The OPAL Framework

Version 2.0

WRITTEN BY

Andreas Adelmann, Christian Baumgarten, Matthias Frey, Achim Gsell, Valeria Rizzoglio, Jochem Snuverink (PSI) Christof Metzger-Kraus, Yves Ineichen, Xiaoying Pang, Steve Russell (LANL), Chuan Wang (CIAE), Suzanne Sheehy, Chris Rogers (RAL) and Daniel Winklehner (MIT)

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Abstract

OPAL is a tool for charged-particle optics in accelerator structures and beam lines. Using the *MAD* language with extensions, *OPAL* is derived from *MAD9P* and is based on the *CLASSIC* 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 ansatz. IPPL was inspired by the POOMA. *OPAL* is built from the ground up as a parallel application exemplifying the fact that HPC (High Performance Computing) is the third leg of science, complementing theory and the experiment. HPC is made possible now through the increasingly sophisticated mathematical models and evolving computer power available on the desktop and in super computer centres. *OPAL* runs on your laptop as well as on the largest HPC clusters available today.

The *OPAL* framework makes it easy to add new features in the form of new *C++* classes. It 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 can be used to model beam lines, linacs, rf-photo injectors and complete XFELs excluding the undulator.

It should be noted that not all features of *OPAL* are available in all flavours. The icon `DOPAL-t` means that a feature is not yet available in *OPAL-t*. Similar icons are used for the other flavours.

Chapter 2

Introduction

2.1 Aim of *OPAL* and History

OPAL is a tool for charged-particle optics in accelerator structures and beam lines. 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 [5]. *OPAL* is built from the ground up as a parallel application exemplifying the fact that HPC (High Performance Computing) is the third leg of science, complementing theory and the experiment. HPC is made possible now through the increasingly sophisticated mathematical models and evolving computer power available on the desktop and in super computer centers. *OPAL* runs on your laptop as well as on the largest HPC clusters available today.

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

OPAL comes in the following flavors:

- *OPAL-cycl*
- *OPAL-t*

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

OPAL-t is a super-set of *Impact-t* [2] and can be used to model guns, injectors, ERLs and complete XFELs excluding the undulator.

It should be noted that not all features of *OPAL* are available in both flavors. The following icon `DOPAL-t` means that a feature is not yet available in *OPAL-t*. A similar icon is used for *OPAL-cycl*.

2.2 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.

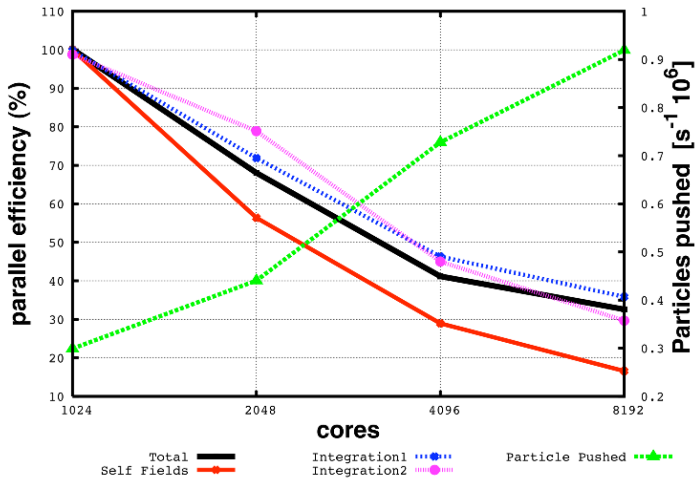


Figure 1: Parallel efficiency and particles pushed per μs as a function of cores

2.3 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.

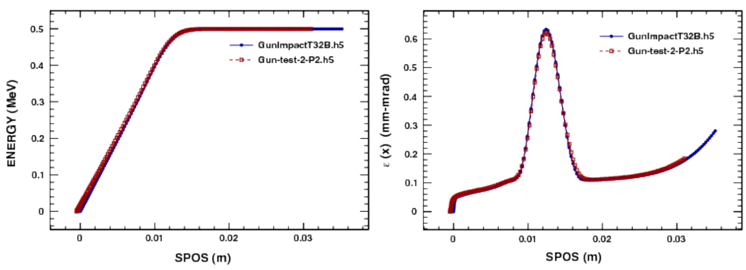


Figure 2: Comparison of energy and emittance in x between *Impact-t* and *OPAL-t*

2.4 Output

The phase space is stored in the H5hut file-format [3] and can be analyzed using e.g. H5root [4]. The frequency of the data output (phase space and some statistical quantities) can be controlled using the `OPTION` statement 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 see Option Statement with the flag STATDUMPFREQ.

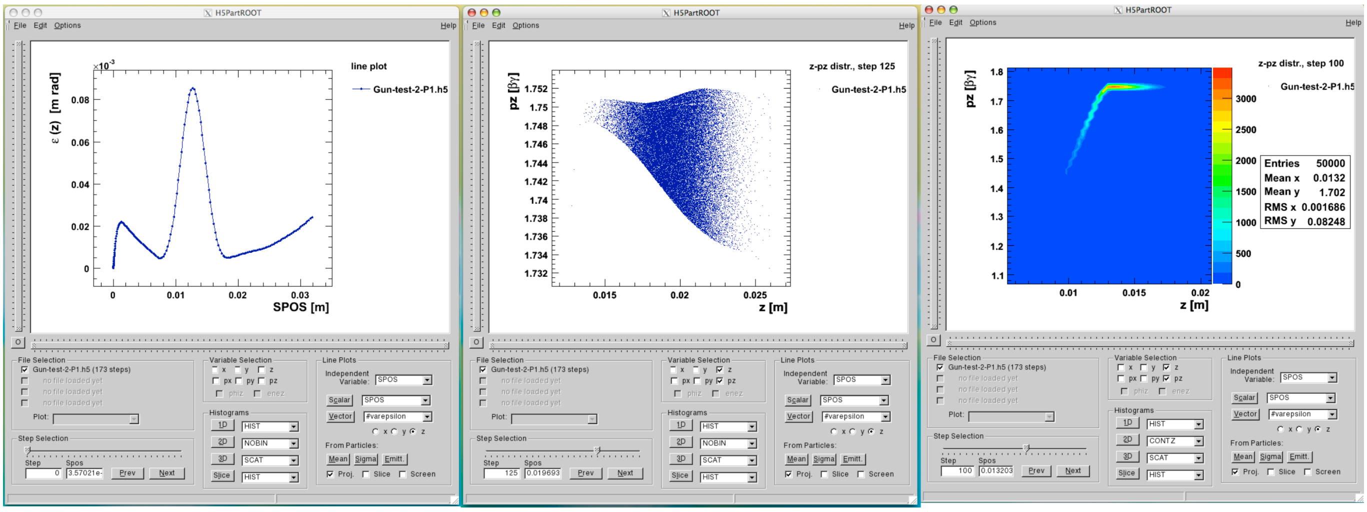


Figure 3: H5root enables a variety of data analysis and post processing task on *OPAL* data

Very important information is displayed on the *stdout* i.e. the *terminal*. The user is strongly advised to consult the stdout frequently.

2.5 Change History

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

2.6 Known Issues and Limitations

See the issue list in the repository.

See also pitfalls and limitations.

2.7 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: Yuanjie Bi, Jianjun Yang, Colwyn Gulliford, Hao Zha, Christopher Mayes, Tulin Kaman, Chuan Wang, Yves Ineichen, Valeria Rizzoglio and Christian Baumgarten.

2.8 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}
}
```

:empty;

2.9 References

[1] F. C. Iselin, *The classic project*, tech. rep. CERN/SL/96-061 (CERN, 1996).

[2] J. Qiang et al., *A three-dimensional quasi-static model for high brightness beam dynamics simulation*, tech. rep. LBNL-59098 (LBNL).

[3] M. Howison et al., *H5hut: A High-Performance I/O Library for Particle-based Simulations*, in IEEE International Conference on Cluster Computing Workshops and Posters (2010), pp. 1–8, 10 . 1109 / CLUSTERWKSP.2010.5613098.

[4] T. Schietinger, *H5root*, 2006.

[5] http://www.nongnu.org/freepooma/

Chapter 3

Conventions

3.1 Physical Units

Throughout the computations *OPAL* uses international units, as defined by SI (Système International).

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
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

3.2 *OPAL*-cycl

The *OPAL*-cycl flavor see Cyclotron is using the so called Cyclotron units. Lengths are defined in (mm), frequencies in (MHz), momenta in ($\beta\gamma$) and angles in (deg), except `RFPHI` which is in (rad).

3.3 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.

Chapter 4

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.

4.1 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.

4.2 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 5

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.

5.1 The Simulation Cycle

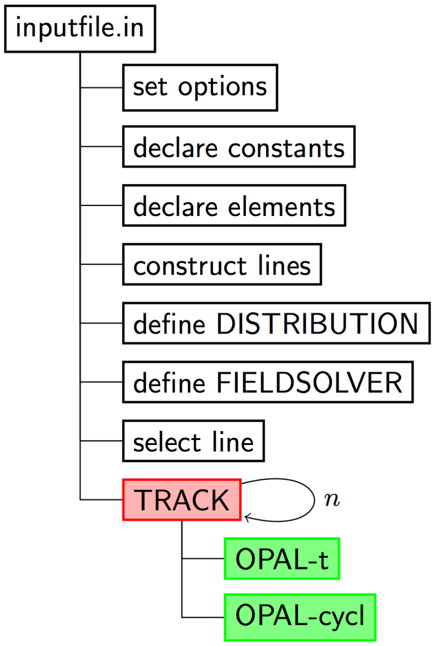


Figure 4: The simulation cycle

5.2 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 following command line arguments:

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. Full support currently only in *OPAL-t*.
--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.
--version		Prints the version and then quits.

Example:

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

5.3 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.

5.4 Examples of Particle Accelerators and Beamlines

OBLA-Gun.in

5.4.1 PSI XFEL 250 MeV Injector

diagnostic.in

5.4.2 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 and other data files.

opal-cycl.in

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

```
opal testinj2-1.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.

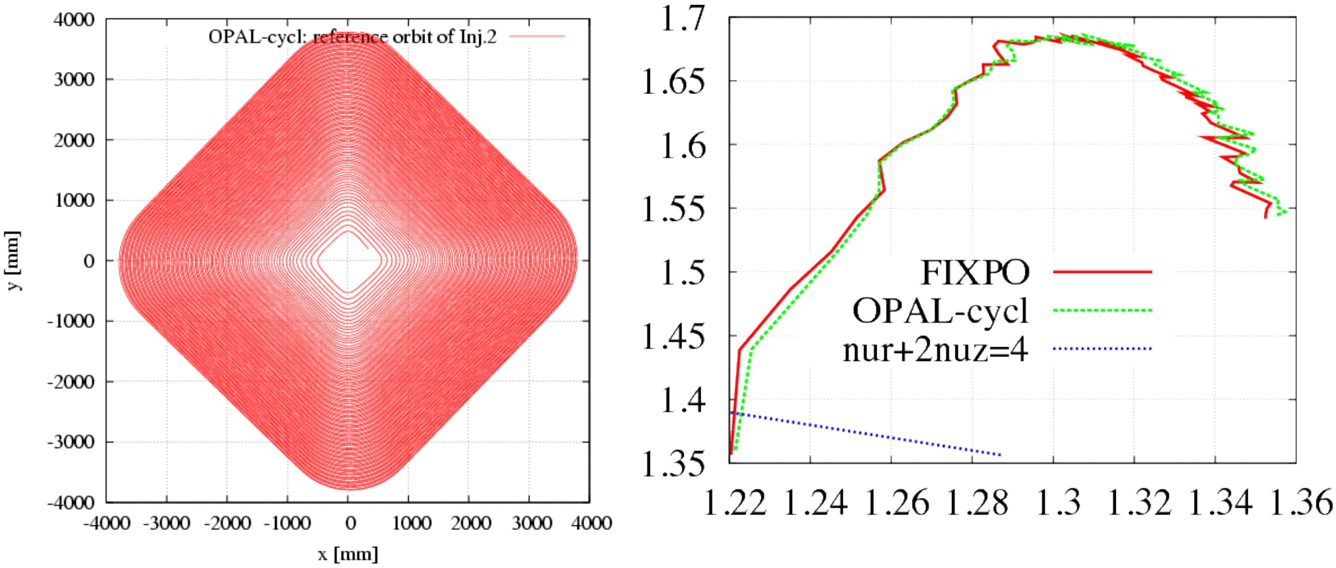


Figure 5: Reference orbit(left) and tune diagram(right) in Injector II

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.

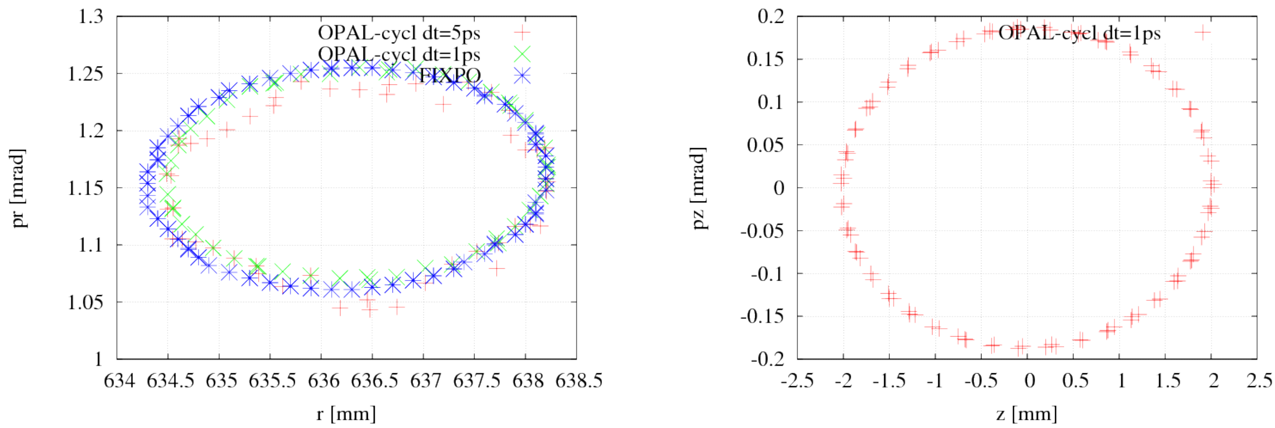


Figure 6: Radial and vertical eigenellipse at 2 MeV of Injector II

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.

opal-cycl-sc.in

To run opal on single node, just use this command:

```
# opal testinj2-2.in
```

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

```
# mpirun -np N opal testinj2-2.in
```

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

```
# mpirun -np N opal testinj2-2.in --restart -1
```

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

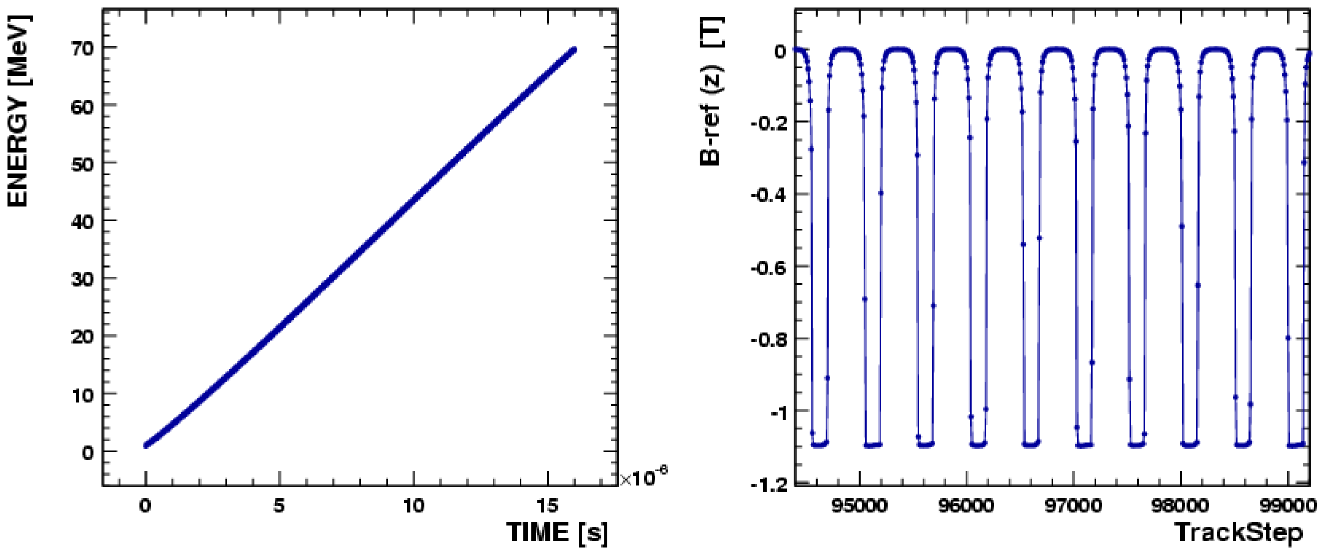


Figure 7: Energy vs. time (left) and external B field vs. track step (Right, only show for about 2 turns)

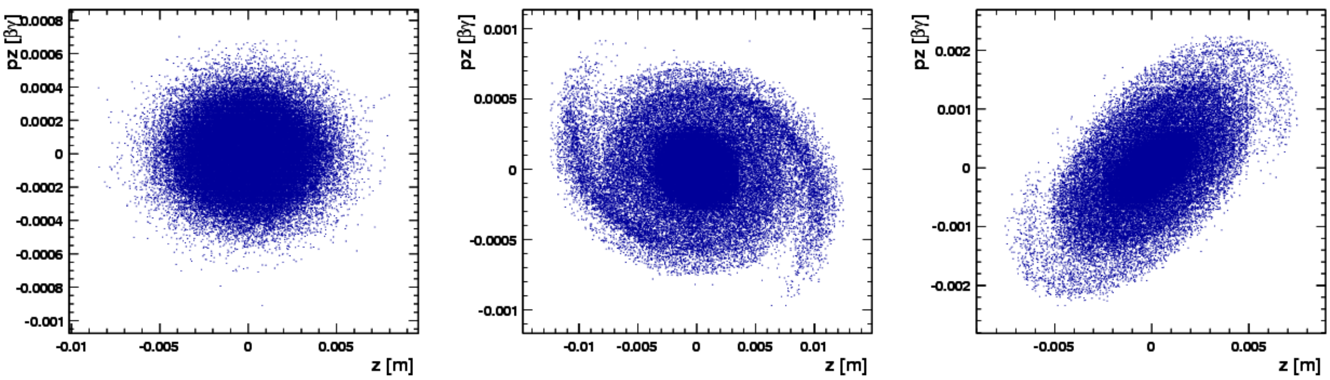


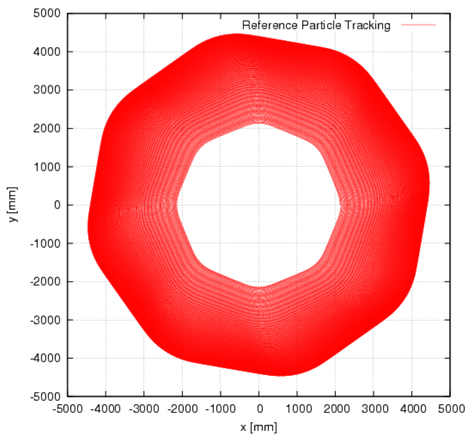
Figure 8: Vertical phase at different energy from left to right: 0.87 MeV, 15 MeV and 35 MeV

5.4.3 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.



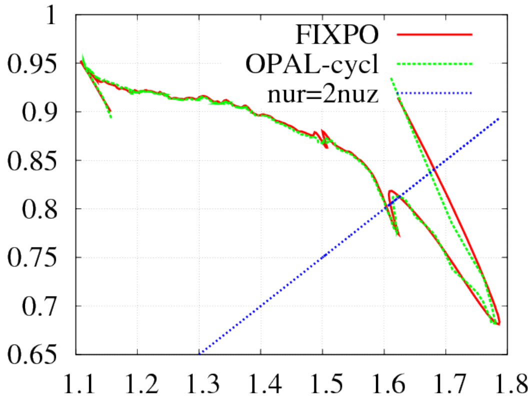


Figure 9: Reference orbit(left) and tune diagram(right) in Ring cyclotron

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.

5.5 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.)

5.5.1 `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 18 to a value that is 10 $\times$ the value of the distribution attribute Table 16 in order for your simulation to behave the same as before.

5.5.2 `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 with one exception. If you are using *OPAL-cycl* then your old input files will work just fine. However, if you are using *OPAL-t* then you will need to set the distribution attribute INPUTMOUNITS to:

```
INPUTMOUNITS = EV
```

Chapter 6

OPAL-t

6.1 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 [6], [7], [8] 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 [9], [6], [7],[8]. 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.

6.2 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 [1].

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

PY $\beta_y\gamma$ Vertical canonical momentum [1].

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

PZ $\beta_z\gamma$ Longitudinal canonical momentum [1].

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

6.3 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 [10].

6.4 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.

6.5 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

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

6.5.1 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 $e_0, \ldots, e_i, \ldots e_n$.

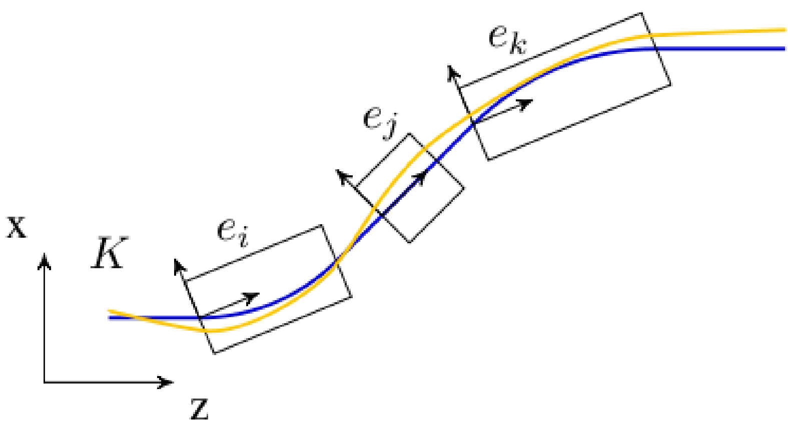


Figure 10: Illustration of local and global coordinates.

6.5.2 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 [11].

The displacement is described by a vector **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). **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.

6.5.3 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.

6.5.4 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).

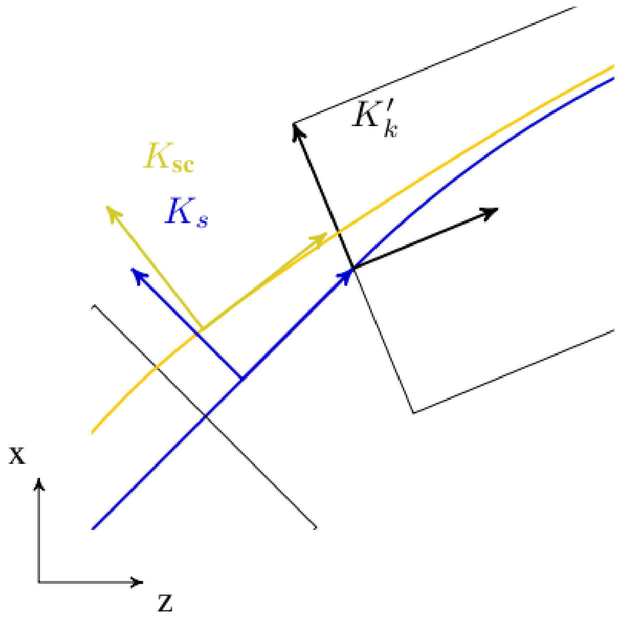


Figure 11: Illustration of K_{sc} and K_s

Both coordinate systems are described in Figure 11.

6.5.5 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.

6.5.6 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.

6.5.7 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 $\mathscr{S}_\text{e} \subset e_0 \ldots e_n$ in case of the example given in Figure 10. An implicit drift is modelled as an empty set $\emptyset$.

6.6 Flow Diagram of *OPAL-t*

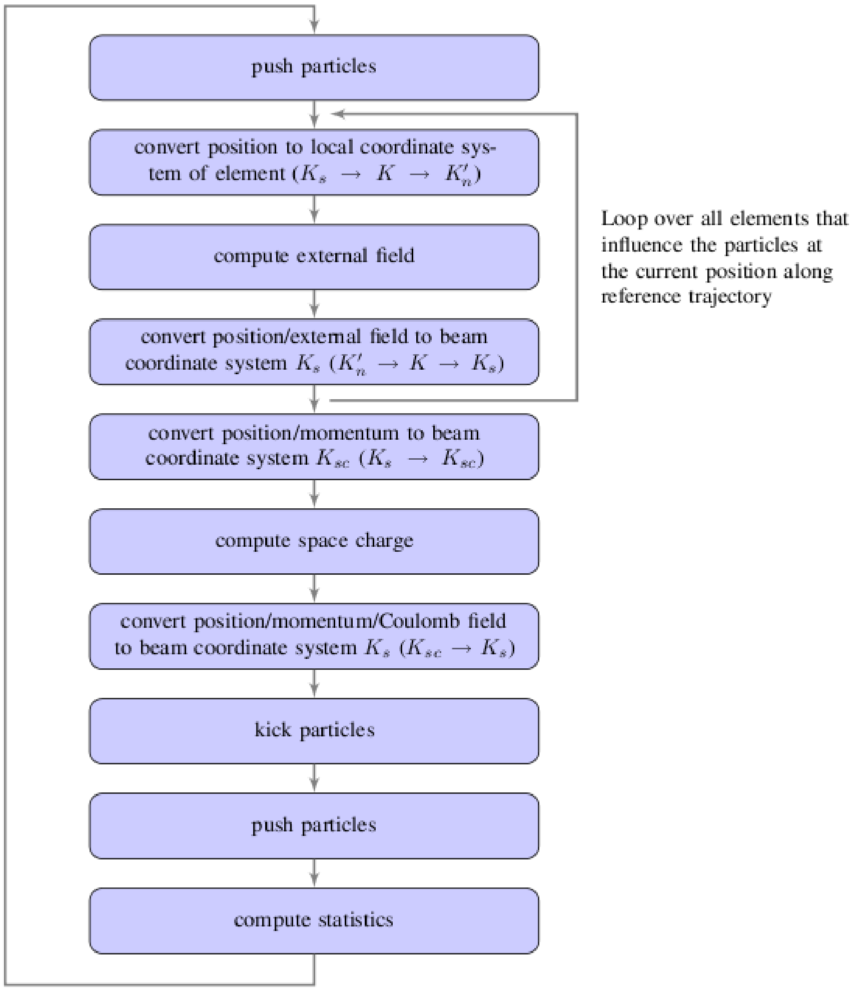


Figure 12: Schematic workflow of *OPAL-t*'s execute method.

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.

6.7 Output

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

6.7.1 *<input_file_name >.stat*

This file is used to log the statistical properties of the bunch in the ASCII variant of the SDDS format [12]. It can be viewed with the SDDS Tools [13] or GNUPLOT. The frequency with which the statistics are computed and written to file can be controlled With the option `STATDUMPFREQ`. The information that is stored are found in the following table.

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`
43	R0_x	m	X-component of position of particle with ID 0 (only when run serial)
44	R0_y	m	Y-component of position of particle with ID 0 (only when run serial)
45	R0_s	m	S-component of position of particle with ID 0 (only when run serial)

Column Nr.	Name	Units	Meaning
46	P0_x	m	X-component of momentum of particle with ID 0 (only when run serial)
47	P0_y	m	Y-component of momentum of particle with ID 0 (only when run serial)
48	P0_s	m	S-component of momentum of particle with ID 0 (only when run serial)

6.7.2 *data/<input_file_name >_Monitors.stat*

OPAL-t computes the statistics of the bunch for every `MONITOR` that it passes. 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

6.7.3 *data/<input_file_name >_3D.opal*

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`.

6.7.4 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.

6.7.5 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 [14], [15] or VisIt [16]. 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 ⇐ r|g|b ⇐ 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`

6.7.6 data/<input_file_name >_ElementPositions.stat

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		Whether the field of a dipole is present
3	quadrupole	1	Whether the field of a quadrupole is present
4	sextupole		Whether the field of a sextupole is present
5	octupole		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

6.7.7 data/<input_file_name >_DesignPath.dat

The trajectory of the reference particle is stored in this ASCII file. The content of the columns are listed in the following table.

Column Nr.	**Name**	**Units**	**Meaning**
1		m	Position in path length

Column Nr.	Name	Units	Meaning
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 m^-1	X-component of electric field at position
9		MV m^-1	Y-component of electric field at position
10		MV m^-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

6.8 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.

6.9 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.

6.9.1 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.

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

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)

$$x = r\cos\varphi \quad y = r\sin\varphi$$
$$z^n = r^n(\cos n\varphi + i\sin n\varphi)$$

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

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

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

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

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).

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

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.

6.9.2 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 6.1: 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 6.2: Maxwell equations

The substitution of Equation 6.1 into Maxwell's equations allows for the derivation of recursion relations. Equation 6.2 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 6.3: a factors

A similar result is obtained from Equation 6.2

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

EQUATION 6.4: c factors

The last equation from $\nabla \times \mathbf{B} = 0$ should be consistent with the two recursion relations obtained. Equation 6.2 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 6.3 and Equation 6.4; therefore the relations are consistent. Furthermore, the last required relations is obtained from the divergence of **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 6.3) 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*.

6.9.3 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 6.1). 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

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

6.9.4 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

$$\psi = z f_0(x,s) + \frac{z^3}{3!} f_1(x,s) + \frac{z^5}{5!} f_3(x,s) + \dots$$

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.

6.10 References

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Chapter 7

OPAL-cycl

7.1 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.

7.2 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.

7.2.1 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 Section 7.2.4.

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.

7.2.2 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.

7.2.3 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 7.7.

7.2.4 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 [eV/c].

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

PY Longitudinal canonical momentum [eV/c].

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

PZ Vertical canonical momentum [eV/c].

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

7.2.4.1 NOTE: 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],

$$(\beta_x\gamma) = \sqrt{(\frac{P_x[eV/c]}{m_0 c}+1)^2-1}.$$

This may be deduced by analogy for the y and z directions.

7.2.5 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 7.2.4. 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 using the starting coordinates r_0 (`RINIT`), ϕ_0 (`PHIINIT`), and z_0 (`ZINIT`), and the starting momenta p_{r0} (`PRINIT`), and p_{z0} (`PZINIT`) of the reference particle, defined in the `CYCLOTRON` element see Cyclotron. Note that $p_{\phi 0}$ is calculated automatically from p_{total}, p_{r0}, and p_{z0}.

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

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

7.3 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).

There are two possible situations. One is the real field map on median plane of the exist cyclotron machine using measurement equipment. Limited by the narrow gaps of magnets, in most cases with cyclotrons, only vertical field B_z on the median plane ($z = 0$) is measured. Since the magnetic field data off the median plane field components is necessary for those particles with $z \neq 0$, the field need to be expanded in Z direction. According to the approach given by Gordon and Taivassalo, 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

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

EQUATION 7.1: Third order field

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

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

All the partial differential coefficients are on the median plane and can be calculated by interpolation. *OPAL-cycl* uses Lagrange's 5-point formula.

The other situation is to calculate the field on the median plane or the 3D fields of the working gap for interesting region numerically by creating 3D model using commercial software, such as TOSCA, ANSOFT and ANSYS during the design phase of a new machine. 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. However, the 3D fields of the entire working gap should be more accurate than the expansion approach especially at the region not so close to the median plane in Z direction.

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

7.3.1 CARBONCYCL type

If `TYPE=CARBONCYCL`, the program requires the B_z data which is stored in a sequence shown in Figure 13.

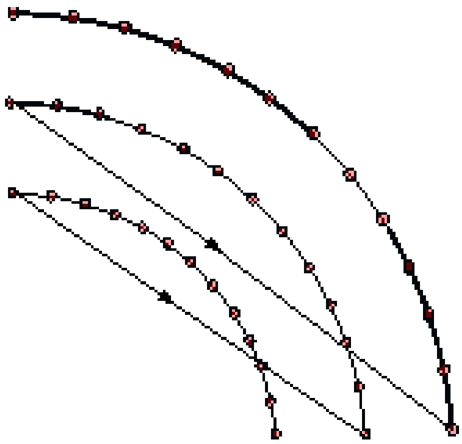

Figure 13: 2D field map on the median plane with primary direction corresponding to the azimuthal direction, secondary direction to the radial direction

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
                       ......
```

7.3.2 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 is the decimal is unlimited. For instance,if $\Delta\theta = \frac{1}{3}^\circ$, the fourth line of the header should be -3.0. In a word, 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
                         ......
```

7.3.3 BANDRF type

If `TYPE=BANDRF`, the program requires the B_z data format which is same as `CARBONCYCL`. But with `BANDRF` type, the program can also read in the 3D electric field(s). For the detail about its usage, please see Cyclotron.

7.3.4 Default PSI format

If the value of `TYPE` is other string rather than above mentioned, 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 is 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
                              ......
```

7.3.5 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).

7.3.6 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.

7.4 RF field

7.4.1 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.

7.4.2 Read 3D RF field-map

The 3D RF field-map can be read from H5hut type file. This is useful for modeling the central region electric fields which usually has complicate shapes. For the detail about its usage, please see Cyclotron.

Please note that in this case, the E field is treated as a part of `CYCLOTRON` element, rather than a independent `RFCAVITY` element.

7.5 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 7.1.

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 $t_2 = \tau - t_1$.

7.6 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.

7.7 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.

7.7.1 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.

7.8 Output

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

7.8.1 *<input_file_name >.stat*

See OPAL-t stat file.

7.8.2 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 see 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 `STEPPERTURN` steps; Otherwise, the particle may not go through a full 360 degrees in `STEPPERTURN` 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.

7.8.3 Tune calculation mode

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

7.8.4 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 [17] and can be analyzed using H5root [18]. The frequency of the data output can be set using the `PSDUMPFREQ` option of `OPTION` statement see 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 see Option Statement.

7.8.5 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 π *mm mrad*.

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

/*
 * try finding a matched distribution
```

```
 */
Dist1:DISTRIBUTION, TYPE=GAUSSMATCHED, LINE=l1, FMAPFN=...,
                    MAGSYM=..., EX = ..., EY = ..., ET = ...;
```

7.8.5.1 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,δ) 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.

7.8.5.1.1 Input file

matchedDistribution.in

7.8.5.1.2 Output

matchedDistribution.output

7.9 References

[17] M. Howison et al., *H5hut: A High-Performance I/O Library for Particle-based Simulations*, in IEEE International Conference on Cluster Computing Workshops and Posters (2010), pp. 1–8, 10 . 1109 / CLUSTERWKSP.2010.5613098.

[18] T. Schietinger, *H5root*, 2006.

Chapter 8

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 *MAD*eight 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.

8.1 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 8.2 and gives a name to the stored command.
2. The `keyword` identifies the action desired. It must be an identifier see Section 8.2.
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 8.2.

- The `attribute-value` gives it a value see Section 8.3. 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 8.3. 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;
```

8.2 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 8.4.

8.3 Command Attribute Types

An object attribute is referred to by the syntax

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

If the attribute is an array see Section 8.13, 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 8.4
Logical	Section 8.5
Real expression	Section 8.6
Deferred expression	Section 8.8.5
Place	Section 8.9.1
Range	Section 8.9.2
Constraint	Section 8.10
Variable Reference	Section 8.11
Regular expression	Section 8.12
Array	Section 8.13
Array of logical	Section 8.13.1
Array of real	Section 8.13.2
Array of string	Section 8.13.3
Array of token lists	Section 8.13.4

See also:

Operators	Table 7
Functions	Table 8
Real functions of arrays	Table 11
Operand	Section 8.8
Random generators	Section 8.8.5

8.4 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 4. An operand in a string can also use the function `STRING` see Table 5. String values can occur in string arrays see Section 8.13.

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 4: 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 5: String Function in *OPAL*

Examples:

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

REAL X=1;
TWISS,LINE=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`.

8.5 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 8.13.1.

A logical expression has the same format and operator precedence as a logical expression in C. It is built from logical operators see Table 6 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 6: 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
```

8.6 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 8.13.2.

A real expression is built from operators see Table 7 and operands see Section 8.8:

```
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 8, Parentheses indicate operator precedence if required. Constant sub-expressions are evaluated immediately, and the result is stored as a constant.

8.7 Operators

An expression can be formed using operators see Table 7 and functions see Table 8 acting on operands see Section 8.8.

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` (`Y` > 0)	real	real,real

Table 7: 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 8: 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 9: 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.
```

8.8 Operands in Expressions

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

8.8.1 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
```

8.8.2 Symbolic constants

OPAL recognizes a few built-in mathematical and physical constants see Table 10. 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	3.1415926535898	1
TWOPI	2π	6.2831853071796	1
RADDEG	$180/\pi$	57.295779513082	rad/deg
DEGRAD	$\pi/180$	.017453292519943	deg/rad
E	e	2.7182818284590	1
EMASS	m_e	.51099906e-3	GeV
PMASS	m_p	.93827231	GeV
HMMASS	m_{h^-}	.939277	GeV
CMASS	m_c	12*0.931494027	GeV
UMASS	m_u	238*0.931494027	GeV
MMASS	m_μ	0.1057	GeV
DMASS	m_d	2*0.931494027	GeV
XEMASS	m_{xe}	124*0.931494027	GeV
CLIGHT	c	299792458	m/s
OPALVERSION		120	for 1.2.0
RANK		$0 \ldots N_p - 1$	1

Table 10: Predefined Symbolic Constants

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

8.8.3 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.

8.8.4 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`.

8.8.5 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.

8.9 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: `DOPAL-t` and `DOPAL-cycl`.

8.9.1 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`.

8.9.2 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`.

8.10 Constraints

Please note this is not yet available in: `DOPAL-t` and `DOPAL-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 ::= "==" | "<" | ">"
```

8.11 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 8.8.3, the second format refers to a named `attribute` of the named `object`. `object` can refer to an element or a command

8.12 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 8.2. 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.."
SAVE,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 saves 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.

8.13 Arrays

An attribute array is a set of values of the same attribute type see Section 8.3. 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
```

8.13.1 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}
```

8.13.2 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 11: 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.

8.13.3 String Arrays

String arrays can only be given as lists of single values. For permissible values String values see Section 8.4.

Example:

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

8.13.4 Token List Arrays

Token list arrays are always lists of single token lists.

Example:

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

Chapter 9

Control Statements

9.1 Getting Help

9.1.1 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=TWISS;
HELP,TWISS;
```

9.1.2 SHOW Command

The `SHOW` statement displays the current attribute values of an object. It has three formats:

```
SHOW;                   // Give help on the "SHOW" command
SHOW,NAME=pattern;      // Show names matching of "pattern"
SHOW,pattern;           // Shortcut for the second format
```

`pattern` is an regular expression see Regular Expressions. If it is non-blank, *OPAL* displays all object names matching the `pattern`. Entering `SHOW` alone displays help on the `SHOW` command.

Examples:

```
SHOW;
SHOW,NAME="QD.*\.L*";
SHOW,"QD.*\.L*";
```

9.1.3 WHAT Command

The `WHAT` statement displays all object names matching a given regular expression. It has three formats:

```
WHAT;                    // Give help on the "WHAT" command
WHAT,NAME=label;         // Show definition of "label"
WHAT,label;              // Shortcut for the second format
```

`label` is an identifier see Identifiers or Labels. If it is non-blank, *OPAL* displays the object `label` in a format similar to the input statement that created the object. Entering `WHAT` alone displays help on the `WHAT` command. Examples:

```
WHAT;
WHAT,NAME=QD;
WHAT,QD;
```

9.2 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 9.7.1, returns to the calling file. Any statement following the `STOP` or `QUIT` statement is ignored.

9.3 OPTION Statement

The `OPTION` command controls global command execution and sets a few global quantities. Starting with version 1.6.0 of *OPAL* the option `VERSION` is mandatory in the *OPAL* input file. Example:

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

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. 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.

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.

TRACE If true, print execution trace. Default false.

WARN If this option is turned off, *OPAL* suppresses all warning messages.

TELL If true, the current settings are listed. Must be the last option in the inputfile in order to render correct results.

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: random values see Deferred Expressions and Random Values.

PSDUMPFREQ Defines after how many time steps the phase space is dumped into the H5hut file. Default value is 10.

STATDUMPFREQ Defines after how many time steps we dump statistical data, such as RMS beam emittance, to the .stat file. The default value is 10. Currently only available for *OPAL-t*.

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 set 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.

- `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.

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

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.

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.

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 LF-2 and RK-4 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.

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. Default value is 1. Making less steps per turn and increasing this value is the recommended way to reduce space charge solve frequency.

REMOTEPARTDEL Artificially delete the remote particle if its distance to the beam mass is larger than `REMOTEPARTDEL` times of the beam rms size, its default values is -1 (no delete)

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.

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

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".

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 -1 then the auto-phasing algorithm isn't run. Default: 6.

PPDEBUG If true, use special initial velocity distribution for parallel plate and print special debug output

SURFDUMPFREQ The frequency to dump surface-partcle interaction data. Default: -1 (no dump).

NUMBLOCKS Maximum number of vectors in the Krylov space (for RCGSolMgr). Default value is 0 and BlockCGSolMgr will be used.

RECYCLEBLOCKS Number of vectors in the recycle space (for RCGSolMgr). Default value is 0 and BlockCGSolMgr will be used.

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

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

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:

1. HALTON
2. SOBOL
3. NIEDERREITER.

For details see the GSL reference manual (18.5).

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

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

BOUNDPDESTROYFQ The frequency to do `boundp_destroy` to delete lost particles. Default 10

BEAMHALOBOUNDARY Defines in terms of sigma where the halo starts. Default: 0.0

CLOTUNEONLY If set to true stop after CLO and tune calculation (not implemented, work in progress).

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`. Default 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/*. Default is false.

VERSION Used to indicate for which version of *OPAL* the input file is written. The versions of *OPAL* and of the input file have to match. 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`. If the version doesn't match then *OPAL* stops immediately and prints instructions on how to convert the input file.

AMR Enable adaptive mesh refinement. Default: FALSE

AMR_YT_DUMP_FREQ The frequency to dump grid and particle data for AMR. Default: 10

MEMORYDUMP If true, it writes the memory consumption of every core to a SDDS file (*.mem). The write frequency corresponds to STATDUMPFREQ. Default: FALSE

Examples:

```
OPTION,ECHO=FALSE,TELL;
OPTION,SEED=987456321
```

ECHO	**= FALSE**	**INFO**	**= TRUE**	**TRACE**	**= FALSE**
WARN	= TRUE	TELL	= FALSE	SEED	= 123456789
PSDUMPFREQ	= 10	STATDUMPFREQ	= 10	PSDUMPEACHTURN	= FALSE
PSDUMPFRAME	= GLOBAL	SPTDUMPFREQ	= 1	REPARTFREQ	= 10
REBINFREQ	= 100	SCSOLVEFREQ	= 1	MTSSUBSTEPS	= 1
REMOTEPARTDEL	= -1	RHODUMP	= FALSE	EBDUMP	= FALSE
CSRDUMP	= FALSE	AUTOPHASE	= 6	PPDEBUG	= FALSE
SURFDUMPFREQ	= -1	NUMBLOCKS	= 0	RECYCLEBLOCKS	= 0
NLHS	= 1	CZERO	= FALSE	RNGTYPE	= RANDOM
ENABLEHDF5	= TRUE	ASCIIDUMP	= FALSE	BOUNDPDESTROYFQ	= 10
BEAMHALOBOUNDARY	= 0.0	CLOTUNEONLY	= FALSE	IDEALIZE	= FALSE
LOGBENDTRAJECTORY	= FALSE	VERSION	= none	AMR	= FALSE

Table 12: Default Settings for Options

9.4 Parameter Statements

9.4.1 Variable Definitions

OPAL recognizes several types of variables.

9.4.1.1 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 9.4.4.

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);
```

9.4.1.2 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.

9.4.1.3 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-expressi` 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.

9.4.2 Symbolic Constants

OPAL recognizes a few build-in built-in mathematical and physical constants see Table 10. 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
```

9.4.3 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.

9.4.4 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
X=0;                   // create variable X with value
                       // zero
WHILE (X <= 0.10) {
  TWISS,LINE=...;      // uses X=0, 0.01, ..., 0.10
  X=EVAL(X+.01);       // increment variable X by 0.01
                       // CANNOT use: X=X+.01;
}
```

9.4.5 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: {0*A,1*A,2*A,3*A,4*A} = {0,4,8,12,16}
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.

9.5 Miscellaneous Commands

9.5.1 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.

9.5.2 SYSTEM: Execute System Command

During an interactive *OPAL* session the command `SYSTEM` allows to execute operating system commands. After execution of the system command, successful or not, control returns to *OPAL*. At present this command is only available under UNIX-like OSes (including Linux and macOS). It has two formats:

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

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

9.5.3 SYSTEM Command under UNIX

Most UNIX commands can be issued directly.

Example:

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

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

9.6 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.

9.7 File Handling

9.7.1 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";
```

9.7.2 SAVE Statement

The `SAVE` command has two formats:

```
SAVE,FILE=file-name
```

`file-name` is a string see String Attributes. The command causes all beam element, beam line, and parameter definitions to be written on the named file.

Examples:

```
SAVE,FILE="structure";
SAVE,"structure";
```

9.8 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.

9.9 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.

9.10 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. Example:

```
// macro definitions:
SHOWIT(X): MACRO {
   SHOW, NAME = X;
}
DOIT(): MACRO {
   DYNAMIC,LINE=RING,FILE="DYNAMIC.OUT";
}

// macro calls:
SHOWIT(PI);
DOIT();
```

Chapter 10

Elements

10.1 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;
```

10.2 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).

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

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.)

PARTICLEMATTERINTERACTION Attach a handler for particle matter interaction, see Chapter Particle Matter Interaction.

X X-component of the position of the element in the laboratory coordinate system.

Y Y-component of the position of the element in the laboratory coordinate system.

Z Z-component of the position of the element in the laboratory coordinate system.

THETA Angle of rotation of the element about the y-axis relative to the default orientation, $\mathbf{n} = (0,0,1)^{\mathbf{T}}$.

PHI Angle of rotation of the element about the x-axis relative to the default orientation, $\mathbf{n} = (0,0,1)^{\mathbf{T}}$

PSI Angle of rotation of the element about the z-axis relative to the default orientation, $\mathbf{n} = (0,0,1)^{\mathbf{T}}$

ORIGIN 3D position vector. An alternative to using `X`, `Y` and `Z` to position the element. Can't be combined with `THETA` and `PHI`. Use `ORIENTATION` instead.

ORIENTATION Vector of Tait-Bryan angles bib.tait-bryan. An alternative to rotate the element instead of using `THETA`, `PHI` and `PSI`. Can't be combined with `X`, `Y` and `Z`, use `ORIGIN` instead.

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.

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

10.3 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: `DOPAL-cycl`. In *OPAL-t* drifts are implicitly given, if no field is present.

10.4 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 10.4.1), `SBEND` (valid in *OPAL-t*, see Section 10.4.3), `RBEND3D`, (valid in *OPAL-t*, see Section 10.4.2) and `SBEND3D` (valid in *OPAL-cycl*, see Section 10.4.7).

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 10.4.1 and Section 10.4.3 describe the geometry and attributes of the *OPAL-t* bend elements `RBEND` and `SBEND`.
2. Section 10.4.4 describes how to implement an `RBEND` or `SBEND` in an *OPAL-t* simulation.
3. Section 10.4.7 is self contained. It describes how to implement an `SBEND3D` element in an *OPAL-cycl* simulation.

Figure 14 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.

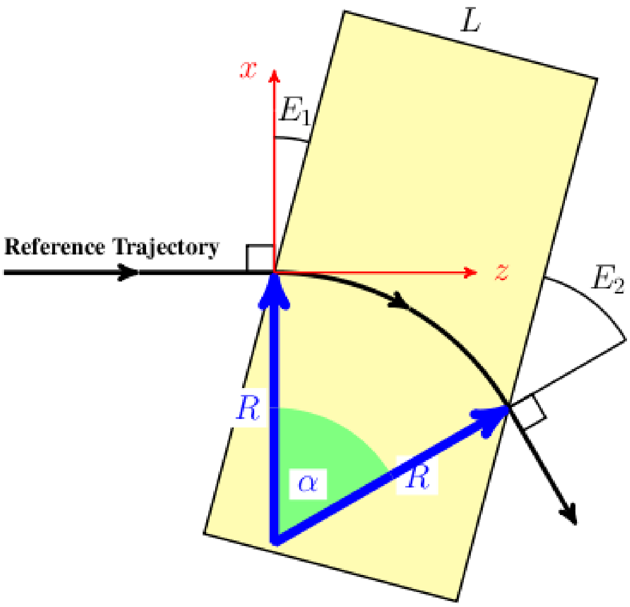

Figure 14: Illustration of a general rectangular bend (`RBEND`) with a positive bend angle α.

10.4.1 RBend (*OPAL-t*)

An `RBEND` is a rectangular bending magnet. The key property of an `RBEND` is that it has parallel pole faces. Figure 14 shows an `RBEND` with a positive bend angle and a positive entrance edge angle.

L Physical length of magnet (meters, see Figure 14).

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 14. Not supported in `DOPAL-t` any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (radians). Figure 14 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 14.

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 10.4.6. The field map is used to describe the fringe fields of the magnet see 1DProfile1.

10.4.2 RBend3D (*OPAL-t*)

An `RBEND3D3D` is a rectangular bending magnet. The key property of an `RBEND3D` is that it has parallel pole faces. Figure 14 shows an `RBEND3D` with a positive bend angle and a positive entrance edge angle.

L Physical length of magnet (meters, see Figure 14).

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 14. Not supported in `DOPAL-t` any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (radians). Figure 14 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 14.

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 10.4.6. The field map is used to describe the fringe fields of the magnet 1DProfile1.

Figure 15 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.

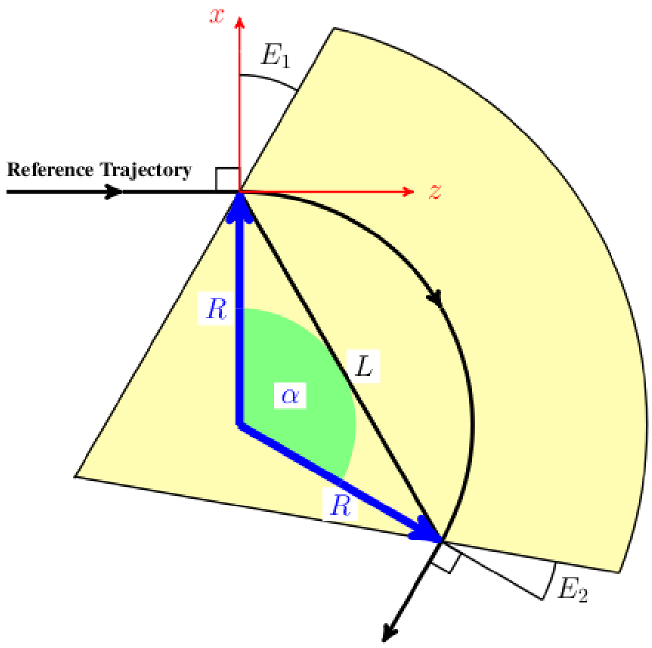

Figure 15: Illustration of a general sector bend(`SBEND`) with a positive bend angle α

10.4.3 SBend (*OPAL-t*)

An `SBEND` is a sector bending magnet. An `SBEND` can have independent entrance and exit edge angles. Figure 15 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 15), 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 degrees) 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 15. Not supported in `DOPAL-t` any more. Superimpose a `Quadrupole` instead.

E1 Entrance edge angle (rad). Figure 15 shows the definition of a positive entrance edge angle.

E2 Exit edge angle (rad). Figure 15 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 15.

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 10.4.6. The field map is used to describe the fringe fields of the magnet see 1DProfile1.

10.4.4 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 sees Section 10.4.1 and Section 10.4.3, and an SBEND has an additional attribute E2 that has no effect on an RBEND, see Section 10.4.3. 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 14 and Figure 15. 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 14 and Figure 15.
5. If the default field map, 1DPROFILE-DEFAULT see Section 10.4.6, 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 10.4.6 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 14). 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 10.4.6 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 14. 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 14) 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 10.4.1 and Section 10.4.3, 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 see 1DProfile1 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.

10.4.5 Bend Fields from 1D Field Maps (*OPAL-t*)

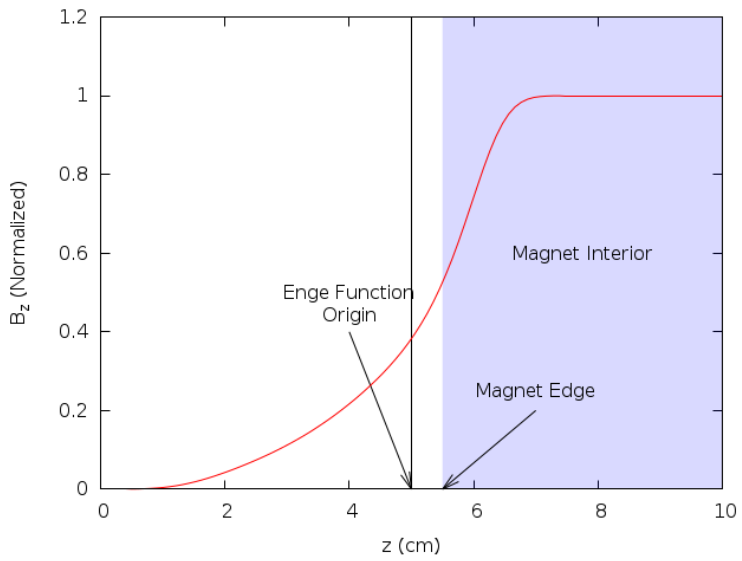

Figure 16: Plot of the entrance fringe field of a dipole magnet along the mid-plane, perpendicular to its entrance face. The field is normalized to 1.0. In this case, the fringe field is described by an Enge function see Equation 10.1 with the parameters from the default `1DProfile1` field map described in Section 10.4.6. 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 38.

The purpose of the `1DProfile1` field map see 1DProfile1 associated with the element is to define the Enge functions (Equation 10.1) 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 10.1: 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 16.

Let us assume we have a correctly defined positive `RBEND` or `SBEND` element as illustrated in Figure 14 and Figure 15. (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 10.1 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.

10.4.6 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 [20] 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 10.4.1 and Section 10.4.3).

10.4.7 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 with the following restrictions/conventions:

1. 3D Field maps have to be generated in the vertical direction (z coordinate in *OPAL-cycl*) from z = 0 upwards. It cannot be generated symmetrically about z = 0 towards negative z values.
2. 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.

Below two examples of a `SBEND3D` which loads a field maps with different units. The `triplet` example has units of cm and fields units of Gauss, where the `Dipole` example (Figure 17) uses meter and Tesla. The first 8 lines in the field map are ignored.

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

The first few links of the field map *fdf-tosca-field-map.table*:

```
     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
```

```
Dipole:SBEND3D,FMAPFN="90degree_Dipole_Magnet.out",LENGTH_UNITS=1000.0, FIELD_UNITS=-10.0;
```

The first few links of the field map *90degree_Dipole_Magnet.out*:

```
    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: *OPAL-cycl*.

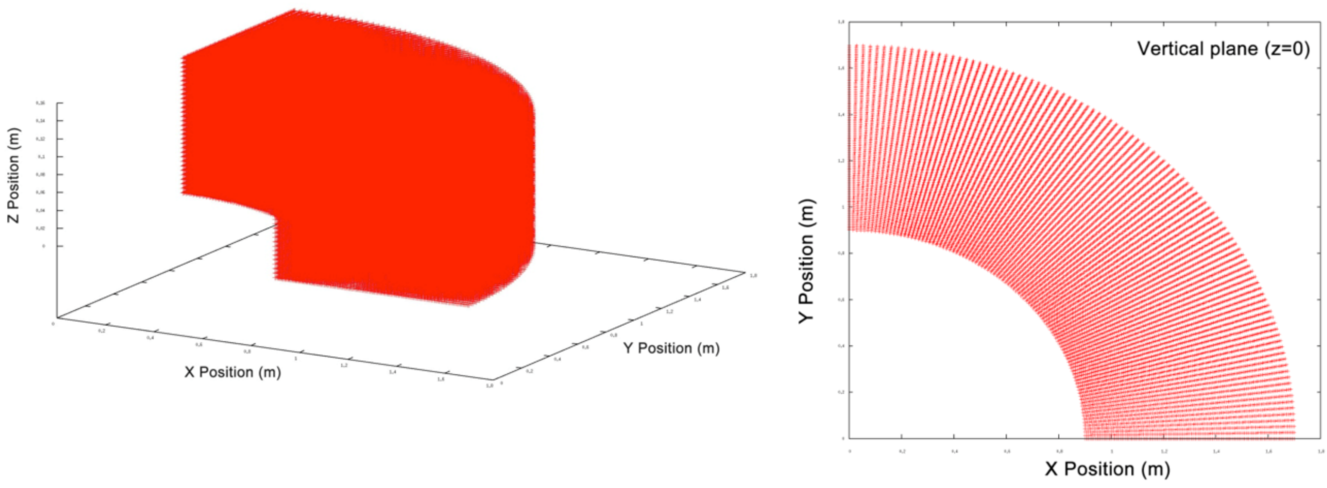

Figure 17: A hard edge model of 90 degree dipole magnet with homogeneous magnetic field. The right figure is showing the horizontal cross section of the 3D magnetic field map when $z = 0$

10.5 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: `DOPAL-cycl`.

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.

Example:

```
QP1: Quadrupole, L=1.20, ELEMEDGE=-0.5265,
     FMAPFN="1T1.T7", K1=0.11;
```

10.6 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.

Example:

```
S:SEXTUPOLE, L=0.4, K2=0.00134;
```

The reference system for a sextupole is a Cartesian coordinate system

10.7 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.

Example:

```
O3:OCTUPOLE, L=0.3, K3=0.543;
```

The reference system for an octupole is a Cartesian coordinate system

10.8 General Multipole

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^{-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^{-n}). A component is negative, if B_x is positive on the positive x-axis.

The order n is unlimited, but all components up to the maximum must be given, even if they are zero. 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 10.5.

```
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.

10.9 General Multipole (will replace Section 10.8 when implemented)

A `MULTIPOLET` is in *OPAL-t* 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, ANGLE=real, VAPERT=real, HAPERT=real,
      LFRINGE=real, RFRINGE=real, TP=real-vector, VARRADIUS=bool;
```

L Physical length of the magnet (meters), without end fields. (Default: 1 m)

ANGLE Physical angle of the magnet (radians). 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 multipole is set from the LENGTH and ANGLE attributes.

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)

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.

MAXFORDER The order of the maximum function f_n used in the field expansion (default: 5). 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).

ROTATION Rotation of the magnet about its central axis (radians, counterclockwise). This enables to obtain skew fields. (Default 0.0 rad)

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. This attribute is only to be set TRUE for a non-zero dipole component. (Default: FALSE)

VARSTEP The step size (meters) used in calculating the reference trajectory for VARRARDIUS = TRUE. It specifies how often the radius of curvature is re-calculated. This has a considerable effect on tracking time. (Default: 0.1 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;
```

The field expansion used in this model is based on the following scalar potential:

$$V = z f_0(x,s) + \frac{z^3}{3!} f_1(x,s) + \frac{z^5}{5!} f_2(x,s) + \dots$$

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.

10.10 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";
```

10.11 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: CARBONCYCL, CYCIAE, AVFEQ, FFAG, BANDRF and default PSI format. For the details of their data format, please read Field Maps.

CYHARMON The harmonic number of the cyclotron h.

RFFREQ The RF system f_{rf} (unit:MHz, default: 0). The particle revolution frequency $f_{rev} = f_{rf} / h$.

FMAPFN File name for the magnetic field map.

SYMMETRY Defines symmetrical fold number of the B field map data.

RINIT The initial radius of the reference particle (unit: mm, default: 0)

PHIINIT The initial azimuth of the reference particle (unit: degree, default: 0)

ZINIT The initial axial position of the reference particle (unit: mm, 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 (unit: mm, default : -10000.0)

MAXZ The maximal vertical extent of the machine (unit: mm, default : 10000.0)

MINR Minimal radial extent of the machine (unit: mm, default : 0.0)

MAXR Minimal radial extent of the machine (unit: 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 <*inputfilename*>*.h5* (or ASCII if ASCIIDUMP is true). 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 h5part file and 4 extra arguments need to specified:

RFMAPFN The file name for the electric field map in h5part binary format.

RFPHI The Initial phase of the electric field map (rad)

ESCALE The scale factor(s) for the electric field map(s)

SUPERPOSE An option whether all of the electric field maps are superposed, The is valid when more than one electric field map is read. (default: true)

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;
```

In this example SUPERPOSE is set to true. Therefore, if a particle locates in multiple field regions, all the field maps are superposed. if SUPERPOSE is set to false, then only one field map, 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 10.14 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

A `TRIMCOIL` object can be defined in two ways:

TYPE Type specifies PSI-RING or PSI-RING-OLD trim coil descriptions. The general PSI-RING description is based on a rational function with polynomials in the nominator and the denominator. The function describes the magnetic field [T] as function of the radius [mm]. The PSI-RING-OLD 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]

BMAX Maximal B field of the trim coils [T]

COEFNUM Coefficients of the numerator, first coefficient is zeroth order (for PSI-RING type only)

COEFDENOM Coefficients of the denominator, first coefficient is zeroth order. If COEFDENOM is not specified, the denominator is 1, and the description will be a normal polynom. (for PSI-RING type only).

SLPTC Slopes of the rising edge [1/mm] (for PSI-RING-OLD type only)

Example:

```
tc1:  TRIMCOIL, TYPE="PSI-RING-OLD", RMIN = 2022.09, RMAX = 2132.09, BMAX=2.0e-4, SLPTC=1;
tc15: TRIMCOIL, TYPE="PSI-RING",     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="RINGCYC", 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*.

10.12 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_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_PRINIT Transverse momentum $\beta\gamma$ for the reference trajectory.

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;
```

10.12.1 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 [mm].

END_POSITION_Y y position of the next element start in the coordinate system of the preceding element [mm].

END_NORMAL_X x component of the normal vector defining the placement of the next element in the coordinate system of the preceding element.

END_NORMAL_Y y component of the normal vector defining the placement of the next element in the coordinate system of the preceding element.

10.13 Source

This element only works in *OPAL-t*. It's only purpose in *OPAL-t* is to indicate that the particle source is contained in the beamline. This is needed to place the elements in three-dimensional space when using `ELEMEDGE`. Otherwise it has no effect on the particles.

10.14 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 (default: 0 m)

VOLT The peak RF voltage (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.

10.14.1 *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 SINGLE GAP 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;
```

10.14.2 *OPAL-cycl* mode

Using a RF Cavity (standing wave) in *OPAL-cycl* mode, the following parameters are defined:

FMAPFN Defines name of file which stores normalized voltage amplitude curve of cavity gap in ASCII format. (See data format in RF field)

VOLT Sets peak value of voltage amplitude curve in MV.

TYPE Defines Cavity type, SINGLEGAP represents cyclotron type cavity.

FREQ Sets the frequency of the RF Cavity in units of MHz.

RMIN Sets the radius of the cavity inner edge in mm.

RMAX Sets the radius of the cavity outer edge in mm.

ANGLE Sets the azimuthal position of the cavity in global frame in degree.

PDIS Set shift distance of cavity gap from center of cyclotron in mm. If its value is positive, the shift direction is clockwise, namely, shift towards the smaller azimuthal angle.

GAPWIDTH Set gap width of cavity in mm.

PHI0 Set initial phase of cavity in degree.

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 18 shows the simplified geometry of a cavity gap and its parameters.

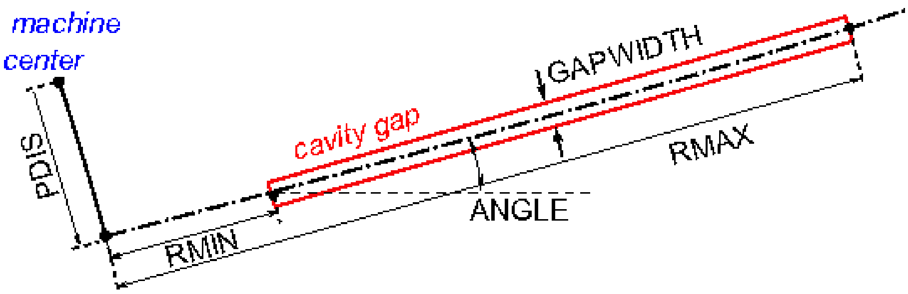

Figure 18: Schematic of the simplified geometry of a cavity gap and parameters

10.15 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.

WIDTH Full width of the cavity [mm].

HEIGHT Full height of the cavity [mm].

L Full length of the cavity [mm].

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.

10.15.1 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:

```
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;

RF_CAVITY: VARIABLE_RF_CAVITY, PHASE_MODEL="RF_PHASE", AMPLITUDE_MODEL="RF_AMPLITUDE",
           FREQUENCY_MODEL="RF_FREQUENCY", L=100., HEIGHT=200., WIDTH=2000.;
```

10.16 Traveling Wave Structure

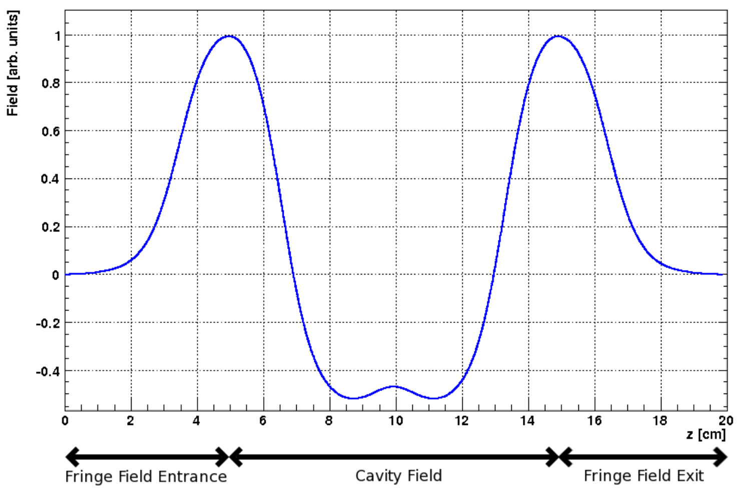

Figure 19: The on-axis field of an S-band (2997.924 MHz) TRAVELINGWAVE structure. The field of a single cavity is shown between its entrance and exit fringe fields. The fringe fields extend one half wavelength ($\lambda/2$) to either side.

An example of a 1D TRAVELINGWAVE structure field map is shown in Figure 19. 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:

$$\mathbf{E}_{\mathbf{entrance}}(\mathbf{r},t) = \mathbf{E}_{\mathbf{from-map}}(\mathbf{r}) \cdot \mathrm{VOLT} \cdot \cos(2\pi \cdot \mathrm{FREQ} \cdot t + \phi_{entrance})$$
$$\mathbf{E}_{\mathbf{exit}}(\mathbf{r},t) = \mathbf{E}_{\mathbf{from-map}}(\mathbf{r}) \cdot \mathrm{VOLT} \cdot \cos(2\pi \cdot \mathrm{FREQ} \cdot t + \phi_{exit})$$

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 19 using

$$\begin{aligned}\mathbf{E}(\mathbf{r},t) = & \frac{\mathrm{VOLT}}{\sin(2\pi \cdot \mathrm{MODE})} \\ & \times \left\{ \mathbf{E}_{\mathbf{from-map}}(x,y,z) \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \mathrm{LAG} + \frac{\pi}{2} \cdot \mathrm{MODE}\right) + \right. \\ & \left. \mathbf{E}_{\mathbf{from-map}}(x,y,z+d) \cdot \cos\left(2\pi \cdot \mathrm{FREQ} \cdot t + \mathrm{LAG} + \frac{3\pi}{2} \cdot \mathrm{MODE}\right) \right\}\end{aligned}$$

where d is the cell length and is defined as $d = \lambda \cdot \mathrm{MODE}$. MODE is an attribute of the element (see below). When calculating the field from the map ($\mathbf{E}_{\mathbf{from-map}}(x,y,z)$), 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.

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;
```

10.17 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.

OUTFN The file name into which the monitor should write the collected data. 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: DOPAL-cycl.

10.18 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 attributes:

L The collimator length (default: 0 m).

OUTFN The file name into which the monitor should write the collected data. The file is an H5hut file.

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.

The reference system for a collimator is a Cartesian coordinate system.

10.18.1 *OPAL-t* mode

The `CCOLLIMATOR` isn't supported. `ECOLLIMATOR`s and `RCOLLIMATOR`s detect all particles which are outside the aperture defined by `XSIZE` and `YSIZE`. For elliptic apertures, `XSIZE` and `YSIZE` denote the half-axes respectively, for rectangular apertures they denote the half-width of the rectangle.

XSIZE The horizontal half-aperture (default: unlimited).

YSIZE The vertical half-aperture (default: unlimited).

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.

ellipse(width, height) An ellipse that is centered at the origin of the 2D coordinate system.

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.

rotate(command, angle) Rotates the holes that are defined by the command about the origin of the 2D coordinate system.

union(command1, command2 [, command3 [, command4 [. . .]]]) Collects the holes that are defined the by the commands.

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.

repeat(command, N, angle) Repeats the holes that are defined by the command rotating each copy successively.

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

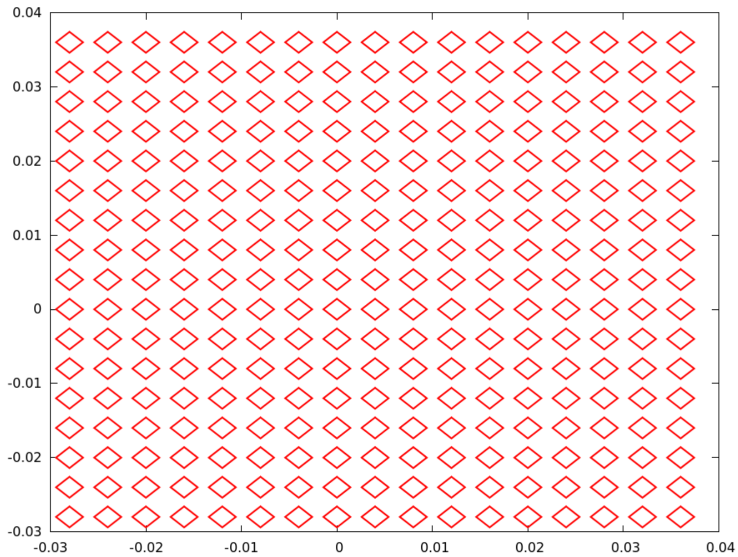

Figure 20: Pepper-pot with rectangle holes

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).

10.18.2 *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. So 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.

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 vertical coordinate of the start point [mm]. Default value is -100mm.

ZEND The vertical coordinate of the end point. [mm]. Default value is -100mm.

WIDTH The width of the collimator. [mm]

PARTICLEMATTERINTERACTION `PARTICLEMATTERINTERACTION` is an attribute of the element. Collimator physics is only a kind of particlematterinteraction. It can be applied to any element. If the type of `PARTICLEMATTERINTERACTION` is `COLLIMATOR`, the material is defined here. The material "Cu", "Be", "Graphite" and "Mo" are defined until now. If this is not set, the particle matter interaction module will not be activated. The particle hitting collimator will be recorded and directly deleted from the simulation.

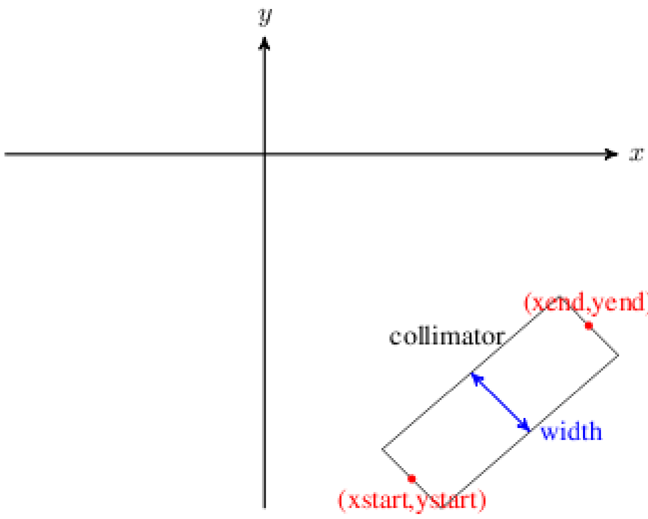

Figure 21: Collimator

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="Collimator", MATERIAL="Cu";
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 *<inputfilename>.h5* (or ASCII if ASCIIDUMP is true).

10.19 Septum (*OPAL-cycl*)

This is a restricted feature: `DOPAL-t`. The particles hitting on the septum is removed from the bunch. 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]

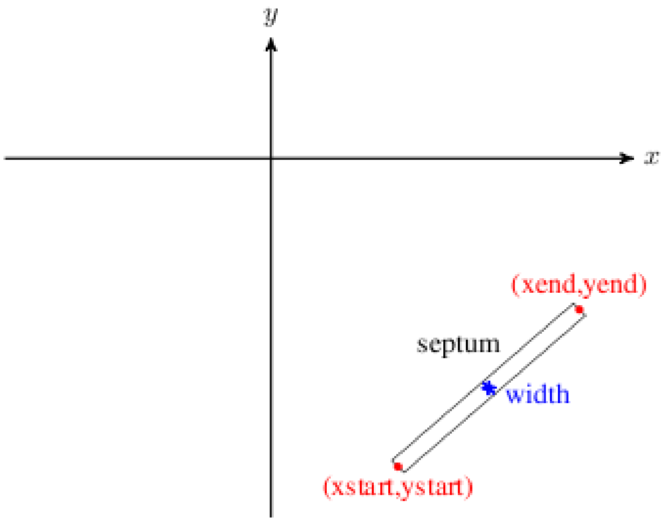

Figure 22: Septum

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 <*inputfilename*>*.h5* (or ASCII if ASCIIDUMP is true).

10.20 Probe (*OPAL-cycl*)

The particles hitting on the probe is recorded. 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]

WIDTH The width of the probe, NOT used yet.

STEP The step size of the probe (for histogram and peak finder output). Default: 1 [mm]

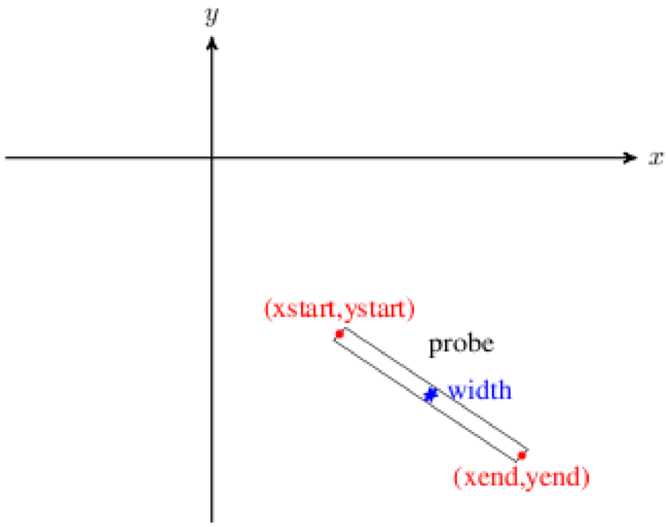

Figure 23: Probe

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 <*inputfilename*>*.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 particles recorded in the PROBE are also 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.

10.21 Stripper (*OPAL-cycl*)

A stripper element strip the electron(s) from a particle. The particle hitting the stripper is recorded in the file, which contains the time, coordinates and momentum of the particle at the moment it hit the stripper. The charge and mass are changed. Its 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]

WIDTH The width of the stripper, NOT used yet.

OPCHARGE Charge number of the out-coming particle. Negative value represents negative charge.

OPMASS Mass of the out-coming particles. [GeV/c^2]

OPYIELD Yield of the out-coming particle (the outcome particle number per income particle) , the default value is 1.

STOP If STOP is true, the particle is stopped and deleted from the simulation; Otherwise, the out-coming particle continues to be tracked along the extraction path.

Example: H_2^+ particle stripping

```
prob1: Stripper, xstart=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 *<inputfilename>.h5* (or ASCII if ASCIIDUMP is true).

10.22 Degrader (*OPAL-t*)

Elliptical degrader with an overall length `L`.

XSIZE Major axis of the transverse elliptical shape, default value is 1e6.

YSIZE Minor axis of the transverse elliptical shape, default value is 1e6.

Example: Graphite degrader of 15 cm thickness.

```
DEGPHYS: PARTICLEMATTERINTERACTION, TYPE="DEGRADER", MATERIAL="Graphite";

DEG1: DEGRADER, L=0.15, ELEMEDGE=0.02, PARTICLEMATTERINTERACTION=DEGPHYS;
```

10.23 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 $E1 = 0$ 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.

10.24 References

[19] *Tait-bryan angles*.

[20] J. E. Spencer and H. A. Enge, *Split-pole magnetic spectrograph for precision nuclear spectroscopy*, Nucl. Instrum. Methods 49, 181–193 (1967).

Chapter 11

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`.

11.1 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

DX Grid step size in x

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

DY Grid step size in y

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

DZ Grid step size in z.

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 0.1 m. 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";
```

11.2 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.

11.2.1 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 [?]
9 Ey [?]
10 Ez [?]
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 Either 'Cartesian' or 'Cylindrical'. 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

DX Grid step size in x

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

DY Grid step size in y

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

DZ Grid step size in z.

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

DT Grid step size in time.

T_STEPS Number of steps in time. It is an error if `T_STEPS` is non-integer or less than 1.

11.2.2 Cylindrical Mode

In Cylindrical mode the format of the field output is:

```
<number of rows>
1 r [m]
2 phi [degree]
3 z [m]
4 t [ns]
5 Br [kGauss]
6 Bphi [kGauss]
7 Bz [kGauss]
8 Er [?]
9 Ephi [?]
10 Ez [?]
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 Either 'Cartesian' or 'Cylindrical'. 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

DR Grid step size in r

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

DPHI Grid step size in phi

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

DZ Grid step size in z.

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

DT Grid step size in time.

T_STEPS Number of steps in time. It is an error if `T_STEPS` is non-integer or less than 1.

Chapter 12

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.

12.1 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.

12.2 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 13

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, BUNCHED=logical, BFREQ=real;
```

The `label` is optional, it defaults to `UNNAMED_BEAM`.

13.1 Particle Definition

The particle mass and charge are defined by:

PARTICLE The name of particles in the machine.

OPAL knows the mass and the charge for the following particles

POSITRON The particles are positrons (`MASS`=m_e, `CHARGE`=1).

ELECTRON The particles are electrons (`MASS`=m_e, `CHARGE`=-1).

PROTON The particles are protons (default, `MASS`=m_p, `CHARGE`=1).

ANTIPROTON The particles are anti-protons (`MASS`=m_p, `CHARGE`=-1).

HMINUS The particles are h- protons (`MASS`=m_{h^-}, `CHARGE`=-1).

CARBON The particles are carbons (`MASS`=m_c, `CHARGE`=12).

URANIUM The particles are of type uranium (`MASS`=m_u, `CHARGE`=35).

MUON The particles are of type muon (`MASS`=m_μ, `CHARGE`=-1).

DEUTERON The particles are of type deuteron (`MASS`=m_d, `CHARGE`=1).

XENON The particles are of type xenon (`MASS`=m_{xe}, `CHARGE`=20).

H2P The particles are of type hydrogen+ (`MASS`=$2 * m_p$, `CHARGE`=1).

For other particle names one may enter:

MASS The particle mass in GeV.

CHARGE The particle charge expressed in elementary charges.

13.2 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.

13.3 Twiss Parameters

The twiss parameters are only used in the twiss calculation. The beam shape and size is in general defined by the distribution command, see Chapter Distribution.

EX Horizontal emittance

EY Vertical emittance

ET Longitudinal emittance

13.4 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

Chapter 14

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).
MATCHEDGAUSS	Initial distribution generated using matched Gaussian distribution(s).
GUNGAUSSFLATTOPTH	Legacy. Special case of `FLATTOP` distribution.
ASTRAFLATTOPTH	Legacy. Special case of `FLATTOP` distribution.

Table 13: 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 13. 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.)

14.1 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 (e.g. 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	EV (default for *OPAL-cycl*)	Use the units eV for the input momentum (e.g. p_x, p_y, p_z).

Table 14: Definition of INPUTMOUNITS attribute.

14.2 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 15: 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.

14.2.1 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 14.8.4.
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 14.1	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 14.1	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 14.1	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 14.1	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 14.1	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 16: Definition of universal distribution attributes. Any distribution type can use these and they are the same whether the beam is *injected* or *emitted*.

14.2.2 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, $\bar{z}$.

Table 17: Definition of distribution attributes that only affect *injected* beams.

14.2.3 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 14.8.

Table 18: Definition of distribution attributes that only affect *emitted* beams.

14.3 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 19 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 19: 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 slightly a slightly different format, depending on whether the distribution is to be *injected* or *emitted*. The *injected* file format is defined in Table 20. The particle coordinates are defined in OPAL-t variables and OPAL-cycl variables. The *emitted* file format is defined in Table 21. 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 20: 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 21: 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 14.8. 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 in Chapter Beam Command must be equal.

14.4 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.

14.4.1 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	RMS length, σ_z, in longitudinal (z) direction. SIGMAZ is used for an *injected* distribution.
SIGMAT	0.0	s	RMS width, σ_t, in time (t). SIGMAT is used for an *emitted* distribution.
SIGMAPX	0.0	Section 14.1	Parameter σ_{px} for defining distribution.
SIGMAPY	0.0	Section 14.1	Parameter σ_{py} for defining distribution.
SIGMAPZ	0.0	Section 14.1	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 22: Definition of the basic distribution attributes for a GAUSS distribution type.

In Table 22 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, $\sigma_x = 1.0$mm, $\sigma_y = 3.0$mm, $\sigma_z = 2.0$mm and an average energy of:

$$W = 1.2\text{MeV}$$

In the x direction, the Gaussian distribution is cutoff at $x = 2.0 \times \sigma_x = 2.0$mm. In the y direction it is cutoff at $y = 2.0 \times \sigma_y = 6.0$mm. This distribution is *injected* into the simulation at an average position of $(\bar{x}, \bar{y}, \bar{z}) = (1.0\text{mm}, -2.0\text{mm}, 10.0\text{mm})$.

14.4.2 `GAUSS` Distribution for Photoinjector

Attribute Name	Default Value	Units	Description
`TPULSEFWHM`	0.0	s	Flat top time see Figure 24.
`TRISE`	0.0	s	Rise time see Figure 24. If defined will override `SIGMAT`.
`TFALL`	0.0	s	Fall time see Figure 24. If defined will override `SIGMAT`.
`FTOSCAMPLITUDE`	0	None	Sinusoidal oscillations can imposed on the flat top in Figure 24. 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 24.

Table 23: 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 24.

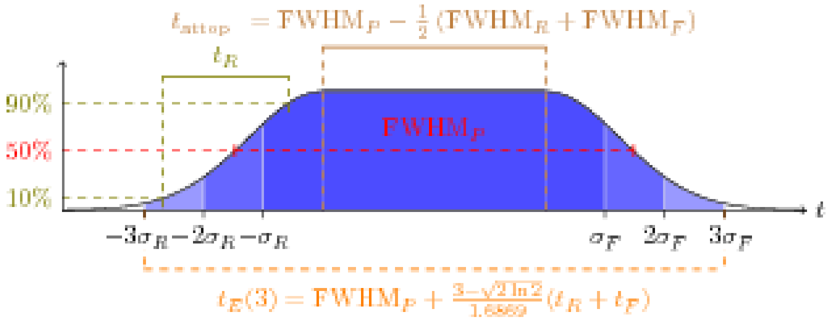

Figure 24: *OPAL* emitted `GAUSS` distribution with flat top.

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 23. Using them, we can create a distribution with the time structure shown in Figure 24. 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 23 do not define RMS quantities, but instead are given by (See also Figure 24):

$$\begin{aligned} \text{TRISE} = t_R &= \left(\sqrt{2\ln(10)} - \sqrt{2\ln\left(\frac{10}{9}\right)} \right) \sigma_R \\ &= 1.6869\sigma_R \\ \text{TFALL} = t_F &= \left(\sqrt{2\ln(10)} - \sqrt{2\ln\left(\frac{10}{9}\right)} \right) \sigma_F \\ &= 1.6869\sigma_F \end{aligned}$$

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 24):

$$\text{TPULSEFWHM} = \text{FWHM}_P = t_{\text{flattop}} + \sqrt{2\ln 2}\,(\sigma_R + \sigma_F)$$

Total emission time, t_E, of this distribution, is a function of the longitudinal cutoff, `CUTOFFLONG` see Table 22, and is given by:

$$\begin{aligned} t_E(\text{CUTOFFLONG}) &= \text{FWHM}_P - \frac{1}{2}(\text{FWHM}_R + \text{FWHM}_F) + \text{CUTOFFLONG}(\sigma_R + \sigma_F) \\ &= \text{FWHM}_P + \frac{\text{CUTOFFLONG} - \sqrt{2\ln 2}}{1.6869}(\text{TRISE} + \text{TFALL}) \end{aligned}$$

Finally, we can also impose oscillations over the flat-top portion of the laser pulse in Figure 24, t_{flattop}. This is defined by the attributes `FTOSCAMPLITUDE` and `FTOSCPERIODS` from Table 23. `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.

14.4.3 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 14.1	x, p_x correlation. (R_{12} in transport notation.)
CORRY	0.0	Section 14.1	y, p_y correlation. (R_{34} in transport notation.)
CORRZ	0.0	Section 14.1	z, p_z correlation. (R_{56} in transport notation.)
CORRT	0.0	Section 14.1	same as and overwritten by CORRZ.
R51	0.0	Section 14.1	x, z correlation. (R_{51} in transport notation.)
R52	0.0	Section 14.1	p_x, z correlation. (R_{52} in transport notation.)
R61	0.0	Section 14.1	x, p_z correlation. (R_{61} in transport notation.)
R62	0.0	Section 14.1	p_x, p_z correlation. (R_{62} in transport notation.)

Table 24: 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;
```

14.5 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.

14.5.1 Injected FLATTOP

The attributes for an *injected* FLATTOP distribution are defined in Table 25 and Table 16. 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 25: Definition of the basic distribution attributes for an *injected* FLATTOP distribution type.

14.5.2 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 24.
TPULSEFWHM	0.0	s	Flat top time. See Figure 24.
TRISE	0.0	s	Rise time. See Figure 24. If defined will override SIGMAT.
TFALL	0.0	s	Fall time. See Figure 24. If defined will override SIGMAT.
FTOSCAMPLITUDE	0	None	Sinusoidal oscillations can imposed on the flat top in Figure 24. 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 24.
LASERPROFFN		None	File name containing measured laser image.
IMAGENAME		None	Name of the file containing the laser image.
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 26: Definition of the basic distribution attributes for an *emitted* FLATTOP distribution type.

The attributes of an *emitted* FLATTOP distribution are defined in Table 26 and Table 16. 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 14.4.2. 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 24.

```
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;
```

14.5.3 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 26. Then, *OPAL-t* will use the laser image as the basis to sample the transverse distribution.

This distribution option is not yet available.

14.5.4 `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`.

14.5.5 `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.

14.6 `BINOMIAL` Distribution Type

The `BINOMIAL` type of distribution is based on [21]. 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 27 and shown in Figure 25.

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 27: Different distributions specified by a single parameter m

TABLE 2: Properties of binomial Phase Space Distributions

m	phase space density $\rho(u,v)$, $u^2+v^2 \equiv a^2 \leq 1$	profile $f(u)=\int_{-\infty}^{+\infty}\rho(u,v)dv$, $u \equiv \frac{x}{x_L}$, $\lvert u \rvert \leq 1$,	profile- form	$\frac{x_L}{2\sigma}$ $(\sigma^2 \equiv \overline{x^2})$	total emittance	$\frac{\Gamma}{2\sigma}$ $\Gamma = \text{FWHM}$	$\frac{\Gamma}{x_L}$	$\frac{f(2\sigma)}{f_{max}}$	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 25: Properties of binomial Phase Space Distributions (taken from [21]).

The attributes of a `BINOMIAL` distribution are defined in Table 28.

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 28: 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,
```

14.7 `MATCHEDGAUSS` Matched Gauss Distribution type

The attributes of a `MATCHEDGAUSS` distribution are defined in Table 29.

Attribute Name	Default Value	Units	Description
`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
`MAGSYM`	0		Number of sector magnets
`FMAPFN`			File for reading fieldmap used to create matched distribution
`FMTYPE`			File format for reading fieldmap used to create matched distribution
`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`	2000		Maximum steps used to find matched distribution

Table 29: Definition of the basic distribution attributes for a `MATCHEDGAUSS` distribution type.

14.8 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.

14.8.1 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 30. 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 30: 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.

14.8.2 Emission Model: ASTRA

The ASTRA emittance model uses the same single parameter as the NONE option as listed in Table 30. However, in this case, the energy defined by the EKIN attribute is added to each emitted particle's momentum in a random way:

$$p_{total} = \sqrt{\left(\frac{\text{EKIN}}{mc^2} + 1\right)^2 - 1}$$
$$p_x = p_{total}\sin(\phi)\cos(\theta))$$
$$p_y = p_{total}\sin(\phi)\sin(\theta))$$
$$p_z = p_{total}|\cos(\theta)|$$

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.

14.8.3 Emission Model: NONEQUIL

The NONEQUIL emission model is based on an actual physical model of particle emission as described in [22], [23], [24]. The attributes needed by this emission model are listed in Table 31.

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 31: 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;
```

14.8.4 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 16). 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 14.3).

14.9 References

[21] W. Joho, Representation of beam ellipses for transport calculations, PSI Internal Report TM-11-14, https://intranet.psi.ch/-pub/AUTHOR_WWW/ABE/TalksDE/TM-11-14.pdf.

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Chapter 15

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.

15.1 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 [25]. 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 [25], [26] and [27]. 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 [28] , [29].

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 15.1: Convolution solution

where

$$G(u,v,w) = \frac{1}{\sqrt{u^2+v^2+w^2}}.$$

A simple discretization of Equation 15.1 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 15.2: 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.

15.1.1 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,

$$\bar{\phi}_j = \sum_{k=0}^{K-1} \bar{\rho}_k \bar{G}_{j-k} \quad , \quad \begin{array}{l} j = 0,\ldots,J-1 \\ k = 0,\ldots,K-1 \\ j-k = -(K-1),\ldots,J-1 \end{array}$$

EQUATION 15.3: 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,

$$\rho_k = \begin{cases} \bar{\rho}_k & \text{if } k = 0,\ldots,K-1 \\ 0 & \text{if } k = K,\ldots,N-1. \end{cases}$$

Define a periodic Green function, G_m, as follows,

$$G_m = \begin{cases} \bar{G}_m & \text{if } m = -(K-1),\ldots,J-1 \\ 0 & \text{if } m = J,\ldots,N-K, \\ G_{m+iN} = G_m & \text{for } i \text{ integer }. \end{cases}$$

EQUATION 15.4: 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 15.5: 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 15.6: Final equation

In the physical (unpadded) region, $j \in [0, J-1]$, so the quantity $j-n$ in Equation 15.6 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 15.5, matches the convolution in Equation 15.3.

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 15.4 – 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 15.4. In that case the approach is identical to the Hockney method [25], [26] and [27]. Lastly, note that the above proof that the convolution, Equation 15.5, is identical to Equation 15.3 in the unpadded region, works even when W^{-jk} and W^{mk} are replaced by W^{jk} and W^{-mk}, respectively, in Equation 15.5. 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 15.7: 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.

15.1.2 Algorithm used in *OPAL*

As a result, the solution of Equation 15.2 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 15.8: 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.

15.1.3 Interpolation Schemes

More details will be given in Version 2.0.0.

15.2 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 [30].

15.3 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.

15.4 The `FIELDSOLVER` Command

See Table 32 for a summary of the Fieldsolver command.

Command	Purpose
`FIELDSOLVER`	Specify a fieldsolver
`FSTYPE`	Specify the type of field solver: `FFT`, `FFTPERIODIC`, `MG`, `FMG` (AMR only) and `NONE`
`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`]
`BCFFTY`	Boundary condition in y [`OPEN`]
`BCFFTZ`	Boundary condition in z [`OPEN,PERIODIC`]
`GREENSF`	Defines the Greens function for the FFT Solver
`BBOXINCR`	Enlargement of the bounding box in %
`GEOMETRY`	Geometry to be used as domain boundary
`ITSOLVER`	Type of iterative solver
`INTERPL`	Interpolation used for boundary points
`TOL`	Tolerance for iterative solver
`MAXITERS`	Maximum number of iterations of iterative solver
`PRECMODE`	Behavior of the preconditioner
`AMR_MAXLEVEL`	Maximum adaptive mesh refinement level (single level if `AMR_MAXLEVEL` is zero)
`AMR_MAXGRID`	Maximum grid size. It has to be smaller than `MX`, `MY`, `MT` when running in parallel
`AMR_TAGGING`	Mesh-refinement strategy

Table 32: Fieldsolver command summary

15.5 Define the Fieldsolver to be used

At present only a FFT based solver is available. Future solvers will include Finite Element solvers and a Multigrid solver with Shortley-Weller boundary conditions for irregular domains.

15.6 Define 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.

15.7 Define Number of Grid Points

Number of grid points in x, y and z for a rectangular grid.

15.8 Define 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.

15.9 Define Greens Function

Two Greens functions can be selected: `INTEGRATED`, `STANDARD`. The integrated Green's function is described in [31], [32], [33]. Default setting is `INTEGRATED`.

15.10 Define 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.

15.11 Define Geometry

The list of geometries defining the beam line boundary. For further details see Chapter Geometry.

15.12 Define Iterative Solver

The iterative solver for solving the preconditioned system: `CG`, `BiCGSTAB` or `GMRES`.

15.13 Define Interpolation for Boundary Points

The interpolation method for grid points near the boundary: `CONSTANT`, `LINEAR` or `QUADRATIC`.

15.14 Define Tolerance

The tolerance for the iterative solver used by the `MG` solver.

15.15 Define Maximal Iterations

The maximal number of iterations the iterative solver performs.

15.16 Define Preconditioner Behavior

The behavior of the preconditioner can be: `STD`, `HIERARCHY` or `REUSE`. This argument is only relevant when using the `MG` solver and should **only be set if the consequences to simulation and solver are evident**. A short description is given in the Table below.

Value	Behavior
`STD`	The preconditioner is rebuilt in every time step (enabled by default)
`HIERARCHY`	The hierarchy (tentative prolongator) is reused
`REUSE`	The preconditioner is reused

Table 33: Preconditioner behavior command summary

15.17 Define the number of Energy Bins to use

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.

15.18 Define AMR Solver

The option `AMR=TRUE` enables further commands to be used in the Fieldsolver command. In order to run a proper AMR simulation one requires following ingredients:

- Upper bound of refinement, specified by `AMR_MAXLEVEL`
- Maximum allowable grid size, specified by `AMR_MAXGRID`. This size holds for all levels in all directions.
- Mesh refinement strategy, specified by `AMR_TAGGING`. Depending on the tagging scheme, further keywords can be used. A summary is given in the Table below.

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 34: Mesh refinement strategies

15.19 References

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Chapter 16

Tracking

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*
NNB	Number of neighbouring bunches in *OPAL-cycl*
name=expression	Parameter relation
RUN	Run particles for specified number of turns or steps
ENDTRACK	Leave tracking mode

Table 35: Commands accepted in Tracking Mode

16.1 Track Mode

Before starting to track, a beam 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 35. 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.

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 `RK-4`, `LF-2` and `MTS`:

- RK-4 the fourth-order Runge-Kutta integrator. This is the default integrator for *OPAL-cycl*.
- LF-2 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 `RK-4` 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 `LF-2` or `RK-4` 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="LF-2";
    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;
```

16.2 Track Particles

This command starts or continues the actual tracking:

```
RUN, METHOD=string, FIELDSOLVER=label, DISTRIBUTION=label-vector, BEAM=label,
FILE=string, TURNS=integer, MBMODE=string, PARAMB=float,
BOUNDARYGEOMETRY=string, MULTIPACTING=logical, OBJECTIVES=string-vector;
```

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.
- `STATISTICAL-ERRORS` This is a method to let *OPAL* run multiple times in parallel while adding imperfections to alignment and other physical quantities.

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.

FILE The name of the file to be written (default="track").

TURNS The number of turns (integer) to be tracked (default: 1, namely single bunch).

In *OPAL-cycl*, this parameter represents the number of bunches those will be injected into the cyclotron. In restart mode, the code firstly read 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 *.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 large 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*.

OBJECTIVES An array of column names from the *.stat* file used in `STATISTICAL-ERRORS` to compute mean value and standard deviation across all runs.

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`.

16.3 STATISTICAL-ERRORS

This method can be used to quantify the effects of imperfections to alignment or other physical quantities such as e.g. the phase or the amplitude. It doesn't propagate the particles directly. Instead it scans through the input file and replaces all occurrences of and with randomly generated values of appropriate distribution. Then one of the other methods, e.g. `PARALLEL-T` is called. These two steps are then repeated many times.

To use this method one has to specify the `METHOD` using the following form:

`STATISTICAL-ERRORS(<trackmethod>, <ncores>, <nruns>),`

where `<trackmethod>` is the method that should track the particles, `<ncores>` is the number of cores used for a run and `<nruns>` is the number of individual runs that should be performed. **It should be noted that the total number of cores available has to be greater or equal to `ncores` + 1.** One core is needed to manage the distribution of tasks and to collect the results. The other cores are used to perform the simulations. If in total $N \times \text{ncores} + 1$ cores are available then N individual runs are processed in parallel each using `ncores`.

For each run of the method `STATISTICAL-ERRORS` a unique base name is generated of the form *foo*. Each individual run is then performed in a directory *foo_run_ddddd*. The files that are produced by the `<trackmethod>` are kept. **This can lead to a large amount of data especially when snapshots of the phase space are stored frequently. The user should make sure that the file system can handle the amount of data or set the option `PSDUMPFREQ` to a big number.**

In the end the method `STATISTICAL-ERRORS` computes the mean and the standard deviation for each variable in the array `OBJECTIVES` along the machine and stores this information in to the *.stat* file.

Chapter 17

Wakefields

OPAL-t provides methods to compute CSR and short-range geometric wakefields.

17.1 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 17.4 - Section 17.13). 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 17.1: 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 17.2: 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 17.3: 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 17.4: 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 17.4:

$$W_T(s) = 10^{-12}\frac{2c}{\pi}Re\left(\int_0^\infty Re(\frac{c}{k}Z_L(k))\cos(ks)dk\right).$$

EQUATION 17.5: Transverse wakefield

To calculate the integrals in Equation 17.4 and Equation 17.5 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.

17.2 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 [34] ,[35]. 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 [36]. 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 [35] and for finite plates [37] can also be calculated. For the infinite plates an impedance can be calculated [36].

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 [38] 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 [39], `1D-CSR-IGF`.

17.3 The WAKE Command

The general input format 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, LONG-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 36: Wakefield command summary

17.4 Define the Wakefield to be used

The WAKE command defines data for a wake function on an element see Common Attributes for all Elements.

17.5 Define the wakefield type

A string value see String Attributes to specify the wake function, either 1D-CSR, 1D-CSR-IGF, LONG-SHORT-RANGE, TRANSV-SHORT-RANGE or LONG-TRANSV-SHORT-RANGE.

17.6 Define the number of bins

The number of bins used in the calculation of the line density.

17.7 Define the bunch length to be constant

With the CONST_LENGTH flag the bunch length can be set to be constant. This has no effect on CSR wakefunctions.

17.8 Define the conductivity

The conductivity of the bunch which can be set to either AC or DC. This has no effect on CSR wakefunctions.

17.9 Define the impedance

The impedance Z_0 of the beam pipe in [Ω]. This has no effect on CSR wakefunctions.

17.10 Define the form of the beam pipe

The form of the beam pipe can be set to `ROUND`. This has no effect on CSR wakefunctions.

17.11 Define the radius of the beam pipe

The radius of the beam pipe in [m]. This has no effect on CSR wakefunctions.

17.12 Define the sigma of the beam pipe

The σ of the beam pipe (material constant), see Equation 17.1. This has no effect on CSR wakefunctions.

17.13 Define the relaxation time (tau) of the beam pipe

The τ defines the relaxation time and is needed to calculate the impedance of the beam pipe see Equation 17.1. This has no effect on CSR wakefunctions.

17.14 Import a wakefield from a file

Since we only need values of the wake function at several discreet 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 [40], [41].

Whenever a file is specified *OPAL* will use the wakefield found in the file and ignore all other commands related to round beam pipes.

17.15 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.

17.16 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`, `RelativFFTLowPass`. 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`, `RelativFFTLowPass`

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.

17.17 References

[34] G. A. Schott, *Electromagnetic Radiation* (Cambridge University Press, 1912).

[35] J. Schwinger, *On the Classical Radiation of Accelerated Electrons*, Phys. Rev. 75, 1912–1925 (1949) 10.1103/PhysRev.75.1912. and http://puhep1.princeton.edu/~kirkmcd/accel/schwinger.pdf

[36] J. B. Murphy, S. Krinsky, and R. L. Gluckstern, *Longitudinal Wakefield for an Electron Moving on a Circular Orbit*, Particle Accelerators 57, 9–64 (1997).

[37] J. S. Nodvick and D. S. Saxon, *Suppression of Coherent Radiation by Electrons in a Synchrotron*, Phys. Rev. 96, 180–184 (1954) 10.1103/PhysRev.96.180.

[38] E. L. Saldin, E. A. Schneidmiller, and M. V. Yurkov, *On the Coherent Radiation of an Electron Bunch Moving in an Arc of a Circle*, Nucl. Instrum. Methods Phys. Res. Sect. A 398, 373–394 (1997) 10.1016/S0168-9002(97)00822-X.

[39] C. E. Mitchell, J. Qiang, and R. D. Ryne, *A fast method for computing 1-d wakefields due to coherent synchrotron radiation*, Nucl. Instrum. Methods Phys. Res. Sect. A 715, 119–125 (2013).

[40] M. Borland, *A self-describing file protocol for simulation integration and shared postprocessors*, in Proc. PAC (1995), pp. 2184–2186.

[41] M. Borland, *A universal postprocessing toolkit for accelerator simulation and data analysis*, in Proc. 1998 ICAP conference (1998), FTU10.

Chapter 18

Geometry

At present the `GEOMETRY` command is still an **experimental feature** which is not to be used by the general user. It can only be used to specify boundaries for the MG Solver. The command can be used in two modes:

1. specify a H5Fed file holding the surface mesh of a complicated boundary geometry
2. specify a cylinder with an elliptic base area

18.1 Geometry Command

Command	Purpose
`GEOMETRY`	Specify a geometry
`FGEOM`	Specifies the H5Fed geometry file
`LENGTH`	Specifies the length of the geometry
`S`	Specifies the start of the geometry
`A`	Specifies the semi-major axis of the elliptic base area
`B`	Specifies the semi-minor axis of the elliptic base area

Table 37: Geometry command summary

FGEOM Define the geometry file, an H5Fed file, containing the surface mesh of the geometry.

LENGTH The length of the specified geometry in [m].

S The start of the specified geometry in [m].

A The semi-major axis of the ellipse in [m].

B The semi-minor axis of the ellipse in [m].

Chapter 19

Physics Models Used in the Particle Matter Interaction Model

The command to define the particle matter interacton is PARTICLEMATTERINTERACTION.

MATERIAL The material of the surface.

ENABLERUTHERFORD Switch to disable Rutherford scattering, default true.

The so defined instance has then to be added to an element using the attribute

19.1 The Energy Loss

The energy loss is simulated using the Bethe-Bloch equation.

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{Kz^2Z}{A\beta^2}\left[\frac{1}{2}\ln\frac{2m_ec^2\beta^2\gamma^2 Tmax}{I^2} - \beta^2\right],$$

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.

The stopping power is compared with PSTAR program of NIST in Figure 26.

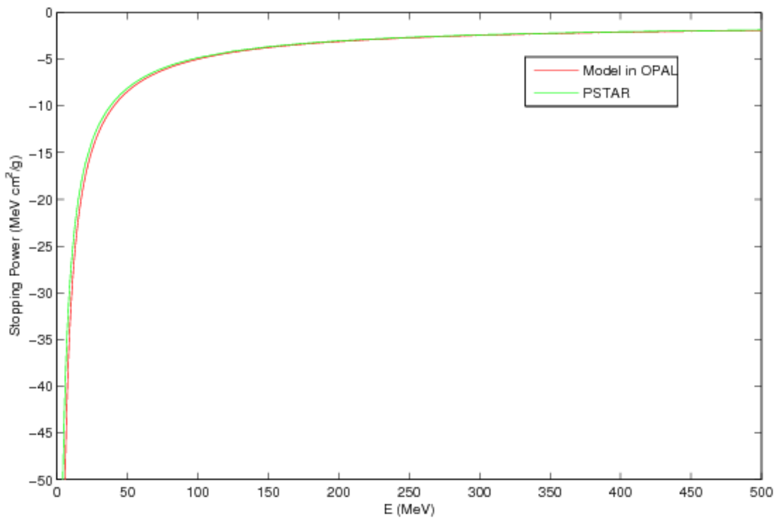

Figure 26: The comparison of stopping power with PSTAR.

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.

19.2 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, 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 $\theta = 2.5\sqrt{2}\theta_0 \approx 3.5\theta_0$,

$$\theta_0 = \frac{13.6MeV}{\beta c p} z \sqrt{\Delta s / X_0}[1 + 0.038\ln(\Delta s / X_0)],$$

where p is the momentum, Δs is the step size, and X_0 is the radiation length.

19.2.1 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,

$$y = y + \Delta s p_y + z_3 \Delta s \theta_0/\sqrt{12} + z_4 \Delta s \theta_0/2,$$

$$p_y = p_y + z_4\theta_0.$$

19.2.2 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 27. 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).

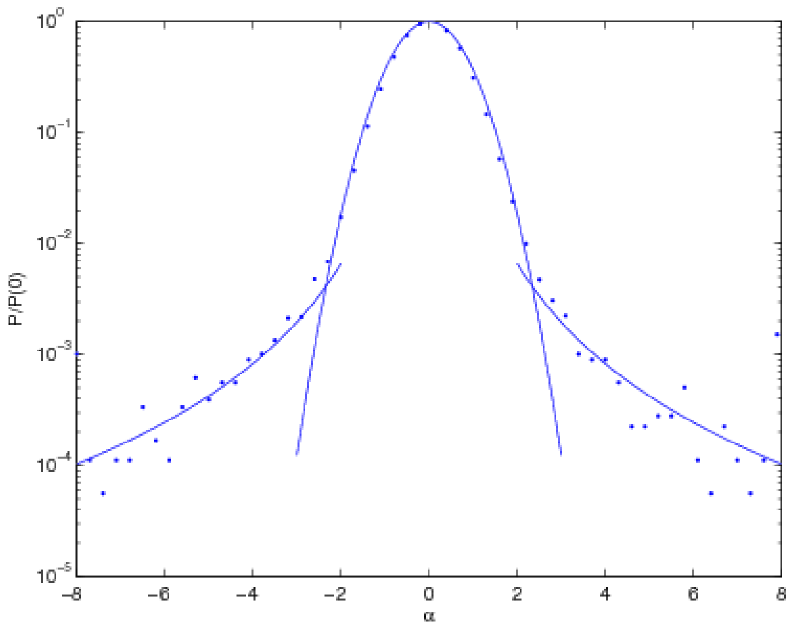

Figure 27: The comparison of Coulomb scattering with Jackson's book.

19.3 The Flow Diagram of *CollimatorPhysics* Class in OPAL

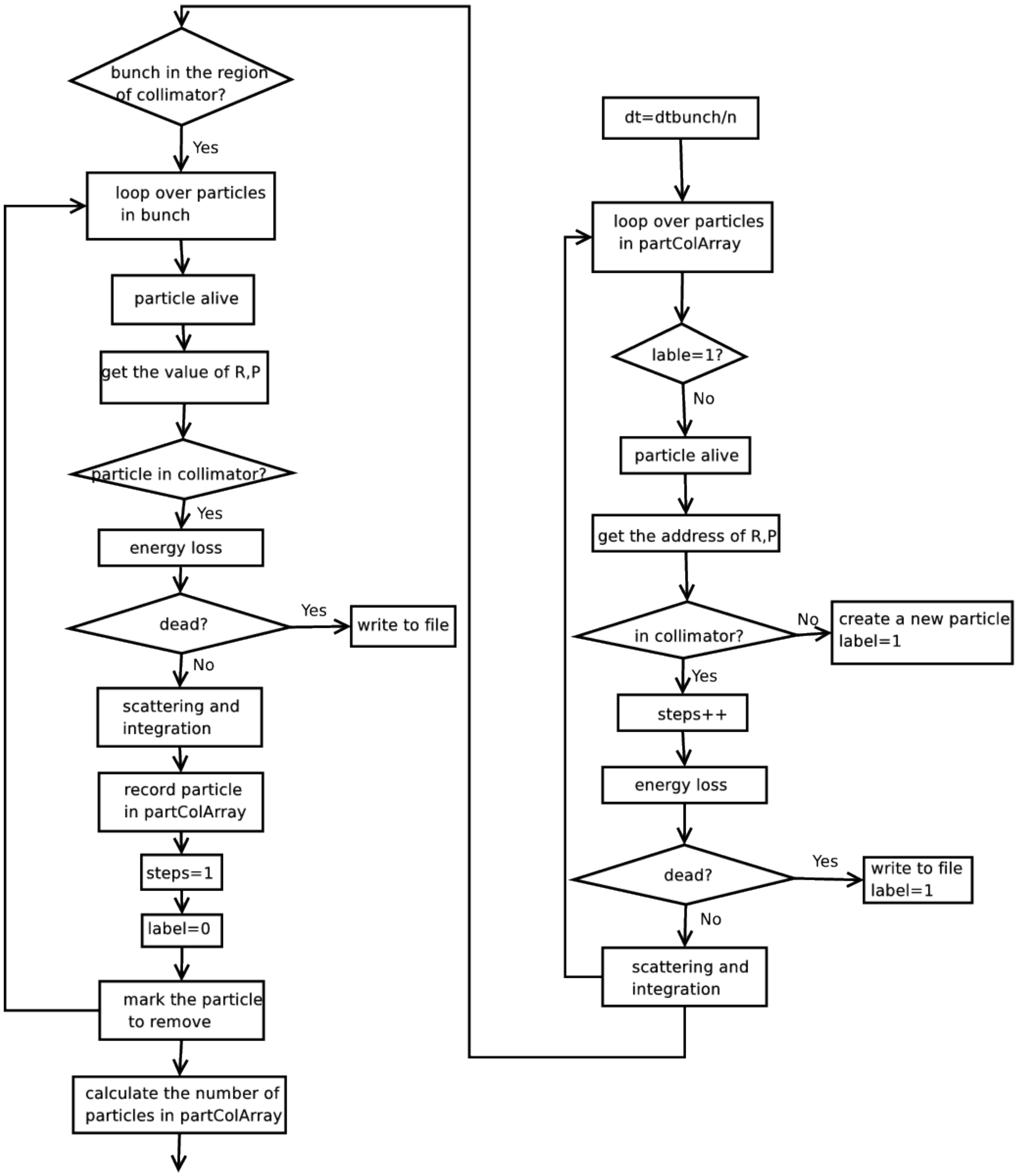

Figure 28: The diagram of CollimatorPhysics in *OPAL*.

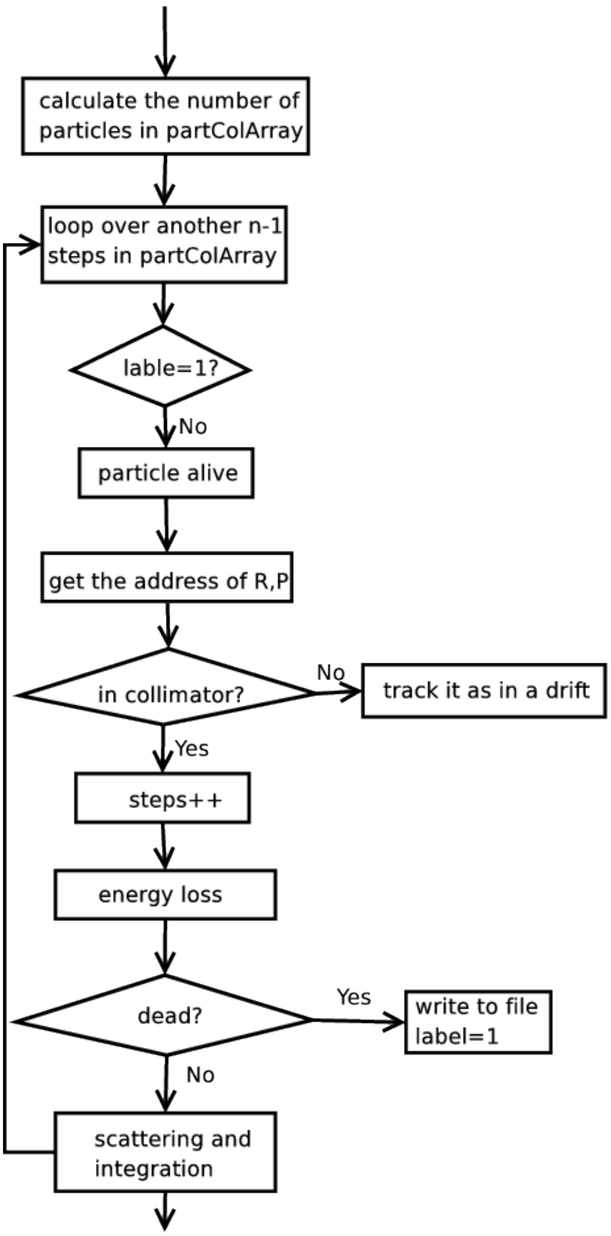

Figure 29: The diagram of CollimatorPhysics in *OPAL* (continued).

19.3.1 The Substeps

Small step is needed in the routine of CollimatorPhysics.

If a large step is given in the main input file, in the file *CollimatorPhysics.cpp*, it is divided by a integer number n to make the step size using for the calculation of collimator physics less than 1.01e-12 s. As shown by Figure 28 and Figure 29 in the previous section, first we track one step for the particles already in the collimator and the newcomers, then another (n-1) steps to make sure the particles in the collimator experience the same time as the ones in the main bunch.

Now, if the particle leave the collimator 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.

19.4 Available Materials in *OPAL*

Material	Z	A	ρ $[g/cm^3]$	X0 $[g/cm^2]$	A2	A3	A4	A5	*OPAL* Name
Aluminum	13	26.98	2.7	24.01	4.739	2766	164.5	2.023E-02	`Aluminum`
BoronCarbide	26	55.25	2.48	50.14	3.963	6065	1243	7.782e-3	`BoronCarbide`
AluminaAl2O3	50	101.96	3.97	27.94	7.227	11210	386.4	4.474e-3	`AluminaAl2O3`
Copper	29	63.54	8.96	12.86	4.194	4649	81.13	2.242E-02	`Copper`
Graphite	6	12.0172	2.210	42.7	2.601	1701	1279	1.638E-02	`Graphite`
GraphiteR6710	6	12.0172	1.88	42.7	2.601	1701	1279	1.638E-02	`GraphiteR6710`
Titan	22	47.8	4.54	16.16	5.489	5260	651.1	8.930E-03	`Titan`
Air	7	14	0.0012	37.99	3.350	1683	1900	2.513E-02	`Air`
Kapton	6	12	1.4	39.95	2.601	1701	1279	1.638E-02	`Kapton`
Gold	79	197	19.3	6.46	5.458	7852	975.8	2.077E-02	`Gold`
Water	10	18	1	36.08	2.199	2393	2699	1.568E-02	`Water`
Mylar	6.702	12.88	1.4	39.95	3.35	1683	1900	2.513E-02	`Mylar`
Berilium	4	9.012	1.848	65.19	2.590	966.0	153.8	3.475E-02	`Berilium`
Molybdenum	42	95.94	10.22	9.8	7.248	9545	480.2	5.376E-03	`Molybdenum`

Table 38: List of materials with their parameters implemented in *OPAL*.

19.5 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.

19.6 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 30 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 31 shows the energy spectrum and angle deviation at z=0.1 m after an elliptic collimator.

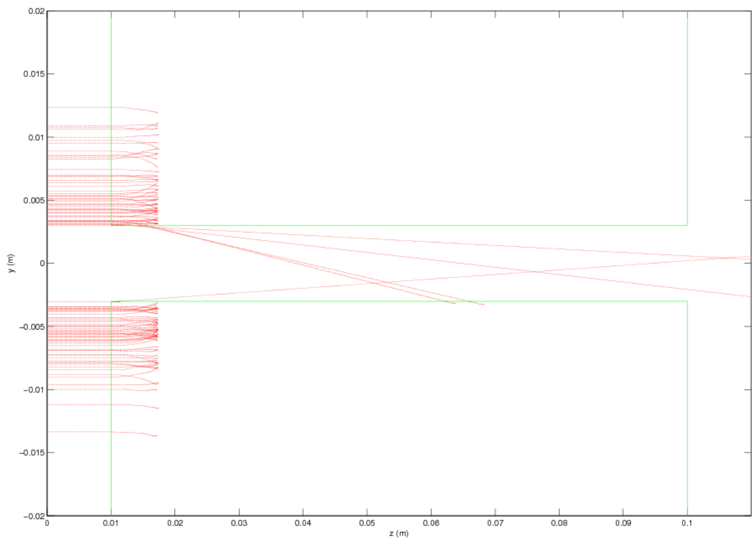

Figure 30: The passage of protons through the collimator.

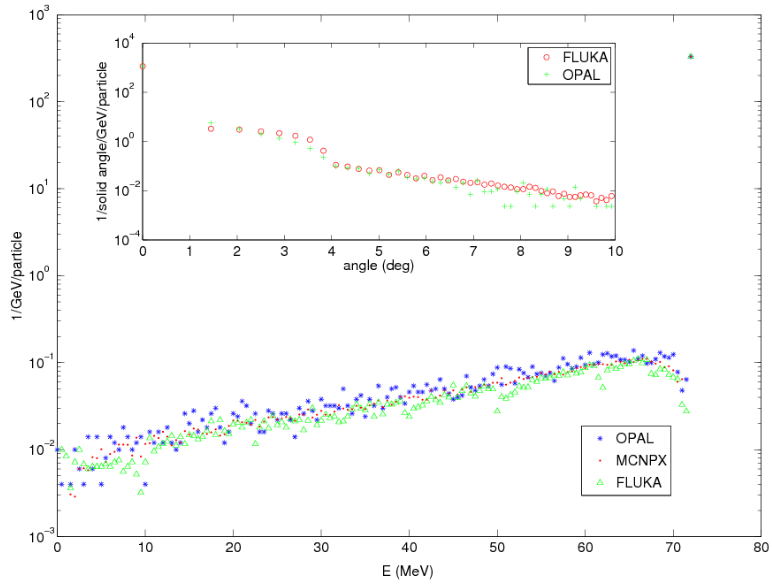

Figure 31: The energy spectrum and scattering angle at z=0.1 m

Chapter 20

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 [pgnl:06,zepv:00,gala:98,yrss:09,basi:05]. 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.

20.1 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

$$\begin{array}{lll} \min & f_m(\mathbf{x}), & m = \{1, \ldots, M\} \\ \text{s.t.} & g_j(\mathbf{x}) \geq 0, & j = \{1, \ldots, J\} \\ & -\infty \leq x_i^L \leq \mathbf{x} = x_i \leq x_i^U \leq \infty, & i = \{0, \ldots, n\}. \end{array}$$

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 32 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.

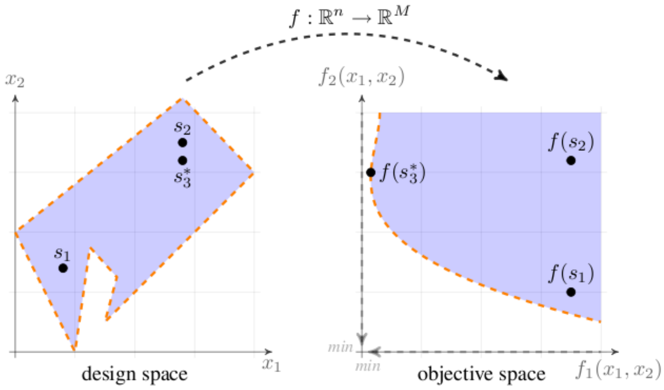

Figure 32: The (often non-linear) mapping $f : \mathbb{R}^n \to \mathbb{R}^M$ from design to objective space. The dashed lines represent the constraints in design space and the set of solutions (Pareto front) in objective space.

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.

20.2 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 [deb:09].

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 33 there exist "weaker" formulations of Pareto optimality. Of special interest is the result shown in [paya:01], 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.

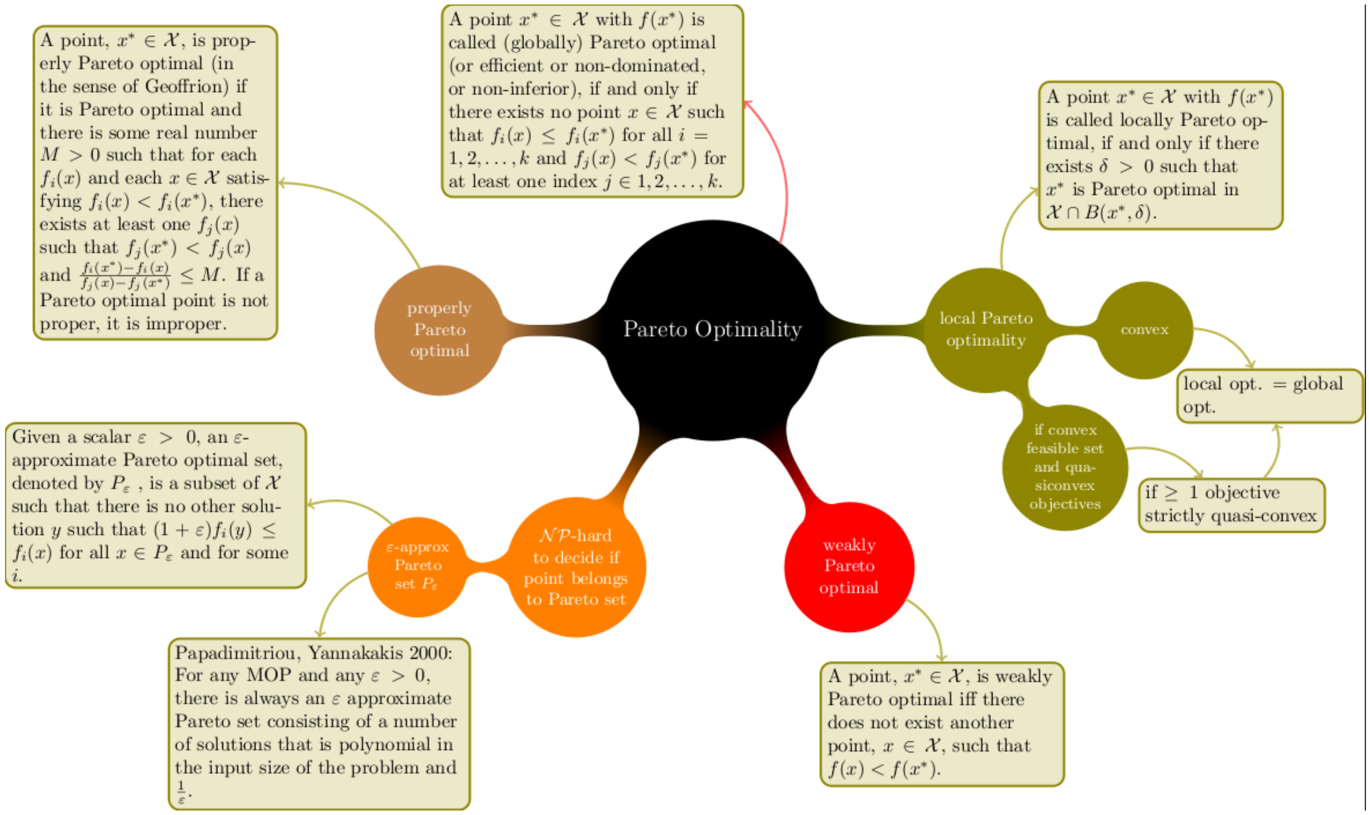

Figure 33: Various definitions regarding Pareto optimality.

20.3 MOGA Theory

Here some facts on “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

20.4 OPAL Commands

20.4.1 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, Also the design variables need to be added to the data file, see also the example files.

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.

20.4.2 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.
NUM_MASTERS	Number of master nodes.
NUM_COWORKERS	Number processors per worker.
SELECTOR	Path of the selector.
DUMP_DAT	Dump old generation data format with frequency.
DUMP_FREQ	Dump old generation data format with frequency.
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.
GENE_MUTATION_PROBABILITY	Mutation probability of individual gene, default: 0.5.
MUTATION_PROBABILITY	Mutation probability of genome, default: 0.5.
RECOMBINATION_PROBABILITY	Probability for genes to recombine, default: 0.5.
SIMBIN_CROSSOVER_NU	Simulated binary crossover, default: 2.0
INITIAL_OPTIMIZATION	Optimize speed of first generation creation (useful when number of infeasible solutions large), default: false
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).

Table 39: Attributes for the command OPTIMIZE.

20.4.3 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 40: Attributes for the command DVAR.

20.4.4 OBJECTIVE Command

The OBJECTIVE command defines an objective for optimization.

Attribute	Description
EXPR	Expression to minimize during optimization.

Table 41: Attributes for the command OBJECTIVE.

20.4.5 CONSTRAINT Command

The CONSTRAINT command defines a constraint for optimization.

Attribute	Description
EXPR	Expression that should be fulfilled during optimization.

Table 42: Attributes for the command CONSTRAINT.

20.4.6 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>, <spos>, <sdds_file>)	A simple expression to get SDDS value near a specific spos for a variable.
statVariableAt(<var>, <spos>)	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).

Table 43: Available functions for the EXPR attributes for OBJECTIVE and CONSTRAINT.

20.4.7 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, SIMBIN_CROSSOVER_NU=2.0,
          NUM_MASTERS=1, NUM_COWORKERS=1, SIMTMPDIR="simtmpdir",
          TEMPLATEDIR="tmpl", FIELDMAPDIR="fieldmaps", OUTPUT="optLinac",
          OUTDIR="results";

QUIT;
```

Data file 05-DL_QN3.data (no function but needed for historical reasons, not needed in later versions)

```
QDX1_K1  17.7   # First  defocusing quadrupole
QFX1_K1 -17.5   # First    focusing quadrupole
QDX2_K1  17.5   # Second defocusing quadrupole
```

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
```

Chapter 21

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).

Be aware of the fact, this is an experimental feature in V2.0.0

21.1 OPAL Commands

It uses almost the same syntax as the optimiser.

21.1.1 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.

21.1.2 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 in output file generation.
OUTDIR	Name of directory used to run and store generation output files.
DVARS	List of design variables to be used.
SAMPLINGS	List of sample methods to be used.
NUM_MASTERS	Number of master nodes (currently only 1 master supported).
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).

Table 44: Attributes for the command SAMPLE.

The difference between `RASTER = TRUE` and `RASTER = FALSE` can be depicted in the following figure.

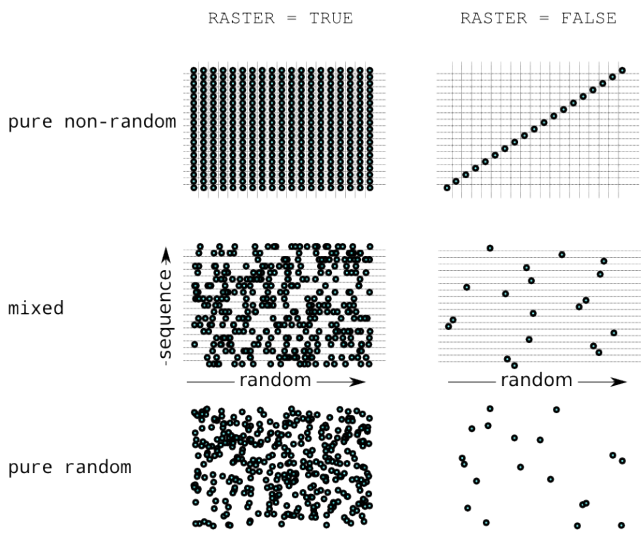

Figure 34: Sampling methods

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.

21.1.3 SAMPLING Command

Attribute	Description
VARIABLE	Name of the design variable.
TYPE	Sampling method (see next section).
RANDOM	Boolean to control whether sampling mode is random or sequential. Default is sequential.
SEED	Seed for random sampling (default: 42).
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 45: Attributes for the command SAMPLING.

21.1.4 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.

Table 46: Available sampling methods.

21.2 Example Input File

opal.in

```
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;
```

Data file opal.data (no function but needed for historical reasons, not needed in later versions)

```
nstep  25
MX     20
```

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 `opal.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="RK-4";
 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 [42] 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 [43] 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 [42]) 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 [43]. 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 [43]. 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 35):

- 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.

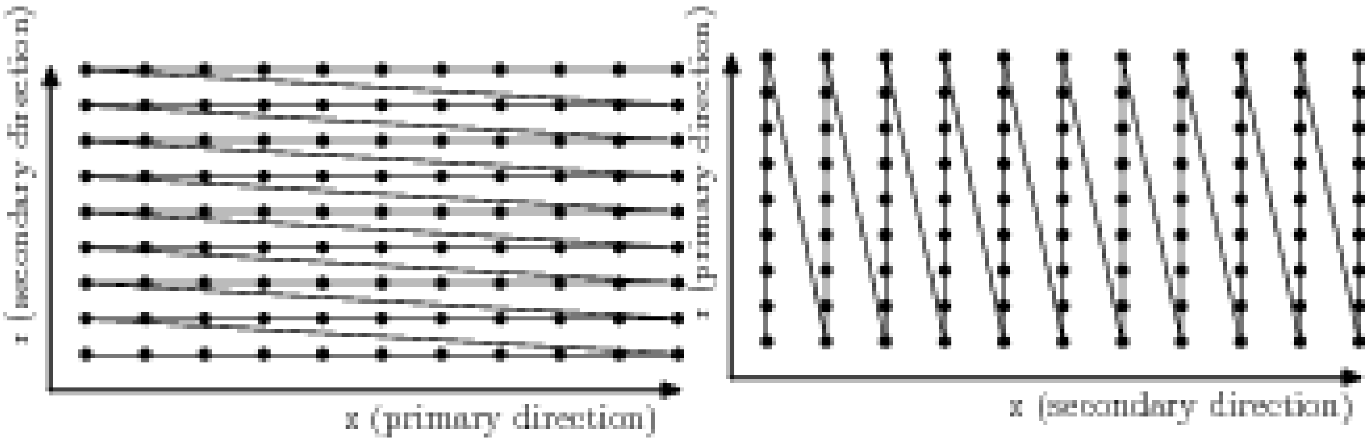

Figure 35: Ordering of points for 2D field maps in T7 files (left XZ orientation, right ZX orientation)

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 36 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 [43]. 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 [43] interpolation algorithm.

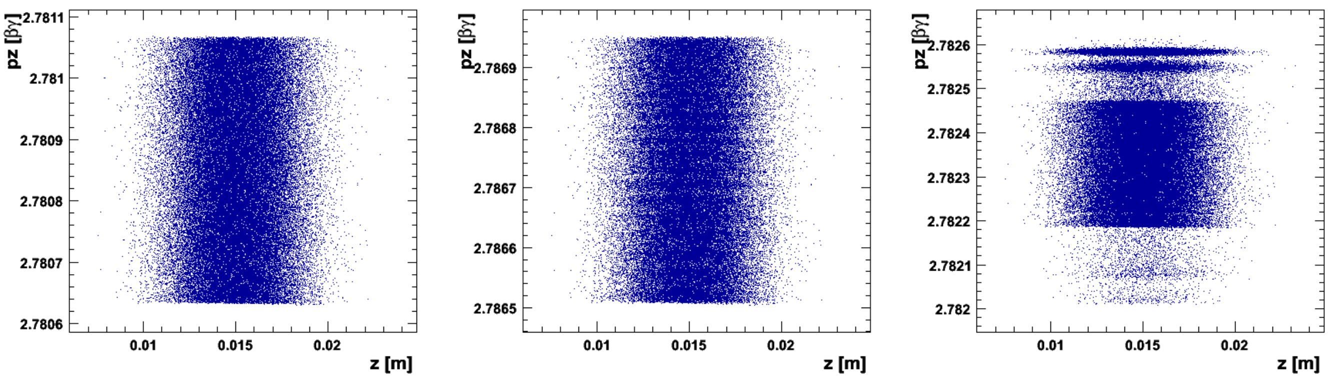

Figure 36: The longitudinal phase space after a gun simulation using a 1D field map (on-axis field) of the gun, a 1D field map (on-axis field) of the gun in combination with the `FAST` switch, and a 2D field map of the gun generated by Superfish [43].

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 $\max(|B_{\text{on axis}}|) = 1.0$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 47: Layout of a `1DMagnetoStatic` field map file.

A `1DMagnetoStatic` field map has the general form shown in Table 47. 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 $\max(|B_{\text{on axis}}|) = 1.0\text{T}$. 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 48: Layout of an `AstraMagnetoStatic` field map file.

An `AstraMagnetoStatic` field map has the general form shown in Table 48. 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 $\max(|E_{onaxis}|) =$

1MV/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 49: Layout of a `1DDynamic` field map file.

A `1DDynamic` field map has the general form shown in Table 49. 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 $\max(|E_{\text{on axis}}|) = 1\text{MV/m}$. The frequency of this field is 2997.924MHz. (*OPAL-t* does not provide a `FAST` version of this map type.)

AstraMagnetoStatic	$N_{Fourier}$	TRUE I 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 50: Layout of an `AstraDynamic` field map file.

An `AstraDynamic` field map has the general form shown in Table 50. 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 [42] 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 38. 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 37 the effect of a negative coefficient for the highest degree in the original data.

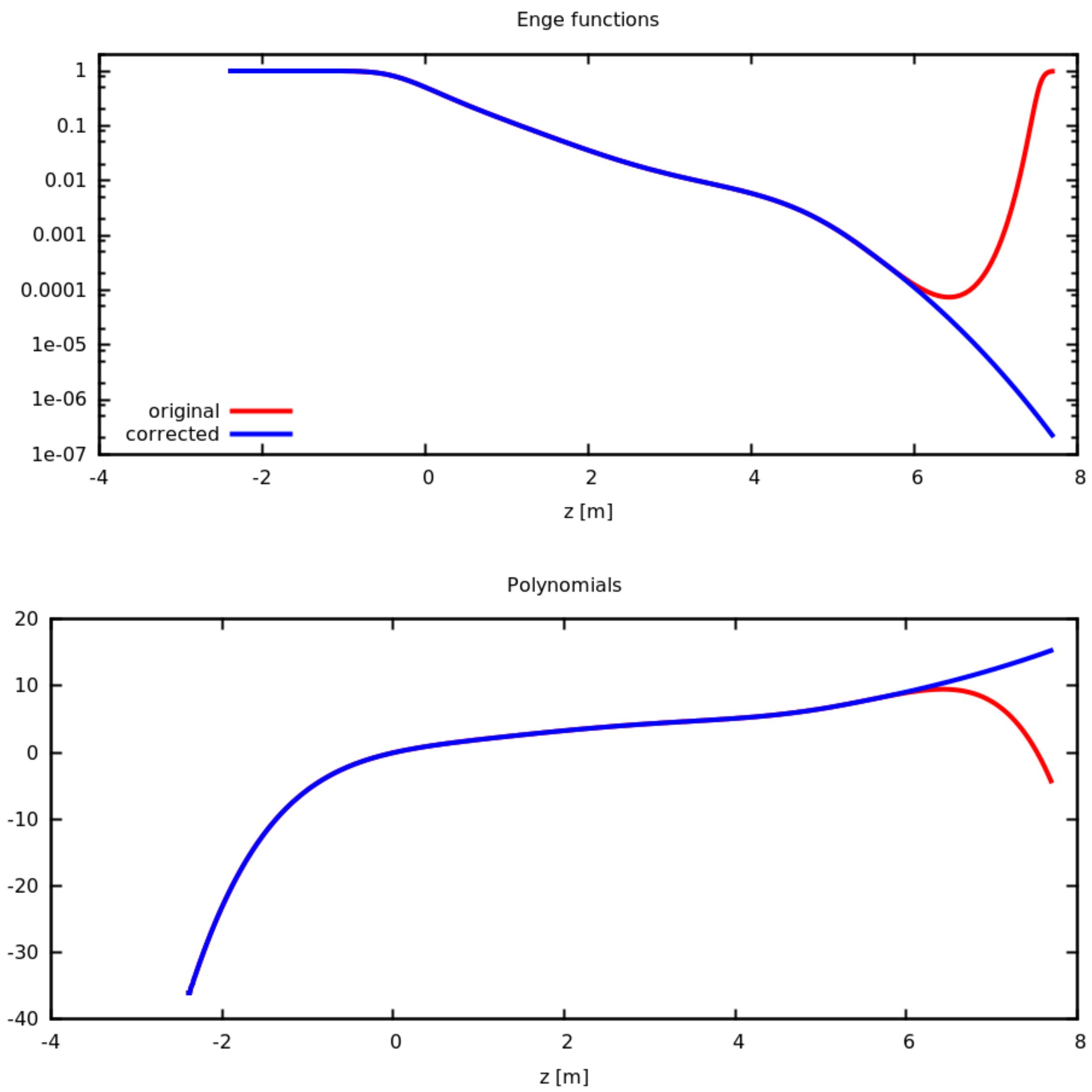

Figure 37: Effect of a negative coefficient for the highest degree in the original data.

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).

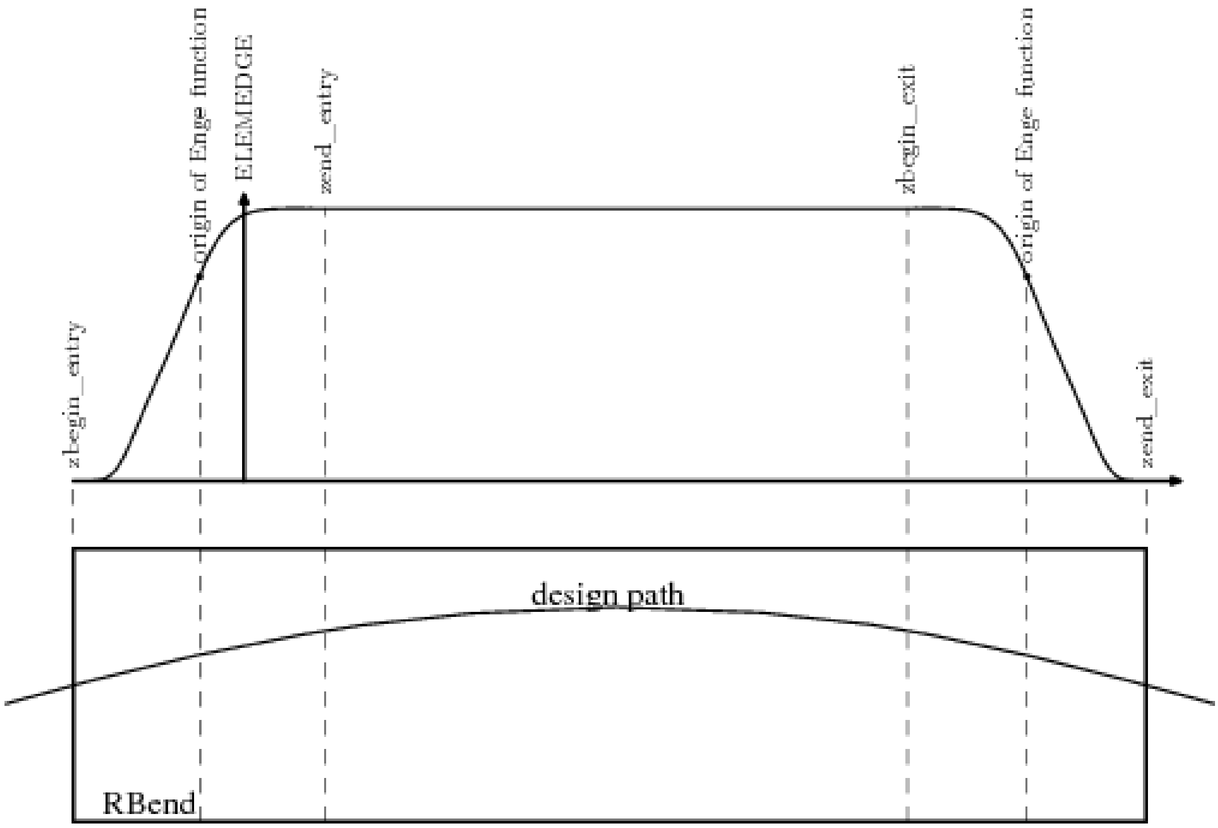

Figure 38: Example of Enge functions describing the entrance and exit fringe fields of a rectangular bend magnet. The top part of the figure shows the relative field strength on the mid-plane. The bottom part of the figure shows an example of a particle trajectory through the magnet. Note that the magnet 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 51. 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 51: Layout of a `1DProfile1` field map file.

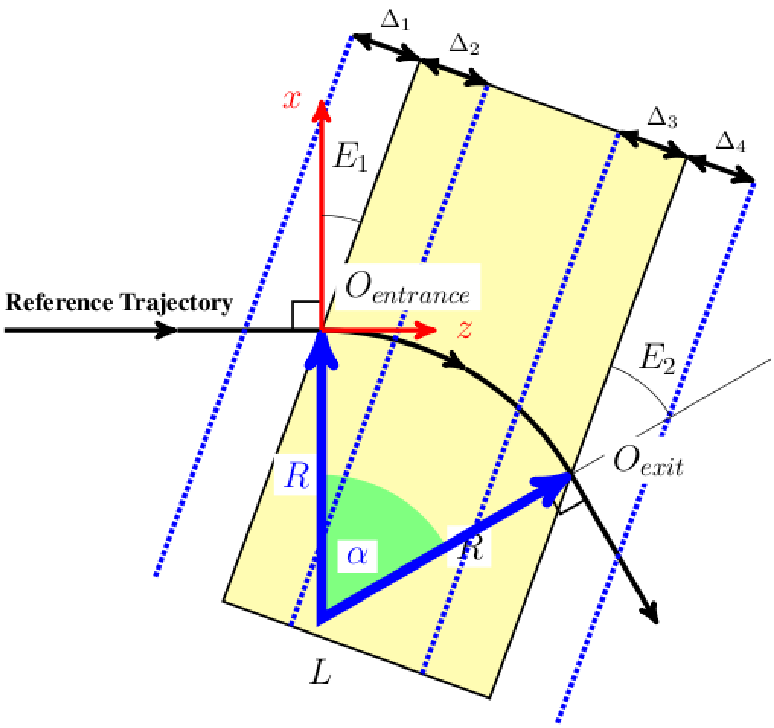

Figure 39: Illustration of a rectangular bend (`RBEND`, see RBend (OPAL-t) showing the entrance and exit fringe field regions. Δ_1 is the perpendicular distance in front of the entrance edge of the magnet where the magnet fringe fields are non-negligible. Δ_2 is the perpendicular distance behind the 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}

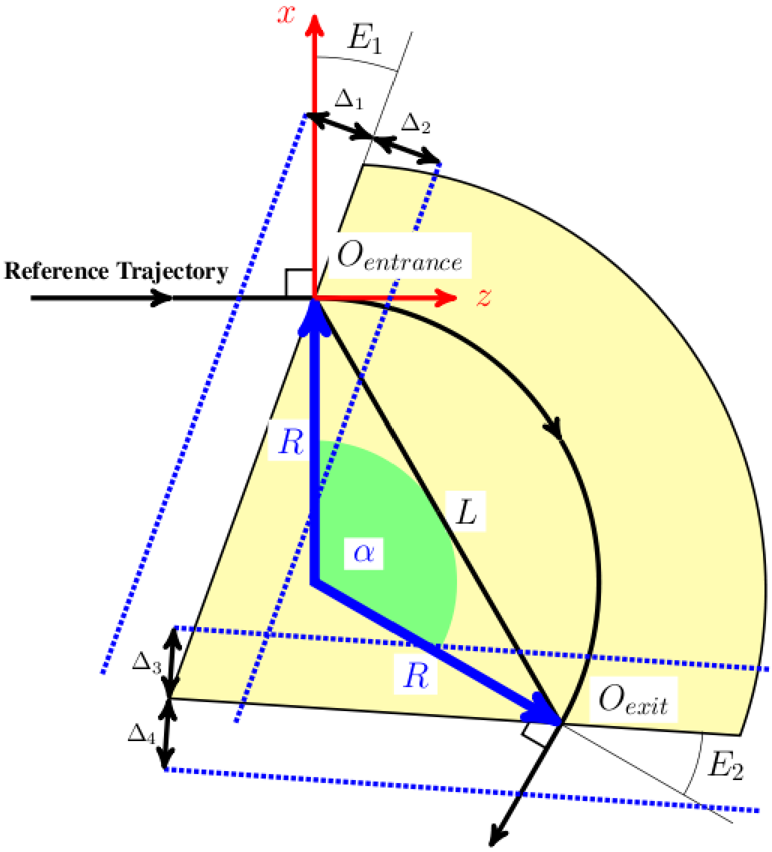

Figure 40: Illustration of a sector bend (SBEND, see SBend (OPAL-t)) showing the entrance and exit fringe field regions. Δ_1 is the perpendicular distance in front of the entrance edge of the magnet where the magnet fringe fields are non-negligible. Δ_2 is the perpendicular distance behind the entrance 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 39 and Figure 40 illustrate the fringe field regions for an RBEND and an SBEND element. Referring to the general field map file shown in Table 51, 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 39 and Figure 40.

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 51 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 52: Layout of a `2DElectroStatic` field map file.

A `2DElectroStatic` field map has the general form shown in Table 52. 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 53: Layout of a `2DMagnetoStatic` field map file.

A `2MagnetoStatic` field map has the general form shown in Table 53. 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 $\max(|E_{z,\text{ on axis}}|) = 1\text{MV/m}$.

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 54: Layout of a `2DDynamic` field map file.

A `2DDynamic` field map has the general form shown in Table 54. 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 55: Layout of a `3DMagnetoStatic` field map file.

A `3DMagnetoStatic` field map has the general form shown in Table 55. 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 56: Layout of a `3DMagnetoStatic_Extended` field map file.

A `3DMagnetoStatic_Extended` field map has the general form shown in Table 56. 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 56.

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 57: Layout of a `3DDynamic` field map file.

A `3DDynamic` field map has the general form shown in Table 57. 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

[42] J. E. Spencer and H. A. Enge, *Split-pole magnetic spectrograph for precision nuclear spectroscopy*, Nucl. Instrum. Methods 49, 181–193 (1967).

[43] 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.

$$\sigma_{beam} = \begin{pmatrix} \sigma_x & \sigma_{xp_x} \\ \sigma_{xp_x} & \sigma_{p_x} \end{pmatrix} = \begin{pmatrix} \sigma_x & \delta \cdot \sqrt{\sigma_x \sigma_{p_x}} \\ \delta \cdot \sqrt{\sigma_x \sigma_{p_x}} & \sigma_{p_x} \end{pmatrix} = \begin{pmatrix} < x^2 > & < xp_x > \\ < xp_x > & < p_x^2 > \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{N}\sum_{i=1}^N x_i^2 & \frac{1}{N}\sum_{i=1}^N x_i p_{x_i} \\ \frac{1}{N}\sum_{i=1}^N x_i p_{x_i} & \frac{1}{N}\sum_{i=1}^N p_{x_i}^2 \end{pmatrix} = \varepsilon \cdot \begin{pmatrix} \beta & -\alpha \\ -\alpha & \gamma \end{pmatrix}$$

$$\bar{p}_x = \sqrt{\frac{1}{N}\sum_{i=1}^N p_{x_i}^2} = \sqrt{\sigma_{p_x}} \qquad \bar{x} = \sqrt{\frac{1}{N}\sum_{i=1}^N x_i^2}$$

$$\bar{p}_y = \sqrt{\frac{1}{N}\sum_{i=1}^N p_{y_i}^2} = \sqrt{\sigma_{p_y}} \qquad \bar{y} = \sqrt{\frac{1}{N}\sum_{i=1}^N y_i^2}$$

$$\gamma = \frac{E_{kin} + m_p}{m_p} \qquad \beta = \sqrt{1 - \frac{1}{\gamma^2}} = \frac{v}{c}$$

$$(\beta\gamma) = \frac{E_{kin} + m_p}{m_p} \cdot \sqrt{1 - \frac{1}{\gamma^2}} = \frac{\beta}{\sqrt{1-\beta^2}} \qquad \mathrm{B}\rho = \frac{(\beta\gamma) \cdot m_p \cdot 10^9}{c} \ [\mathrm{T\ m}]$$

$$m_p = 0.939277[GeV] \qquad c = 299792458[m/s]$$

Quantity	`MADX`		Conversion			*OPAL-Output*	
Momenta	$\bar{p}_x$	[rad]	$\bar{p}_x[\beta\gamma]$	=	$(\bar{p}_x\,[\mathrm{rad}])\cdot(\beta\gamma)$	$\bar{p}_x$	$[\beta\gamma]$
Correlation of $\bar{x}$,$\bar{p}_x$	δ	[1]	δ	=	$(\sigma_{xp_x}\,[\mathrm{m\ rad}])\,/\,((\bar{p}_x\,[\mathrm{rad}])\cdot(\bar{x}\,[\mathrm{m}]))$	δ	[1]
				=	$(\sigma_{xp_x}\,[\mathrm{m\ rad}])\,/\sqrt{(\sigma_x\,[\mathrm{m}^2])\cdot\left(\sigma_{p_x}\left[\mathrm{rad}^2\right]\right)}$		
Emittance	ε_x	[m rad]	$\varepsilon_x[\mathrm{m}\ \beta\gamma]$	=	$\sqrt{(\bar{p}_x\,[\beta\gamma])^2\cdot(\bar{x}\,[\mathrm{m}])^2-(\delta\cdot(\bar{x}\,[\mathrm{m}])\cdot(\bar{p}_x\,[\beta\gamma]))^2}$	ε_x	$[\mathrm{m}\ \beta\gamma]$
				=	$\sqrt{\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)\cdot(\sigma_x\,[\mathrm{m}^2])-\left(\delta\cdot\sqrt{(\sigma_x\,[\mathrm{m}^2])\cdot\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)}\right)^2}$		
				=	$\sqrt{\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)\cdot(\sigma_x\,[\mathrm{m}^2])-(\sigma_{xp_x}\,[\mathrm{m}\ \beta\gamma])^2}$		
Twiss Parameter α	α	[1]	$\alpha\,[1]$	=	$-\delta\cdot(\bar{x}\,[\mathrm{m}])\cdot(\bar{p}_x\,[\beta\gamma])\,/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$	α_T	[1]
				=	$-\delta\cdot\sqrt{(\sigma_x\,[\mathrm{m}^2])\cdot\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)}\,/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$		
Twiss Parameter β_T	β_T	[m/rad]	$\beta_T\,[\mathrm{m}/\beta\gamma]$	=	$(\bar{x}\,[\mathrm{m}])^2\,/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$	β_T	$[\mathrm{m}/\beta\gamma]$
				=	$\left(\sigma_x\left[\mathrm{m}^2\right]\right)/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$		
Twiss Parameter γ_T	γ_T	[rad/m]	$\gamma_T\,[\beta\gamma/\mathrm{m}]$	=	$(\bar{p}_x\,[\beta\gamma])^2\,/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$	γ_T	$[\beta\gamma/\mathrm{m}]$
				=	$\left(\sigma_{p_x}\left[(\beta\gamma)^2\right]\right)/\,(\varepsilon_x\,[\mathrm{m}\ \beta\gamma])$		
Focusing strength	k_1	$\left[\mathrm{m}^{-2}\right]$	$k_1\,[\mathrm{T/m}]$	=	$\left(k_1\left[\mathrm{m}^{-2}\right]\right)\cdot(\mathrm{B}\rho\,[\mathrm{T\ m}])$	k_1	[T/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:

$$\begin{aligned}
\mathrm{d}\Delta E(\varphi,r)\varphi = &- \int_{z_\text{begin}}^{z_\text{end}} (1+\omega\frac{\partial t(z,\varphi)}{\partial\varphi}) \sin(\omega t(z,\varphi)+\varphi) E_z(z,r) \\
&= -\cos(\varphi) \int_{z_\text{begin}}^{z_\text{end}} (1+\omega\frac{\partial t(z,\varphi)}{\partial\varphi}) \sin(\omega t(z,\varphi)) E_z(z,r) dz \\
&- \sin(\varphi) \int_{z_\text{begin}}^{z_\text{end}} (1+\omega\frac{\partial t(z,\varphi)}{\partial\varphi}) \cos(\omega t(z,\varphi)) E_z(z,r) dz \equiv 0.
\end{aligned}$$

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

```
K[i] = K[i-1] + q Δz[i](cos(φ)(Ez[i-1](Γ21[i] - Γ22[i]) + Ez[i]Γ22[i])
                         - sin(φ)(Ez[i-1](Γ11[i] - Γ12[i]) + Ez[i]Γ12[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

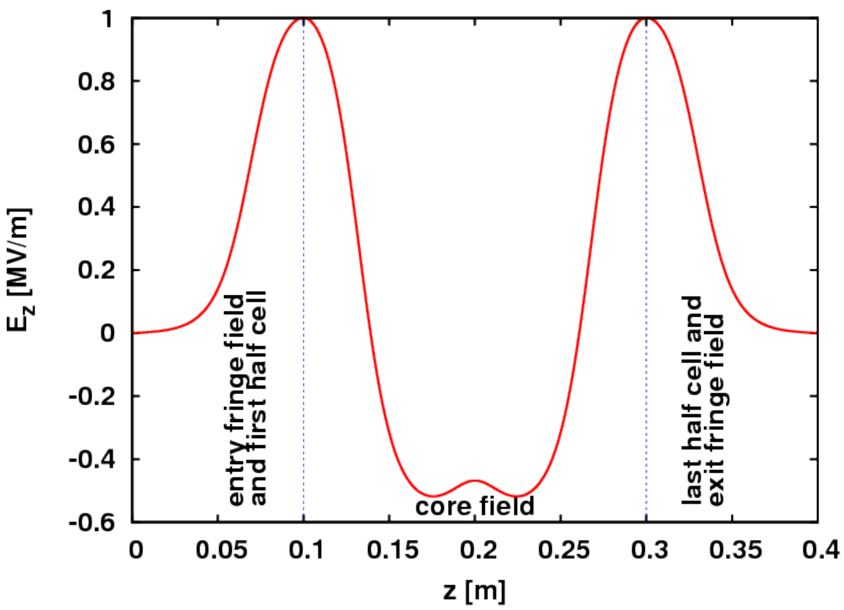

Figure 41: Field map 'FINLB02-RAC.T7' of type 1DDynamic

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 41.

$$\Delta E(\varphi, r) = qV_0 \int_{z_{\text{begin}}}^{z_{\text{beginCore}}} \cos(\omega t(z,\varphi) + \varphi) E_z(z,r)dz$$

$$+ qV_{\text{core}} \int_{z_{\text{beginCore}}}^{z_{\text{endCore}}} \cos(\omega t(z,\varphi) + \varphi_{\text{c1}} + \varphi) E_z(z,r)dz$$

$$+ qV_{\text{core}} \int_{z_{\text{beginCore}}}^{z_{\text{endCore}}} \cos(\omega t(z,\varphi) + \varphi_{\text{c2}} + \varphi) E_z(z+s,r)dz$$

$$+ qV_0 \int_{z_{\text{endCore}}}^{z_{\text{end}}} \cos(\omega t(z,\varphi) + \varphi_{\text{ef}} + \varphi) E_z(z,r)dz,$$

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

$$
\begin{aligned}
\Delta E(\varphi, r) = q\,V_0 \int_0^{1.5\cdot s} \cos\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \varphi\right) E_z(z,r)\,dz \\
+ \frac{2q\,V_0}{\sqrt{3}} \int_{1.5\cdot s}^{40.5\cdot s} \cos\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \frac{\pi}{6} + \varphi\right) E_z(z \quad\quad, r) dz \\
+ \frac{2q\,V_0}{\sqrt{3}} \int_{1.5\cdot s}^{40.5\cdot s} \cos\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \frac{\pi}{2} + \varphi\right) E_z(z+s, r) dz \\
+ q\,V_0 \int_{40.5\cdot s}^{42\cdot s} \cos\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \varphi\right) E_z(z,r)\,dz.
\end{aligned}
$$

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 ($z' = z + s$)

$$\int_0^{3\cdot s} \sin\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \frac{3\pi}{2} + \varphi\right) E_z^{(1)}((z+s) \bmod(3s), r) dz$$

$$= \int_s^{4\cdot s} \sin\left(\omega\left(\frac{z'-s}{\beta c} + t_0\right) + \frac{3\pi}{2} + \varphi\right) E_z^{(1)}(z' \bmod(3s), r) dz'$$

$$= \int_0^{3\cdot s} \sin\left(\omega\left(\frac{z}{\beta c} + t_0\right) + \frac{5\pi}{6} + \varphi\right) E_z^{(1)}(z, r)\, dz.$$

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 [44]. 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 [44] 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 42.

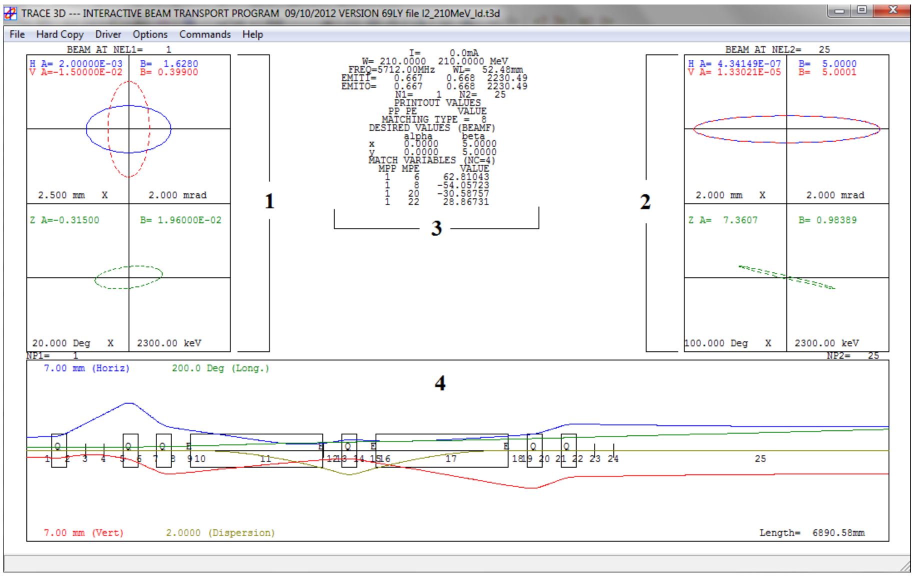

Figure 42: TRACE 3D graphic interface where: (1) input beam in transverse plane (above) and longitudinal plane (below); (2) output beam in transverse plane (above) and longitudinal plane (below); (3) summary of beam parameters such as input and output emittances and desired value for matching function; (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 [45]. The TRANSPORT version for Windows provides a graphic beam profile diagram, as well as a sigma matrix description of the simulated beam and line [46]. 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 [45] 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 43.

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 43: Sigma-matrix structure in TRACE 3D [44]

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 [46] is shown in Figure 44.

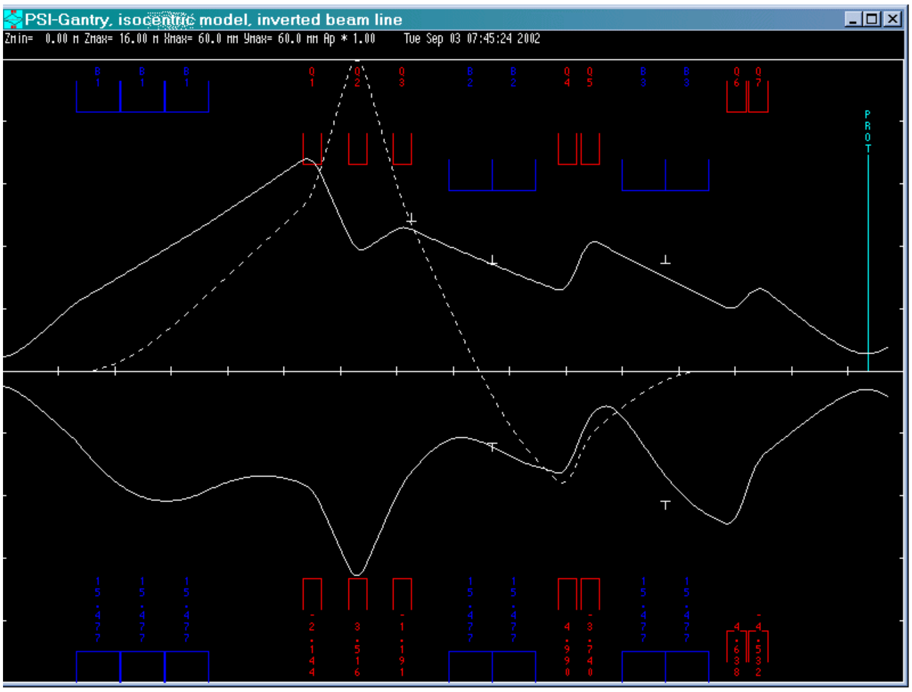

Figure 44: GUI TRANSPORT graphic interface [47]. The continuous lines describe the beam envelope in the vertical plane (above) and horizontal plane (below). The dashed line displays the dispersion. The elements in the beam line are drawn as blue and red rectangles

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 45.

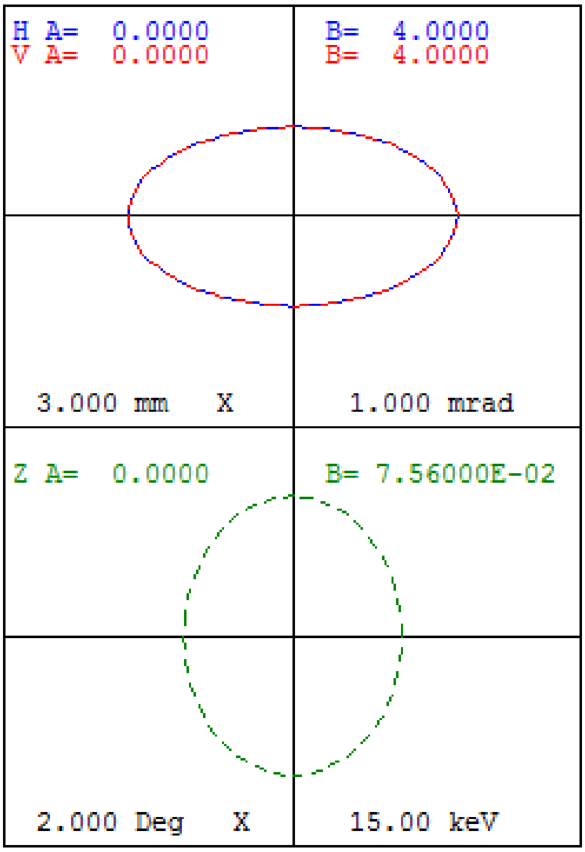

Figure 45: TRACE 3D input beam in the transversal plane (above) and in the longitudinal plane (below)

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 46: 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 46. 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 58: 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 59: 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 47.

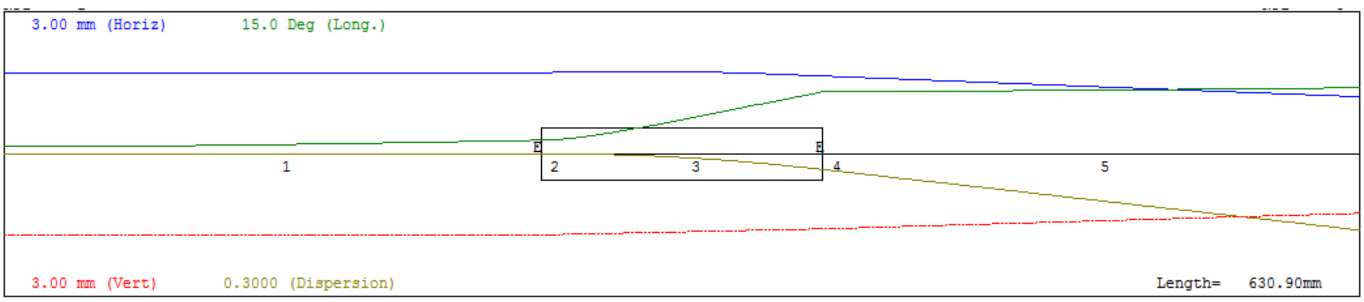

Figure 47: Beam envelopes in TRACE 3D for a SBEND with entrance and exit edge angles. The blue line describes the beam envelope in the horizontal plane, the red line in the vertical plane, the green line in the longitudinal plane. The yellow line displays the dispersion

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 60: 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 61.

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 61: 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 48.

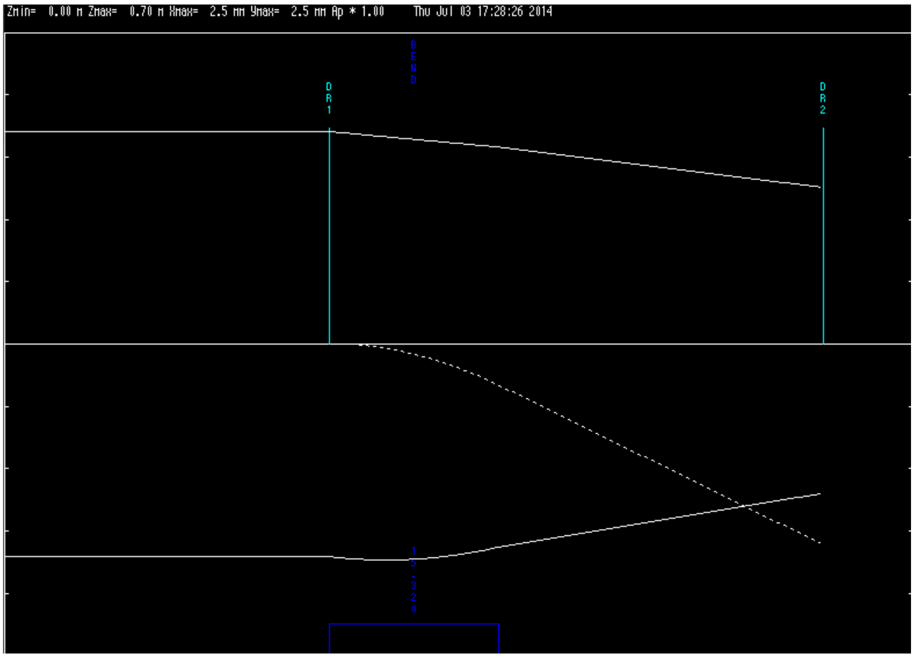

Figure 48: Beam envelopes in TRANSPORT for a SBEND with entrance and exit edge angles. The continuous lines describe the beam envelope in the vertical plane (above) and horizontal plane (below). The dashed line displays the dispersion.

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 62: 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 49.

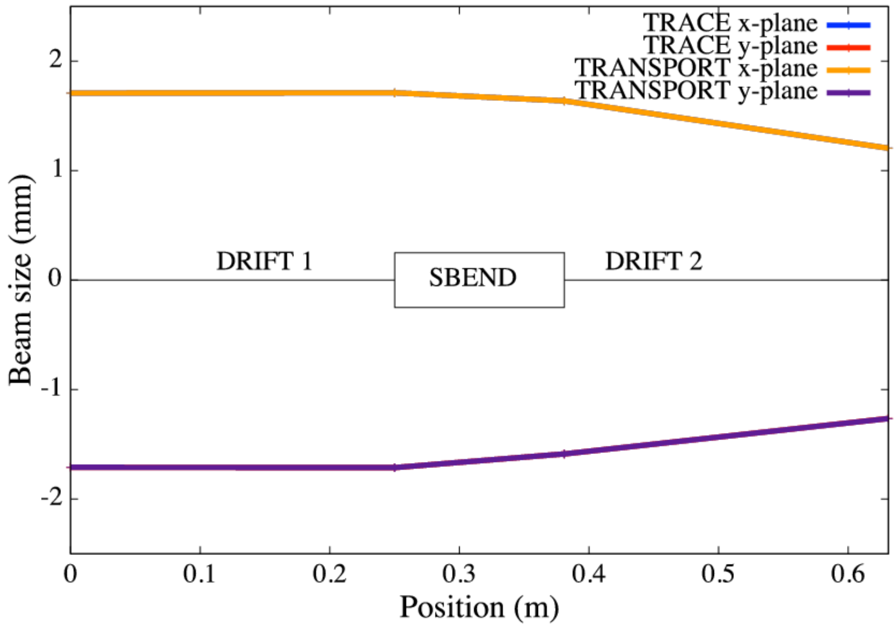

Figure 49: Transversal beam size comparison between TRACE 3D and TRANSPORT

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 63 and in Figure 50.

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 63: Horizontal and longitudinal emittance comparison between TRACE 3D and TRANSPORT, both expressed in π-mm-mrad

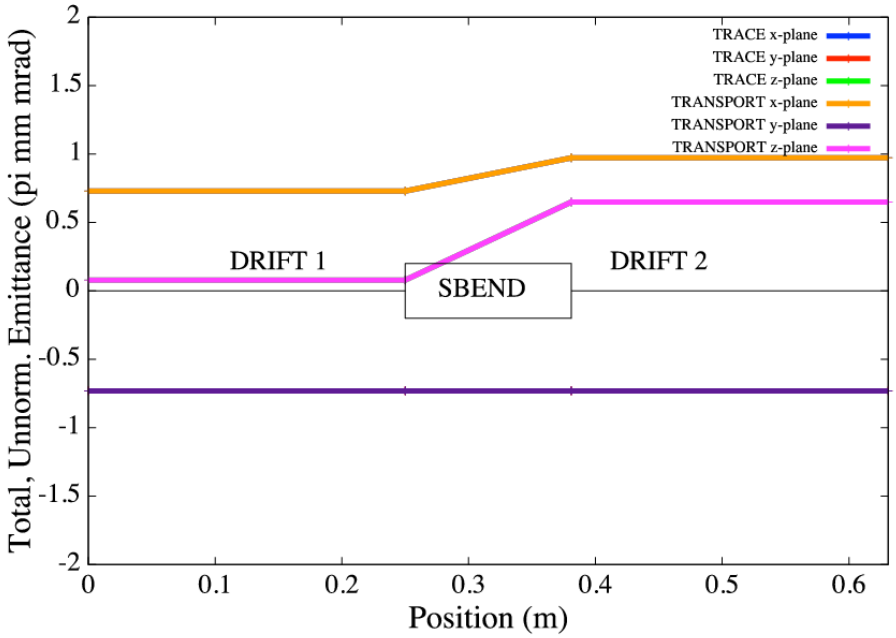

Figure 50: Emittance comparison between TRACE and TRANSPORT

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 64: 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 65.

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 65: 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 46, 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 58 and Table 59 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,
```

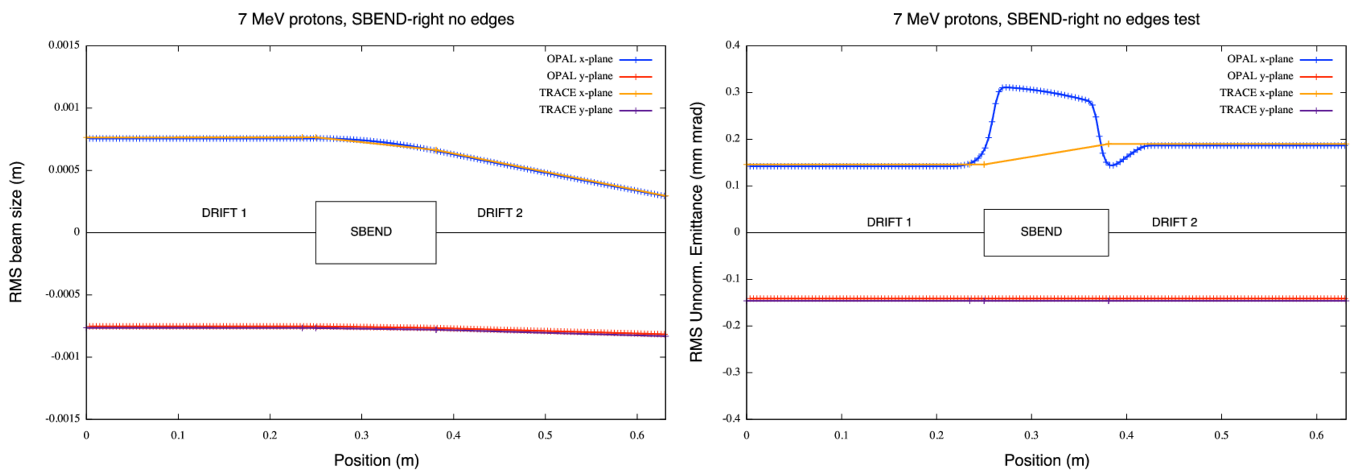

Figure 51: TRACE 3D and *OPAL* comparison: SBEND without edge angles,

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,
```

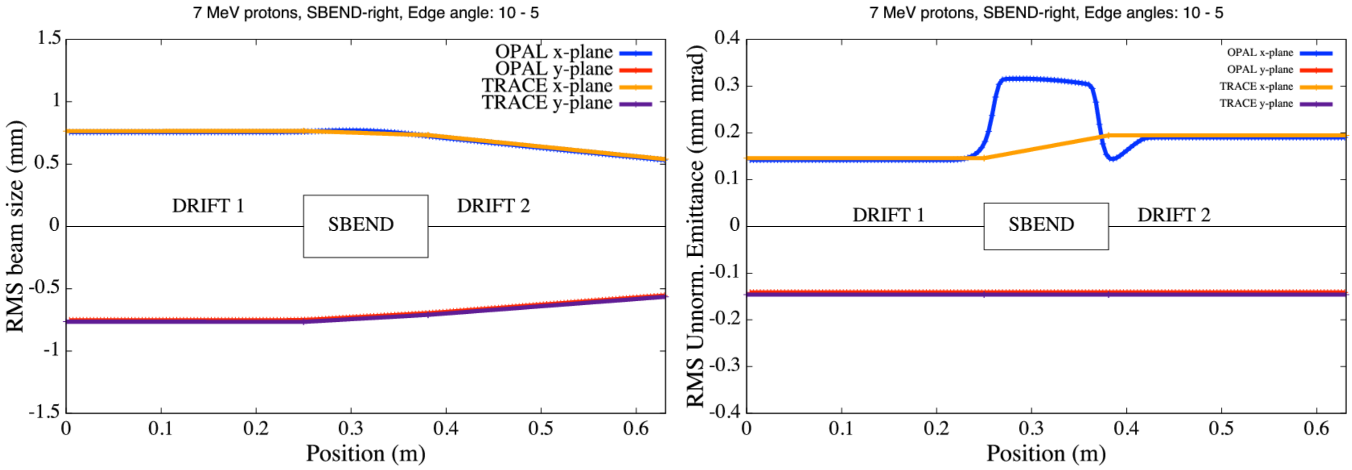

Figure 52: TRACE 3D and *OPAL* comparison: SBEND with edge angles

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 53 using:

```
// Bending magnet configuration:
K1=1.5
E1=0, E2=0,
```

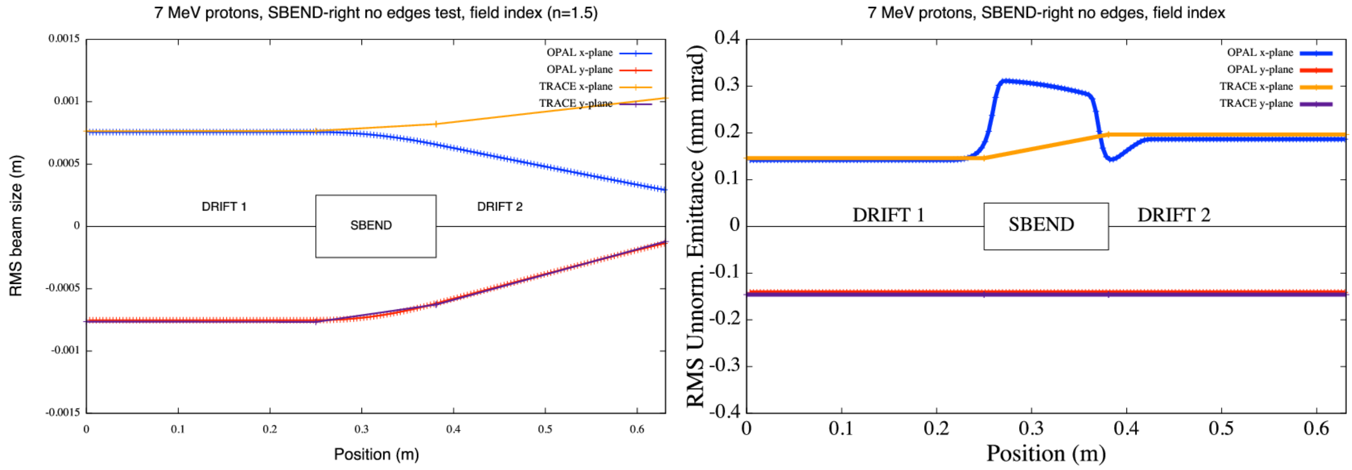

Figure 53: TRACE 3D and *OPAL* comparison: SBEND with field index and default field map

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 54, is achieved using a test field map in which the fringe field extension has been changed in the thin lens approximation.

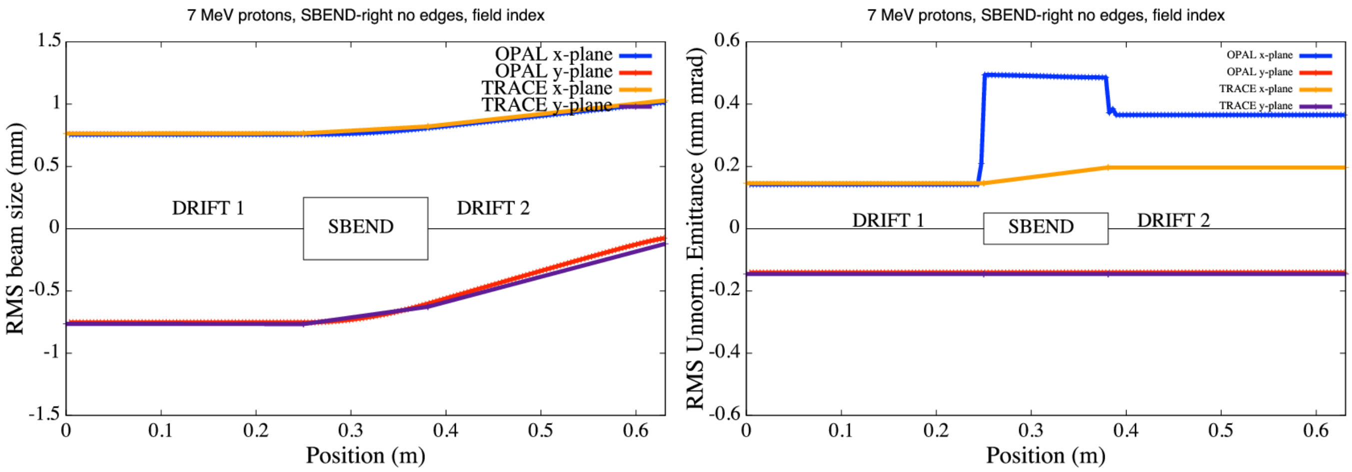

Figure 54: TRACE 3D and *OPAL* comparison: SBEND with field index and test field map

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 66: 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 54.

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.

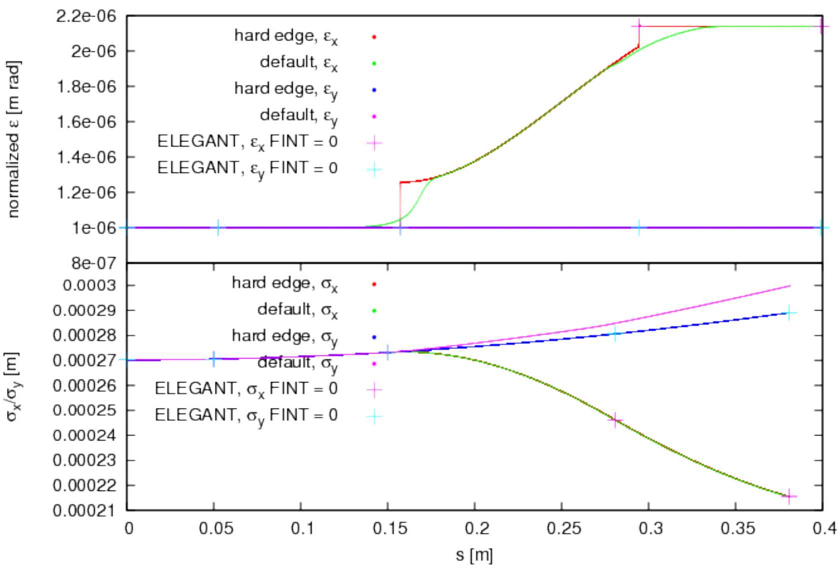

Figure 55: Compare emittances and beam sizes obtained by using the hard edge map (*OPAL*), the default map (*OPAL*), and the ELEGANT

Figure 55 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 56 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 56, 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.

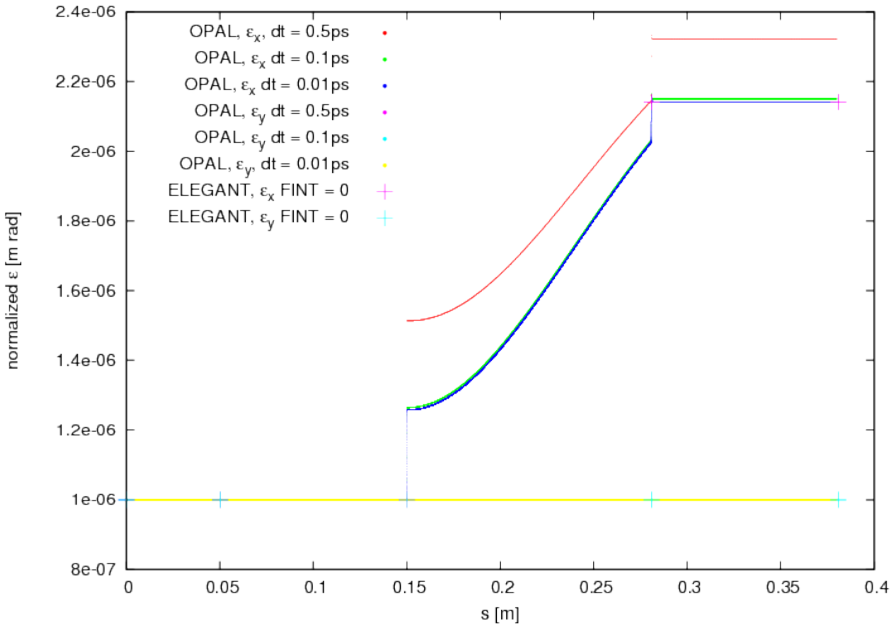

Figure 56: Horizontal and vertical normalized emittances for different integration time steps

Figure 57 and Figure 58 examine the effects of the fringe field range and the integration time step on the simulation accuracy. Figure 58 is a zoom-in plot of Figure 57. We can conclude that the size of the integration time step has more influence on the accuracy of the simulation.

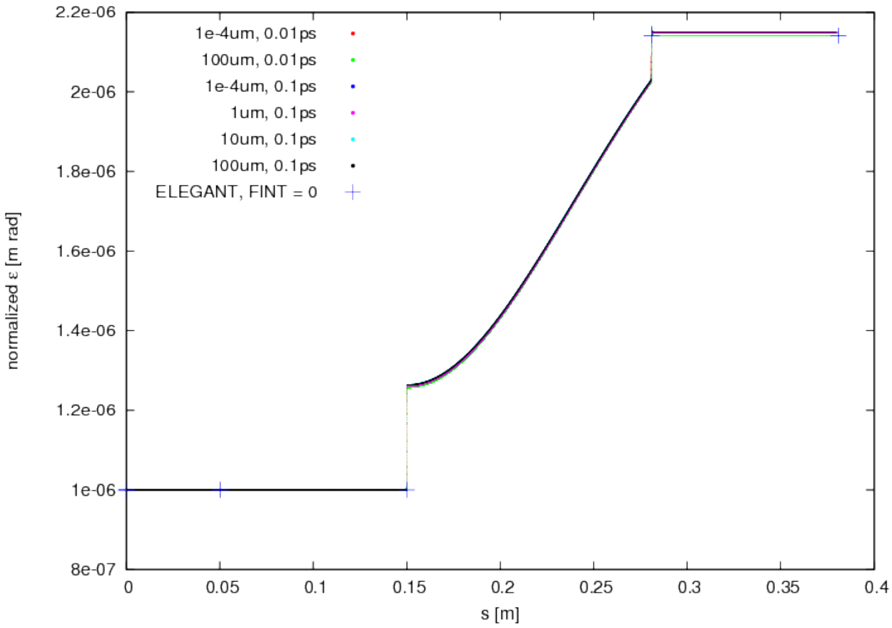

Figure 57: Normalized horizontal emittance for different fringe field ranges and integration time steps

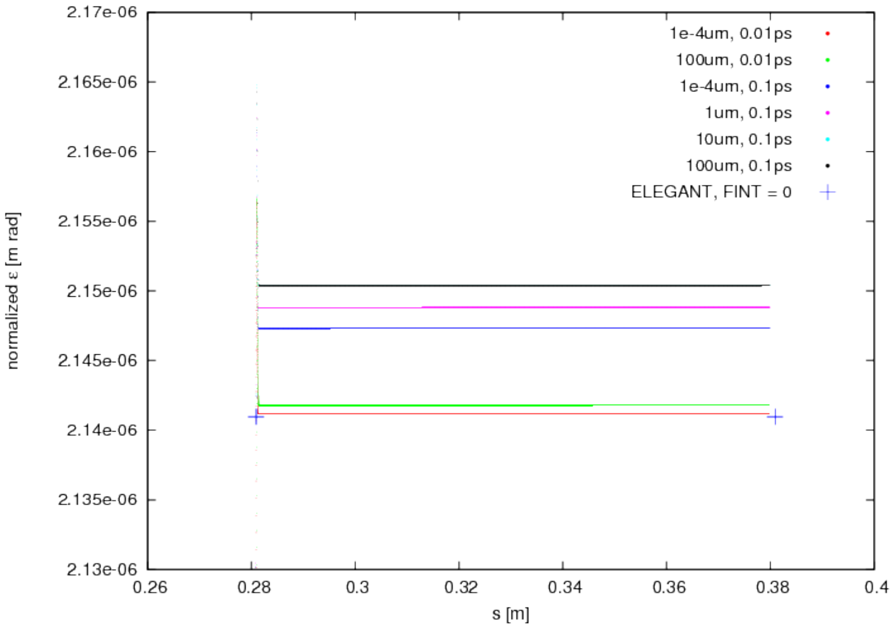

Figure 58: Zoom in on the final emittance in Figure 57

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 [48] 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,δ) 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.

$$\begin{aligned} P_x &= x'\beta\gamma, \\ P_y &= y'\beta\gamma, \\ s &= (\bar{t}-t)\beta c. \end{aligned}$$

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 59 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.

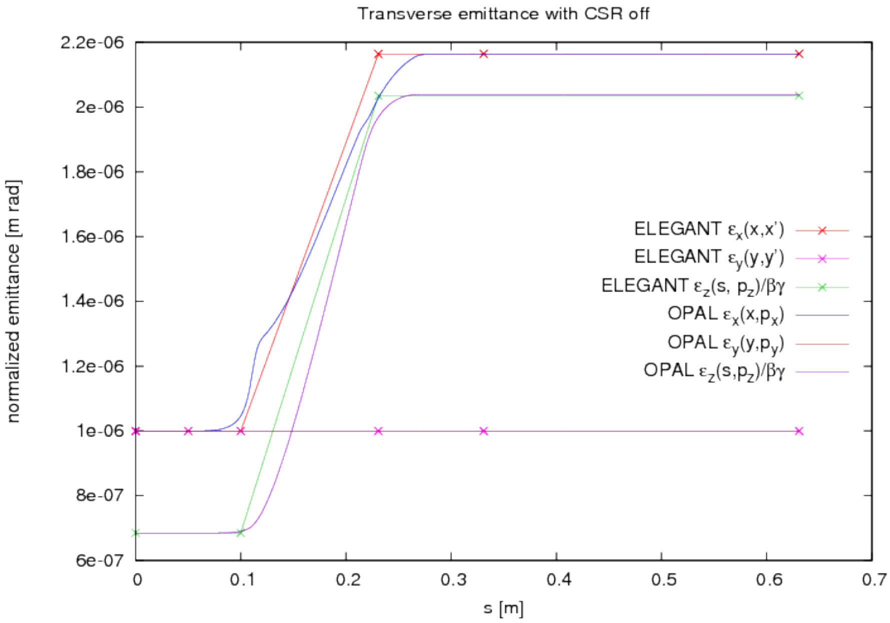

Figure 59: Comparison of the trace space using ELEGANT and *OPAL*

When CSR calculations are enabled for both the bending magnet and the following drift, Figure 60 shows the average δ or $\frac{\Delta p}{p}$ change along the beam line, and Figure 61 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 $\frac{\Delta p}{p} = \frac{1}{\beta^2}\frac{\Delta \overline{E}}{\overline{E}+mc^2}$, where $\Delta \overline{E}$ is the average kinetic energy from the *.stat* output file.

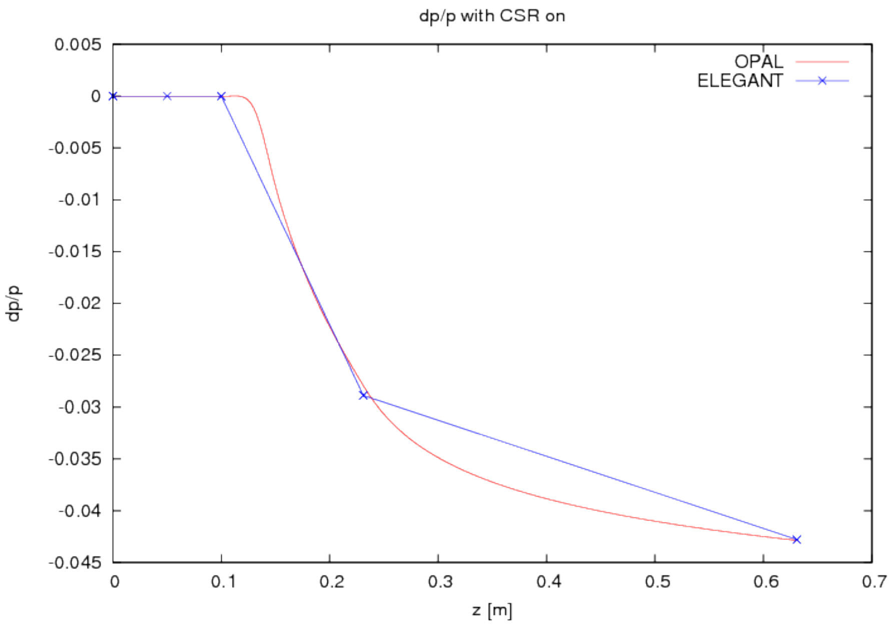

Figure 60: $\frac{\Delta p}{p}$ in Elegant and *OPAL*

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 61.

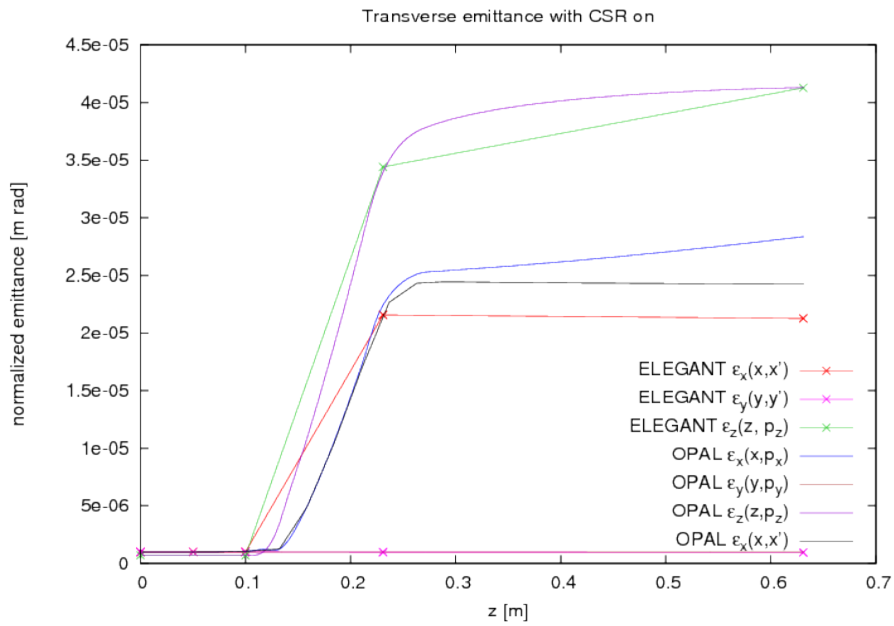

Figure 61: Transverse emittances in ELEGANT and *OPAL*

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 $\varepsilon_x(x, P_x) = \sqrt{\langle x^2 \rangle \langle P_x^2 \rangle - \langle x P_x \rangle^2}$ where $P_x = \beta\gamma x'$, not the trace-like emittance which is calculated as $\varepsilon_x(x, x') = \beta\gamma\sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle x x' \rangle^2}$ [prstab2003]. In Figure 61, 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. $Q_{\rm tot} = \frac{I}{\nu_{\rm rf}}$. For the simulation we use a grid with 16^3 grid point and open boundary condition. The number of macro particles is $N_{\rm p} = 10^5$.

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 62 and Figure 63. This proves to some extend the compatibility of the space charge solvers of *OPAL* and `Impact-t`.

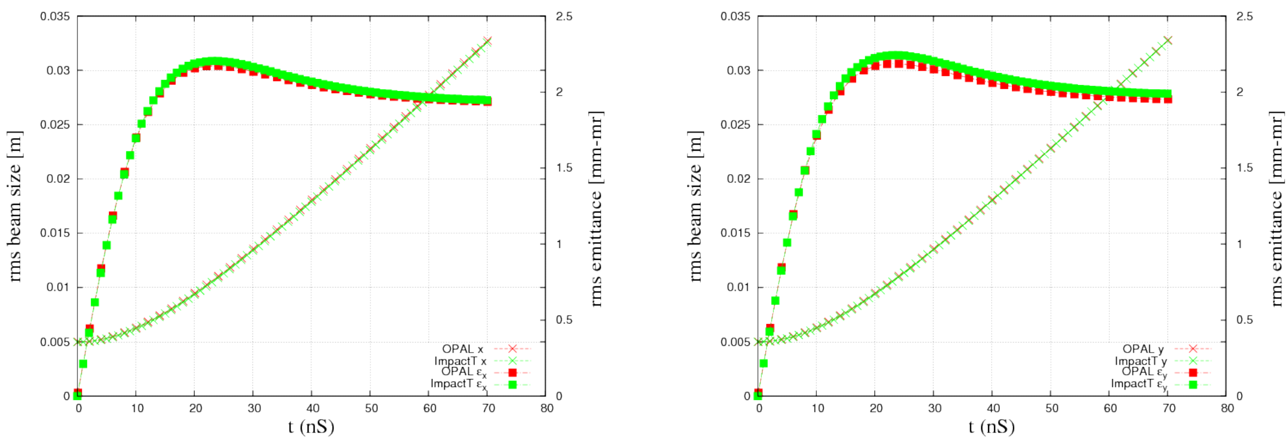

Figure 62: Transverse beam sizes and emittances in `Impact-t` and *OPAL*

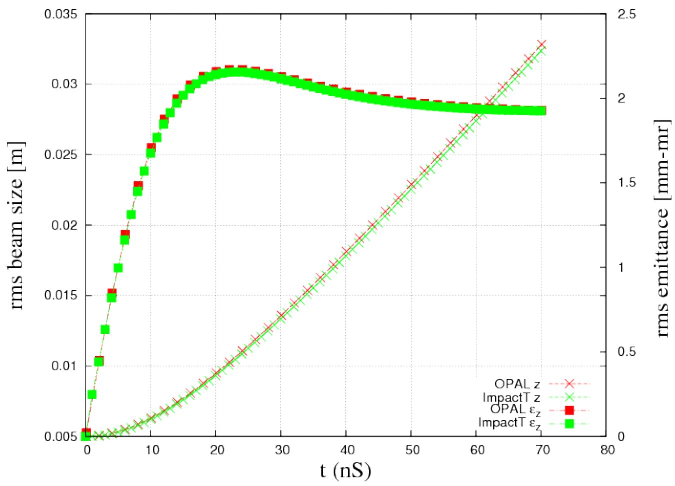

Figure 63: Longitudinal beam size and emittance in `Impact-t` and *OPAL*

E.5 References

[44] K. Crandall and D. Rusthoi, *Documentation for trace: an interactive beam-transport code*, tech. rep. (Los Alamos National Laboratory).

[45] K. L. Brown et al., *TRANSPORT - A Computer Program for Designing Charged Particle Beam Transport Systems*, tech. rep. CERN 73-16, revised as CERN 80-4 (CERN, 1980).

[46] U. Rohrer, *PSI graphic transport framework based on a cern-slac-fermilab version by K.L. Brown et al*, tech. rep. (PSI).

[47] U. Rohrer, http://aea.web.psi.ch/Urs_Rohrer/MyWeb/moregifs/gantryb.gif.

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