SOFT Documentation

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You have reached the Quickstart documentation of SOFT, the Synchrotron-detecting Orbit Following Toolkit. To get the source code of SOFT, check the SOFT website or SOFT GitHub repository. If you're looking for the gory mathematical details of how SOFT is implemented, you should look into the SOFT Manual.



Introduction

SOFT is a synthetic synchrotron diagnostic that can be applied to study the synchrotron radiation emitted by runaway electrons in tokamaks. By solving the guiding-center equations of motion in a numeric magnetic equilibrium, the physics of the system are utilized and allows SOFT to be applied to experimental scenarios.

Compiling

SOFT is written in C, and as such is straightforward to setup on a Linux system. While SOFT hasn't been tested on any other system, it should be possible compile and run on for example Windows and Mac with some additional effort.

2.1 Dependencies

SOFT depends on a number other technologies, some of which are required for compilation, while others can be compiled in optionally. Technologies that are absolutely mandatory in order to compile SOFT are

- CMake, for preparing necessary build files.
- A C compiler with OpenMP support (such as gcc).
- GNU Scientific Library, for various mathematical operations. If a version of GSL older than 2.0 is used, the GSL extension interp2d must also be installed.

A number of libraries are also optional for compilation, and can be compiled in for additional functionality. The optional libraries are

- HDF5 for reading/writing data in HDF5 format.
- MATLAB, for reading/writing data in MATLAB's *.mat format.
- An MPI library, such as MPICH or OpenMPI. Compiling in support for MPI allows running SOFT across multiple computers, such as on a supercomputer cluster.

2.2 Obtaining the code

You may clone the latest build from the SOFT GitHub repository via the command line:

\$ git clone https://github.com/hoppe93/SOFT.git

or if you have your ssh keys configured with GitHub:

\$ git clone git@github.com:hoppe93/SOFT.git

2.3 Compiling

Once the SOFT source code has been obtained and all required and desired dependencies have been installed, navigate to the directory cloned from GitHub:

\$ cd SOFT

Next, to compile SOFT, create a build directory, navigate to it, run CMake followed by make, using the following set of commands:

```
$ mkdir build
$ cd build
$ cmake ../ -DUSE_HDF5=ON -DUSE_MATLAB=ON -DUSE_MPI=OFF
$ make
```

If the build was successful, the SOFT binary will be found under build/src/soft. The flags starting with -D specify configuration options, and in the command above we see that in this case SOFT would be configured with HDF5 and MATLAB support, but without MPI support. This is the default, and would have happened even if those flags were not specified. To enable/disable compilation for either of these libraries, simply specify ON/OFF as appropriate in the above.

2.4 Usage

All configuration of a SOFT run is done in a separate script file, commonly referred to as a pi file (for *Particle Information*). As such, running SOFT is as simple as

\$./soft pi

assuming the pi file has been setup appropriately. There are a large number of options that can be specified in the pi file, and for this reason the details of using SOFT are left to the *How to run SOFT*.

How to run SOFT

All configuration of a SOFT run is done in a separate configuration file, commonly referred to as a pi file. In this section the basic structure of a pi file will be explained in detail. For detailed information about which options can be set, pleaes consult the SOFT manual.

3.1 Examples

The best way to learn how to set up run scripts for SOFT is to see examples of such run scripts. A basic pi file can look like the following:

```
# Basic SOFT pi file
useequation=guiding-center-relativistic
usetool=sycamera
# Specify magnetic field
magnetic_field=circular
                          # Use analytic magnetic field
magnetic circular { B0=5; major_radius=0.68; minor_radius=0.22; safety_factor=1; }
domain_has_outer_wall=no # Remove outer device walls to prevent from blocking_
⇔radiation
# Set phase-space
particles {
   t = 0, -1
   rdyn=0.84,1000
   p=3e7,3e7,1
   pitch=0.15,0.15,1
}
# Specify properties for the sycamera tool
tool sycamera {
                                   # Side length (in m) of (square) detector
   aperture=0.006
   cone=delta
                                   # Use the cone model (not full angular_
→distribution)
```

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```
direction=0,1,0
                                  # Normal vector of detector surface (not.
← necessarily normalized)
   position=0,-1.069,0
                                  # Position vector of detector, relative tokamak ...
→point of symmtetry
   product=image
                                  # Output a synchrotron image when done
   radiation=synchrotron_spectrum # Take spectrum of radiation into account
   spectrum=5e-7,1e-6 # Detector spectral range
   toroidal_resolution=3500  # Number of steps in toroidal integral
   vision_angle=2.0
                                  # Size of field-of-view
}
# Specify properties for the 'image' sycout
sycout image {
   pixels=1000
   name=image.dat
}
```

The settings available for SOFT are many more, and for a detailed list of which settings are available, please consult the SOFT manual. Further examples of pi files for different purposes are:

- distpi Illustrates how SOFT can be run together with a runaway distribution function.
- hollowpi An example of simulating a hollow electron beam.
- simplepi The basic example shown above, setting just the most important options.
- orbitpi Shows how to use the orbit following part of SOFT to simulate particle orbits.

3.2 Basic syntax

Options in a pi file are specified by first giving the name of the option, followed by an equal sign, followed by the value to assign to the option. White-space around the equal sign is ignored. Typically, everything between the equal sign and the end-of-line marker is considered part of the assigned value, except for any white-space coming either directly after the equal sign, or directly before the end-of-line-marker. It is however possible to put several settings on the same line by separating them with semi-colons (;).

Comments can be given by preceding the comment text with a hashtag symbol (#). Any text following the hashtag on the same line will be ignored. Note that comments *cannot* be ended with a semi-colon.

Some options should be assigned vectors of data, such as the direction and rdyn options (among others) in the above example. Each component of the vector must be separated by a comma, and any white-space surrounding commas is ignored. Note that all floating-point numbers can be specified using either decimal form (i.e. 1000 or 0.68) or C scientific notation (i.e. 5e-7).

3.3 Environments

Some options in SOFT are considered *global* and are specified directly in the file, such as for example useequation and usetool in the example above. Many options are however specific to certain modules of SOFT, and they are instead specified inside the appropriate option *environment*.

There are four different environments in SOFT, all of which are syntactically similar. With the exception of the particles environment (which really just sets what could be considered global options), they are also conceptually similar.

The magnetic, tool and sycout environments specify options for a particular SOFT module, and the name of the module must be specified in the environment *header*. The settings are then wrapped within curly brackets ({ and }) and given to the specified module. Note that even if an environment for a module is present in the configuration file, it does not mean that the module will automatically used. Other options must be set to enable modules.

The basic syntax for an environment environment configuring the module named module is:

```
environment module {
    ...
}
```

The particles environment does not require any module name to specified.

3.3.1 magnetic

The magnetic environment specifies settings for the magnetic equilibrium to use, as well as the surrounding walls. Currently, there are two different so called *magnetic handler* modules that can be used. The first and simplest is the circular magnetic handler which implements simple analytic circular magnetic field with a constant safety factor. The second magnetic handler, named numeric, allows the specification of a magnetic field numerically from for example an HDF5 or MATLAB *.mat file.

3.3.2 particles

The particles environment sets a number of options relating to the phase-space of the run. Since it is necessarily tied to the *particles* module of SOFT, the module name part of the environment specification given above should be omitted.

In addition to specifying the bounds of and number of points in phase-space, the particles environment can also be used to specify a different mass or charge of the simulated particle species.

Note: The orbit tool for tracing particle orbits only allows simulating a single point of phase-space at a time, and can otherwise give rise to some very anonymous errors.

3.3.3 tool

The tool environment sets the options for particular tool. A tool, in SOFT, is a module which receives information about a computed orbit and processes it. Currently, there are two tools in SOFT, and these are the orbit and sycamera tools. The orbit tool simply traces a particle or guiding-center orbit, keeps track of a few addiational parameters, and outputs it all to a CSV file.

The sycamera tool is the synchrotron camera (or rather detector) tool which gives SOFT its name. A large part of the SOFT code is dedicated to this module, and the options set by this tool include for example the type of synchrotron radiation model to use, the number of toroidal steps to take, various detector properties among many other things.

3.3.4 sycout

Due to the great versatility of the sycamera tool, the types of output that could be obtained it are numerous. Since each of the output types requires its own set of settings, a separate environment for specifying settings to the output handler of the sycamera tool was created.

The sycout environment thus specifies settings of a sycamera output handler module. To date there are five different *sycout* modules, namely

Mod-	Description
ule	
name	
green	Generates a Green's function which relates the distribution of runaways to the resulting spectrum or
	image. (Can) allow fast computation of image/spectrum.
image	Generates a synthetic synchrotron image.
space3d	Stores 3D information about all particles contributing to a synchrotron image allows visualizing the
	corresponding surface-of-visibility.
spec-	Generates a spectrum curve.
trome-	
ter	
topview	Stores information about where particles where located in the xy-plane when when they emitted towards
	the detector. Allows visualizing the toroidal distribution of particles that are visible to the detector.

Magnetic equilibria

There are currently two magnetic handler modules available for SOFT. The circular handler implements a simple circular magnetic field with a constant safety factor, and is somewhat faster than the alternative. The numeric allows the magnetic field to be loaded from numeric data, which is interpolated. This handler is often the desired one as it allows complicated magnetic geometries to be simulated.

4.1 Analytic circular

The circular magnetic handler implements the magnetic field:

$$\boldsymbol{B}(r,\theta) = \frac{B_0}{1 - (r/R_m)\cos\theta} \left(\frac{r}{q(r)R_m}\hat{\boldsymbol{\theta}} - \hat{\boldsymbol{\phi}}\right)$$

where r is the minor radius, θ the poloidal angle, B_0 the magnetic field strength on the magnetic axis (r = 0), R_m is the major radius, q is the safety factor, $\hat{\theta}$ is a unit vector in the poloidal direction and $\hat{\phi}$ is a unit vector in the toroidal direction. While this formula allows arbitrary q-profiles, SOFT currently only implements this magnetic field with a linear q-profile.

The magnetic field shown above has three free parameters, namely the field strength B_0 , the tokamak major radius R_m and safety factor $q(r) = q_0$. These parameters must be specified by the user, and are set by specifying the options B0, major_radius and safety_factor respectively in the magnetic circular environment. For SOFT to be able to determine when a particle escapes confinement and hits the wall, the minor radius of the device must also be specified. A circular cross section is assumed. All options for the *circular* magnetic handler are set according to

```
magnetic circular {
    B0 = 5
    major_radius = 0.68
    minor_radius = 0.22
    safety_factor = 1
}
```

4.2 Numeric

One of the great strengths of SOFT is that magnetic equilibrias can be specified as numeric data, allowing complicated magnetic configurations, and in particular, experimentally measured data, to be plugged into SOFT. Specifying a numeric equilibrium in the pi file is as simple as

```
magnetic_handler=numeric
magnetic numeric {
    name=/path/to/magnetic/equilibrium.mat
}
```

Currently, the equilibrium data can be stored in either a HDF5, (MATLAB) MAT or SDT file. Both HDF5 and MATLAB files can be created easily with user-friendly tools such as Python or MATLAB, while SDT (for *Semi-Descriptive Text*) is a SOFT-specific text-based format which is likely the best choice if the magnetic equilibrium is generated using a small C/C++ program which is difficult to interface with HDF5 or MATLAB.

Since SOFT assumes the magnetic field to be toroidally symmetric, the magnetic field components in a poloidal plane must be specified. SOFT uses a cylindrical coordinate system for specifying the magnetic field, so that $\boldsymbol{B} = B_r \hat{\boldsymbol{r}} + B_z \hat{\boldsymbol{z}} + B_\phi \hat{\boldsymbol{\phi}}$, where $B_r \hat{\boldsymbol{r}}$ denotes the component radially out from the point of symmetry of the tokamak, $B_z \hat{\boldsymbol{z}}$ denotes the component in the vertical direction, and $B_\phi \hat{\boldsymbol{\phi}}$ denotes the component in the toroidal direction, perpendicular to the poloidal plane in which the magnetic field is given.

4.2.1 Variables

Both HDF5, MATLAB and SDT files have a *variable* concept where data within the file is named. Because of this, SOFT looks for certain variables in the datasets, loads them and gives them meaning in the code. The following variables must be present in all SOFT magnetic equilibrium files:

Variable	Туре	Description
Br	m-by-n matrix	Radial component of magnetic field (radius-by-z).
Bphi	m-by-n matrix	Toroidal component of magnetic field (radius-by-z).
Bz	m-by-n matrix	Vertical component of magnetic field (radius-by-z).
desc	String	A longer description of the equilibrium. Must be present, but may be empty.
maxis	1-by-2 vector	Specifies the location of the magnetic axis in the (R, z) -plane.
name	String	Name of the equilibrium. Must be present, but may be empty.
r	1-by-m vector	List radial points in which the components of the magnetic are given.
separatrix	2-by-many vec-	List of contour points marking the separatrix in the (R, z) -plane.
	tor	
wall	2-by-many vec-	List of contour points marking the bounds of the device in the poloidal plane.
	tor	
Z	1-by-n vector	List of vertical points in which the components of the magnetic field are
		given.

Note: Only one of the separatrix and wall variables is required to be present in the equilibrium file. Both may be present, and in that case the domain contour to use can be specified as an additional option to the numeric magnetic handler. By default the wall contour will be used if available.

Distribution functions

In SOFT, distribution functions depend on three variables, namely the major radius ρ at which the guiding-center orbit was initiated, the momentum p of the particle, as well as the cosine of the pitch angle $\xi = \cos \theta_p$ in the outer midplane.

5.1 File format

Distribution functions are given to SOFT as Matlab MAT-files. SOFT expects the following variables to be present in the file:

Name	Description
description String describing the distribution function.	
f	Actual distribution function. An n_r -by- $n_p n_{\xi}$ matrix (see below).
name	String naming the distribution function.
р	Vector containing points of momentum. Size 1-by- n_p .
punits	String describing the units of p. Either ev, normalized or si.
r	Vector containing radial points. Size 1-by- n_r .
xi	Vector containing (cosine of) pitch angle points. Size 1-by- n_{ξ} .

The most important variable in a SOFT distribution function file is f, which is the actual distribution function. The variable is stored as a matrix with each row representing a momentum-space distribution function, i.e. with the radial coordinate changing along the row index.

Each row of f corresponds to a momentum-space distribution function, shaped as one long $n_p \times n_{\xi}$ vector. The elements are ordered into n_{ξ} groups of n_p elements, so that the first n_p elements of the vector corresponds to holding ξ fixed and varying p.

The name and description variables are fairly arbitrary and are only included to provide the user with basic information about the distribution function.

The p, r and xi variables are vectors consisting of n_p , n_r and n_{ξ} elements respectively. Together, the vectors specify the grid in momentum, radius and (cosine of) pitch angle on which the distribution function is defined.

To allow users to specify momentum coordinates in the units most convenient for them, and more importantly to prevent mix-ups of used units, the variable punits must be provided specifying the units used for the momentum variable. Allowed values are ev (for momentum in eV/mc), normalized (for $p \equiv \gamma\beta$, where γ is the electron's Lorentz factor and β is the electron's speed normalized to the speed of light) and si (for SI units, i.e. kg · m/s).

Note: Even though CODE is commonly used to generate distribution functions for SOFT, plain CODE distribution functions are not directly compatible with SOFT. The distribution function given as output by CODE consists of a set of Legendre polynomial coefficients used in evaluating the distribution function $f(p, \xi)$. SOFT on the other hand requires the function values to be already evaluated.

5.2 Helper tools for CODE/NORSE

A nice graphical helper tool has been developed for analyzing CODE/NORSE distributions and generating distributions readable by SOFT. The tool is called codeviz and is available on GitHub.

Geometric kernels

The way SOFT is constructed makes it possible to rewrite the "SOFT equation" on the form

$$I_{ij} = \int \mathrm{d}\rho \mathrm{d}p_{\parallel} \mathrm{d}p_{\perp} f(\rho, p_{\parallel}, p_{\perp}) \hat{I}_{ij}(\rho, p_{\parallel}, p_{\perp}, \boldsymbol{x}_{0})$$

where I_{ij} is the brightness of pixel (i, j), and \hat{I}_{ij} denotes the *geometric kernel function* for a particular detector/tokamak combination, that connects the distribution of runaways of a particular velocity and initial position, with the image seen by a particular camera in a specific tokamak. The great benefit of this formulation is that only a set of multiplications are required to produce the synchrotron radiation image seen by a camera. A similar formulation for the synchrotron spectrum exists.

The format of the Green's function is specified in the pi-file using the dimensions option. The value of this option is a set of characters denoting each of the variables that should appear in the Green's function. For example, dimensions = r12ij would generate a Green's function containing information about radius, velocity coordinate 1, velocity coordinate 2 as well as both pixels of the image. The possible characters and their meaning are:

Function Description	
1	Velocity coordinate 1. Depends on which coordinates are used in the pi-file.
2	Velocity coordinate 2. Depends on which coordinates are used in the pi-file.
i	The "y"-axis of the image.
j	The "x"-axis of the image.
r	Radial coordinate.
W	Spectrum wavelength.

To generate a geometric kernel function with SOFT, create a new sycout environment in your pi file with the format

```
sycout green {
   format=mat
   output=greenW.mat
   function=r12ij
   pixels=60
}
```

All options for the green sycout are documented in the Parameter reference.

6.1 Output file

The file generated by SOFT containing the geometric kernel function will contain the variables listed in the table below. The actual geometric kernel functions is found as a vector named func which can be reshaped to be handled more easily.

Variable	Туре	Description
func	1-by- $n_{\rho}n_1n_2n_{\lambda}n_in_j$	Geometric kernel function
	vector	
paraml	1-by- n_1 vector	Velocity parameter #1
paramlname	String	Name of velocity parameter #1. E.g. ppar.
param2	1-by- n_2 vector	Velocity parameter #2
param2name	String	Name of velocity parameter #2. E.g. pperp.
pixels	Integer	Number of pixels
r	1-by- n_{ρ} vector	List of radial points
stokesparams	Integer	1 if elements are Stokes parameters. 0 if only intensities are stored.
type	String	Type of geometric kernel. Either of the functions listed in the table
		above.
wavelengths	1-by- n_{λ} vector	List of wavelength points.

6.2 Working with kernel function

To more easily work with the geometric kernel function it should be reshaped into an appropriately dimensioned array. In Matlab, this can be done through

```
load softOutput % Kernel function assumed to be located in 'softOutput.mat'
% Get number of elements in each dimension
nw = length(wavelengths);
n1 = length(param1);
n2 = length(param2);
nr = length(r);
% Reshape kernel function
Ihat = reshape(func, [pixels, pixels, nw, n2, n1, nr]);
% Access image at radius #1, param1 #2, param2 #3 and wavelength #4
I = squeeze(Ihat(:, :, 4, 3, 2, 1));
```

and similarly in Python

```
import numpy as np
import scipy.io
# Load mat-file
matfile = scipy.io.loadmat('softOutput.mat')
# Set variables
func = matfile['func'][0]
pixels = matfile['pixels'][0][0]
param1 = matfile['param1name'][0]
```

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```
# ...and the same for all other variables...
# Get number of elements in each dimension
nr = r.size
n1 = param1.size
n2 = param2.size
nw = wavelengths.size
# Reshape kernel function
That = np.reshape(func, (nr, n1, n2, nw, pixels, pixels))
```

Note: The order in which the number of elements are given to reshape is very significant!

The above examples are for a function of type r12ij.

Polarization information

When radiation=synchrotron_spectrum SOFT will also store information about the polarization of the detected radiation. Using the polimage and polspectrometer sycouts, it is possible to generate output files containing the polarization information in image or spectrum format. In this section usage and interpretation of the data will be briefly be discussed.

7.1 What information does SOFT store?

SOFT stores the four Stokes parameters, S, Q, U and V, averaged over the relevant parameters (depending on which model is being used). The emitted synchrotron power per unit frequency, per unit solid angle, can be written in terms of the two quantities A_{\parallel} and A_{\perp} as

$$rac{\mathrm{d}^2 P}{\mathrm{d}\omega\mathrm{d}\Omega} \propto \left|-oldsymbol{\epsilon}_{\parallel}A_{\parallel}+oldsymbol{\epsilon}_{\perp}A_{\perp}
ight|^2.$$

where ϵ_{\parallel} is a vector corresponding to polarization in the gyration plane, and ϵ_{\perp} to polarization in the plane orthogonal to that. It can be shown that the Stokes parameters can be expressed using A_{\parallel} and A_{\perp} through

$$\begin{split} I \propto A_{\parallel}^{2} + A_{\perp}^{2}, \\ Q \propto \left(A_{\perp}^{2} - A_{\parallel}^{2}\right) \cos 2\beta, \\ U \propto \left(A_{\perp}^{2} - A_{\parallel}^{2}\right) \sin 2\beta, \\ V \propto 2A_{\parallel}A_{\perp} \cos 2\beta. \end{split}$$

The angle β is the angle between the plane of parallel polarization and the plane in which the horizontal polarization is *measured*. The first Stokes parameter, *I*, is just the intensity of the radiation as obtained also from the SOFT image sycout.

The fourth Stokes parameter V is often quoted as identically zero in the literature, a result stemming from that the object $A_{\parallel}A_{\perp}$ is odd in the angle ψ between the guiding-center's emission cone and a line-of-sight. When averaged over all emission angles, the contribution to V therefore cancels identically. In the angular and spectral distribution implemented in SOFT however, we do not neglect the finite emission width, and therefore obtain a finite contribution

to the V parameter, since it is possible for only part of the emission cone to overlap the detector (corresponding to "cut-offs" in the integration over emission angle).

For a derivation of the full $\frac{d^2 P}{d\omega d\Omega}$, see for example Jackson's "Electrodynamics", Landau-Lifshitz "The Classical Theory of Fields" or Mathias Hoppe's Master's thesis (link).

7.2 File format

The polimage sycout of SOFT outputs a variable-based file (such as SDT, HDF5 or Matlab) containing the following variables:

Variable	Description
detectorPosition	Vector specifying the position of the detector
detectorDirection	Central viewing direction of the detector
detectorVisang	Vision angle of the detector
StokesI	Stokes I parameter
StokesQ	Stokes Q parameter
StokesU	Stokes U parameter
StokesV	Stokes V parameter
wall	Wall data used for the simulation

3D emission maps

Due to the highly anisotropic nature of bremsstrahlung and synchrotron radiation combined with the fact that radiation is only detected if it's emitted directly at the detector, a given detector can only measure radiation from particles in a certain regions of space. It can be shown that these regions of space all satisfy (approximately) the condition

$$\hat{\boldsymbol{b}}(\boldsymbol{x}) \cdot \frac{\boldsymbol{x} - \boldsymbol{X}}{|\boldsymbol{x} - \boldsymbol{X}|} = \cos \theta_{\mathrm{p}},$$
(8.1)

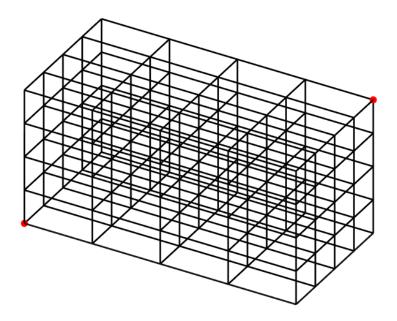
where \hat{b} is the magnetic field unit vector, x is the particle's position, X is the detector's position and θ_p denotes the particle's pitch angle (note that the pitch angle also varies as the particle moves in the inhomogeneous magnetic field, and therefore picks up a dependence on x). The solution to this equation, i.e. the points x satisfying it, trace out a surface in real space which we refer to as the *surface-of-visibility*. When the detector is located in the midplane, this surface typically takes the shape of a twisted cylinder.

8.1 Solving for surface-of-visibility

Using SOFT it is possible to solve (8.1), accounting for the finite detector size. This is done by adding the sycout space3d (see space3d for a parameter reference) to your SOFT runscript. As with every sycout, you must also add a line product=space3d to the tool sycamera block. One example definition of the sycout is a follows

```
sycout space3d {
    output=outfile.mat
    type=pixels
    pixels=200
    point0=-0.5,-0.25,-0.25
    point1=0.5,0.25,0.25
}
```

The output parameter specifies the name of the output file, and the type parameter specifies the algorithm to use for storing 3D information. Setting type=pixels means SOFT will divide the space into N^3 cells, where N is the value assigned to the pixels parameter, between the two edge points point0 and point1 (see the figure below; the red dots indicate the locations of the edge points). During the SOFT run, each cell records the radiation being emitted from the box and accumulates it.



The other value available for type is real, which stores the exact coordinates of each point that contributes to the final image. This means that the output will be more detailed, but it will also grow with each particle.

8.2 Visualizing

Visualization of space3d files is complicated by the fact that each point represents emitted light, which adds together along lines of sights. A simple C program has been written by Mathias for generating sequences of PNG images from S3D output files. The program is available on GitHub: s3dvid.

Parameter reference

There are a number of settings that can be specified in a pi file, and each of the SOFT modules introduces its own set of options. In this section a complete list of all the options that can be set in a pi file are given.

Contents

- Global options
- Particle settings
- Magnetic settings
 - circular
 - numeric
- sycout settings
 - green
 - image
 - space3d
 - spectrometer
 - topview

9.1 Global options

debug

Default value: 0 **Example line:** debug=1 Allowed values: 0 or 1

If set to 1, debug output will be generated and written to stdout during the run. Default value is 0.

domain_has_outer_wall

Default value: yes Example line: domain_has_outer_wall=no Allowed values: yes or no

If set to no, ignores all points of the wall/separatrix outside $R = R_m$, where R_m denotes the radial coordinate of the magnetic axis. This will allows the placement of a detector outside the device. The mid-pole will still be present to block out radiation.

interptimestep

Default value: Example line: Allowed values: TODO

magnetic_field

Default value: None Example line: magnetic_field=numeric Allowed values: circular and numeric

Specifies the name of the magnetic field handler module to use. Either circular or numeric.

maxtimestep

Default value: None Example line: maxtimestep=le-11 Allowed values: Any positive real value

Sets the maximum allowed size of a timestep in the equation solver (whichever it may be). If the adaptive timestep becomes larger than this, it is automatically adjusted to this value. By default there is no limit on how long the timestep can be.

nodrifts

Default value: no Example line: nodrifts=yes Allowed values: yes or no

If set to yes, ignores the drift terms in the first-order guiding-center equations of motion (effectively solving the zeroth-order guiding-center equations of motion). This option only influences behaviour of the code when the guiding-center equations of motion are solved. By default the value of this option is no so that the drift terms are kept.

progress

Default value: 0 **Example line:** progress=10 Allowed values: Any non-negative integer

Specifies how many times during the run SOFT should print information about the current progress. Information will be printed in uniform steps as particles (defined as points in phase-space) are completed.

threads

Default value: Number of threads suggested by OpenMP **Example line:** threads=3 **Allowed values:** Any positive integer (no upper limit)

Overrides the number of threads started by each (MPI) process. By default, SOFT will start the number of threads indicated by the OMP_NUM_THREADS environment variable in each process.

tolerance

Default value: 1e-12 **Example line:** tolerance=4e-13 **Allowed values:** Any positive real number

Specifices the tolerance in the RKF45 solver. The default tolerance is set by the tool used in the run. The orbit tool defaults to a tolerance of 10^{-7} , while the sycamera defaults to a tolerance of 10^{-12} .

useequation

Default value: None Example line: useequation=guiding-center-relativistic Allowed values: guiding-center, guiding-center-relativistic, particle, particle-relativistic.

Determines which set of equations of motion to solve. Note that the sycamera tool requires that the (relativistic) guiding-center equations of motion be solved. Possible values for this option are particle, particle-relativistic, guiding-center and guiding-center-relativistic.

usetool

Default value: None Example line: usetool=sycamera Allowed values: orbit, sycamera

Sets the name of the tool to use. Can either be orbit (which traces orbits), or sycamera (which computes various synchrotron-radiation quantities for runaway electrons).

9.2 Particle settings

```
charge
```

Default value: One electron charge (i.e. -1) **Example line:** charge=4 **Allowed values:** orbit, sycamera

The charge of the particle to simulate, in units of the elementary charge ($e \approx 1.602 \times 10^{-19}$ C). The default value is -1, i.e. the electron charge.

cospitch

Default value: None **Example line:** cospitch=1, 0.95, 100**Allowed values:** A number $\in [0, 1]$; A number $\in [0, 1]$; any positive integer

Specifies the range of cosines of the particle's pitch anle with which to initiate orbits. The first argument specifies the first value in the range to give to particles, while the second argument argument specifies the last value in the range. The third argument specifies the total number of values to simulate. Example: cospitch = 0.999, 0.97, 10, while initiate ten particles with cosine of the pitch angle values between 0.97 and 0.999.

gc_position

Default value: Yes Example line: gc_position=no Allowed values: yes or no

If set to yes, assumes that the position given specifies the guiding-center position when solving the guiding-center equations of motion. If set to no, the program instead assumes that the particle position is specified and compensates accordingly when solving the guiding-center equations of motion. Has no effect when solving the full particle orbit.

mass

Default value: One electron mass (0.000548579909 u) **Example line:** mass=2 **Allowed values:** Any positive real number

The particle mass in unified atomic mass units (u). The default value is 0.000548579909, corresponding to the electron mass.

p

Default value: None **Example line:** p=1e6, 1.2e7, 10 **Allowed values:** Any real number; any real number; any positive integer

Specifies the range of momenta with which to initiate orbits. The first argument specifies the first momentum value to give to particles while the second argument specifies the last momentum value. The third argument specifies the total number of momentum values to simulate. Example: p = 3e7, 4e7, 5.

pitch

Default value: None **Example line:** pitch=0.05, 0.15, 14 **Allowed values:** A number $\in [0, \pi]$; a number $\in [0, \pi]$; any positive integer

Specifies the range of pitch angles with which to initiate orbits. The first argument specifies the first pitch angle to give to particles while the second argument specifies the last pitch angle. The third argument specifies the total number of pitch angles to simulate. Example: pitch = 0.03, 0.25, 15.

ppar

Default value: None

Example line: ppar=1e6,1.2e7,14

Allowed values: Any real number; any real number; any positive integer

Specifies the range of parallel momenta with which to initiate orbits. The first argument specifies the first parallel momentum to give to particles while the second argument specifies the last momentum value. The third argument specifies the total number of momentum values to simulate. Example: ppar = 3e7, 4e7, 5.

pperp

Default value: None

Example line: pperp=1e6, 1.2e7, 14

Allowed values: Any real number; any real number; any positive integer

Specifies the range of perpendicular momenta with which to initiate orbits. The first argument specifies the first perpendicular momentum to give to particles while the second argument specifies the last momentum value. The third argument specifies the total number of momentum values to simulate. Example: pperp = 3e6, 7e6, 15.

r

Default value: None

Example line: r=0.68,0.84,14

Allowed values: Any real number inside device; any real number inside device; any positive integer

Specifies the range of radii with which to initiate orbits. The first argument specifies the first radius to give to particles while the second argument specifies the last radius. The third argument specifies the total number of radii to simulate. Example: r = 0.68, 0.84, 80.

rdyn

Default value: None

Example line: rdyn=0.84,14

Allowed values: Any real number inside device; any positive integer

Specifies the outermost radius at which to initiate orbits, as well as the number of radii to drop particles on. The innermost radius is automatically set as the magnetic axis, and particles will only be dropped at a radius in the interval if their "effective magnetic axis" radial location is less than the currently simulated. The "effective magnetic axis" arises due to orbit drifts, and if it's presence is not properly accounted for, weird bright or dark spots will show up in synchrotron image (when orbit drifts are taken into account). Example: rdyn = 0.84, 80.

t

Default value: 0, -1 **Example line:** t=0, 1e-6 **Allowed values:** Any real number; any real number

The first argument of this parameter specifies the reference time. For most purposes this parameter is most conveniently set to 0. The second argument specifies the end time, at which point an orbit should be considered finished and no longer followed. If the second argument is less than the reference time (the first argument), the orbit will be followed for one full *poloidal* orbit, or until the simulation clock is greater than minus the end time.

9.3 Magnetic settings

Two different magnetic handler modules are provided with SOFT. These are the circular module, implementing a simple analytical magnetic field with a circular cross-section and constant safety factor, as well as the numeric module, which loads 2D numeric magnetic fields.

Performance-wise, the numeric module is somewhat slower than the circular model, due to that the former interpolates the 2D magnetic field with a cubic spline. The difference is however only about a factor of two.

9.3.1 circular

в0

Default value: 1 **Example line:** B0=5.2 **Allowed values:** Any real number

Specifies the magnetic field strength on the magnetic axis, i.e. on the circle $R = R_m, Z = 0$. In units of Tesla.

major_radius

Default value: 1 Example line: major_radius=2 Allowed values: Any positive real number

Specifies the major radius of the tokamak. In units of meter.

minor_radius

Default value: 1 Example line: minor_radius=1 Allowed values: Any real number

Specifies the minor radius of the device. In units of meter. This parameter only influences the location of the walls of the tokamak, and does not affect the magnetic field.

safety_factor

Default value: 1 **Example line:** B0=1 **Allowed values:** Any real number

The safety factor, or q-factor of the tokamak magnetic field. In this analytical model of the magnetic field, the safety factor is a constant.

9.3.2 numeric

axis

Default value: Set in equilibrium file **Example line:** axis=0.68, -0.002 **Allowed values:** Any positive real number; any real number Specifies the location of the magnetic axis in a poloidal plane. The first coordinate specifies the major radial location (R) of the axis, and the second coordinate specifies the vertical location (Z) of the axis. SOFT requires the magnetic equilibrium data file to give this value, but under some circumstances it may be desirable to override the value set in the equilibrium file, in which case this parameter can be used.

file

Default value: None

Example line: file=/path/to/magnetic/equilibrium.mat
Allowed values: Any real number

Specifies the name of the file containing the magnetic equilibrium data to use. The format that this file must have is described under *Magnetic equilibria*. The format of the file is determined by analyzing the file name extension. All file formats supported by the SOFT file interface can be used.

format

Default value: auto Example line: format=mat Allowed values: auto, hdf5 or mat

Overrides the format specifier for the magnetic equilibrium data file. auto is the default, which causes SOFT to determine the file format based on the filename extension. hdf5 causes SOFT to interpret the data file as an HDF5 file. mat causes SOFT to interpret the data file as a Matlab MAT file.

wall

Default value: any Example line: wall=separatrix Allowed values: any, separatrix, wall

Specifies which type of wall should be used. Equilibrium data files can contain two types of "walls", namely the actual tokamak wall cross-section or the separatrix/last closed flux surface. SOFT only requires one of these two types to be present in the data file, and with any set, the tokamak wall will be first be considered, but if it's not present in the file, the separatrix will be used instead. The wall and separatrix options forces the use of either of the two types. *The wall is the structure beyond which particles will be considered as lost and no longer followed*.

9.4 sycout settings

A sycout (short for *SYnchrotron Camera OUTput*) is an output module that is coupled to the sycamera tool of SOFT. Currently the following sycouts are available:

- green Generates a Green's function
- image Generates a camera image
- polimage Generates a camera image with polarization information
- polspectrometer Generates a spectrum with polarization information
- space3d Stores 3D information about the contributions to an image
- spectrometer Generates a spectrum
- topview Stores X and Y coordinates of contributions to an image. Creates a top-down "map" of contributions.

9.4.1 green

The green sycout allows you to generate Green's functions for images, spectra or any kind of function you can imagine. Green's functions are sometimes also known as weight functions and are essentially mappings from a distribution function to a quantity such as an image, spectrum or combination thereof.

Instructions on how to use this sycout are available under :ref: 'geomkern'.

format

Default value: Auto-determined from output filename extension **Example line:** format=mat **Allowed values:** h5, hdf5, mat, out, sdt

Overrides the default setting for what file format to store the output in. If not set, the output file format is determined based on the filename extension of the output file. h5 and hdf5 forces HDF5 output. mat forces Matlab MAT output. out and sdt forces SOFT self-descriptive text (SDT) format output (text-based).

function

Default value: None

Example line: function=r12ij

Allowed values: Any (non-repeating) combination of the characters 1, 2, i, j, r, w

Sets the shape and contents of the Green's function. A more detailed description of how this option works can be found under *Geometric kernels*.

output

Default value: None

Example line: output=outputfile.mat
Allowed values: Any non-line-breaking string

Sets the name of the output file. The format of the output file is determined based on the extension part of this setting unless the format option has also been specified. By extension is meant everything that comes after the last dot (.).

pixels

Default value: None Example line: pixels=520 Allowed values: Any positive integer

Sets the number of pixels of the image, i.e. the number of elements in each of the i and j dimensions. Only required if either i or j appears in the function option.

stokesparams

Default value: no Example line: stokesparams=yes Allowed values: yes or no

If set to yes, each of the four Stokes parameters I, U, Q and V will be stored in the Green's function (thereby giving it an extra dimension with four elements). If set to no, only the intensity parameter is stored, which is the value commonly measured by spectrometers and cameras.

suboffseti

suboffsetj

Default value: 0 Example line: suboffseti=20 Allowed values: Any non-negative integer

Green's functions for images tend to become quite large, and in many cases much of the Green's function is zero and provides no interesting information. In these cases, a subset of the image can be stored so that the correct wide-angle image distortion is still present. These offset parameters specify the offsets in the i and j directions respectively from which the image that is to be stored should start.

subpixels

Default value: Same as ''pixels'' Example line: subpixels=30 Allowed values: Any positive integer

Specifies the number of pixels in each of the i and j directions of the subset image. Since the subset image must lie within the full image, suboffseti``+``subpixels and suboffsetj``+``subpixels must both be less than or equal to pixels.

9.4.2 image

The image sycout generates a camera image.

brightness

Default value: intensity Example line: brightness=histogram Allowed values: bw, histogram, intensity

Specifies how pixels should be colored. With bw (for black-and-white), pixels are simply marked if they receive a contribution. Thus, if any radiation hits the pixel during the run, the pixel will contain the value 1 at the end of the run and 0 otherwise.

The histogram option specifies that each hit in a pixel should increase the value of the pixel by 1. The radiation intensity reaching the pixel is not considered.

The intensity option takes the emitted radiation intensity into account, including spectral effects (if enabled through other options).

includese paratrix

Default value: yes Example line: includeseparatrix=no Allowed values: no and yes

Specifies whether or not to include separatrix data from the input magnetic equilibrium data file in the output. By default, it is set to yes. If no separatrix data is available, the separatrix variable is omitted from the output file.

includewall

Default value: yes Example line: includewall=no Allowed values: no and yes

Specifies whether or not to include wall data from the input magnetic equilibrium data file in the output. By default, it is set to yes. If no wall data is available, the wall variable is omitted from the output file.

name

Default value: None

Example line: name=output-file.mat

Allowed values: Any string allowed by the underlying file system

Specifies the name of the file to which the output will be written. The output is written through the SOFT file interface which means it will be either in a HDF5 file, a Matlab MAT file or a SOFT SDT (Self-Descriptive Text) format. The file format is determined based on the filename extension. For HDF5, use either *.h5* or *.hdf5*, for Matlab MAT use *.mat*, and for SDT any other extension (though *.sdt* is recommended).

pixels

Default value: None Example line: pixels=300 Allowed values: Any positive integer

Sets the number of pixels in the image. Images are always square and have the same number of pixels in the x (i) direction as in the y (j) direction.

9.4.3 space3d

The space3d can be used to store 3D data about the points of space that contribute to an image. A description about how to use it can be found in space3d.

output

Default value: None

Example line: output=name-of-outputfile.mat

Allowed values: Any string allowed by the underlying file system

Name of the file to which output should be written. The space3d module uses the SOFT file interface, meaning output can be written in either HDF5, Matlab MAT or SOFT SDT (Self-Descriptive Text) format. The format of the output file is determined based on the filename extension. For HDF5 use *.h5* or *.hdf5*, for Matlab MAT use *.mat*, and for SDT use any other extension (though *.sdt* is recommended).

pixels

Default value: None Example line: pixels=300 Allowed values: Any positive integer

When type=pixels, sets the number of pixels in each direction of the bounding box. A value of for example 100 means that there will be a total of $100 \times 100 \times 100 = 1\,000\,000$ "pixels" in the box.

point0

Default value: None **Example line:** point0=.40,-.75,.20 **Allowed values:** Any real number; any real number; any real number

Specifies one of the two defining edge points of the bounding box.

point1

Default value: None **Example line:** point1=.63,-.15,-.20 **Allowed values:** Any real number; any real number; any real number

Specifies one of the two defining edge points of the bounding box.

type

Default value: None Example line: type=pixels Allowed values: pixels, real

Specifies the type of 3D object to store. pixels divides the bounding box into a number of smaller boxes and collects the contribution in each of those (the number of boxes is determined by the pixels option). This 3D type is fixed in size and is represented as a simple 3D array.

The real type stores the real location of each particle that contributes to the image. This 3D grows in size with the number of particles that hit the detector, and is stored as a sparse matrix. It's usually very difficult to determine the final size of this 3D type, but it gives much more detailed data and can sometimes be the more space-efficient option.

9.4.4 spectrometer

The spectrometer sycout stores spectra.

name

Default value: None Example line: name=spectrum.mat Allowed values: Any string allowed by the file system

Name of the output file.

9.4.5 topview

The topview sycout generates a top map of the tokamak, showing where in the xy-plane radiation comes from. Note that the image is line-integrated along the z direction, and bright areas in the top view therefore do not necessarily correspond to bright areas in the image.

brightness

Default value: intensity Example line: brightness=histogram Allowed values: bw, histogram, intensity Specifies how pixels should be colored. With bw (for black-and-white), pixels are simply marked if they receive a contribution. Thus, if any radiation hits the pixel during the run, the pixel will contain the value 1 at the end of the run and 0 otherwise.

The histogram option specifies that each hit in a pixel should increase the value of the pixel by 1. The radiation intensity reaching the pixel is not considered.

The intensity option takes the emitted radiation intensity into account, including spectral effects (if enabled through other options).

name

Default value: None

Example line: name=output-file.mat

Allowed values: Any string allowed by the underlying file system

Specifies the name of the file to which the output will be written. The output is written through the SOFT file interface which means it will be either in a HDF5 file, a Matlab MAT file or a SOFT SDT (Self-Descriptive Text) format. The file format is determined based on the filename extension. For HDF5, use either *.h5* or *.hdf5*, for Matlab MAT use *.mat*, and for SDT any other extension (though *.sdt* is recommended).

pixels

Default value: None Example line: pixels=300 Allowed values: Any positive integer

Sets the number of pixels in the topview. Topviews are always square and have the same number of pixels in the x (i) direction as in the y (j) direction.

The SDT format

The SDT format (for *SOFT Descriptive Text* or *Self-Descriptive Text* or *Semi-Descriptive Text*) was developed in order to import magnetic field data from systems with no HDF5 or MATLAB support. It is a very simple text-based format without fancy features and with little safety. It is recommended that users stick to HDF5 or MATLAB files whenever possible.

10.1 Basic structure

Just as MATLAB files (and in a sense, HD5 files), SDT files contains a set of variables. Each variable consists of a *header* and a *body*. The header is always one line and specifies the name and dimensions of the variable. The body (which comes on the very next line) is at least one line and contains the data of the variable, in ASCII format. Variables are separated by empty lines.

The header always consists of two integers and a string, all separated by spaces. The first integer specifies the number of rows in the data. The second integer specifies the number of columns in the data (or number of characters, in the case of strings). The name is an ASCII string of arbitrary length (but without any whitespace characters).

Note that strings and numeric variables are, technically, encoded differently. Data should always be readable by a human in a text-editor, meaning that numeric values are converted to their ASCII equivalent, while strings are stored directly without converting every single character to an ASCII digit. There is no indication in the header about which type of data a variable contains and so it is up to the user to read variables using the correct decoder.

Matrices are stored by converting each element to its ASCII equivalent. Elements in the same row are separated by single spaces, while rows are separated by (Unix) newlines (i.e. just one $\n or 0xA$ character).

10.2 Example SDT file

An example SDT file containing three variables is shown below:

1 2 maxis
1.688510 0.048496
3 3 someMatrix
1.1 2.2 3.3
4.4 5.5 6.6
7.7 8.8 9.9
1 29 someString
This is an SDT example string

Troubleshooting

Images contain very sharp, very bright lines. Are particles with large pitch angles being simulated? If so, there's a numerical issue that could potentially arise. In the calculation of a synchrotron image, the Jacobian for the orbit $J = (\partial R/\partial \rho)(\partial Z/\partial \tau) - (\partial R/\partial \tau)(\partial Z/\partial \rho)$ must be computed. The derivatives with respect to τ are straightforward, but to find the derivatives with respect to ρ (the radius at which the particle is initiated) we must compute one additional orbit, at $\rho + \epsilon$, where ϵ is an arbitrarily small number. Internally, this number is fixed to 10^{-6} , which should be sufficient for most cases. If however the orbits corresponding to ρ and $\rho + \epsilon$ lie on opposite sides of the trapped-passing boundary, this will lead to a large error in the computations of the derivatives which will amplify one particular orbit. Currently, the best approach for fixing this should be to make the value of macro JACOBIAN_ORBIT_STEP in src/include/global.h smaller.

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