity in the horizontal emittance when the hard edge map is used in the calculation. This discontinuity comes from the fact that *OPAL* emittance is calculated at an instant time. Once the beam or part of the beam gets into the dipole, its P_x gets a kick which will result in a sudden emittance change.

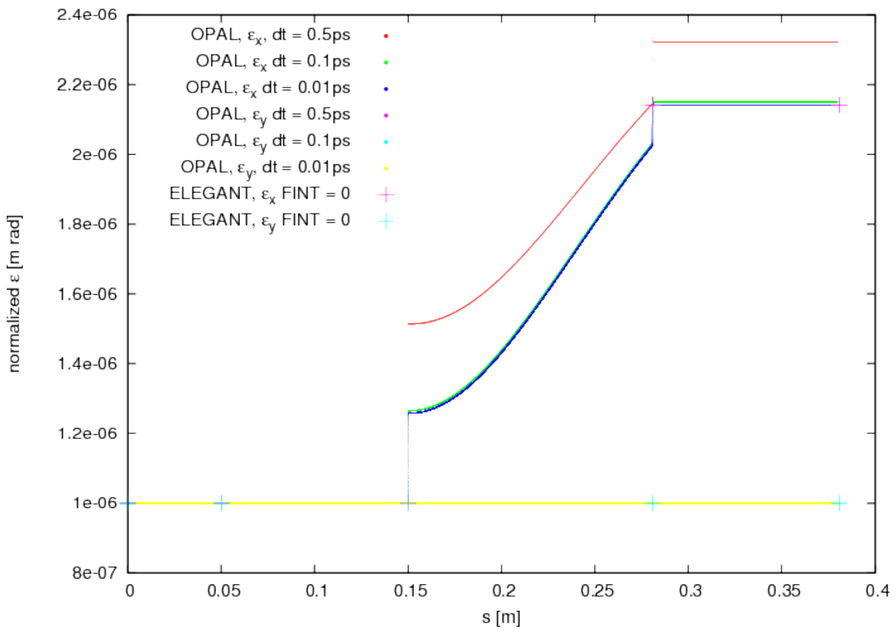


Figure 63: Horizontal and vertical normalized emittances for different integration time steps

Figure 64 and Figure 65 examine the effects of the fringe field range and the integration time step on the simulation accuracy. Figure 65 is a zoom-in plot of Figure 64. We can conclude that the size of the integration time step has more influence on the accuracy of the simulation.

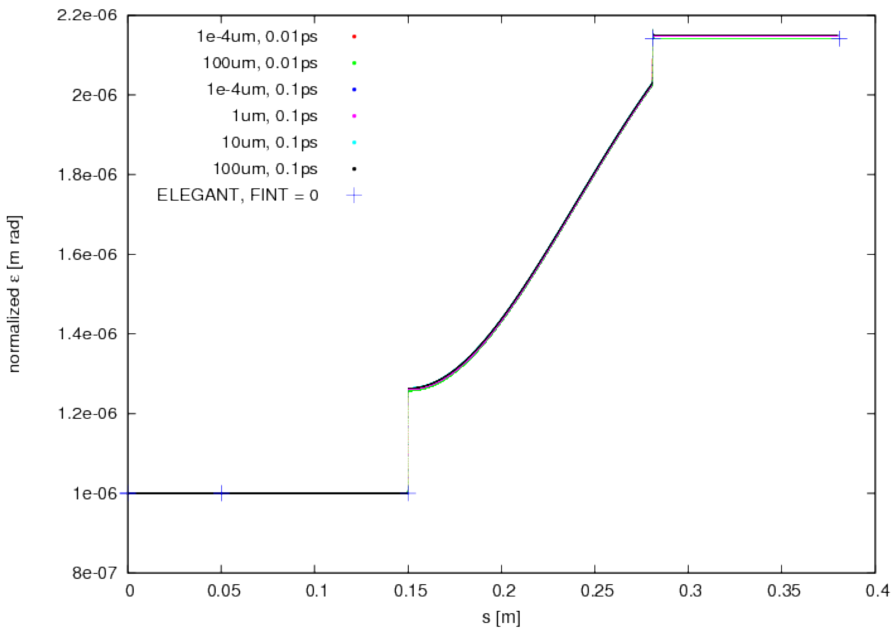


Figure 64: Normalized horizontal emittance for different fringe field ranges and integration time steps

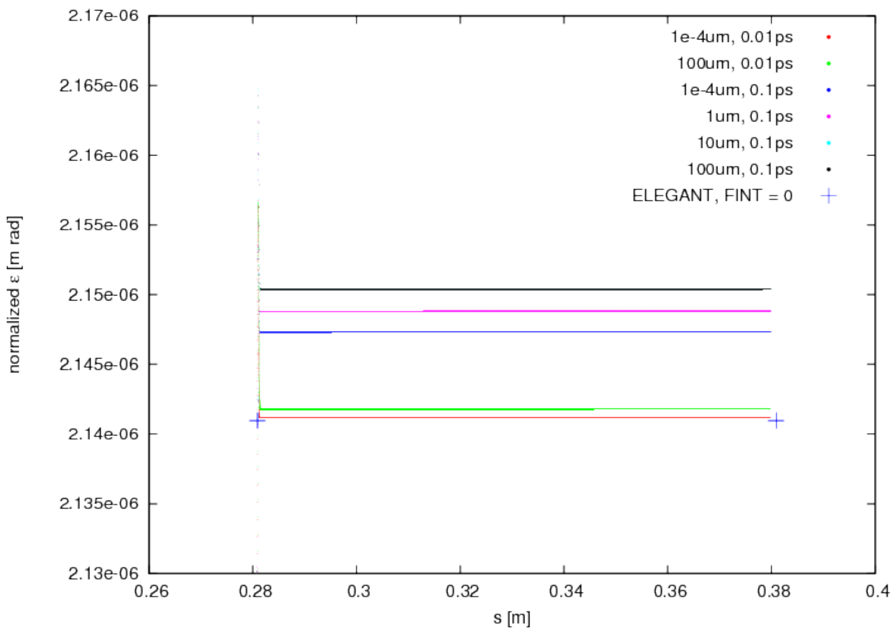


Figure 65: Zoom in on the final emittance in Figure 64

E.3 1D CSR comparison with ELEGANT

1D-CSR wake function can now be used for the drift element by defining its attribute `WAKEF = FS_CSR_WAKE`. In order to calculate the CSR effect correctly, the drift has to follow a bending magnet whose CSR calculation is also turned on.

```
bend1: SBEND, ANGLE = bend_angle,
E1 = 0, E2 = 0,
FMAPFN = "1DPROFILE1-DEFAULT",
ELEMEDGE = drift_before_bend,
DESIGNENERGY = bend_energy,
L = bend_length,
WAKEF = FS_CSR_WAKE;
```

```
drift1: DRIFT, L=0.4, ELEMEDGE = drift_before_bend +
bend_length, WAKEF = FS_CSR_WAKE;
```

E.3.1 Benchmark

The *OPAL* dipoles all have fringe fields. When comparisons are done between *OPAL* and ELEGANT [86] for example, one needs to appropriately set the FINT attribute of the bending magnet in ELEGANT in order to represent the field correctly. Although ELEGANT tracks in the $(x, x', y, y', s, \delta)$ phase space, where $\delta = \frac{\Delta p}{p_0}$ and p_0 is the momentum of the reference particle, the watch point output beam distributions from the ELEGANT are list in $(x, x', y, y', t, \beta\gamma)$. If one wants to compare ELEGANT watch point output distribution to *OPAL*, unit conversion needs to be performed, i.e.

$$\begin{aligned} P_x = & \quad x'\beta\gamma, \\ P_y = & \quad y'\beta\gamma, \\ s = & \quad (\bar{t} - t)\beta c. \end{aligned}$$

To benchmark the CSR effect, we set up a simple beamline with 0.1 m drift, 30 degree sbend and a 0.4 m drift. When the CSR effect is turn off, Figure 66 shows that the normalized emittances calculated using both *OPAL* and ELEGANT agree. The emittance values from *OPAL* are obtained from the *.stat* file, while for ELEGANT, the transverse emittances are obtained from the sigma output file (enx, and eny), the longitudinal emittance is calculated using the watch point beam distribution output.

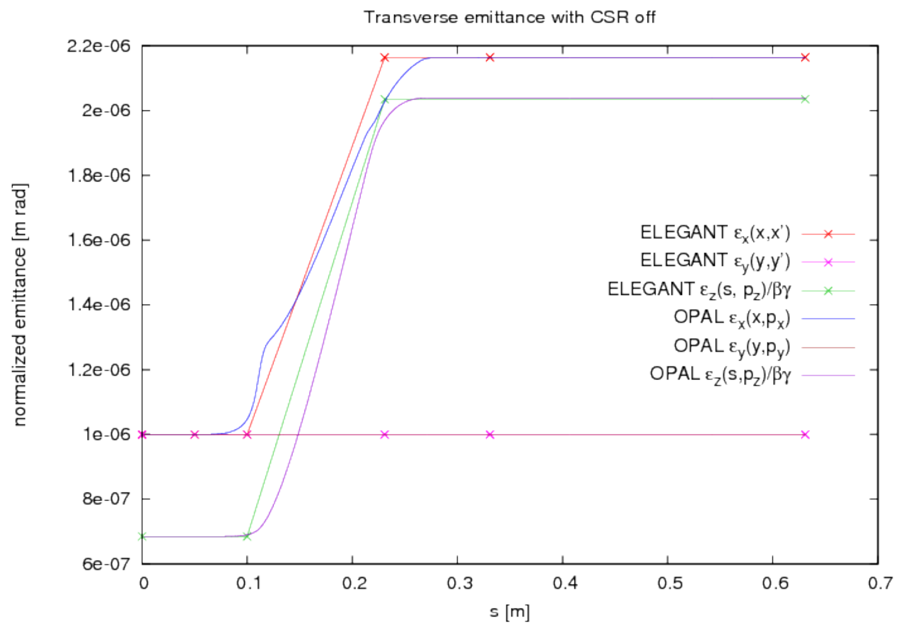


Figure 66: Comparison of the trace space using ELEGANT and *OPAL*

When CSR calculations are enabled for both the bending magnet and the following drift, Figure 67 shows the average δ or $\frac{\Delta p}{p}$ change along the beam line, and Figure 68 compares the normalized transverse and longitudinal emittances obtained by these two codes. The average $\frac{\Delta p}{p}$ can be found in the centroid output file (Cdelta) from ELEGANT, while in *OPAL*, one can calculate it using $\frac{\Delta p}{p} = \frac{1}{\beta^2}\frac{\Delta \bar{E}}{\bar{E}+mc^2}$, where $\Delta\bar{E}$ is the average kinetic energy from the *.stat* output file.

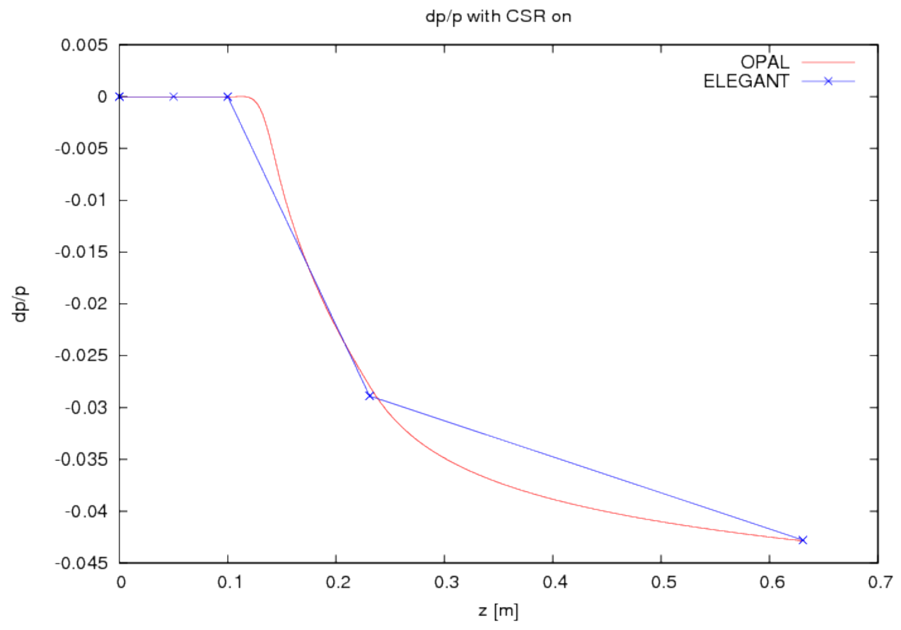


Figure 67: $\frac{\Delta p}{p}$ in Elegant and *OPAL*

In the drift space following the bending magnet, the CSR effects are calculated using Stupakov's algorithm with the same setting in both codes. The average fractional momentum change $\frac{\Delta p}{p}$ and the longitudinal emittance show good agreements between these codes. However, they produce different horizontal emittances as indicated in Figure 68.

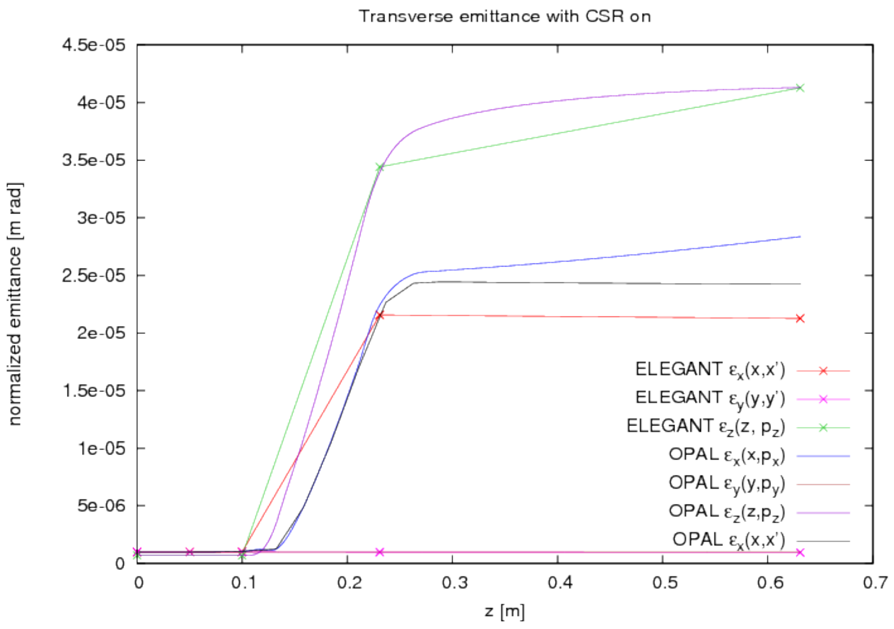


Figure 68: Transverse emittances in ELEGANT and *OPAL*

One important effect to notice is that in the drift space following the bending magnet, the normalized emittance $\varepsilon_x(x,P_x)$ output by *OPAL* keeps increasing while the trace-like emittance $\varepsilon_x(x,x')$ calculated by ELEGANT does not. This can be explained by the fact that with a relatively large energy spread (about 3% at the end of the dipole due to CSR), **a correlation** between transverse position and energy can build up in a drift thereby induce emittance growth. However, this effect can only be observed in the normalized emittance calculated with $\varepsilon_x(x,P_x) = \sqrt{\langle x^2\rangle\langle P_x^2\rangle - \langle xP_x\rangle^2}$ where $P_x = \beta\gamma x'$, not the trace-like emittance which is calculated as $\varepsilon_x(x,x') = \beta\gamma\sqrt{\langle x^2\rangle\langle x'^2\rangle - \langle xx'\rangle^2}$ [prstab2003]. In Figure 68, a trace-like horizontal emittance is also calcualted for the *OPAL* output beam distributions. Like the ELEGANT result, this trace-like emittance doesn't grow in the drift. However, their differences come from the ELEGANT's lack of CSR effect in the fringe field region.

E.4 *OPAL* & `Impact-t`

This benchmark compares rms quantities such as beam size and emittance of *OPAL* and `Impact-t` [qiang2005, qiang2006-1, qiang2006-2]. A **cold** 10mA H+ bunch is expanding in a 1m drift space. A Gaussian distribution, with a cut at 4 σ is used. The charge is computed by assuming a 1MHz structure i.e. $Q_{\mathrm{tot}} = \frac{I}{\nu_{\mathrm{rf}}}$. For the simulation we use a grid with 16^3 grid point and open boundary condition. The number of macro particles is $N_{\mathrm{p}} = 10^5$.

E.4.1 *OPAL* Input

```
OPTION, ECHO = FALSE, PSDUMPFREQ = 10,
STATDUMPFREQ = 10, REPARTFREQ = 1000,
PSDUMPFRAME = GLOBAL, VERSION=10600;

TITLE, string="Gaussian bunch drift test";

REAL Edes    = 0.001;        // GeV
REAL CURRENT = 0.01;  // A
REAL gamma=(Edes+PMASS)/PMASS;
REAL beta=sqrt(1-(1/gamma^2));
REAL gambet=gamma*beta;
REAL P0 = gamma*beta*PMASS;

D1: DRIFT, ELEMEDGE = 0.0, L = 1.0;

L1: LINE = (D1);

Fs1: FIELDSOLVER, FSTYPE = FFT, MX = 16, MY = 16, MT = 16, BBOXINCR=0.1;

Dist1: DISTRIBUTION, TYPE = GAUSS,
       OFFSETX = 0.0, OFFSETY = 0.0, OFFSETZ = 15.0e-3,
       SIGMAX = 5.0e-3, SIGMAY = 5.0e-3, SIGMAZ = 5.0e-3,
       OFFSETPX = 0.0, OFFSETPY = 0.0, OFFSETPZ = 0.0,
       SIGMAPX = 0.0 , SIGMAPY = 0.0 , SIGMAPZ = 0.0 ,
       CORRX = 0.0, CORRY = 0.0, CORRZ = 0.0,
       CUTOFFX = 4.0, CUTOFFY = 4.0, CUTOFFLONG = 4.0;

Beam1: BEAM, PARTICLE = PROTON, CHARGE = 1.0, BFREQ = 1.0, PC = P0,
               NPART = 1E5, BCURRENT = CURRENT, FIELDSOLVER = Fs1;

SELECT, LINE = L1;

TRACK, LINE = L1, BEAM = Beam1, MAXSTEPS = 1000, ZSTOP = 1.0, DT = 1.0e-10;
 RUN, METHOD = "PARALLEL-T", BEAM = Beam1, FIELDSOLVER = Fs1, DISTRIBUTION = Dist1;
ENDTRACK;
STOP;
```

E.4.2 `Impact-t` Input

```
!Welcome to Impact-t input file.
!All comment lines start with "!" as the first character of the line.
! col row
1 1
!
! information needed by the integrator:
! step-size, number of steps, and number of bunches/bins (??)
!
!   dt    Ntstep  Nbunch
1.0e-10   700     1
!
! phase-space dimension, number of particles, a series of flags
! that set the type of integrator, error study, diagnostics, and
! image charge, and the cutoff distance for the image charge
!
! PSdim  Nptcl   integF  errF  diagF  imchgF  imgCutOff (m)
6 100000  1 0 1 0 0.016
!
! information about mesh: number of points in x, y, and z, type
! of boundary conditions, transverse aperture size (m),
! and longitudinal domain size (m)
!
!  Nx  Ny  Nz  bcF   Rx    Ry    Lz
16 16 16 1 0.15 0.15 1.0e5
!
!
! distribution type number (2 == Gauss), restart flag, space-charge substep
! flag, number of emission steps, and max emission time
```

```
!
! distType  restartF  substepF  Nemission  Temission
2           0         0         -1          0.0
!
!  sig*   sigp*  mu*p*  *scale  p*scale  xmu*      xmu*
!
0.005 0.0 0.0  1. 1. 0.0 0.0
0.005 0.0 0.0  1. 1. 0.0 0.0
0.005 0.0 0.0  1. 1. 0.0 0.0462
!
! information about the beam: current, kinetic energy, particle
! rest energy, particle charge, scale frequency, and initial cavity phase
!
! I/A   Ek/eV     Mc2/eV          Q/e  freq/Hz  phs/rad
0.010   1.0e6     938.271998e+06  1.0  1.0e6      0.0
!
!
! ======= machine description starts here =======
! the following lines, which must each be terminated with a '/',
! describe one beam-line element per line; the basic structure is
! element length, ???, ???, element type, and then a sequence of
! at most 24 numbers describing the element properties
!   0  drift tube    2      zedge radius
!   1  quadrupole    9      zedge, quad grad, fileID,
!                             radius, alignment error x, y
!                             rotation error x, y, z
! L/m  N/A N/A  type  location of starting edge  v1  <B0><B0><B0>  v23 /
1.0    0   0    0    0.0                           0.5            /
```

E.4.3 Results

A good agreement is shown in the Figure 69 and Figure 70. This proves to some extend the compatibility of the space charge solvers of *OPAL* and `Impact-t`.

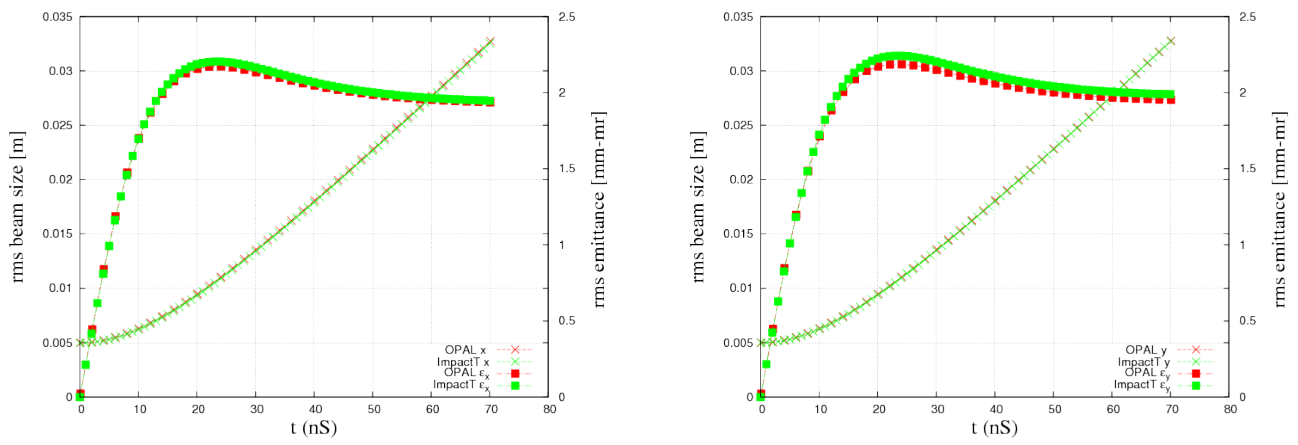


Figure 69: Transverse beam sizes and emittances in `Impact-t` and *OPAL*

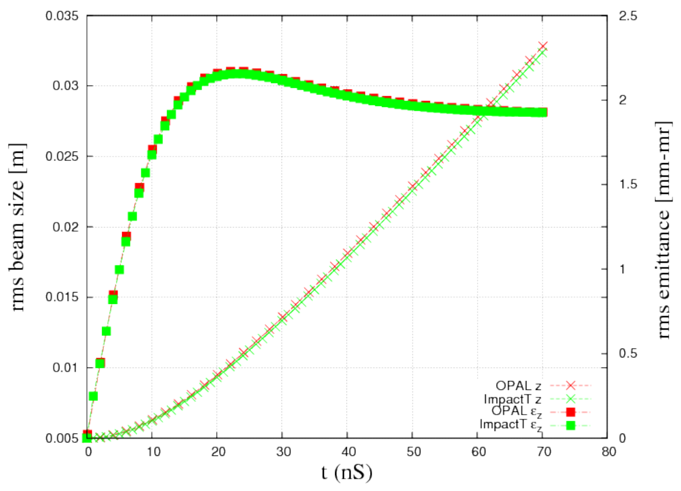


Figure 70: Longitudinal beam size and emittance in `Impact-t` and *OPAL*

E.5 References

[82] K. Crandall and D. Rusthoi, *Documentation for TRACE: An Interactive Beam-Transport Code*, Tech. Rep. LA—10235-MS, Los Alamos National Laboratory (1985).

[83] K. L. Brown et al., *TRANSPORT - A Computer Program for Designing Charged Particle Beam Transport Systems*, Tech. Rep. CERN 80-4, European Organization for Nuclear Research (1980).

[84] U. Rohrer, *PSI graphic transport framework based on a CERN-SLAC-FERMILAB version by K.L. Brown et al*.

[85] U. Rohrer, http://aea.web.psi.ch/Urs_Rohrer/MyWeb/moregifs/gantryb.gif.

[86] M. Borland, *elegant: a flexible SDDS-compliant code for accelerator simulation*, Tech. Rep. LS-287, Advanced Photon Source (2000).