EPOCH

An open source PIC code for high energy density physics

Users Manual

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Users Manual for the EPOCH PIC codes

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1 FAQs

1.1 Is this manual up to date?

Whenever a new milestone version of EPOCH is finalised, the version number is changed and this manual is updated accordingly. The version number of the manual should match the first two digits for that of the EPOCH source code. This version number is printed to screen when you run the code. The line looks something like the following:

```
Welcome to EPOCH2D Version 4.3.3   (commit v4.3.3-3-g3ed1a0e--clean)
```

Here, only the number "4.3" is important.

Since version 3.1 of the manual, new additions and changes are mentioned in the appendix.

1.2 What is EPOCH?

EPOCH is a plasma physics simulation code which uses the Particle in Cell (PIC) method. In this method, collections of physical particles are represented using a smaller number of pseudoparticles, and the fields generated by the motion of these pseudoparticles are calculated using a finite difference time domain technique on an underlying grid of fixed spatial resolution. The forces on the pseudoparticles due to the calculated fields are then used to update the pseudoparticle velocities, and these velocities are then used to update the pseudoparticle positions. This leads to a scheme which can reproduce the full range of classical micro-scale behaviour of a collection of charged particles.

1.2.1 Features of EPOCH

- MPI parallelised, explicit, second-order, relativistic PIC code.
- Dynamic load balancing option for making optimal use of all processors when run in parallel.
- MPI-IO based output, allowing restart on an arbitrary number of processors.
- Data analysis and visualisation options include ITT IDL, LLNL VisIt and Mathworks MatLab.
- Control of setup and runs of EPOCH through a customisable input deck.

1.3 The origins of the code

The EPOCH family of PIC codes is based on the older PSC code written by Hartmut Ruhl and retains almost the same core algorithm for the field updates and particle push routines. EPOCH was written to add more modern features and to structure the code in such a way that future expansion of the code is made as easy as possible.

1.4 What normalisations are used in EPOCH?

Since the idea from the start was that EPOCH would be used by a large number of different users and that it should be as easy as possible to "plug in" different modules from different people into a given copy of the code, it was decided to write EPOCH in SI units. There are a few places in the code where some quantities are given in other units for convenience (for example charges are specified in multiples of the electron charge), but the entire core of the code is written in SI units.

1.5 What are those _num things doing everywhere?

Historically using the compiler auto-promotion of `REAL` to `DOUBLE PRECISION` was unreliable, so EPOCH uses "kind" tags to specify the precision of the code. The `_num` suffixes and the associated definition of `REAL`s as `REAL(num)` are these "kind" tags in operation. The `_num` tags force numerical constants to match the precision of the code, preventing errors due to precision conversion. The important thing is that all numerical constants should be tagged with an `_num` tag and all `REAL`s should be defined as `REAL(num)`.

1.6 What is an input deck?

An input deck is text file which can be used to set simulation parameters for EPOCH without needing to edit or recompile the source code. It consists of a list of blocks which start as **begin:blockname** and end with **end:blockname**. Within the body of each block is a list of key/value pairs, one per line, with key and value separated by an equals sign. Most aspects of a simulation can be controlled using an input deck, such as the number of grid points in the simulation domain, the initial distribution of particles and initial electromagnetic field configuration. It is designed to be relatively easy to read and edit. For most projects it should be possible to set up a simulation without editing the source code at all. For more details, read "**3**" (Section 3).

1.7 I just want to use the code as a black box, or I'm just starting. How do I do that?

Begin by reading "**5**" (Section 5). There's quite a lot to learn in order to get started, so you should plan to read through all of this section. You will also need to refer to "**3**" (Section 3). Next, look at the code and have a play with some test problems. After that re-read this section. This should be enough for testing simple problems.

1.8 What is the auto-loader?

Throughout this document we will often refer to the "auto-loader" when setting up the initial particle distribution. In the input deck it is possible to specify a functional form for the density and temperature of a particle species. EPOCH will then place the particles to match the density function and set the velocities of the particles so that they match the Maxwellian thermal distribution for the temperature. The code which performs this particle set up is called the "auto-loader".

At present, there is no way to specify a non-Maxwellian particle distribution from within the input deck. In such cases, it is necessary to edit and recompile the EPOCH source code. The recommended method for setting the initial particle properties is to use the "`manual_load`" function as described in Section 4.2.

1.9 What is a maths parser?

As previously mentioned, the behaviour of EPOCH is controlled using an input deck which contains a list of key/value pairs. The value part of the pair is not restricted to simple constants but can be a complex mathematical expression. It is evaluated at run time using a section of code called the "maths parser". There is no need for the end user to know anything about this code. It is just there to enable the use of mathematical expressions in the input deck. Further information about this facility can be found in Section 3.15.

1.10 I am an advanced user, but I want to set up the code so that less experienced users can use it. How do I do that?

See "**4.6**" (Section 4.6).

1.11 I want to develop an addition to EPOCH. How do I do that?

A slightly outdate developers manual exists which should be sufficient to cover most aspects of the code functionality. However, the code is written in a fairly modular and consistent manner, so reading through that is the best source of information. If you get stuck then you can post questions on the CCPForge forums.

1.12 I want to have a full understanding of how EPOCH works. How do I do that?

If you really want to understand EPOCH in full, the only way is to read all of this manual and then read through the code. Most of it is commented.

2 EPOCH for end users

This manual aims to give a complete description of how to set up and run EPOCH as an end user. Further details on the design and implemetation of the code may be found in Arber et al. [1] and Ridgers et al. [2].

We begin by giving a brief overview of the EPOCH code-base, how to compile and run the code. Note that throughout this user manual, instructions are given assuming that you are typing commands at a UNIX terminal.

2.1 Structure of the EPOCH codes

When obtained, the EPOCH codes all have a similar structure. If the tarred and gzipped archive (commonly referred to as a tarball) is downloaded and unpacked into the user's `$HOME` directory, then the extracted contents will consist of a directory named "`$HOME/epoch-4.3.3`" (with "4.3.3" substituted by the current version number) and the subdirectories and files listed below.

Alternatively, if the code is checked out from the CCPForge subversion repository with the command

```
svn checkout --username <user> http://ccpforge.cse.rl.ac.uk/svn/epoch
```

then the directory will be "`$HOME/epoch/trunk`". In this case, the directories "`$HOME/epoch/branches`" and "`$HOME/epoch/tags`" will also be created. These two directories are entirely unnecessary. You can avoid creating them by checking out the subversion repository using the following command

```
svn co --username <user> http://ccpforge.cse.rl.ac.uk/svn/epoch/trunk epoch
```

All the required source code will then be contained in a directory named "`$HOME/epoch`".

Once the code has been obtained, the top-level directory will contain the following 5 directories and two files

- epoch1d - Source code and other files required for the 1D version of EPOCH.
- epoch2d - Source code and other files required for the 2D version of EPOCH.
- epoch3d - Source code and other files required for the 3D version of EPOCH.
- MatLab - The files for creating a plug-in for the Mathworks MatLab visualisation tool for reading SDF files generated by an EPOCH run.
- VisIt - The files for creating a plug-in for the LLNL VisIt parallel visualisation tool for reading SDF files generated by an EPOCH run.
- CODING_STYLE - This document contains the conventions which must be used for any code being submitted for inclusion in the EPOCH project.
- epoch_tarball.ssh - This is a shell script which is used for creating the tarred and gzipped archives of EPOCH which are posted to CCPForge each time a new release is made.

The three EPOCH subdirectories all have a similar structure. Inside each of the epoch{1,2,3}d directories, there are 4 sub-directories:

- src - The EPOCH source code.
- IDL - The IDL routines needed to open the SDF files which the code outputs.
- example_decks - A sample data directory containing example input deck files.
- Data - This is an empty directory to use for running simulations.

there are also 5 files:

- COMMIT - Contains versioning information for the code.

- Changelog.txt - A brief overview of the change history for each released version of EPOCH.
- Makefile - A standard makefile.
- Start.pro - An IDL script which starts the IDL visualisation routines. Execute it using "idl Start".
- unpack_source_from_restart - Restart dumps can be written to contain a copy of the input decks and source code used to generate them. This script can be used to unpack that information from a given restart dump. It is run from the command line and must be passed the name of the restart dump file.

2.2 Libraries and requirements

The EPOCH codes are written using MPI for parallelism, but have no other libraries or dependencies. Currently, the codes are written to only require MPI1.2 compatible libraries, although this may change to require full MPI2 compliance in the future. Current versions of both MPICH and OpenMPI implement the MPI2 standard and are known to work with this code. The SCALI MPI implementation is only compliant with the MPI1.2 specification and may loose support soon. There are no plans to write a version of EPOCH which does not require the MPI libraries.

The code is supplied with a standard GNU make Makefile, which is also compatible with most other forms of the **make** utility. In theory it is possible to compile the code without a **make** utility, but it is much easier to compile the code using the supplied makefile.

2.3 Compiling and running EPOCH

To compile EPOCH in the supplied state, you must first change to the correct working directory. As explained in Section 2.1, the root directory for EPOCH contains several subdirectories, including separate directories for each of the 1D, 2D and 3D versions of the code. To compile the 2D version of the code, you first switch to the "epoch2d" directory using the command

```
cd $HOME/epoch/epoch2d
```

and then type

```
make
```

and the code will compile. There are certain options within the code which are controlled by compiler preprocessors and are described in the next section. When the code is compiled, it creates a new directory called "bin" containing the compiled binary which will be called `epoch1d`, `epoch2d` or `epoch3d`. To run the code, just execute the binary file by typing:

```
./bin/epoch2d
```

or whatever the correct binary is for the dimensionality of the code that you have. You should be given a screen which begins with the EPOCH logo, and then reads:

```
Welcome to EPOCH2D Version 4.3.3   (commit v4.3.3-3-g3ed1a0e--clean)

The code was compiled with the following compile time options
*************************************************************
Per particle weighting -DPER_PARTICLE_WEIGHT
Tracer particle support -DTRACER_PARTICLES
Particle probe support -DPARTICLE_PROBES
*************************************************************
Code is running on 1 processing elements

Specify output directory
```

At this point, the user simply types in the name of the (already existing) output directory and the code will read the input deck files inside the specified directory and start running. To run the code in parallel, just use the normal mpirun or mpiexec scripts supplied by your MPI implementation. If you want the code to run unattended, then you will need to pipe in the output directory name to be used. The method for doing this varies between MPI implementations. For many MPI implementations (such as recent versions of OpenMPI) this can be achieved with the following:

```
echo Data | mpirun -np 2 ./bin/epoch2d
```

Some cluster setups accept the following instead:

```
mpirun -np 2 ./bin/epoch2d < deck.file
```

where "deck.file" is a file containing the name of the output directory. Some cluster queueing systems do not allow the use of input pipes to mpirun. In this case, there is usually a "-stdin" command line option to specify an input file. See your cluster documentation for more details.

As of version 4.2.12, EPOCH now checks for the existence of a file named "USE_DATA_DIRECTORY" in the current working directory before it prompts the user for a Data directory. If such a file exists, it reads it to obtain the name of the data directory to use and does not prompt the user. If no such file exists, it prompts for a data directory name as before. This is useful for cluster setups in which it is difficult or impossible to pipe in the directory name using a job script.

The "Makefile" supplied with EPOCH is setup to use the Intel compiler by default. However, it also contains configurations for gfortran, pgi, g95, hector and ibm (the compiler suite used on IBM's BlueGene machines). In order to compile using one of the listed configurations, add the "`COMPILER=`" option to the "`make`" command. For example

```
make COMPILER=gfortran
```

will compile the code using the gfortran compiler and appropriate compiler flags. You can also compile the code with debugging flags by adding "`MODE=debug`" and can compile using more than one processor by using "`-j<n>`", where "`<n>`" is the number of processors to use. Note that this is just to speed up the compilation process; the resulting binary can be run on any number of processors.

2.4 Compiler flags and preprocessor defines

As already stated, some features of the code are controlled by compiler preprocessor directives. The flags for these preprocessor directives are specified in "Makefile" and are placed on lines which look like the following:

```
DEFINES += $(D)PER_PARTICLE_WEIGHT
```

On most machines "`$(D)`" just means "`-D`" but the variable is required to accommodate more exotic setups.

Most of the flags provided in the "Makefile" are commented out by prepending them with a "`#`" symbol (the "make" system's comment character). To turn on the effect controlled by a given preprocessor directive, just uncomment the appropriate "DEFINES" line by deleting this "`#`" symbol. The options currently controlled by the preprocessor are:

- PER_PARTICLE_WEIGHT - Instead of running the code where each pseudoparticle represents the same number of real particles, each pseudoparticle can represent a different number of real particles. Many of the codes more advanced features require this and it is turned on by default. It can be turned off to save on memory, but this is recommended only for advanced users.
- TRACER_PARTICLES - Gives the option to specify one or more species as tracer particles. Tracer particles are specified like normal particles, and move about as would a normal particle with the same charge and mass, but tracer particles do not generate any current and are therefore passive elements in the simulation. Any attempt to add particle collision effects should remember

that tracer species should not interact through collisions. The implementation of tracer particles requires an additional "IF" clause in the particle push, so it is not activated by default.

- PARTICLE_PROBES - For laser plasma interaction studies it can sometimes be useful to be able to record information about particles which cross a plane in the simulation. Since this requires the code to check whether each particles has crossed the plane in the particles pusher and also to store copies of particles until the next output dump, it is a heavyweight diagnostic. Therefore, this diagnostic is only enabled when the code is compiled with this directive.
- PARTICLE_SHAPE_TOPHAT - By default, the code uses a first order b-spline (triangle) shape function to represent particles giving third order particle weighting. Using this flag changes the particle representation to that of a top-hat function (0th order b-spline yielding a second order weighting).
- PARTICLE_SHAPE_BSPLINE3 - This flag changes the particle representation to that of a 3rd order b-spline shape function (5th order weighting).
- PARTICLE_ID - When this option is enabled, all particles are assigned a unique identification number when writing particle data to file. This number can then be used to track the progress of a particle during the simulation.
- PARTICLE_ID4 - This does the same as the previous option except it uses a 4-byte integer instead of an 8-byte one. Whilst this saves storage space, care must be taken that the number does not overflow.
- PHOTONS - This enables support for photon particle types in the code. These are a pre-requisite for modelling synchrotron emission, radiation reaction and pair production (see Section 3.12).
- TRIDENT_PHOTONS - This enables support for virtual photons which are used by the Trident process for pair production.
- PARTICLE_COUNT_UPDATE - Makes the code keep global particle counts for each species on each processor. This information isn't needed by the core algorithm, but can be useful for developing some types of additional physics packages. It does require one additional MPI_ALL_REDUCE per species per timestep, so it is not activated by default.
- PREFETCH - This enables an Intel-specific code optimisation.
- PARSER_DEBUG - The code outputs more detailed information whilst parsing the input deck. This is a debug mode for code development.
- PARTICLE_DEBUG - Each particle is additionally tagged with information about which processor it is currently on, and which processor it started on. This is a debug mode for code development.
- MPI_DEBUG - This option installs an error handler for MPI calls which should aid tracking down some MPI related errors.
- NO_IO - This option disables all file I/O which can be useful when doing benchmarking.
- PER_PARTICLE_CHARGE_MASS - By default, the particle charge and mass are specified on a per-species basis. With this flag enabled, charge and mass become a per-particle property. This is a legacy flag which will be removed soon.

If a user requests an option which the code has not been compiled to support then the code will give an error message as follows:

```
*** WARNING ***
The element "particle_probes" of block "output" cannot be set
because the code has not been compiled with the correct preprocessor options.
Code will continue, but to use selected features, please recompile with the
-DPARTICLE_PROBES option
```

It is also possible to pass other flags to the compiler. In “Makefile” there is a line which reads
`FFLAGS = -O3 -fast`
The two commands to the right are compiler flags and are passed unaltered to the FORTRAN compiler. Change this line to add any additional flags required by your compiler.

By default, EPOCH will write a copy of the source code and input decks into each restart dump. This can be very useful since a restart dump contains an exact copy of the code which was used to generate it, ensuring that you can always regenerate the data or continue running from a restart. The output can be prevented by using “dump_source_code = F” and “dump_input_deck = F” in the output block. However, the functionality is difficult to build on some platforms so the Makefile contains a line for bypassing this section of the build process. Just below all the DEFINE flags there is the following line:

```
# ENCODED_SOURCE = dummy_encoded_source.o
```

Just uncomment this line and source code in restart dumps will be permanently disabled.

2.5 Running EPOCH and basic control of EPOCH1D

When the code is run, the output is

Command line output

```
       d#########P d#########b       .#######b         d#######  d##P      d##P
      d#########P d###########    d###########     .##########  d##P      d##P
     ----        ----     ----  -----     ----   -----         ----      -- P
    d#########P d####,,,####P ####.      .#### d###P          d############P
   d#########P d#########P   ####       .###P ####.          d############P
  d##P        d##P           ####     d####   ####.         d##P      d##P
 d#########P d##P            ###########P     ##########P  d##P      d##P
d#########P d##P              d######P          #######P  d##P      d##P

Welcome to EPOCH2D Version 4.3.3   (commit v4.3.3-3-g3ed1a0e--clean)

The code was compiled with the following compile time options
*************************************************************
Per particle weighting -DPER_PARTICLE_WEIGHT
Tracer particle support -DTRACER_PARTICLES
Particle probe support -DPARTICLE_PROBES
*************************************************************
Code is running on 1 processing elements

Specify output directory
```

At which point the end user should simply type in the name of the directory where the code output is to be placed. This directory must also include the file “`input.deck`” which controls the code setup, specifies how to set the initial conditions and controls the I/O. Writing an input deck for EPOCH is fairly time consuming and so the code is supplied with some example input decks which include all the necessary sections for the code to run.

3 The EPOCH input deck

Most of the control of EPOCH is through a text file called `input.deck`. The input deck file must be in the output directory which is passed to the code at runtime and contains all the basic information which is needed to set up the code, including the size and subdivision of the domain, the boundary conditions, the species of particles to simulate and the output settings for the code. For most users this will be capable of specifying all the initial conditions and output options they need. More complicated initial conditions will be handled in later sections.

The input deck is a structured file which is split into separate blocks, with each block containing several "parameter" = "value" pairs. The pairs can be present in any order, and not all possible pairs must be present in any given input deck. If a required pair is missing the code will exit with an error message. The blocks themselves can also appear in any order. The input deck is case sensitive, so true is always "T", false is always "F" and the names of the parameters are always lower case. Parameter values are evaluated using a maths parser which is described in Section 3.15.

If the deck contains a "\" character then the rest of the line is ignored and the next line becomes a continuation of the current one. Also, the comment character is "`#`"; if the "`#`" character is used anywhere on a line then the remainder of that line is ignored.

There are three *input deck directive* commands, which are:

- begin:*block* - Begin the block named *block*.
- end:*block* - Ends the block named *block*.
- import:*filename* - Includes another file (called *filename*) into the input deck at the point where the directive is encountered. The input deck parser reads the included file exactly as if the contents of the included file were pasted directly at the position of the import directive.

Each block must be surrounded by valid *begin:* and *end:* directives or the input deck will fail. There are currently fourteen valid blocks hard coded into the input deck reader, but it is possible for end users to extend the input deck. The fourteen built in blocks are:

- control - Contains information about the general code setup.
- boundaries - Contains information about the boundary conditions for this run.
- species - Contains information about the species of particles which are used in the code. Also details of how these are initialised.
- laser - Contains information about laser boundary sources.
- fields - Contains information about the EM fields specified at the start of the simulation.
- window - Contains information about the moving window if the code is used in that fashion.
- output - Contains information about when and how to dump output files.
- output_global - Contains parameters which should be applied to all output blocks.
- dist_fn - Contains information about distribution functions that should be calculated for output.
- probe - Contains information about particle probes used for output.

- collisions - Contains information about particle collisions.
- qed - Contains information about QED pair production.
- subset - Contains configuration for filters which can be used to modify the data to be output.
- constant - Contains information about user defined constants and expressions. These are designed to simplify the initial condition setup.

3.1 control block

The control block sets up the basic code properties for the domain, the end time of the code, the load balancer and the types of initial conditions to use.

The control block of a valid input deck for EPOCH2D reads as follows:

control block

```
begin:control
   # global number of gridpoints
   nx = 512 # in x
   ny = 512 # in y
   # global number of particles
   npart = 10 * nx * ny

   # final time of simulation
   t_end = 1.0e-12
   # nsteps = -1

   # size of domain
   x_min = -0.1e-6
   x_max = 400.0e-6
   y_min = -400.0e-6
   y_max = 400.0e-6

   # dt_multiplier = 0.95
   # dlb_threshold = 0.8

   # restart_snapshot = 98

   # field_order = 2
   # stdout_frequency = 10
end:control
```

As illustrated in the above code block, the “#” symbol is treated as a comment character and the code ignores everything on a line following this character.

The allowed entries are as follows:

nx, ny, nz - Number of grid points in the x,y,z direction. This parameter is mandatory.

npart - The global number of pseudoparticles in the simulation. This parameter does not need to be given if a specific number of particles is supplied for each particle species by using the “npart” directive in each species block (see Section 3.3). If both are given then the value in the control block will be ignored.

nsteps - The number of iterations of the core solver before the code terminates. Negative numbers instruct the code to only terminate at t_end. If nsteps is not specified then t_end must be given.

t_end - The final simulation time in simulation seconds before the code terminates. If t_end is not specified then nsteps must be given. If they are both specified then the first time restriction to be satisfied takes precedence. Sometimes it is more useful to specify the time in picoseconds or femtoseconds. To accomplish this, just append the appropriate multiplication factor. For example, "t_end = 3 * femto" specifies 3 femtoseconds. A list of multiplication factors is supplied in Section 3.15.1.

{x,y,z}_min - Minimum grid position of the domain in metres. These are required parameters. Can be negative. "{x,y,z}_start" is accepted as a synonym. In a similar manner to that described above, distances can be specified in microns using a multiplication constant. eg. "x_min = 4 * micron" specifies a distance of 4μm.

{x,y,z}_max - Maximum grid position of the domain in metres. These are required parameters. Must be greater than {x,y,z}_min. "{x,y,z}_end" is accepted as a synonym.

dt_multiplier - Factor by which the timestep is multiplied before it is applied in the code, i.e. a multiplying factor applied to the CFL condition on the timestep. Must be less than one. If no value is given then the default of 0.95 is used.

dlb_threshold - The minimum ratio of the load on the least loaded processor to that on the most loaded processor allowed before the code load balances. Set to 1 means always balance, set to 0 means never balance. If this parameter is not specified then the code will only be load balanced at initialisation time.

restart_snapshot - The number of a previously written restart dump to restart the code from. If not specified then the initial conditions from the input deck are used.
Note that as of version 4.2.5, this parameter can now also accept a filename in place of a number. If you want to restart from "0012.sdf" then it can either be specified using "restart_snapshot = 12", or alternatively it can be specified using "restart_snapshot = 0012.sdf". This syntax is required if output file prefixes have been used (see Section 3.7).

field_order - Order of the finite difference scheme used for solving Maxwell's equations. Can be 2, 4 or 6. If not specified, the default is to use a second order scheme.

stdout_frequency - If specified then the code will print a one line status message to stdout after every given number or timesteps. The default is to print nothing to screen (ie. "`stdout_frequency = 0`").

use_random_seed - The initial particle distribution is generated using a random number generator. By default, EPOCH uses a fixed value for the random generator seed so that results are repeatable. If this flag is set to "T" then the seed will be generated using the system clock.

nproc{x,y,z} - Number of processes in the x,y,z directions. By default, EPOCH will try to pick the best method of splitting the domain amongst the available processors but occasionally the user may wish to override this choice.

smooth_currents - This is a logical flag. If set to "T" then a smoothing function is applied to the current generated during the particle push. This can help to reduce noise and self-heating in a simulation. The smoothing function used is the same as that outlined in Buneman [3]. The default value is "F".

field_ionisation - Logical flag which turns on field ionisation. See Section 3.3.2.

use_bsi - Logical flag which turns on barrier suppression ionisation correction to the tunnelling ionisation model for high intensity lasers. See Section 3.3.2. This flag should always be enabled when using field ionisation and is only supplied for testing purposes. The default is “T”.

use_multiphoton - Logical flag which turns on modelling ionisation by multiple photon absorption. This should be set to “F” if there is no laser attached to a boundary as it relies on laser frequency. See Section 3.3.2. This flag should always be enabled when using field ionisation and is only supplied for testing purposes. The default is “T”.

particle_tstart - Specifies the time at which to start pushing particles. This allows the field to evolve using the Maxwell solver for a specified time before beginning to move the particles.

use_exact_restart - Logical flag which makes a simulation restart using exactly the same configuration as the original simulation. If set to “T” then the domain split amongst processors will be identical along with the seeds for the random number generators. Note that the flag will be ignored if the number of processors does not match that used in the original run. The default value is “F”.

allow_cpu_reduce - Logical flag which allows the number of CPUs used to be reduced from the number specified. In some situations it may not be possible to divide the simulation amongst all the processors requested. If this flag is set to “T” then EPOCH will continue to run and leave some of the requested CPUs idle. If set to “F” then code will exit if all CPUs cannot be utilised. The default value is “T”.

check_stop_file_frequency - Integer parameter controlling automatic halting of the code. The frequency is specified as number of simulation cycles. Refer to description later in this section. The default value is 10.

stop_at_walltime - Floating point parameter controlling automatic halting of the code. Refer to description later in this section. The default value is -1.0.

stop_at_walltime_file - String parameter controlling automatic halting of the code. Refer to description later in this section. The default value is an empty string.

simplify_deck - If this logical flag is set to “T” then the deck parser will attempt to simplify the maths expressions encountered after the first pass. This can significantly improve the speed of evaluation for some input deck blocks. The default value is “F”.

print_constants - If this logical flag is set to “T”, deck constants are printed to the “deck.status” file as they are parsed. The default value is “F”.

use_migration - Logical flag which determines whether or not to use particle migration. The default is “F”. See Section 3.3.1.

migration_interval - The number of timesteps between each migration event. The default is 1 (migrate at every timestep). See Section 3.3.1.

Most of the control block is self explanatory, but there are two parts which need further description.

3.1.1 Dynamic Load Balancing

The first is the **dlb_threshold** flag. “dlb” stands for Dynamic Load Balancing and, when turned on, it allows the code to rearrange the internal domain boundaries to try and balance the workload on each processor. This rearrangement is an expensive operation, so it is only performed when the maximum load imbalance reaches a given critical point. This critical point is given by the parameter “dlb_threshold” which is the ratio of the workload on the least loaded processor to the most loaded processor. When the calculated load imbalance is less than “dlb_threshold” the code performs a re-balancing sweep, so if “dlb_threshold = 1.0” is set then the code will keep trying to re-balance the workload at almost every timestep. At present the workload on each processor is simply calculated from the number of particles on each processor, but this will probably change in future. If the “dlb_threshold” parameter is not specified then the code will only be load balanced at initialisation time.

3.1.2 Automatic halting of a simulation

It is sometimes useful to be able to halt an EPOCH simulation midway through execution and generate a restart dump. Two methods have been implemented to enable this.

The first method is to check for the existence of a “STOP” file. Throughout execution, EPOCH will check for the existence of a file named either “STOP” or “STOP_NODUMP” in the simulation output directory. The check is performed at regular intervals and if such a file is found then the code exits immediately. If “STOP” is found then a restart dump is written before exiting. If “STOP_NODUMP” is found then no I/O is performed.

The interval between checks is controlled by the integer parameter “check_stop_frequency” which can be specified in the “control” block of the input deck. If it is less than or equal to zero then the check is never performed.

The next method for automatically halting the code is to stop execution after a given elapsed walltime. If a positive value for “stop_at_walltime” is specified in the control block of an input deck then the code will halt once this time is exceeded and write a restart dump. The parameter takes a real argument which is the time in seconds since the start of the simulation.

An alternative method of specifying this time is to write it into a separate text file. “stop_at_walltime_file” is the filename from which to read the value for “stop_at_walltime”. Since the walltime will often be found by querying the queueing system in a job script, it may be more convenient to pipe this value into a text file rather than modifying the input deck.

3.2 boundaries block

The **boundaries** block sets the boundary conditions of each boundary of the domain. Some types of boundaries allow EM wave sources (lasers) to be attached to a boundary. Lasers are attached at the initial conditions stage.

An example boundary block for EPOCH2D is as follows:

boundaries block
```
begin:boundaries
   bc_x_min = simple_laser
   bc_x_max_field = simple_outflow
   bc_x_max_particle = simple_outflow
   bc_y_min = periodic
   bc_y_max = periodic
end:boundaries
```

The **boundaries** accepts the following parameters:

bc_{x,y,z}_min - The condition for the lower boundary for both fields and particles. "xbc_left", "ybc_down" and "zbc_back" are accepted as a synonyms.

bc_{x,y,z}_min_{field,particle} - The condition for the lower boundary for {fields,particles}. "xbc_left_{field,particle}", "ybc_down_{field,particle}" and "zbc_back_{field,particle}" are accepted as a synonyms.

bc_{x,y,z}_max - The condition for the upper boundary for both fields and particles. "xbc_right", "ybc_up" and "zbc_front" are accepted as a synonyms.

bc_{x,y,z}_max_{field,particle} - The condition for the upper boundary for {fields,particles}. "xbc_right_{field,particle}", "ybc_up_{field,particle}" and "zbc_front_{field,particle}" are accepted as a synonyms.

cpml_thickness - The thickness of the CPML boundary in terms of the number of grid cells (see Section 3.2.1). The default value is 6.

cpml_kappa_max - A tunable CPML parameter (see Section 3.2.1).

cpml_a_max - A tunable CPML parameter (see Section 3.2.1).

cpml_sigma_max - A tunable CPML parameter (see Section 3.2.1).

There are ten boundary types in EPOCH and each boundary of the domain can have one and only one of these boundaries attached to it. These boundary types are:

periodic - A simple periodic boundary condition. Fields and/or particles reaching one edge of the domain are wrapped round to the opposite boundary. If either boundary condition is set to periodic then the boundary condition on the matching boundary at the other side of the box is also assumed periodic.

simple_laser - A characteristic based boundary condition to which one or more EM wave sources can be attached. EM waves impinging on a simple_laser boundary are transmitted with as little reflection as possible. Particles are fully transmitted. The field boundary condition works by allowing outflowing characteristics to propagate through the boundary while using the attached lasers to specify the inflowing characteristics. The particles are simply removed from the simulation when they reach the boundary.

simple_outflow - A simplified version of simple_laser which has the same properties of transmitting incident waves and particles, but which cannot have EM wave sources attached to it. These boundaries are about 5% more computationally efficient than simple_laser boundaries with no attached sources. This boundary condition again allows outflowing characteristics to flow unchanged, but this time the inflowing characteristics are set to zero. The particles are again simply removed from the simulation when they reach the boundary.

reflect - This applies reflecting boundary conditions to particles. When specified for fields, all field components are clamped to zero.

conduct - This applies perfectly conducting boundary conditions to the field. When specified for particles, the particles are reflected.

open - When applied to fields, EM waves outflowing characteristics propagate through the boundary. Particles are transmitted through the boundary and removed from the system.

cpml_laser - See Section 3.2.1.

cpml_outflow - See Section 3.2.1.

thermal - See Section 3.2.2.

NOTE: If simple_laser, simple_outflow, cpml_laser, cpml_outflow or open are specified on one or more boundaries then the code will no longer necessarily conserve mass.

Note also that it is possible for the user to specify contradictory, unphysical boundary conditions. It is the users responsibility that these flags are set correctly.

3.2.1 CPML boundary conditions

There are now Convolutional Perfectly Matched Layer boundary conditions in EPOCH. The implementation closely follows that outlined in the book "Computational Electrodynamics: The Finite-Difference Time-Domain Method" by Taflove and Hagness [4]. See also Roden and Gedney [5].

CPML boundaries are specified in the input deck by specifying either "cpml_outflow" or "cpml_laser" in the boundaries block. "cpml_outflow" specifies an absorbing boundary condition whereas "cpml_laser" is used to attach a laser to an otherwise absorbing boundary condition.

There are also four configurable parameters:

cpml_thickness - The thickness of the CPML boundary in terms of the number of grid cells. The default value is 6.

cpml_kappa_max, **cpml_a_max**, **cpml_sigma_max** - These are tunable parameters which affect the behaviour of the absorbing media. The notation follows that used in the two references quoted above. Note that the "cpml_sigma_max" parameter is normalised by σ_{opt} which is taken to be 3.2/dx (see Taflove and Hagness [4] for details). These are real valued parameters which take the following default values: cpml_kappa_max=20, cpml_a_max=0.15, cpml_sigma_max=0.7

An example usage is as follows:

```
begin:boundaries
   cpml_thickness = 16
   cpml_kappa_max = 20
   cpml_a_max = 0.2
   cpml_sigma_max = 0.7
   bc_x_min = cpml_laser
   bc_x_max = cpml_outflow
   bc_y_min = cpml_outflow
   bc_y_max = cpml_outflow
end:boundaries
```

3.2.2 Thermal boundaries

Thermal boundary conditions have been added to the "boundaries" block. These simulate the existence of a "thermal bath" of particles in the domain adjacent to the boundary. When a particle leaves the simulation it is replace with an incoming particle sampled from a Maxwellian of a temperature corresponding to that of the initial conditions. It is requested using the keyword "thermal". For example:

```
begin:boundaries
   bc_x_min = laser
   bc_x_max = thermal
end:boundaries
```

3.3 species block

The next section of the input deck describes the particle species used in the code. An example species block for any EPOCH code is given below.

species block
```
begin:species
   name = Electron
   charge = -1.0
   mass = 1.0
   frac = 0.5
   # npart = 2000*100
   # tracer = F
   density = 1.e4
   temp = 1e6

   temp_x = 0.0
   temp_y = temp_x(Electron)
   density_min = 0.1 * den_max
   density = if(abs(x) lt thick, den_max, 0.0)
   density = if((x gt -thick) and (abs(y) gt 2e-6), 0.0, density(Carbon))
end:species

begin:species
   name = Carbon
   charge = 4.0
   mass = 1836.0*12
   frac = 0.5

   density = 0.25*density(Electron)
   temp_x = temp_x(Electron)
   temp_y = temp_x(Electron)

   dumpmask = full
end:species
```

Each species block accepts the following parameters:

name - This specifies the name of the particle species defined in the current block. This name can include any alphanumeric characters in the basic ASCII set. The name is used to identify the species in any consequent input block and is also used for labelling species data in any output dumps. It is a mandatory parameter.

NOTE: IT IS IMPOSSIBLE TO SET TWO SPECIES WITH THE SAME NAME!

charge - This sets the charge of the species in multiples of the electron charge. Negative numbers are used for negatively charged particles. This is a mandatory parameter.

mass - This sets the mass of the species in multiples of the electron mass. Cannot be negative. This is a mandatory parameter.

npart - This specifies the number of pseudoparticles which should be loaded into the simulation domain for this species block. Using this parameter is the most convenient way of loading particles for simulations which contain multiple species with different number densities. If **npart** is specified in a species block then any value given for **npart** in the **control** block is ignored. **npart** should not be specified at the same time as **frac** within a **species** block.

frac - This specifies what fraction of **npart** (the global number of particles specified in the control block) should be assigned to the species.

NOTE: frac should not be specified at the same time as npart for a given species.

npart_per_cell - Integer parameter which specifies the number of particles per cell to use for the initial particle loading. At a later stage this may be extended to allow "npart_per_cell" to be a spatially varying function.

If per-species weighting is used then the value of "npart_per_cell" will be the average number of particles per cell. If "npart" or "frac" have also been specified for a species, then they will be ignored.

To avoid confusion, there is no globally used "npart_per_species". If you want to have a single value to change in the input deck then this can be achieved using a constant block.

dumpmask - Determines which output dumps will include this particle species. The dumpmask has the same semantics as those used by variables in the "output" block, described in Section 3.7. The actual dumpmask from the output block is applied first and then this one is applied afterwards. For example, if the species block contains "dumpmask = full" and the output block contains "vx = always" then the particle velocity will be only be dumped at full dumps for this particle species. The default dumpmask is "always".

dump - This logical flag is provided for backwards compatibility. If set to "F" it has the same meaning as "dumpmask = never". If set to "T" it has the same meaning as "dumpmask = always".

tracer - Logical flag switching the particle species into tracer particles. Tracer particles are enabled with the correct precompiler option, and when set for a given species make that species move correctly for its charge and mass, but contribute no current. This means that these particles are passive tracers in the plasma. "tracer = F" is the default value.

identify - Used to identify the type of particle. Currently this is used primarily by the QED routines. See Section 3.12 for details.

immobile - Logical flag. If this parameter is set to "T" then the species will be ignored during the particle push. The default value is "F".

The species blocks are also used for specifying initial conditions for the particle species. The initial conditions in EPOCH can be specified in various ways, but the easiest way is to specify the initial conditions in the input deck file. This allows any initial condition which can be specified everywhere in space by a number density and a drifting Maxwellian distribution function. These are built up using the normal maths expressions, by setting the density and temperature for each species which is then used by the autoloader to actually position the particles.

The elements of the species block used for setting initial conditions are:

density - Particle number density in m^{-3}. As soon as a density= line has been read, the values are calculated for the whole domain and are available for reuse on the right hand side of an expression. This is seen in the above example in the first two lines for the Electron species, where the density is first set and then corrected. If you wish to specify the density in parts per cubic metre then you can divide by the "cc" constant (see Section 3.15.1). This parameter is mandatory.

density_min - Minimum particle number density in m^{-3}. When the number density in a cell falls below density_min the autoloader does not load any pseudoparticles into that cell to minimise the number of low weight, unimportant particles. If set to 0 then all cells are loaded with particles. This is the default.

density_max - Maximum particle number density in m^{-3}. When the number density in a cell rises above density_max the autoloader clips the density to density_max allowing easy implementation of exponential rises to plateaus. If it is a negative value then no clipping is performed. This is the default.

mass_density - Particle mass density in $kg\, m^{-3}$. The same as "density" but multiplied by the particle mass. If you wish to use units of $g\, cm^{-3}$ then append the appropriate multiplication factor. For example: "`mass_density = 2 * 1e3 / cc`".

temp_{x,y,z} - The temperature in each direction for a thermal distribution in Kelvin.

temp - Sets an isotropic temperature distribution in Kelvin. If both temp and a specific temp_x, temp_y, temp_z parameter is specified then the last to appear in the deck has precedence. If neither are given then the species will have a default temperature of zero Kelvin.

temp_{x,y,z}_ev, temp_ev - These are the same as the temperature parameters described above except the units are given in electronvolts rather than Kelvin.

drift_{x,y,z} - Specifies a momentum space offset in $kg\ ms^{-1}$ to the distribution function for this species. By default, the drift is zero.

offset - File offset. See below for details.

It is also possible to set initial conditions for a particle species using an external file. Instead of specifying the initial conditions mathematically in the input deck, you specify in quotation marks the filename of a simple binary file containing the information required.

external initial conditions
```
begin:species
   name = Electron
   density = 'Data/ic.dat'
   offset = 80000
   temp_x = 'Data/ic.dat'
end:species
```

An additional element is also introduced, the offset element. This is the offset in bytes from the start of the file to where the data should be read from. As a given line in the block executes, the file is opened, the file handle is moved to the point specified by the offset parameter, the data is read and the file is then closed. Therefore, unless the offset value is changed between data reading lines the same data will be read into all the variables. The data is read in as soon as a line is executed, and so it is perfectly possible to load data from a file and then modify the data using a mathematical expression.

The file should be a simple binary file consisting of floating point numbers of the same precision as `_num` in the core EPOCH code. For multidimensional arrays, the data is assumed to be written according to FORTRAN array ordering rules (ie. column-major order).

NOTE: The files that are expected by this block are SIMPLE BINARY files, NOT FORTRAN unformatted files. It is possible to read FORTRAN unformatted files using the offset element, but care must be taken!

3.3.1 Particle migration between species

It is sometimes useful to separate particle species into separate energy bands and to migrate particles between species when they become more or less energetic. A method to achieve this functionality has been implemented. It is specified using two parameters to the "control" block:

use_migration - Logical flag which determines whether or not to use particle migration. The default is "F".

migration_interval - The number of timesteps between each migration event. The default is 1 (migrate at every timestep).

The following parameters are added to the "species" block:

migrate - Logical flag which determines whether or not to consider this species for migration. The default is "F".

promote_to - The name of the species to promote particles to.

demote_to - The name of the species to demote particles to.

promote_multiplier - The particle is promoted when its energy is greater than "promote_multiplier" times the local average. The default value is 1.

demote_multiplier - The particle is demoted when its energy is less than "demote_multiplier" times the local average. The default value is 1.

promote_density - The particle is only considered for promotion when the local density is less than "promote_density". The default value is the largest floating point number.

demote_density - The particle is only considered for demotion when the local density is greater than "demote_density". The default value is 0.

3.3.2 Ionisation

EPOCH now includes field ionisation which can be activated by defining ionisation energies and an electron for the ionising species. This is done via the species block using the following parameters:

ionisation_energies - This is an array of ionisation energies (in Joules) starting from the outermost shell. It expects to be given all energies down to the fully ionised ion; if the user wishes to exclude some inner shell ionisation for some reason they need to give this a very large number. Note that the ionisation model assumes that the outermost electron ionises first always, and that the orbitals are filled assuming ground state. When this parameter is specified it turns on ionisation modelling. If you wish to specify the values in Electron-Volts, add the "ev" multiplication factor (see Section 3.15.1).

ionisation_electron_species - Name of the electron species. This can be specified as an array in the event that the user wishes some levels to have a different electron species which can be handy for monitoring ionisation at specific levels. "electron" and "electron_species" are accepted as synonyms.

For example, ionising carbon species might appear in the input deck as:

```
begin:species
   charge = 0.0
   mass = 1837.2
   name = carbon
   ionisation_energies = (11.26*ev,24.38*ev,47.89*ev,64.49*ev,392.1*ev,490.0*ev)
   ionisation_electron_species = \
       (electron,electron,electron,fourth,electron,electron)
   rho = den_gas
end:species

begin:species
   charge = -1.0
   mass = 1.0
   name = electron
   rho = 0.0
end:species

begin:species
   charge = -1.0
   mass = 1.0
   name = fourth
   rho = 0.0
end:species
```

If "ionisation_electron_species" is not specified then the electron species are created automatically and are named according to the ionising species name with a number appended. For example

```
begin:species
   name = Helium
   ionisation_energies = (24.6*ev,54.4*ev)
   dump = F
end:species
```

With this species block, the electron species named "Helium1" and "Helium2" are automatically created. These species will also inherit the "dump" parameter from their parent species, so in this example they will both have "dump = F" set. This behaviour can be overridden by explicitly adding a species block of the same name with a differing dumpmask. eg.

```
begin:species
   name = Helium1
   dump = T
end:species
```

Field ionisation consists of three distinct regimes; multiphoton in which ionisation is best described as absorption of multiple photons, tunnelling in which deformation of the atomic Coulomb potential is the dominant factor, and barrier suppression ionisation in which the electric field is strong enough for an electron to escape classically. It is possible to turn off multiphoton or barrier suppression ionisation through the input deck using the following control block parameters:

use_multiphoton - Logical flag which turns on modelling ionisation by multiple photon absorption. This should be set to "F" if there is no laser attached to a boundary as it relies on laser frequency. The default is "T".

use_bsi - Logical flag which turns on barrier suppression ionisation correction to the tunnelling ionisation model for high intensity lasers. The default is "T".

3.4 laser block

Laser blocks attach an EM wave source to a boundary which is set as simple_laser.

laser block

```
begin:laser
   boundary = x_min
   id = 1
   intensity_w_cm2 = 1.0e15
   lambda = 1.06 * micron
   pol_angle = 0.0
   phase = 0.0
   t_profile = gauss(time,40.0e-15,40.0e-15)
   t_start = 0.0
   t_end = 80.0e-15
end:laser
```

As already mentioned in the discussion of laser boundaries in the boundaries block, lasers are attached to compatible boundaries here in the initial conditions deck.

boundary - The boundary on which to attach the laser. In 1D, the directions can be either x_min or x_max. "left" and "right" are accepted as a synonyms. In 2D, y_min and y_max may also be specified. These have synonyms of "down" and "up". Finally, 3D adds z_min and z_max with synonyms of "back" and "front".

amp - The amplitude of the E field of the laser in V/m.

intensity - The intensity of the laser in W/m^2. There is no need to specify both intensity and amp and the last specified in the block is the value used. It is mandatory to specify at least one. The amplitude of the laser is calculated from intensity using the formula `amp = sqrt(2*intensity/c/epsilon0)`. "irradiance" is accepted as a synonym.

intensity_w_cm2 - This is identical to the **intensity** parameter described above, except that the units are specified in W/cm^2.

id - An id code for the laser. Used if you specify the laser time profile in the EPOCH source rather than in the input deck. Does not have to be unique, but all lasers with the same id will have the same time profile. This parameter is optional and is not used under normal conditions.

omega - Angular frequency (rad/s not Hz) for the laser.

frequency - Ordinary frequency (Hz not rad/s) for the laser.

lambda - Wavelength in a vacuum for the laser specified in m. If you want to specify in μm then you can multiply by the constant "micron". One of **lambda** or **omega** (or **frequency**) is a required parameter.

pol_angle - Polarisation angle for the electric field of the laser in radians. This parameter is optional and has a value of zero by default. The angle is measured with respect to the right-hand triad of propagation direction, electric and magnetic fields. Although the 1D code has no y or z spatial axis, the fields still have y and z components. If the laser is on **x_min** then the default E field is in the y-direction and the B field is the z-direction. The polarisation angle is measured clockwise about the x-axis with zero along the E_y direction. If the laser is on **x_max** then the angle is anti-clockwise.
Similarly, for propagation directions:
y_min - angle about y-axis, zero along z-axis
z_min - angle about z-axis, zero along x-axis
y_max - angle anti-clockwise about y-axis, zero along z-axis
z_max - angle anti-clockwise about z-axis, zero along x-axis

pol - This is identical to **pol_angle** with the angle specified in degrees rather than radians. If both are specified then the last one is used.

phase - The phase profile of the laser wavefront given in radians. Phase may be a function of both space and time. The laser is driven using $\sin(\omega t + \phi)$ and **phase** is the ϕ parameter. There is zero phase shift applied by default.

profile - The spatial profile of the laser. This should be a spatial function not including any values in the direction normal to the boundary on which the laser is attached, and the expression will be evaluated at the boundary. It may also be time-dependant. The laser field is multiplied by the profile to give its final amplitude so the intention is to use a value between zero and one. By default it is a unit constant and therefore has no affect on the laser amplitude. This parameter is redundant in 1D and is only included for consistency with 2D and 3D versions of the code.

t_profile - Used to specify the time profile for the laser amplitude. Like **profile** the laser field is multiplied by this parameter but it is only a function of time and not space. In a similar manner to **profile**, it is best to use a value between zero and one. Setting values greater than one is possible but will cause the maximum laser intensity to grow beyond **amp**. In previous versions of EPOCH, the **profile** parameter was only a function of space and this parameter was used to impose time-dependance. Since **profile** can now vary in time, **t_profile** is no longer needed but it has been kept to facilitate backwards compatibility. It can also make input decks clearer if the time dependance is given separately. The default value of **t_profile** is just the real constant value of 1.0.

t_start - Start time for the laser in seconds. Can be set to the string "start" to start at the beginning of the simulation. This is the default value. When using this parameter, the laser start is hard. To get a soft start use the t_profile parameter to ramp the laser up to full strength.

t_end - End time for the laser in seconds, can be set to the string "end" to end at the end of the simulation. This is the default value. When using this parameter, the laser end is clipped straight to zero at t>t_end. To get a soft end use the t_profile parameter to ramp the laser down to zero.

If you add multiple laser blocks to the initial conditions file then the multiple lasers will be additively combined on the boundary.

In theory, any laser time profile required is possible, but the core FDTD solver for the EM fields in EPOCH produces spurious results if sudden changes in the field intensity occur. This is shown in Figures 1 and 2. The pulse shown in Figure 1 used a constant t_profile and used t_end to stop the laser after 8fs. Since the stopping time was not an exact multiple of the period, the result was to introduce spurious oscillations behind the pulse. If the laser had a finite phase shift so that the amplitude did not start at zero, a similar effect would be observed on the front of the pulse.

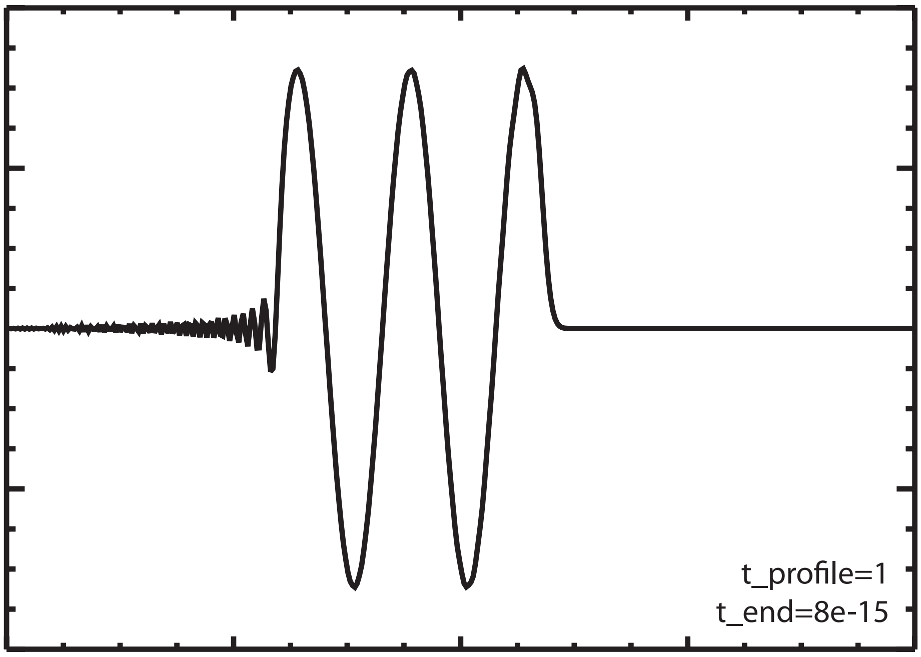


Figure 1: A laser pulse with a sharp cutoff shows numerical artefacts behind the pulse.

Figure 2 instead used a Gaussian window function with a characteristic width of 8fs as well as using t_end to introduce a hard cutoff. It can clearly be seen that there are no spurious oscillations and the wave packet propagates correctly, showing only some dispersive features.

There is no hard and fast rule as to how rapid the rise or fall for a laser can be, and the best advice is to simply test the problem and see whether any problems occur. If they do then there are various solutions. Essentially, the timestep must be reduced to the point where the sharp change in amplitude can be accommodated. The best solution for this is to increase the spatial resolution (with a comparable increase in the number of pseudoparticles), thus causing the timestep to drop via the CFL condition.

This is computationally expensive, and so a cheaper option is simply to decrease the input.deck option dt_multiplier. This artificially decreases the timestep below the timestep calculated from the internal stability criteria and allows the resolution of sharp temporal gradients. This is an inferior solution since the FDTD scheme has increased error as the timestep is reduced from that for EM waves. EPOCH includes a high order field solver to attempt to reduce this.

3.5 fields block

The next type of block in the EPOCH input deck is the fields block. This allows you to specify the electric and magnetic fields at any point in the domain. An example block is shown below:

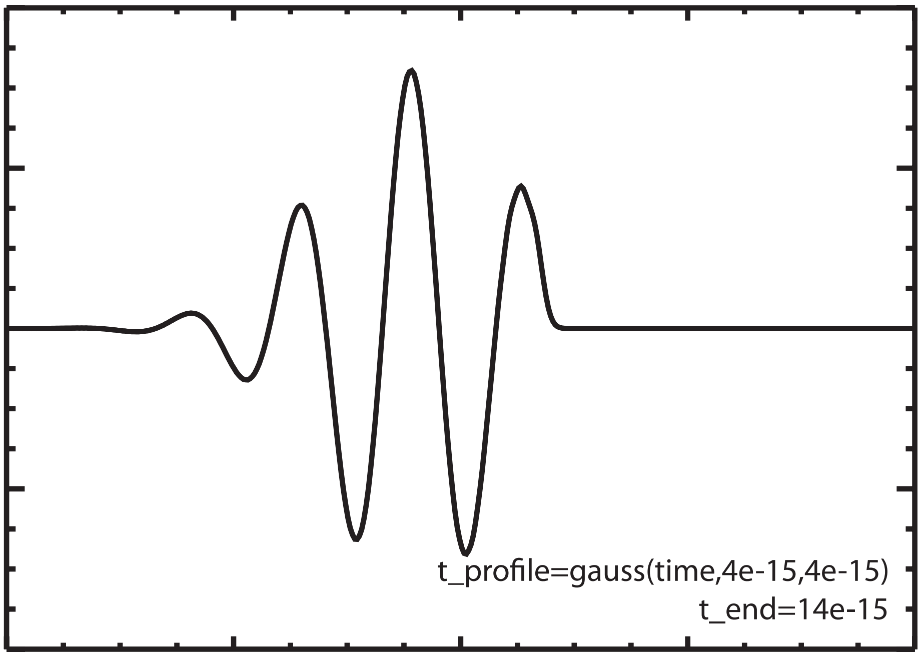


Figure 2: A laser pulse with a smooth temporal profile shows no artefacts.

fields block

```
begin:fields
   ex = sin(pi*x/length_x)
   ey = cos(pi*x/length_x)
   ez = 0
   bx = 1.0
   by = -1.0
   bz = 0
end:fields
```

Once again, this is a very simple block needing only limited explanation. All field variables are accessible by name and can be read back using the appropriate commands from the maths parser (see Section 3.15). The possible parameters are as follows:

ex, ey, ez - The electric field vectors pointing in all three directions. The default value is zero.

bx, by, bz - The magnetic field vectors pointing in all three directions. The default value is zero.

offset - File offset. The field values may also be specified using a binary file in a similar way to that used for species variables. See Section 3.3 for more details.

Any valid maths parser expression can be used to set up the fields, and no check is made to ensure that the $\nabla.B = 0$ is satisfied.

3.6 window block

EPOCH can include an optional block which causes the simulation domain to operate as a moving window. At present, it is only possible to have the window moving at a constant speed parallel to the x direction, although the window does not have to start moving at t = 0. When the window moves, the code removes particles from the left hand edge of the domain and introduces new particles at the right hand edge. The new particles are placed by re-evaluating the species density, temperature and drift using the new time and spatial coordinates. The block looks like:

```
begin:window
   move_window = T
   window_v_x = 3.0e8
   window_start_time = 7.0e-13
   bc_x_min_after_move = simple_outflow
   bc_x_max_after_move = simple_outflow
end:window
```

move_window - Logical flag determining whether or not to move the window. If the window block is absent then this is the same as setting move_window to "F".

window_v_x - The speed in m/s of the window.

window_start_time - The time in seconds at which the window should start moving.

bc_x_min_after_move - The boundary condition which should apply to the left boundary after the window has started moving. This is to allow the swapping of a laser boundary to a simple outflow boundary. Boundary codes are the same as when just specifying normal boundaries. If a boundary value isn't specified then it is assumed that the boundary isn't changed when the window starts moving. "xbc_left_after_move" is accepted as a synonym.

bc_x_max_after_move - The boundary condition which should apply to the right boundary after the window has started moving. "xbc_right_after_move" is accepted as a synonym.

3.7 output block

Output in EPOCH is handled using the custom designed SDF file format (Self Describing Format). A detailed specification of this format is available elsewhere, although this is only of interest to developers wishing to write new libraries. EPOCH comes with readers for ITT IDL, LLNL VisIt and Mathworks MatLab. The IDL reader is also compatible with the open source GDL tool.

There are two styles of output block supported by EPOCH. The first style, which will be referred to as the "traditional" style, is the method that has been supported by EPOCH since its inception. With this method, a single output block governs all the output dumps which are to be performed. There are a few levels of output which give some small amount of flexibility over what gets dumped but these do not allow for a very fine-grained control.

In version 4.0 of EPOCH, a new style was introduced in which multiple named output blocks may be specified allowing for much greater flexibility. The existence of a "name" parameter is what determines that an output block is the new style rather than the traditional style.

Most of the parameters are shared by both styles. The following sections document the traditional style of output block and any differences between the two styles are described in Section 3.7.9.

What the code should output and when it should output it is specified in the "output" block of the input deck. An example output block is shown below:

output block
```
begin:output
   # If use_offset_grid is true then the code dumps a grid which
   # displays positions relative to the left hand edge of the window
   use_offset_grid = F
   # number of timesteps between output dumps
   dt_snapshot = 1.0e-14
   # Number of dt_snapshot between full dumps
   full_dump_every = 10
```

```
  restart_dump_every = -1
  force_final_to_be_restartable = T

  # Properties at particle positions
  particles = never
  px = never
  py = never
  pz = never
  vx = never
  vy = never
  vz = never
  charge = never
  mass = never
  particle_weight = never

  # Properties on grid
  grid = always
  ex = always
  ey = always
  ez = always
  bx = always
  by = always
  bz = always
  jx = always
  jy = always
  ekbar = always + species
  mass_density = never + species
  charge_density = always
  number_density = always + species
  temperature = always + species

  distribution_functions = always
  particle_probes = never
end:output
```

There are three types of output dump in EPOCH which are used for different purposes. These types are:

- normal - The most frequent type of output dump in EPOCH is a normal dump.
- full - A full dump is usually written every 10 or so normal dumps. A full dump contains all the data that a normal dump contains and should also contain any information which is needed only infrequently, whether this is the full particle information or a large distribution function. It is possible to turn off full dumps completely.
- restart - A restart dump is a dump where the code guarantees to write enough data to allow the code to restart from the output. Output dumps are guaranteed to contain all the information in a normal dump and, if they coincide with the timing for a full dump, will also contain the full dump information.

Information will never be written into a file twice, even if two conditions for it being written are satisfied (i.e even if px should be dumped both because it is a full dump and a restart dump, px will only be written once).

Note that these dump levels only really make sense for the traditional style of output block and are not really required when the new style is used.

3.7.1 Dumpmask

When specifying which type of output dump to write a variable to there are eight options which can be specified for each variable and can be combined by addition. Some combinations make no sense but are formally valid. The first four options specify at which output types the variable is to be dumped:

never - If the variable is not a required restart variable then it will never be written. If it is a required restart variable then it will be written only at restart dumps.

full - This variable will be written at full dumps only.

always - This variable will be written at full, normal and restart dumps.

restart - This variable will be written at restart dumps only. Note that variables required for restarting the code are always written to restart dumps. This flag is to enable the writing of additional variables into such dump files.

For grid variables derived from summing over particles (ie. "ekbar", "mass_density", "charge_density", "number_density", "temperature") the following two parameters also apply.

species - The derived variable should be output on a species by species basis. It is combined with a dumpmask code by addition as in:
`charge_density = always + species`.

no_sum - The output for this derived variable should not be summed over all species. By default, derived variables are summed over all species. If you don't want to include this sum, you must use the "no_sum" flag. It is combined with a dumpmask code by addition as in:
`charge_density = always + species + no_sum`.

Most grid variables may be averaged over time. A more detailed description of this is given in Section 3.7.7. Data averaging is specified using the following dumpmask parameters.

average - The output for this variable should be averaged over time. The time span over which the variable will be averaged is controlled using flags described in Section 3.7.2.

snapshot - By default, the "average" parameter replaces the variable with an averaged version of the data. Adding this flag specifies that the non-averaged variable should also be dumped to file.

When applied to a variable, these codes are referred to as a dumpmask.

3.7.2 Directives

The first set of options control the type and frequency of output dumps. They are used as follows

disabled - Logical flag. If this is set to "T" then the block is ignored and never generates any output. The default value is "F".

dt_snapshot - Sets the interval between normal output dumps in simulation seconds. Setting zero or negative means that the code will output every step of the core solver. The code does NOT guarantee that outputs will be exactly dt_snapshot apart, what is guaranteed is that the next output will be after the first iteration which takes the simulation to a time $\geq$ **dt_snapshot** from the last output. As with other variables which specify a unit of time, it can be specified in more convenient unit by using a multiplication factor (see Section 3.15.1). For example, "dt_snapshot = 5 * femto" will set it to be 5 femtoseconds. The default value is a large number which will never trigger an output.

nstep_snapshot - Sets the number of timesteps between normal output dumps. Setting zero or negative means that the code will output every step of the core solver. If **dt_snapshot** is also specified then both conditions are considered and output will be generated when either condition is met. The default value is a large integer which will never trigger an output.

full_dump_every - The number of normal output dumps between full output dumps. Setting to zero makes every dump a full dump. Setting to a negative number stops the code from producing any full dumps. This is the default.

restart_dump_every - The number of normal output dumps between restart dumps. Setting to zero makes every dump a restart dump. Setting to a negative number stops the code from producing any restart dumps. This is the default.

force_first_to_be_restartable - Logical flag which determines whether the file written at time zero is a restart dump. The default value is "F".

force_last_to_be_restartable - Force the code to override other output settings and make the last output dump it writes be a restart dump. Any internal condition which causes the code to terminate will make the code write a restart dump, but code crashes or scheduler terminations will not cause the code to write a restart dump. "force_final_to_be_restartable" is accepted as a synonym. The default value is "T".

dump_first - Logical flag which determines whether to write an output file immediately after initialising the simulation. The default is "T".

dump_last - Logical flag which determines whether to write an output file just before ending the simulation. The default is "T" if an output block exists in the input deck and "F" otherwise. "dump_final" is accepted as a synonym.

time_start - Floating point parameter which specifies the simulation time at which to start considering output for the block. Note that if "dump_first" or "dump_last" are set to true for this block then dumps will occur at the first or last timestep regardless of the value of the **time_start** parameter. This also applies to the three following parameters. The default value is 0.

time_stop - Floating point parameter which specifies the simulation time at which to stop considering output for the block. The default value is the largest possible float.

nstep_start - Integer parameter which specifies the step number at which to start considering output for the block. The default value is 0.

nstep_stop - Integer parameter which specifies the step number at which to stop considering output for the block. The default value is the largest possible integer.

dump_cycle - If this is set to a positive integer then the output file number will be reset to zero after the specified cycle number is reached. eg. if "dump_cycle = 2" then the sequence of output dumps will be 0000.sdf, 0001.sdf, 0002.sdf, 0000.sdf, 0001.sdf, etc. The default is 0, so dump cycling never occurs.

dump_cycle_first_index - If this is set to a positive integer then the value is used as the first index to use when cycling output dumps due to the "dump_cycle" parameter. For example, if "dump_cycle = 2" and "dump_cycle_first_index = 1" then the sequence of output dumps will be 0000.sdf, 0001.sdf, 0002.sdf, 0001.sdf, 0002.sdf, 0001.sdf, etc. The default is 0.

dump_source_code - EPOCH has the ability to write its own source code into restart dumps. This is generated at compile time and embedded into the binary and so is guaranteed to match that corresponding to the running code. EPOCH comes with a script called unpack_source_from_restart which can be used to unpack the source code from a restart dump. To use this script, just type

```
unpack_source_from_restart <sdf_filename>
```

at the command-line. If this logical flag is set to false then the feature will be disabled. The default value is "T".

dump_input_decks - If this logical flag is set to true then a copy of the input decks for the currently running simulation is written into the restart dumps. The default value is "T".

dt_average - When averaged variables are being output to file, this parameter specifies the simulation time period over which averaging is to occur. "averaging_period" is accepted as a synonym.

nstep_average - When averaged variables are being output to file, this parameter specifies the number of time steps over which averaging is to occur. "min_cycles_per_average" is accepted as a synonym. If both dt_average and nstep_average are specified, the code will use the one which gives the longest simulation time-span.

use_offset_grid - When using moving windows some visualisation programs (notably VisIt) show the motion of the window by moving the visualisation window rather than by changing the x-axis. Setting this option to "T" causes the code to write another grid which always gives the offset relative to the left hand edge of the window rather than the true origin. Performs no function when not using the moving window. The default value is "F".

filesystem - String parameter. Some filesystems can be unreliable when performing parallel I/O. Often this is fixable by prefixing the filename with 'ufs' or 'nfs'. This parameter supplies the prefix to be used. The default value is an empty string.

file_prefix - Although this parameter is supported by the traditional style of output block, its primary purpose is for use with multiple output blocks so it is documented in Section 3.7.9.

A few additional parameters have been added for use with the new style of output block. These are documented in Section 3.7.9.

3.7.3 Particle Variables

The next set are per particle properties. If you wish to plot these according to their spatial positions, you must include the "particle_grid" in your output variables. All entries have a default dumpmask of "never".

particle_grid - Requests the output of particle positions. This is a restart variable. No particle variables can be plotted in VisIt unless this is dumped. If any particle variables are written then the "particle_grid" is automatically written unless "particle_grid = never" is specified. The synonym "particles" may also be used.

px, py, pz - The dumpmasks for the particle momenta. Restart variable.

vx, vy, vz - The dumpmasks for the particle velocities.

charge - The dumpmask for the charge of a given particle. This has no effect if the code is not compiled with the flag "-DPER_PARTICLE_CHARGE_MASS" (see Section 2.4).

mass - The dumpmask for the mass of a given particles. This has no effect if the code is not compiled with the flag "-DPER_PARTICLE_CHARGE_MASS" (see Section 2.4). The synonym "rest_mass" may also be used.

particle_weight - The dumpmask for the weighting function which describes how many real particles each pseudoparticle represents. Restart variable.

ejected_particles - If requested then all the particles which have left the simulation domain since the last output dump of this type are included in the output. The list of ejected particles is treated as if it were a separate species and the particle variables which get written are requested using the other particle variable flags (ie. "particle_grid", etc). Once the data has been written, the ejected particle lists are reset and will accumulate particles until the next requested output dump.

particle_energy - The dumpmask for per-particle kinetic energy.

relativistic_mass - The dumpmask for per-particle relativistic mass (ie. not rest mass).

gamma - The dumpmask for per-particle relativistic gamma (ie. $[1-(v/c)^2]^{-1/2}$).

optical_depth - The dumpmask for per-particle optical depth. Restart variable. This option is only supplied for debugging purposes and should not be required by most users.

trident_optical_depth - The dumpmask for per-particle optical depth used by the Trident model. Restart variable. This option is only supplied for debugging purposes and should not be required by most users.

qed_energy - The dumpmask for per-particle QED-related particle energy. Restart variable. This option is only supplied for debugging purposes and should not be required by most users.

id - Global particle ID. See below for details.

Particle IDs are useful if you want to track the progress of each particle throughout the simulation. Since they increase the size of each particle data structure, they are disabled by default and must be enabled using a compiler flag. The "PARTICLE_ID" flag will use an 8-byte integer to represent the ID and "PARTICLE_ID4" uses a 4-byte integer. They are written to file using the "id" flag.

Note: In the current implementation, the particle IDs are passed between processors and written to file using REAL numbers. This means that in double precision the maximum particle ID is $2^{53} \sim 10^{16}$. This should be ample for the foreseeable future. However, if the code is compiled for single precision then the maximum ID is $2^{24} = 16777216$. Probably not big enough.

3.7.4 Grid Variables

The next set of parameters specify properties which are defined on a regular cartesian mesh. All entries have a default dumpmask of "never".

grid - The dumpmask for the Cartesian grid which defines the locations of the grid variables. No grid variables can be plotted in VisIt unless this variable is output. If any grid variables are written then the "grid" is automatically written unless "grid = never" is specified. The synonym "field_grid" may also be used.

ex, ey, ez - The electric field vectors pointing in all three directions. Restart variables.

bx, by, bz - The magnetic field vectors pointing in all three directions. Restart variables. In 1D bx is a trivial variable because of the Solenoidal condition. It is included simply for symmetry with higher dimension codes.

jx, jy, jz - The current densities pointing in all three directions. Restart variables.

3.7.5 Derived Variables

The final set of parameters specify properties which are not variables used in the code but are derived from them. The first six variables are derived by summing properties of all the particles in each grid cell. The resulting quantities are defined on the regular cartesian mesh used for grid variables. All entries have a default dumpmask of "never".

ekbar - Mean kinetic energy on grid. Can have species dumpmask.

ekflux - Mean kinetic energy flux in each direction on the grid. Can have species dumpmask.

mass_density - Mass density on grid. Can have species dumpmask.

charge_density - Charge density on grid. Can have species dumpmask.

number_density - Number density on grid. Can have species dumpmask.

temperature - Isotropic temperature on grid. Can have species dumpmask.

poynt_flux - Poynting flux in each direction.

3.7.6 Other Variables

distribution_functions - Dumpmask for outputting distribution functions specified in the input deck. Each individual distribution function can have its own dumpmask and these will be applied after the value of "distribution_functions" has been considered. For example, if the output block contains "distribution_functions = full" and the dist_fn block (see Section 3.9) contains "dumpmask = always" then the distribution function will only be output at full dumps.

particle_probes - Dumpmask for outputting particle probes specified in the input deck. Each individual particle probe can have its own dumpmask and these will be applied after the value of "particle_probes" has been considered. For example, if the output block contains "particle_probes = always" and the dist_fn block contains "dumpmask = full" then the particle probe will only be output at full dumps.

absorption - This is a two-valued output variable. It accepts a dumpmask in the same manner as other output variables. When selected, two numbers will be calculated and written to file:

1. "Absorption/Laser_enTotal" - The total amount of energy injected into the simulation by laser boundaries.
2. "Absorption/Abs_frac" - The fraction of the total laser energy being absorbed by the open boundaries.

total_energy_sum - This is also a two-valued output variable. It accepts a dumpmask in the same manner as other output variables. When selected, the following two numbers will be calculated and written to file:

1. "Total Particle Energy in Simulation (J)"
2. "Total Field Energy in Simulation (J)"

3.7.7 Data Averaging

EPOCH can accumulate an average value for field variables to be written to output dumps. These may be requested by using the "average" keyword when specifying a dump variable. The non-averaged variable will still be written to restart dumps where required for restarting the code but not full or normal dumps. If you also want the non-averaged variable to be written then you can add the "snapshot" option.

The period of time over which averaging occurs can be specified using the "dt_average" keyword. Alternatively, you may specify the number of cycles over which to perform the averaging using the "nstep_average" keyword. If both "dt_average" and "nstep_average" are specified then the averaging will be performed over the longest of the two intervals.

Note that previous versions of the code would alter the time step to ensure that there were enough cycles between output dumps to satisfy the "nstep_average" parameter. However, since it affects the accuracy of the result, this is no longer the case and only a warning message is issued.

The following shows an example use of averaging in the output block.

```
begin:output
   dt_snapshot = 1.0e-15
   full_dump_every = 10
   dt_average = 1.0e-17

   charge_density = always + average + snapshot
   mass_density = full + average + snapshot
   ekbar = full + average
end:output
```

With this configuration, "charge_density" will be written in both normal and averaged form at normal, full and restart dumps. "mass_density" will be written in both forms at full dumps. Only the average value of "ekbar" will be written at full dumps.

Only field and derived variables can be averaged currently in EPOCH. Particle properties, distribution functions and particle probes cannot currently be averaged.

3.7.8 Single-precision output

By default, EPOCH is compiled and run using double precision arithmetic. This is the only method which has been fully tested and the method that we recommend to other users of the code. However, this also means that data files can get very large.

To avoid this problem, it is possible to run the code in double precision but convert the data to single precision when writing to disk. This is done by adding the "single" field the the dumpmask of an output variable. It can be specified on a per-variable basis.

```
begin:output
   dt_snapshot = 8 * femto

   grid = always
   ex = always
   ey = always + single
end:output
```

In this example, the grid variable "ex" will be written as a double precision array and "ey" will be converted to single precision.

Dumping variable averages adds an extra field variable for each average requested. These take up memory during runtime but do not influence the simulation behaviour in any way. For this reason, if the average is to be written out in single precision then it may as well be stored in a single precision variable. This behaviour can be requested using the "average_single" dumpmask flag.

3.7.9 Multiple output blocks

In more recent versions of EPOCH, it is now possible to have multiple "output" blocks in the input deck, each with their own "dt_snapshot" or "nstep_snapshot" and their own set of output variables.

The syntax remains the same as the original "output" block syntax with the addition of "name" and "restartable" fields.

The "name" field specifies the file name to use for the output list. Each time EPOCH generates an output dump, it writes an entry into the file "`<name>.visit`". This can be used to find all the output dumps of a specific output block. It is named with a ".visit" suffix to enable its use as a file grouping list in the VisIt data analysis tool, but it is just a plain text file so it can equally be used by any other program.

If two output blocks are written at the same time, the output will be combined into a single file.

The "restartable" field specifies that the output block should generate output dumps containing all the information necessary to restart a simulation.

The following parameters are supported by the new style of output block in addition to those for the traditional style:

name - Identifies the output block with a name which is required when multiple output blocks are used.

restartable - Specifies whether or not the output for this block is a restartable dump.

dump_at_times - Floating point parameter which specifies a set of simulation times at which to write the current output block. This can only be used with named output blocks. The values are given as a comma separated list. eg. "dump_at_time = 0, 0.15, 1.1". The name "times_dump" is accepted as a synonym. By default the list is empty.

dump_at_nsteps - Integer parameter which specifies a set of step numbers at which to write the current output block. This can only be used with named output blocks. The values are given as a comma separated list. eg. "dump_at_nsteps = 5, 11, 15". The name "nsteps_dump" is accepted as a synonym. By default the list is empty.

file_prefix - String parameter. It is sometimes useful to distinguish between dumps generated by the different output blocks. This parameter allows the user to supply a file prefix to be prepended to all dumps generated by the current output block. See below for further details. The default value is an empty string.

rolling_restart - Logical flag. If set to "T", this sets the parameters required for performing rolling restarts on the current block. It is a shorthand for setting the following flags: "dump_cycle = 1", "restartable = T" and "file_prefix = roll". With rolling restarts enabled the first file will be named "roll0000.sdf" and the second will be "roll0001.sdf". The third dump will again be named "roll0000.sdf", overwriting the first one. In this way, restart dumps can be generated throughout the duration of the simulation whilst limiting the amount of disk space used.

The following parameters cannot be used in conjunction with the new style of output block:

- full_dump_every
- restart_dump_every
- force_first_to_be_restartable
- force_last_to_be_restartable
- use_offset_grid

The "file_prefix" parameter warrants some further discussion. This parameter prepends the given prefix to all files generated by the output block in which it is specified. For example, if "file_prefix = aa" is set then files generated by the output block will be named "aa0000.sdf", etc. instead of just "0000.sdf".

This also allows different variables to different files at the same time step. For example, here are two output blocks which do not use file prefixes:

```
begin:output
   name = o1
   nstep_snapshot = 1
   charge_density = always
end:output

begin:output
   name = o2
   dump_at_nsteps = 10
   restartable = T
end:output
```

With this input deck, we want to have the "charge_density" derived variable at every snapshot and then periodically write a restart dump. The problem is that the dump file "0010.sdf" contains both the restart information and the "charge_density" variable. At the end of the run we can't just delete the large restart dumps without losing the smaller variables at that time step.

With the new version we would add a prefix to one or both blocks:

```
begin:output
   name = o1
   file_prefix = small
   nstep_snapshot = 1
   charge_density = always
end:output

begin:output
   name = o2
   nstep_snapshot = 10
   restartable = T
end:output
```

Now the "charge_density" will be written to "small0000.sdf", etc. At step 10, two files will be written: "small0010.sdf" containing just the charge_density and "0000.sdf" containing all the restart variables.

Note that some care must be taken, since if the same variable is in the output block for multiple file prefixes then multiple copies will be written to file. This obviously uses more disk space and is more time consuming than necessary.

It should also be noted that if multiple output blocks use the same file stem then their output will be combined. eg:

```
begin:output
   name = o1
   file_prefix = a
   dump_at_nsteps = 2,4
   ex = always
end:output

begin:output
   name = o2
   file_prefix = a
   dump_at_nsteps = 3,4
   ey = always
end:output

begin:output
   name = o3
   file_prefix = b
   dump_at_nsteps = 4
   ez = always
end:output
```

In this example, at step 2 a0000.sdf contains ex, step 3 a0001.sdf contains ey, step 4 a0002.sdf contains ex, ey and b0000.sdf contains ez.

3.8 output_global block

With the introduction of multiple output blocks, there are now a few parameters that only make sense to be applied globally across all output blocks. To accommodate this, a new block named "output_global" has been added. Most of the parameters accepted by this block have the same meaning as those in the "output" block except that they are applied to all "output" blocks.

The parameters that can be specified in the "output_global" block are as follows:

force_first_to_be_restartable - Logical flag which determines whether the file written at time zero is a restart dump. The default value is "F".

force_last_to_be_restartable - Force the code to override other output settings and make the last output dump it writes be a restart dump. Any internal condition which causes the code to terminate will make the code write a restart dump, but code crashes or scheduler terminations will not cause the code to write a restart dump. "force_final_to_be_restartable" is accepted as a synonym. The default value is “T”.

dump_first - Logical flag which determines whether to write an output file immediately after initialising the simulation. The default is “F”.

dump_last - Logical flag which determines whether to write an output file just before ending the simulation. The default is “T” if an output block exists in the input deck and “F” otherwise. “dump_final” is accepted as a synonym.

time_start - Floating point parameter which specifies the simulation time at which to start considering output for the block. Note that if “dump_first” or “dump_last” are set to true for this block then dumps will occur at the first or last timestep regardless of the value of this parameter. This also applies to the three following parameters. The default value is 0.

time_stop - Floating point parameter which specifies the simulation time at which to stop considering output for the block. The default value is the largest possible float.

nstep_start - Integer parameter which specifies the step number at which to start considering output for the block. The default value is 0.

nstep_stop - Integer parameter which specifies the step number at which to stop considering output for the block. The default value is the largest possible integer.

sdf_buffer_size - Integer parameter. When writing particle data to an SDF file, the data is first transferred into an output buffer. The size of this buffer can have a big impact on the overall speed of writing dump files. This parameter allows the size of the buffer to be specified in bytes. The default value is 67108864 (64 MB).

filesystem - String parameter. Some filesystems can be unreliable when performing parallel I/O. Often this is fixable by prefixing the filename with ‘ufs’ or ‘nfs’. This parameter supplies the prefix to be used. The default value is an empty string.

use_offset_grid - When using moving windows some visualisation programs (notably VisIt) show the motion of the window by moving the visualisation window rather than by changing the x-axis. Setting this option to “T” causes the code to write another grid which always gives the offset relative to the left hand edge of the window rather than the true origin. Performs no function when not using the moving window. The default value is “F”.

3.9 dist_fn block

Sometimes it is useful to reconstruct part of the full phase space for one or more particle species. This functionality is provided through a dist_fn block. The distribution function is integrated over all dimensions which are not axes of the distribution function.

Calculating distribution functions requires some degree of integration of data leading to various possible ways of normalising the resulting distribution function. In EPOCH, distribution functions are normalised so that the value at every point of the distribution function is the number of particles within that cell of the distribution function, ignoring all phase space directions which are not considered as an axis of the distribution function. Summing the distribution function should give the total number of real particles (as opposed to computational pseudoparticles) in the simulation.

An example dist_fn block is given below:

dist_fn block

```
begin:dist_fn
   name = x_px
   ndims = 2
   dumpmask = always

   direction1 = dir_x
   direction2 = dir_px

   # range is ignored for spatial coordinates
   range1 = (1,1)
   range2 = (-50.0e-20,50.0e-20)

   # resolution is ignored for spatial coordinates
   resolution1 = 1
   resolution2 = 5000

   restrict_py = (-3.0e-20,3.0e-20)

   include_species:Electron
   include_species:Carbon
end:dist_fn
```

name - The name of the distribution function when it is output. This name is appended with the name of each species for which the data is output and so, for example, when applied to a species named carbon the output is called **x_px_Carbon**. The Cartesian grid which describes the axes of the distribution function would then be called **grid_x_px_Carbon**.

ndims - The number of dimensions in this phase space reconstruction. Due to difficulties in visualising data in more than three dimensions, this is restricted to being 1, 2 or 3.

dumpmask - Determines which output dumps will include this distribution function. The dumpmask has the same semantics as those used by variables in the "output" block, described in Section 3.7. The dumpmask from "distribution_functions" in the output block is applied first and then this one is applied afterwards. For example, if the dist_fn block contains "dumpmask = full" and the output block contains "distribution_functions = always" then this distribution function will be only be dumped at full dumps. The default dumpmask is "always".

direction*n* - This is the phase space to sample along axis **n**. This can be any one of: dir_x, dir_y, dir_z, dir_px, dir_py, dir_pz, dir_en, dir_gamma_m1, dir_xy_angle, dir_yz_angle, dir_zx_angle with spatial codes only being available in dimensionalities of the code which have that direction. Therefore dir_z does not exist in EPOCH1D or EPOCH2D and dir_y does not exist in EPOCH1D.

The flags "dir_xy_angle", "dir_yz_angle" and "dir_zx_angle" calculate the distribution of particle momentum directions in the X-Y, Y-Z and Z-X planes.

range*n* - The range between which this axis should run. This is in the form of (minimum, maximum). Any particle which exceeds the range is ignored. In the current version of EPOCH, the "range$n$" parameter is ignored when applied to a spatial direction. For momentum directions this parameter is specified in $kg\ ms^{-1}$. If the range of a momentum direction is set so that the maximum and the minimum are equal then the code will automatically set the range to exactly span the range of particle momenta at the point of writing the dump.

NOTE: Currently the range parameters have to be simple floating point numbers and NOT maths parser expressions.

resolutionn - The number of gridpoints in a given direction. Once again this is ignored for spatial dimensions where the resolution is always the same as the resolution of the underlying simulation.

include_species - Specifies a species which should be included in the output. This is useful since it is rare that momentum limits are appropriate for both electrons and ions, so usually for a given dist_fn block only electrons or ions are considered. It is possible to have two dist_fn blocks with the same name but different momentum ranges and different include_species settings produce the effect of a single diagnostic for all species in the output file.

restrict_{x,y,z,px,py,pz} - Restrictions are specified in the same way as ranges, but have a subtly different behaviour. Ranges specify the range of a visible axis on the resulting distribution function, whereas restrictions allow you to specify minimum and maximum values for each spatial and momentum direction and use only particles which fall within this range when calculating the distribution function. Restrictions can be specified even for properties which are not being used as axes. It is possible to set a restriction that is more restrictive than the range applied. This is not trapped as an error and such parts of the distribution function are guaranteed to be empty. The available spatial restrictions depend on the dimensionality of the code. Therefore, attempting to set restrict_z in EPOCH1D will produce a warning.

At present, the code to calculate the distribution functions has one limitation: it ignores particle shape functions when calculating properties on the spatial axis, meaning that the result is less smooth than normal properties from the code.

3.10 probe block

Sometimes it is useful to consider all the properties of particle which pass through a point/line/plane (depending on dimension) in the simulation. To allow this, it is possible to specify one or more *Particle Probe* blocks in the input deck. These record copies of all particles which cross a point/line/plane in a given direction which meet minimum and maximum kinetic energy criteria and output the particle properties into the normal output files. Particle probes record the positions, momenta and weight of all particles passing through the plane. To use particle probes, the code must be compiled with the `-DPARTICLE_PROBES` compiler option. This is a fairly heavyweight diagnostic since each particle position must be tested from within the particle push. The code will run faster if it is not compiled in.

The probe is specified in terms of a point in the plane and the normal vector to the plane which is to be monitored. Particles are only recorded if they cross the plane in the direction given by the normal vector. If you want to record particles travelling in both directions then use two particle probes, one with an opposite signed normal vector to the other.

```
begin:probe
   name = electron_back_probe

   point = (50.0e-6, -50.0e-6)
   normal = (1.0, 0.0)

   ek_min = 0.0
   ek_max = -1.0
   include_species:s1

   dumpmask = always
end:probe
```

name - The name that the probe should have in output dumps. Output variables are then named this as a prefix. For example, the block shown above will result in the name **`electron_back_probe_px`** for the x momentum. The particle positions would just be called **`electron_back_probe`**.

point - An arbitrary point in the plane of the probe.

normal - A vector normal to the plane of the probe, in the direction of crossings you wish to monitor.

include_species - The species to which this probe should be applied. To probe several species, use several probe blocks in the input deck. "probe_species" is accepted as a synonym.

ek_min - The minimum kinetic energy of particles to store information about. Set to 0 for no minimum kinetic energy.

ek_max - The maximum kinetic energy of particles to store information about. Set to -1 for no maximum kinetic energy.

dumpmask - The dump code for this particle probe. This is the same as that for the main output controls in **`input.deck`**. Note that the code has to store copies of particles which pass through the probe until a dump occurs. This means that the code's memory requirements can increase drastically if this code only dumps probe information infrequently. If this is set to **`never`** then the code effectively never uses the probe.

3.11 collisions block

EPOCH has a particle collision routine based on the model presented by Sentoku and Kemp [6]. This adds a new output block named "collisions" which accepts the following three parameters.

use_collisions - This is a logical flag which determines whether or not to call the collision routine. If omitted, the default is "T" if any of the frequency factors are non-zero (see below) and "F" otherwise.

coulomb_log - This may either be set to a real value, specifying the Coulomb logarithm to use when scattering the particles or to the special value "auto". If "auto" is used then the routine will calculate a value based on the local temperature and density of the particle species being scattered, along with the two particle charges. If omitted, the default value is "auto".

collide - This sets up a symmetric square matrix of size nspecies × nspecies containing the collision frequency factors to use between particle species. The element (s1,s2) gives the frequency factor used when colliding species s1 with species s2. If the factor is less than zero, no collisions are performed. If it is equal to one, collisions are performed normally. For any value between zero and one, the collisions are performed using a frequency multiplied by the given factor.
If "collide" has a value of "all" then all elements of the matrix are set to one. If it has a value of "none" then all elements are set to minus one.
If the syntax "species1 species2 <value>" is used, then the (species1,species2) element of the matrix is set to the factor "<value>". This may either be a real number, or the special value "on" or "off". The "collide" parameter may be used multiple times.
The default value is "all" (ie. all elements of the matrix are set to one).

collisional_ionisation - If this logical flag is set to "T" then the collisional ionisation model is enabled. This process is independent of **field_ionisation** (Section 3.3.2). However, in order to set up **collisional_ionisation** you must also specify ionisation energies and electrons in a **species** block (see Section 3.3.2). The default value is "F".

For example:

```
collisions
begin:collisions
   use_collisions = T
   coulomb_log = auto
   collide = all
   collide = spec1 spec2 off
   collide = spec2 spec3 0.1
end:collisions
```

With this block, collisions are turned on and the Coulomb logarithm is automatically calculated. All values of the frequency array are set to one except (spec1,spec2) is set to minus one (and also (spec2,spec1)) and (spec2,spec3) is set to 0.1

3.12 qed block

EPOCH can model QED pair production, synchrotron emission and radiation reaction as described in Duclous et al. [7]. It is enabled using the compiler flag "-DPHOTONS". Additionally, the Trident process is enabled using "-DTRIDENT_PHOTONS".
A new input deck block named "qed" has been added which accepts the following parameters:

use_qed - Logical flag which turns QED on or off. The default is "F".

qed_start_time - Floating point value specifying the time after which QED effects should be turned on. The default is 0.

produce_photons - Logical flag which specifies whether to track the photons generated by synchrotron emission. If this is "F" then the radiation reaction force is calculated but the properties of the emitted photons are not tracked. The default is "F".

photon_energy_min - Minimum energy of produced photons. Radiation reaction is calculated for photons of all energies, but photons with energy below this cutoff are not tracked. The default is 0.

photon_dynamics - Logical flag which specifies whether to push photons. If "F" then photons are generated, but their motion through the domain is not simulated and they stay where they were generated. The default is “F”.

produce_pairs - Logical flag which determines whether or not to simulate the process of pair generation from gamma ray photons. Both produce_photons and photon_dynamics must be “T” for this to work. The default is “F”.

qed_table_location - EPOCH’s QED routines use lookup tables to calculate gamma ray emission and pair production. If you want to use tables in a different location from the default, specify the new location using this parameter. The default is “src/physics_packages/TABLES”.

use_radiation_reaction - Logical flag which determines whether or not to calculate the radiation reaction force. If set to “F” then the force is not calculated. This should nearly always be enabled when using the QED model. It is only provided for testing purposes. The default value is “T”.

QED also requires that the code now know which species are electrons, positrons and photons. The species type is specified using a single “identify” tag in a species block. To specify an electron the block in the deck would look like

```
begin:species
   name = electron
   frac = 0.5
   rho = 7.7e29
   identify:electron
end:species
```

Once the identity of a species is set then the code automatically assigns mass and charge states for the species. Possible identities are:

electron - A normal electron species. All species of electrons in the simulation must be identified in this way or they will not generate photons.

positron - A normal positron species. All species of positron in the simulation must be identified in this way or they will not generate photons.

photon - A normal photon species. One species of this type is needed for photon production to work. If multiple species are present then generated photons will appear in the first species of this type.

bw_electron - The electron species for pair production by the Breit-Wheeler process. If a species of this type exists then electrons from the pair production module will be created in this species. If no species of this type is specified then pair electrons will be generated in the first electron species.

bw_positron - As above but for positrons.

trident_electron - The electron species for pair production by the Trident process. If a species of this type exists then electrons from the pair production module will be created in this species. If no species of this type is specified then pair electrons will be generated in the first electron species.

trident_positron - As above but for positrons.

proton - A normal proton species. This is for convenience only and is not required by the pair production routines.

A species should be identified only once, so a "bw_electron" species does not need to also be identified as an "electron" species. If the code is running with "produce_photons=T" then a photon species must be created by the user and identified. If the code is running with "produce_pairs=T" then the code must specify at least one electron (or bw_electron) species and one positron (or bw_positron) species. These species will usually be defined with zero particles from the start of the simulation and will accumulate particles as the simulation progresses. The code will fail to run if the needed species are not specified.

The basic input deck has now been considered fully but it is possible for an end user to add new blocks to the input deck As a result, a version of the code which you have obtained from a source other than CCPForge may include other input deck blocks. These should be described in additional documentation provided with the version of the code that you have.

3.13 subset block

It is possible to restrict the number of particles written to file according to various criteria. For example, you can now output the momentum of all particles which have a gamma lower than 1.8 or the positions of a randomly chosen subset of a given species.

A new input deck block named "subset" is defined which accepts the following parameters:

name - The name given to this subset. This is used to identify the subset in the output block and is also used when labelling the data in the SDF files.

include_species - Add the given particle species to the set of particles that this subset applies to. By default, no particle species are included.

dumpmask - The dumpmask to use when considering this subset in an output block. This takes the same form as the output block dumpmask. The default value is "always".

random_fraction - Select a random percentage of the particle species. This is a real value between zero and one. If 0 is specified, no particles are selected. If 1 is specified, all the particles are selected. If 0.2 is specified, 20% of the particles are selected.

{px,py,pz,weight,charge,mass,gamma}_min - Select only the particles with momentum, weight, charge, mass or gamma which is greater than the given value.

{px,py,pz,weight,charge,mass,gamma}_max - Select only the particles with momentum, weight, charge, mass or gamma which is less than the given value.

{x,y,z}_min - Select only the particles whose position lies above the given value.

{x,y,z}_max - Select only the particles whose position lies below the given value.

id_min,max - Select only the particles whose "id" is greater than or less than the given values. The "id" field is explained below.

Once a subset has been defined, the subset name can then be used in place of (or in addition to) the dumpmask in an "output" block. For example:

```
begin:subset
   name = background
   random_fraction = 0.1
   include_species:electron
   include_species:proton
end:subset

begin:subset
   name = high_gamma
   gamma_min = 1.3
   include_species:electron
end:subset

begin:output
   particles = background + high_gamma + always
   px = background + high_gamma
   py = background
   pz = always
end:output
```

In this example, three "px" blocks will be written: "Particles/background/electron/Px", "Particles/background/proton/Px" and "Particles/high_gamma/electron/Px". The "background" blocks will contain 10% of the each species, randomly selected. The "high_gamma" block will contain all the electrons with a gamma greater than 1.3.

There will also be "Particles/background/electron/Py" and "Particles/background/proton/Py" block containing y-momentum for the same 10% random subset of particles. Finally, the "Particles/All/electron/Pz" and "Particles/All/proton/Pz" will contain the z-momentum for all particles.

The final selection criteria given in the list above is "id_min" and "id_max". As of EPOCH version 4.0, the code can now assign a unique ID field to every particle in the simulation. This can be useful for tracking specific particles as they move through a simulation. As this field adds extra memory requirements to the particles, it is disabled by default and must be compiled in using the "-DPARTICLE_ID" compiler flag.

Particle IDs can be written to file using the "id" variable name in the "output" block. Eg.

```
begin:output
   particles = always
   id = always
end:output
```

3.14 constant block

The constant block type helps to make the input deck more flexible and maintainable. It allows you to define constants and maths parser expressions (see Section 3.15) which can be used by name later in the deck.

Constants are simply maths parser expressions which are assigned to a name as shown above. When the name is used on the right hand side of a deck expression it is replaced by the expression it was assigned with. This expression may be a simple numerical constant, a mathematical expression or a function. Constants may contain spatially varying information without having to pre-calculate them at every location in the domain. To those familiar with FORTRAN codes which use statement functions, parameters appearing in the “constant” block are fairly similar.

If a constant name is reused in a constant block then the old constant is deleted and replaced with the new one. This happens without warning.

constant block

```
begin:constant
   lambda = 1.06 * micron
   omega = 2.0*pi*c/lambda
   den_crit = critical(omega)
   scale = 3.5 * micron
   den_max = 5.0*den_crit
   thick = 300e-9
   pplength = 6000e-9
   widscale = 5.0e-6

   t_wid = (10.0e-6)/c
   amax = 1.0
   wy = 1e-6
   y = 0.0

   slope = exp(-2.0*(y/wy)^2)
   blob = gauss(sqrt(x^2+y^2),0.0,1.0e-6)
end:constant
```

Using constants can be very helpful when dealing with long, complicated expressions since they allow the expression to be broken down into much simpler parts. They can also be used to get around the FORTRAN string length limitation built into many compilers which prevents deck lines being longer then 512 characters long. As a general rule, it is a good idea to break down complicated expressions using constants or by other means, in order to make the deck look more readable.

Constants are persistent for the entire runtime of the code, allowing them to be used when specifying time profiles for lasers, and also allowing developers to use maths parser expressions for other internal parts of the code where needed.

In the above example, several pre-defined constants have been used (**pi** and **c**) and also several functions (**critical**, **exp**, **gauss** and **sqrt**). These are described in Section 3.15.1 and Section 3.15.2.

3.15 The maths parser

A discussion of the input deck for EPOCH would not be complete without consideration of the maths parser. The maths parser is the code which reads the input decks. The parser makes it possible that any parameter taking a numerical value (integer or real) can be input as a mathematical expression rather than as a numerical constant. The maths parser is fairly extensive and includes a range of mathematical functions, physical and simulation constants and appropriately prioritised mathematical operators.

3.15.1 Constants

The maths parser in EPOCH has the following constants

- pi - The ratio of the circumference of a circle to its diameter.
- kb - Boltzmann’s constant.

- me - Mass of an electron.
- qe - Charge of an electron.
- c - Speed of light.
- epsilon0 - Permeability of free space.
- mu0 - Permittivity of free space.
- ev - Electronvolt.
- kev - Kilo-Electronvolt.
- mev - Mega-Electronvolt.
- micron - A convenience symbol for specifying wavelength in microns rather than metres.
- milli - 10^{-3}
- micro - 10^{-6}
- nano - 10^{-9}
- pico - 10^{-12}
- femto - 10^{-15}
- atto - 10^{-18}
- cc - A convenience symbol for converting from cubic metres to cubic centimetres (ie. 10^{-6})
- time - Initial simulation time.
- x,y,z - Grid coordinates in the x,y,z direction.
- ix,iy,iz - Grid index in the x,y,z direction.
- nx,ny,nz - Number of grid points in the x,y,z direction.
- dx,dy,dz - Grid spacing in the x,y,z direction.
- {x,y,z}_min - Grid coordinate of the minimum x,y,z boundary.
- {x,y,z}_max - Grid coordinate of the maximum x,y,z boundary.
- length_{x,y,z} - The length of the simulation box in the x,y,z direction.
- nproc_{x,y,z} - The number of processes in the x,y,z directions.
- nsteps - The number of timesteps requested.
- t_end - The end time of the simulation.

It is also possible for an end user to specify custom constants both within the code and from the input deck. These topics are covered later in this subsection. An example of using a constant would be:

```
length_x = pi
```

3.15.2 Functions

The maths parser in EPOCH has the following functions

- abs(a) - Absolute value.
- floor(a) - Convert real to integer rounding down.
- ceil(a) - Convert real to integer rounding up.
- nint(a) - Convert real to integer rounding to nearest integer.
- sqrt(a) - Square root.
- sin(a) - Sine.
- cos(a) - Cosine.
- tan(a) - Tangent.
- asin(a) - Arcsine.
- acos(a) - Arccosine.
- atan(a) - Arctangent.
- sinh(a) - Hyperbolic sine.
- cosh(a) - Hyperbolic cosine.
- tanh(a) - Hyperbolic tangent.
- exp(a) - Exponential.
- loge(a) - Natural logarithm.
- log10(a) - Base-10 logarithm.
- log_base(a,b) - Base-b logarithm.
- gauss(x, x_0, w) - Calculate a Gaussian profile in variable x centred on x_0 with a characteristic width w. $f(x) = \exp\left(-((x - x_0)/w)^2\right)$. In this expression the full width at half maximum is given by $fwhm = 2w\sqrt{\ln 2}$
- supergauss(x, x_0, w, n) - This is identical to "gauss" except it takes a fourth parameter, n, which is the power to raise the exponential argument to.
- semigauss(t, A, A_0, w) - Calculate a semi Gaussian profile in variable t with maximum amplitude A, amplitude at $t = 0$ A_0 and width w. The parameter A_0 is used to calculate t_0, the point at which the Gaussian reaches its maximum value. For t less than t_0 the profile is Gaussian and for t greater than t_0 it is the constant A.

$$t_0 = w\sqrt{-\ln\left(A_0/A\right)}$$

$$f(t) = \begin{cases} A\exp\left(-((t - t_0)/w)^2\right), & t < t_0 \\ A, & \text{otherwise} \end{cases}$$

- interpolate(interp_var,....,n_pairs) - Linear interpolation function, explained later.
- if(a,b,c) - Conditional function. If a != 0 the function returns b, otherwise the function returns c.

- density(a) - Returns the density for species a.
- temp_{x,y,z}(a) - Returns temperature in the x, y or z direction for species a.
- temp(a) - Returns the isotropic temperature for species a.
- e{x,y,z}(x,y,z) - Returns the x, y or z component of the electric field at the specified location.
- b{x,y,z}(x,y,z) - Returns the x, y or z component of the magnetic field at the specified location.
- critical(ω) - Returns the critical density for the given frequency ω. ie. $n_{crit}(\omega) = \omega^2 m_0 \epsilon_0 / e^2$

It is also possible for an end user to specify custom functions within the code. An example of using a function would be:

```
length_x = exp(pi)
```

The use of most of these functions is fairly simple, but "interpolate" requires some additional explanation. This function allows a user to specify a set of position,value pairs and have the code linearly interpolate the values between these control points. This function is mainly intended for ease of converting initial conditions from other existing PIC codes, and the same effect can usually be obtained more elegantly using the "if" command. The structure of the "interpolate" command is as follows: The first parameter is the variable which is to be used as the axis over which to interpolate the values. This can in general be any valid expression, but will normally just be a coordinate axis. The next 2n entries are the position,value pairs and the final parameter is the number of position,value pairs. The slightly clunky syntax of this command is unfortunately necessary to allow it to work with some fairly fundamental features of the maths parser used in EPOCH.

3.15.3 Operators

The maths parser in EPOCH allows the following operators

- a + b - Addition operator.
- a - b - Subtraction operator or unary negation operator (auto-detected).
- a * b - Multiplication operator.
- a / b - Division operator.
- a^b - Power raise operator.
- a e b - Power of ten operator (1.0e3 = 1000).
- a lt b - Less than operator. Returns 1 if a < b, otherwise returns 0. Intended for use with if.
- a gt b - Greater than operator. Returns 1 if a > b, otherwise returns 0.
- a eq b - Equality operator. Returns 1 if a == b, otherwise returns 0.
- a and b - Logical and operator. Returns 1 if a != 0 and b != 0, otherwise returns 0.
- a or b - Logical or operator. Returns 1 if a != 0 or b != 0, otherwise returns 0.

These follow the usual rules for operator precedence, although it is best to surround more complex expressions in parenthesis if the precedence is important. It is not possible at this time to specify custom operators without major changes to the code. An example of using an operator would be:

```
length_x = 10.0 + 12.0
```

4 EPOCH use in practice

4.1 Specifying initial conditions for particles using the input deck

If the initial conditions for the plasma you wish to model can be described by a number density and temperature profile on the underlying grid then EPOCH can create an appropriate particle distribution for you. The set of routines which accomplish this task are known as the autoloader. For many users, this functionality is sufficient to make use of the code and there is no need to deal with the internal representation of particles in EPOCH.

The autoloader randomly loads particles in space to reproduce the number density profile that was requested. It then sets the momentum components of the particles to approximate a Maxwell-Boltzmann distribution corresponding to the temperature profile. Sometimes this is not the desired behaviour, for example you may wish to model a bump-on-tail velocity distribution. It is currently not possible to specify these initial conditions from the input deck and the particles must be setup by modifying the source code.

There are two stages to the particle setup in EPOCH

- auto_load - This routine is called after reading and parsing the input deck. It takes care of allocating particles and setting up their initial positions and momenta using the initial conditions supplied in deck file. It is not necessary to recompile the code, or even have access to the source to change the initial conditions using this method.
- manual_load - Once particles have been allocated they can have their properties altered in this routine. By default it is an empty routine which does nothing.

4.1.1 Setting autoloader properties from the input deck

To illustrate using the autoloader in practice, we present an example for setting up an isolated plasma block in 2D. This would look like:

```
begin:species
   name = s1
   # first set density in the range 0->1
   # cut down density in x direction
   density = if ((x gt -1) and (x lt 1),1.0,0.2)
   # cut down density in y direction
   density = if ((y gt -1) and (y lt 1),density(s1),0.2)

   # multiply density by real particle density
   density = density(s1)*100.0

   # Set the temperature to be zero
   temp_x = 0.0
   temp_y = temp_x(s1)

   # Set the minimum density for this species
   density_min = 0.3*100.0
end:species

begin:species
   # Just copy the density for species s1
   density = density(s1)
   # Just copy the temperature from species s1
   temp_x = temp_x(s1)
   temp_y = temp_y(s1)

   # Set the minimum density for this species
   density_min = 0.3*100.0
end:species
```

An important point to notice is that the two parts of the logical expressions in the input deck are enclosed within their own brackets. This helps to remove some ambiguities in the functioning of the input deck parser. It is hoped that this will soon be fixed, but at present ALWAYS enclose logical expressions in brackets.

4.2 Manually overriding particle parameters set by the autoloader

Since not all problems in plasma physics can be described in terms of an initial distribution of thermal plasma, it is also possible to manually control properties of each individual pseudoparticle for an initial condition. This takes place in the subroutine **manual_load** in the file user_interaction/ic_module.f90. Manual loading takes place after all the autoloader phase, to allow manual tweaking of autoloader specified initial conditions.

4.2.1 EPOCH internal representation of particles

Before we can go about manipulating particle properties in **manual_load**, we first need an overview of how the particles are defined in EPOCH. Inside the code, particles are represented by a Fortran90 TYPE called "particle". The current definition of this type (in 2D) is:

```
  TYPE particle
    REAL(num), DIMENSION(3) :: part_p
    REAL(num), DIMENSION(c_ndims) :: part_pos
#ifdef PER_PARTICLE_WEIGHT
    REAL(num) :: weight
#endif
#ifdef PER_PARTICLE_CHARGE_MASS
    REAL(num) :: charge
    REAL(num) :: mass
#endif
    TYPE(particle), POINTER :: next, prev
#ifdef PARTICLE_DEBUG
    INTEGER :: processor
    INTEGER :: processor_at_t0
#endif
  END TYPE particle
```

Note the presence of the preprocessor directives, meaning that charge and mass only exist if the **-DPER_PARTICLE_CHARGE_MASS** define was put in the makefile. If you want to access a property that does not seem to be present, check the preprocessor defines.

The "particle" properties can be explained as follows:

- part_p - The momentum in 3 dimensions for the particle. This is always of size 3.
- part_pos - The position of the particle in space. This is of the same size as the dimensionality of the code.

- weight - The weight of this particle. The number of real particles represented by this pseudoparticle.
- charge - The particle charge. If the code was compiled without per particle charge, then the code uses the charge property from TYPE(particle_species).
- mass - The particle rest mass. If the code was compiled without per particle mass, then the code uses the mass property from TYPE(particle_species).
- next, prev - The next and previous particle in the linked list which represents the particles in the current species. This will be explained in more detail later.
- processor - The rank of the processor which currently holds the particle.
- processor_at_t0 - The rank of the processor on which the particle started.

Collections of particles are represented by another Fortran TYPE, called **`particle_list`**. This type represents all the properties of a collection of particles and is used behind the scenes to deal with inter-processor communication of particles. The definition of the type is:

```
TYPE particle_list
  TYPE(particle), POINTER :: head
  TYPE(particle), POINTER :: tail
  INTEGER(KIND=8) :: count
  ! Pointer is safe if the particles in it are all unambiguously linked
  LOGICAL :: safe

  TYPE(particle_list), POINTER :: next, prev
END TYPE particle_list
```

- head - The first particle in the linked list.
- tail - The last particle in the linked list.
- count - The number of particles in the list. Note that this is NOT MPI aware, so reading count only gives you the number of particles on the local processor.
- safe - Any particle_list which a user should come across will be a safe particle_list. Don't change this property.
- next, prev - For future expansion it is possible to attach particle_lists together in another linked list. This is not currently used anywhere in the code.

An entire species of particles is represented by another Fortran TYPE, this time called **`particle_species`**. This represents all the properties which are common to all particles in a species. There are lots of entries which are only compiled in when compile-time flags are specified. The definition without any such flags is:

```
TYPE particle_species
  ! Core properties
  CHARACTER(string_length) :: name
  TYPE(particle_species), POINTER :: next, prev
  INTEGER :: id
  INTEGER :: dumpmask

  REAL(num) :: charge
```

```
    REAL(num) :: mass
    REAL(num) :: weight
    INTEGER(KIND=8) :: count
    TYPE(particle_list) :: attached_list

    ! Injection of particles
    INTEGER(KIND=8) :: npart_per_cell
    REAL(num), DIMENSION(:), POINTER :: density
    REAL(num), DIMENSION(:,:), POINTER :: temperature
  END TYPE particle_species
```

This definition is for the 2D version of the code. The only difference for the other two versions is the number of dimensions in the density and temperature arrays.

- name - The name of the particle species, used in the output dumps etc.
- next, prev - Particle species are also linked together in a linked list. This is used internally by the output dump routines, but should not be used by end users.
- id - The species number for this species. This is the same number as is used in the input deck to designate the species.
- dumpmask - Determine when to include this species in output dumps. Note that the flag is ignored for restart dumps.
- charge - The charge in Coulombs. Even if PER_PARTICLE_CHARGE_MASS is specified, this is still populated from the input deck, and now refers to the reference charge for the species.
- mass - The mass in kg.
- weight - The per-species particle weight.
- count - The global number of particles of this species (NOTE may not be accurate). This will only ever be the number of particles on this processor when running on a single processor. While this property will be accurate when setting up initial conditions, it is only guaranteed to be accurate for the rest of the code if the code is compiled with the correct preprocessor options.
- attached_list - The list of particles which belong to this species.

The last three entries are only used by the particle injection model.

4.2.2 Setting the particle properties

The details of exactly what a linked list means in EPOCH requires a more in-depth study of the source code. For now, all we really need to know is that each species has a list of particles. A pointer to the first particle in the list is contained in `species_list(ispecies)%attached_list%head`. Once you have a pointer to a particle (eg. `current`), you advance to the next pointer in the list with `current => current%next`.

After all the descriptions of the types, actually setting the properties of the particles is fairly simple. The following is an example which positions the particles uniformly in 1D space, but doesn't set any momentum.

```
SUBROUTINE manual_load

  TYPE(particle), POINTER :: current
  INTEGER :: ispecies
  REAL(num) :: rpos, dx

  DO ispecies = 1, n_species
    current => species_list(ispecies)%attached_list%head
    dx = length_x / species_list(ispecies)%attached_list%count
    rpos = x_min
    DO WHILE(ASSOCIATED(current))
      current%part_pos = rpos
      current%weight = 1.0_num
      rpos = rpos + dx
      current => current%next
    ENDDO
  ENDDO

END SUBROUTINE manual_load
```

This will take the particles which have been placed at random positions by the autoloader and repositions them in a uniform manner. In order to adjust the particle positions, you need to know about the grid used in EPOCH. In this example we only required the length of the domain, "length_x" and the minimum value of x, "x_min". A more exhaustive list is given in the following section. Note that I completely ignored the question of domain decomposition when setting up the particles. The code automatically moves the particles onto the correct processor without user interaction.

In the above example, note that particle momentum was not specified and particle weight was set to be a simple constant. Setting particle weight can be very simple if you can get the pseudoparticle distribution to match the real particle distribution, or quite tricky if this isn't possible. The weight of a pseudoparticle is calculated such that the number of pseudoparticles in a cell multiplied by their weights equals the number of physical particles in that cell. This can be quite tricky to get right, so in more complicated cases it is probably better to use the autoloader than to manually set up the number density distribution.

4.2.3 Grid coordinates used in EPOCH.

When setting up initial conditions within the EPOCH source (rather than using the input deck) there are several constants that you may need to use. These constants are:

- nx - Number of gridpoints on the local processor in the x direction.
- ny - Number of gridpoints on the local processor in the y direction (2D and 3D).
- nz - Number of gridpoints on the local processor in the z direction (3D).
- length_{x,y,z} - Length of domain in the x, y, z directions.
- {x,y,z}_min - Minimum value of x, y, z for the whole domain.
- {x,y,z}_max - Maximum value of x, y, z for the whole domain.
- n_species - The number of species in the code.

There are also up to three arrays which are available for use.

- x(-2:nx+3) - Position of a given gridpoint in real units in the x direction.
- y(-2:ny+3) - Position of a given gridpoint in real units in the y direction (2D and 3D).
- z(-2:nz+3) - Position of a given gridpoint in read units in the z direction (3D).

4.2.4 Loading a non-thermal particle distribution.

While the autoloader is capable of dealing with most required initial thermal distributions, you may want to set up non-thermal initial conditions. The code includes a helper function to select a point from an arbitrary distribution function which can be used to deal with most non-thermal distributions. To use the helper function, you need to define two 1D arrays which are the x and y axes for the distribution function. An example of using the helper function is given below.

```
SUBROUTINE manual_load

  TYPE(particle), POINTER :: current
  INTEGER, PARAMETER :: np_local = 1000
  INTEGER :: ispecies, ip
  REAL(num) :: temperature, stdev2, tail_width, tail_height, tail_drift
  REAL(num) :: frac, tail_frac, min_p, max_p, dp_local, p2, tail_p2
  REAL(num), DIMENSION(np_local) :: p_axis, distfn_axis

  temperature = 1e4_num
  tail_width = 0.05_num
  tail_height = 0.2_num
  tail_drift = 0.5_num

  DO ispecies = 1, n_species
    stdev2 = kb * temperature * species_list(ispecies)%mass
    frac = 1.0_num / (2.0_num * stdev2)
    tail_frac = 1.0_num / (2.0_num * stdev2 * tail_width)

    max_p = 5.0_num * SQRT(stdev2)
    min_p = -max_p

    dp_local = (max_p - min_p) / REAL(np_local-1, num)
    DO ip = 1, np_local
      p_axis(ip) = min_p + (ip - 1) * dp_local
      p2 = p_axis(ip)**2
      tail_p2 = (p_axis(ip) - tail_drift * max_p)**2
      distfn_axis(ip) = EXP(-p2 * frac) &
          + tail_height * EXP(-tail_p2 * tail_frac)
    ENDDO

    current=>species_list(ispecies)%attached_list%head
    DO WHILE(ASSOCIATED(current))
      current%part_p(1) = sample_dist_function(p_axis, distfn_axis)
      current=>current%next
    ENDDO
  ENDDO

END SUBROUTINE manual_load
```

This example will set the particles to have a bump-on-tail velocity distribution, a setup which is not possible to do using only the input deck. It is not necessary to normalise the distribution function, as this is done automatically by the **sample_dist_function** function.

4.3 Lasers

EPOCH has the ability to add EM wave sources such as lasers at boundaries. To use lasers, set the boundary that you wish to have a laser on to be of type **`simple_laser`** and then specify one or more lasers attached to that boundary. Lasers may be specified anywhere initial conditions are specified.

4.4 laser blocks in multiple dimensions.

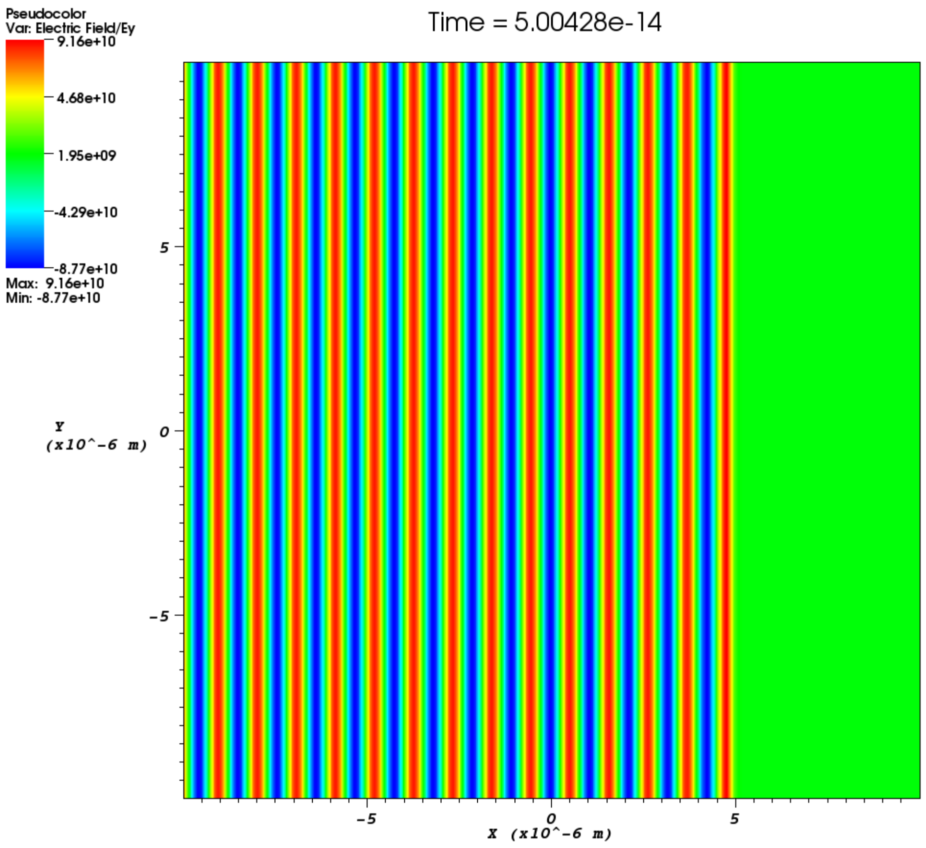


Figure 3: Constant laser profile

When running EPOCH in 2D or 3D, the laser can be modified spatially via the profile and phase parameters. These are briefly outlined in Section 3.4 but in this section we will describe them in a little more depth.

profile - The spatial profile for the laser. This is essentially an array defined along the edge (or surface) that the laser is attached to. It is clear that the spatial profile is only meaningful perpendicular to the laser's direction of travel and so it is just a single constant in 1D. The laser profile is evaluated as an initial condition and so cannot include any temporal information which must be encoded in t_profile. The spatial profile is evaluated at the boundary where the laser is attached and so only spatial information in the plane of the boundary is significant. This is most clearly explained through a couple of examples. In these examples the spatial profile of the laser is set to vary between a flat uniform profile (**profile = 1**) and a Gaussian profile in y (**profile = gauss(y,0,2.5e-6)**). The difference between these profiles is obvious but the important point is that a laser travelling parallel to the x-direction has a profile in the y direction. Similarly a laser propagating in the y-direction has

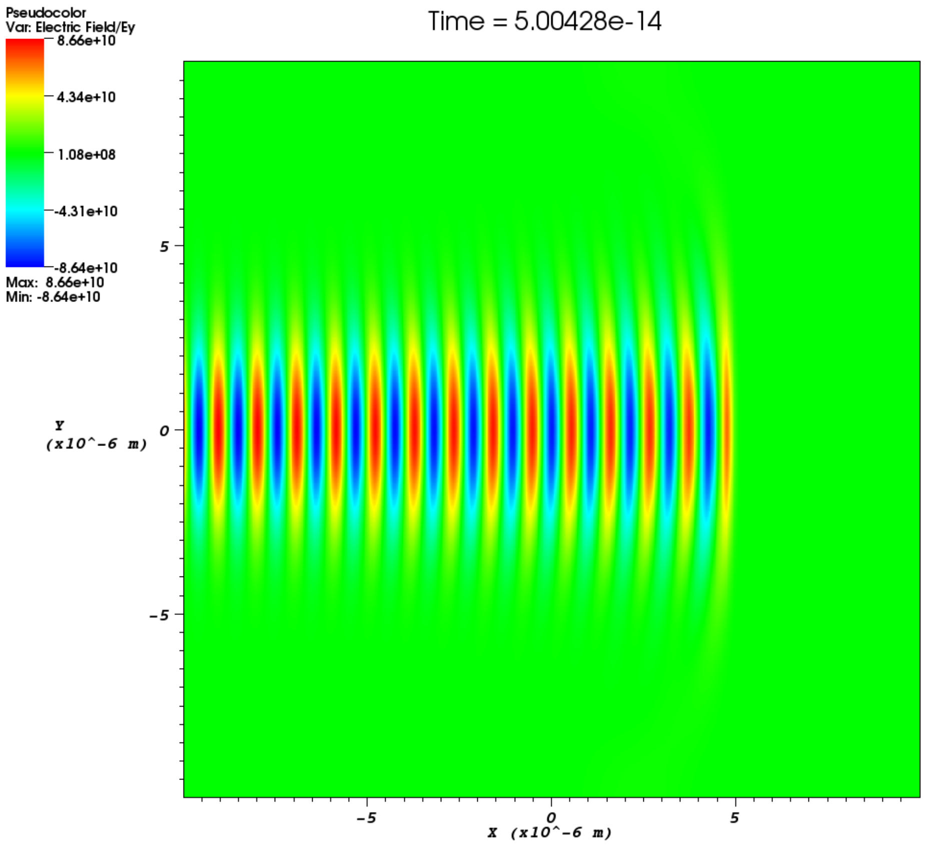


Figure 4: Gaussian laser profile

a profile in the x direction. In 3D this is extended so that a laser propagating in a specified direction has a profile in both orthogonal directions. So a laser travelling parallel to the x axis in 3D would have a profile in y and z. Since 3D lasers are very similar to 2D lasers, they will not be considered here in greater detail, but in 3D, it is possible to freely specify the laser profile across the entire face where a laser is attached.

phase - Phase shift for the laser in radians. This is a spatial variable which is also defined across the whole of the boundary on which the laser is attached. This allows a user to add a laser travelling at an angle to a boundary as shown in Figure 5. The setup for this is not entirely straightforward and requires a little bit of explanation. Figure 6 illustrates a laser being driven at an angle on the x_min boundary. Different wave fronts cross the y-axis at different places and this forms a sinusoidal profile along y that represents the phase. The wavelength of this profile is given by $\lambda_\phi = \lambda / \sin\theta$, where λ is the wavelength of the laser and θ is the angle of the propagation direction with respect to the x-axis. The actual phase to use will be $\phi(y) = -k_\phi y = -2\pi y/\lambda_\phi$. It is negative because the phase of the wave is propagating in the positive y direction. It is also necessary to alter the wavelength of the driver since this is given in the direction perpendicular to the boundary. The new wavelength to use will be $\lambda \cos\theta$. Figure 5 shows the resulting E_y field for a laser driven at an angle of $\pi/8$. Note that since the boundary conditions in the code are derived for propagation perpendicular to the boundary, there will be artefacts on the scale of the grid for lasers driven at an angle.

Using this technique it is also possible to focus a laser. This is done by using the same technique as above but making the angle of propagation, θ, a function of y such that the laser is focused to a point along the x-axis.

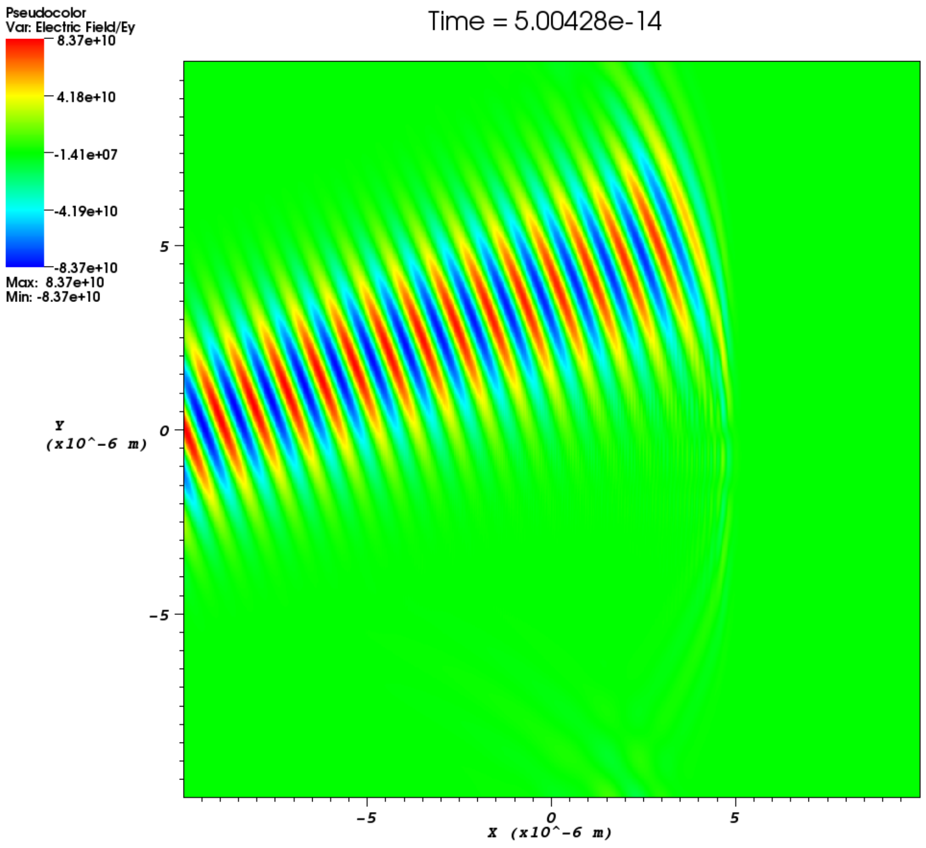


Figure 5: Angled laser profile

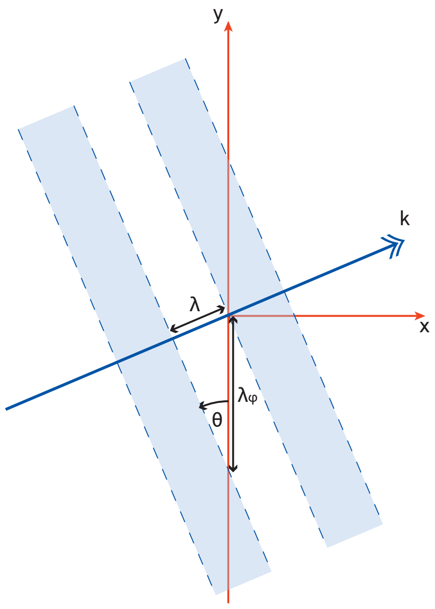


Figure 6: Laser at an angle

4.5 Restarting EPOCH from previous output dumps

Another possible way of setting up initial conditions in EPOCH is to load in a previous output dump and use it to specify initial conditions for the code. The effect of this is to restart the code from the state that it was in when the dump was made. To do this, you just set the field "restart_snapshot" to the number of the output dump from which you want the code to restart. Because of the way in which the code is written you cannot guarantee that the code will successfully restart from any output dump. To restart properly, the following *must* have been dumped

- Particle positions.
- Particle momenta.
- Particle species.
- Particle weights.
- Relevant parts of the electric field (If for example it is known that ez == 0 then it is not needed).
- Relevant parts of the magnetic field.

It is possible to use the manual particle control part of the initial conditions to make changes to a restarted initial condition after the restart dump is loaded. The output files don't include all of the information needed to restart the code fully since some of this information is contained in the input deck. However, a restart dump also contains a full copy of the input deck used and this can be unpacked before running the code.

If specific "restart" dumps are specified in the input deck, or the "force_final_to_be_restartable" flag is set then in some cases the output is forced to contain enough information to output all the data. These restart dumps can be very large, and also override the "dumpmask" parameter specified for a species and output the data for that species anyway.

4.6 Parameterising input decks

The simplest way to allow someone to use EPOCH as a black box is to give them the input.deck files that control the setup and initial conditions of the code. The input deck is simple enough that a quick read through of the relevant section of the manual should make it fairly easy for a new user to control those features of the code, but the initial conditions can be complex enough to be require significant work on the part of an unfamiliar user to understand. In this case, it can be helpful to use the ability to specify constants in an input deck to parameterise the file. So, to go back to a slight variation on an earlier example:

```
begin:species
   name = s1

   # first set density in the range 0->1
   # cut down density in x direction
   density = if ((x gt -1) and (x lt 1),1.0,0.2)
   # cut down density in y direction
   density = if ((y gt -1) and (y lt 1),density(s1),0.2)

   # multiply density by real particle density
   density = density(s1)*100.0

   # Set the temperature to be zero
   temp_x = 0.0
   temp_y = temp_x(s1)

   # Set the minimum density for this species
   density_min = 0.3*100.0
end:species

begin:species
```

```
   name = s2

   # Just copy the density for species s1
   density = density(s1)

   # Just copy the temperature from species s1
   temp_x = temp_x(s1)
   temp_y = temp_y(s1)

   # Set the minimum density for this species
   density_min = 0.3*100.0
end:species
```

The particle density (100.0) is hard coded into the deck file in several places. It would be easier if this was given to a new user as:

```
begin:constant
   particle_density = 100.0 # Particle number density
end:constant

begin:species
   name = s1

   # first set density in the range 0->1
   # cut down density in x direction
   density = if ((x gt -1) and (x lt 1),1.0,0.2)
   # cut down density in y direction
   density = if ((y gt -1) and (y lt 1),density(s1),0.2)

   # multiply density by real particle density
   density = density(s1)*particle_density

   # Set the temperature to be zero
   temp_x = 0.0
   temp_y = temp_x(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species

begin:species
   name = s2

   # Just copy the density for species s1
   density = density(s1)

   # Just copy the temperature from species s1
   temp_x = temp_x(s1)
   temp_y = temp_y(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species
```

It is also possible to parameterise other elements of initial conditions in a similar fashion. This is generally a good idea, since it makes the initial conditions easier to read an maintain.

4.7 Using spatially varying functions to further parameterise initial conditions

Again, this is just a readability change to the normal input.deck file, but it also makes changing and understanding the initial conditions rather simpler. In this case, entire parts of the initial conditions are moved into a spatially varying constant in order to make changing them at a later date easier. For example:

```
begin:constant
   particle_density = 100.0 # Particle number density
   profile_x = if((x gt -1) and (x lt 1),1.0,0.2)
   profile_y = if((y gt -1) and (y lt 1),1.0,0.2)
end:constant

begin:species
   name = s1

   # multiply density by real particle density
   density = particle_density * profile_x * profile_y

   # Set the temperature to be zero
   temp_x = 0.0
   temp_y = temp_x(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species

begin:species
   name = s2

   # Just copy the density for species s1
   density = density(s1)

   # Just copy the temperature from species s1
   temp_x = temp_x(s1)
   temp_y = temp_y(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species
```

This creates the same output as before. It is now trivial to modify the profiles later. For example:

```
begin:constant
   particle_density = 100.0 # Particle number density
   profile_x = gauss(x,0.0,1.0)
   profile_y = gauss(y,0.0,1.0)
end:constant

begin:species
   name = s1

   # multiply density by real particle density
   density = particle_density * profile_x * profile_y

   # Set the temperature to be zero
   temp_x = 0.0
   temp_y = temp_x(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species

begin:species
   name = s2

   # Just copy the density for species s1
   density = density(s1)

   # Just copy the temperature from species s1
   temp_x = temp_x(s1)
   temp_y = temp_y(s1)

   # Set the minimum density for this species
   density_min = 0.3*particle_density
end:species
```

This changes the code to run with a Gaussian density profile rather then a step function. Again, this can be extended as far as required.

5 Basic examples of using EPOCH

In this section we outline a few worked examples of setting up problems using the EPOCH input deck.

5.1 Electron two stream instability

An obvious simple test problem to do with EPOCH is the electron two stream instability. An example of a nice dramatic two stream instability can be obtained using EPOCH1D by setting the code with the following input deck files.

input.deck

```
begin:control
   nx = 400
   npart = 20000
   #final time of simulation
   t_end = 1.5e-1

   #size of domain
   x_min = 0
   x_max = 5.0e5
end:control


begin:boundaries
   bc_x_min = periodic
   bc_x_max = periodic
end:boundaries


begin:constant
   drift_p = 2.5e-24
   temp = 273
   dens = 10
end:constant


begin:species
   # Rightwards travelling electrons
   name = Right
   charge = -1
   mass = 1.0
   frac = 0.5
   temp_x = temp
   drift_x = drift_p
   rho = dens
end:species


begin:species
   # Leftwards travelling electrons
   name = Left
   charge = -1
   mass = 1.0
   frac = 0.5
   temp_x = temp
   drift_x = -drift_p
   rho = dens
end:species


begin:output
   # number of timesteps between output dumps
   dt_snapshot = 1.5e-3
   # Number of dt_snapshot between full dumps
   full_dump_every = 1
```

```
    # Properties at particle positions
    particles = always
    px = always

    # Properties on grid
    grid = always
    ex = always
    ey = always
    ez = always
    bx = always
    by = always
    bz = always
    jx = always
    ekbar = always
    mass_density = never + species
    charge_density = always
    number_density = always + species
    temperature = always + species

    # extended io
    distribution_functions = always
end:output
```

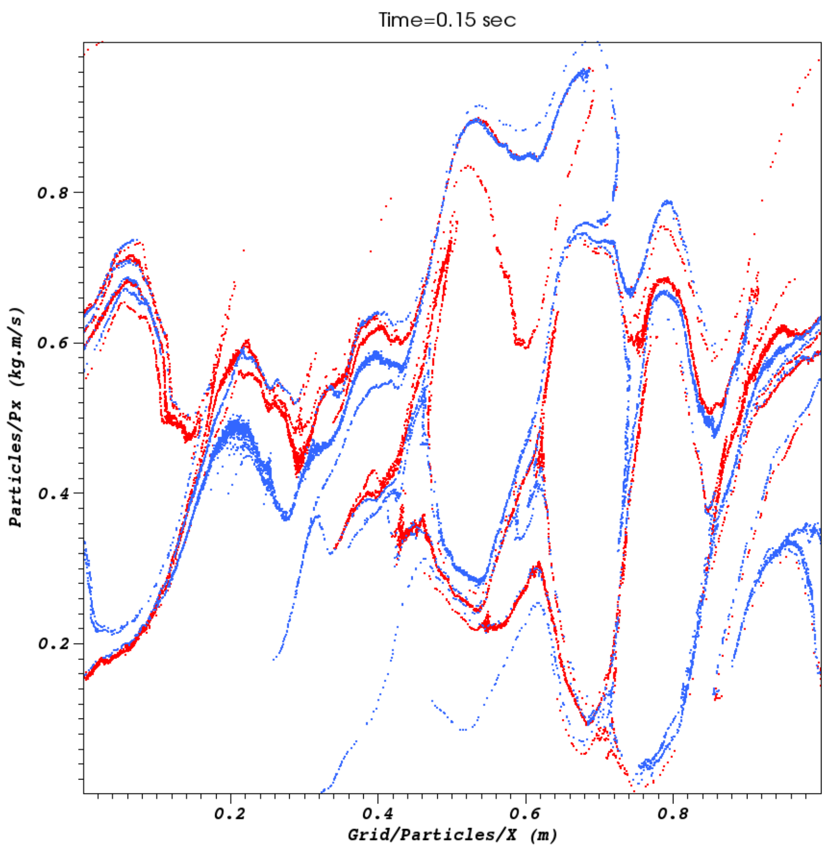


Figure 7: The final state of the electron phase space for the two stream instability example.

While the input.deck file is rather long, most of it is the basic standard input deck that is supplied with EPOCH, with only the length of the domain, the final time and the time between snapshots specific to this problem. ic.deck, the initial conditions file, is very simple indeed. The first block sets up constants for the momentum space drift, the temperature and the electron number density. The second and third blocks set up the two drifting Maxwellian distributions and the constant density profile. Note that we have written this example as two separate files simply to demonstrate how this is done. The same result would be obtained by appending the contents of "ic.deck" to the end of "input.deck" and removing the "import" line. The final output from this simulation is shown in Figure 7.

5.2 Structured density profile in EPOCH2D

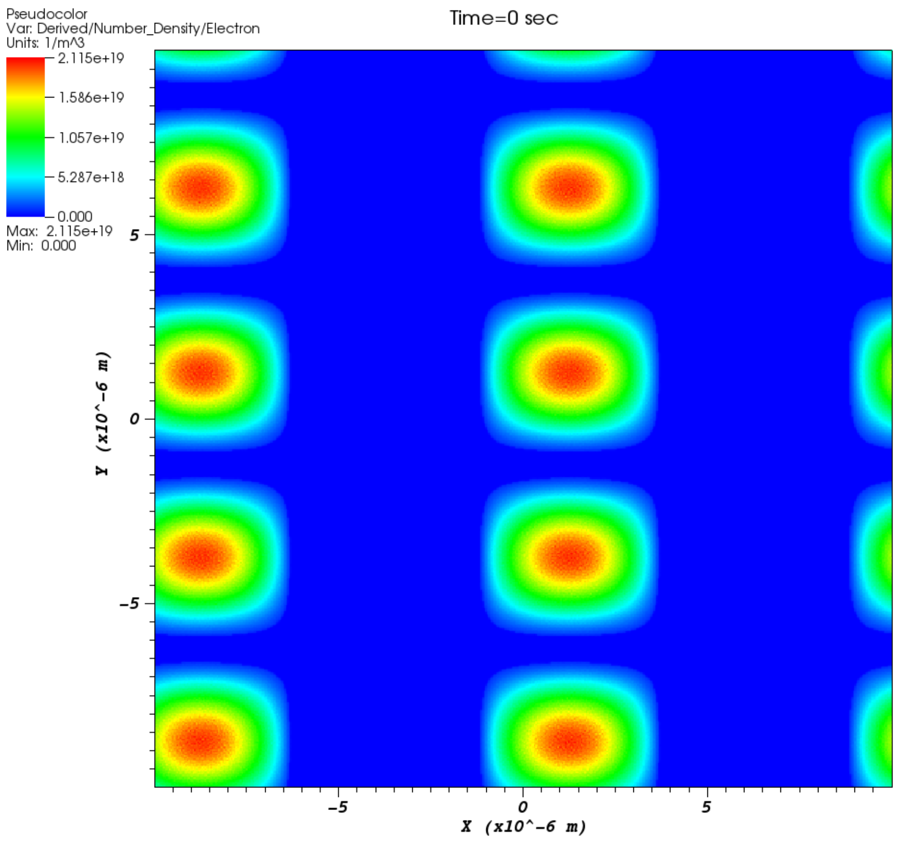


Figure 8: Complex 2D density structure

A simple but useful example for EPOCH2D is to have a highly structured initial condition to show that this is still easy to implement in EPOCH. A good example initial condition would be:

input.deck
```
begin:control
   nx = 500
   ny = nx
   x_min = -10 * micron
   x_max = -x_min
   y_min = x_min
   y_max = x_max
   nsteps = 0
   npart = 40 * nx * ny
end:control

begin:boundaries
   bc_x_min = periodic
   bc_x_max = periodic
   bc_y_min = periodic
   bc_y_max = periodic
end:boundaries

begin:constant
   den_peak = 1.0e19
end:constant

begin:species
   name = Electron
   density = den_peak*(sin(4.0*pi*x/length_x+pi/4))*(sin(8.0*pi*y/length_y)+1)
   density_min = 0.1*den_peak
   charge = -1.0
   mass = 1.0
   frac = 0.5
end:species

begin:species
   name = Proton
   density = density(Electron)
   charge = 1.0
   mass = 1836.2
   frac = 0.5
end:species

begin:output
   number_density = always + species
end:output
```

The species block for **Electron** is specified first, setting up the electron density to be a structured 2D sinusoidal profile. The species block for **Proton** is then set to match the density of **Electron**, enforcing charge neutrality. On its own this initial condition does nothing and so only needs to run for 0 timesteps (**nsteps = 0** in input.deck). The resulting electron number density should look like Figure 8

5.3 A hollow cone in 3D

A more useful example of an initial condition is to create a hollow cone. This is easy to do in both 2D and 3D, but is presented here in 3D form.

input.deck
```
begin:control
   nx = 250
   ny = nx
   nz = nx
   npart = 2 * nx * ny * nz
   x_min = -10 * micron
   x_max = -x_min
   y_min = x_min
   y_max = x_max
   z_min = x_min
   z_max = x_max
   nsteps = 0
end:control

```

```
begin:boundaries
   bc_x_min = simple_laser
   bc_x_max = simple_outflow
   bc_y_min = periodic
   bc_y_max = periodic
   bc_z_min = periodic
   bc_z_max = periodic
end:boundaries

begin:output
   number_density = always + species
end:output

begin:constant
   den_cone = 1.0e22
   ri = abs(x - 5.0e-6) - 0.5e-6
   ro = abs(x - 5.0e-6) + 0.5e-6
   xi = 3.0e-6 - 0.5e-6
   xo = 3.0e-6 + 0.5e-6
   r = sqrt(y^2 + z^2)
end:constant

begin:species
   name = proton
   charge = 1.0
   mass = 1836.2
   frac = 0.5
   rho = if((r gt ri) and (r lt ro), den_cone, 0.0)
   rho = if((x gt xi) and (x lt xo) and (r lt ri), den_cone, rho(proton))
   rho = if(x gt xo, 0.0, rho(proton))
end:species

begin:species
   name = electron
   charge = -1.0
   mass = 1.0
   frac = 0.5
   rho = rho(proton)
end:species
```

To convert this to 2D, simply replace the line **`r = sqrt(y^2+z^2)`** with the line **`r = abs(y)`**. The actual work in these initial conditions is done by the three lines inside the block for the **Proton** species. Each of these lines performs a very specific function:

1. Creates the outer cone. Simply tests whether **`r`** is within the range of radii which corresponds to the thickness of the cone and if so fills it with the given density. Since the inner radius is x dependent this produces a cone rather than a cylinder. On its own, this line produces a pair of cones joined at the tip.

2. Creates the solid tip of the cone. This line just tests whether the point in space is within the outer radius of the cone and within a given range in x, and fills it with the given density if true.

3. Cuts off all of the cone beyond the solid tip. Simply tests if x is greater than the end of the cone tip and sets the density to zero if so.

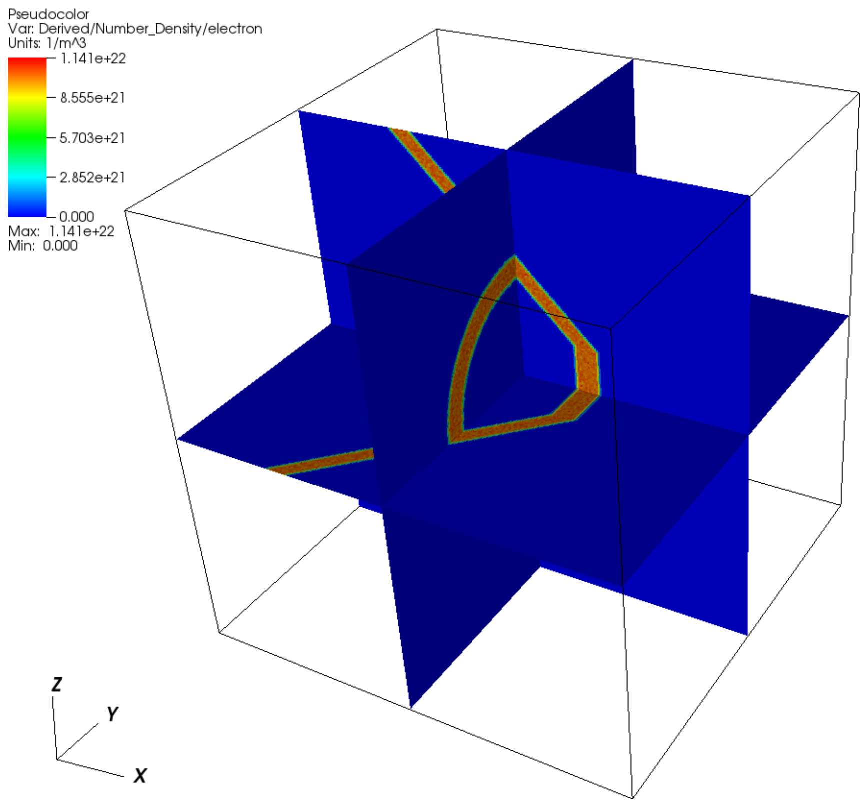


Figure 9: Cone initial conditions in 3D

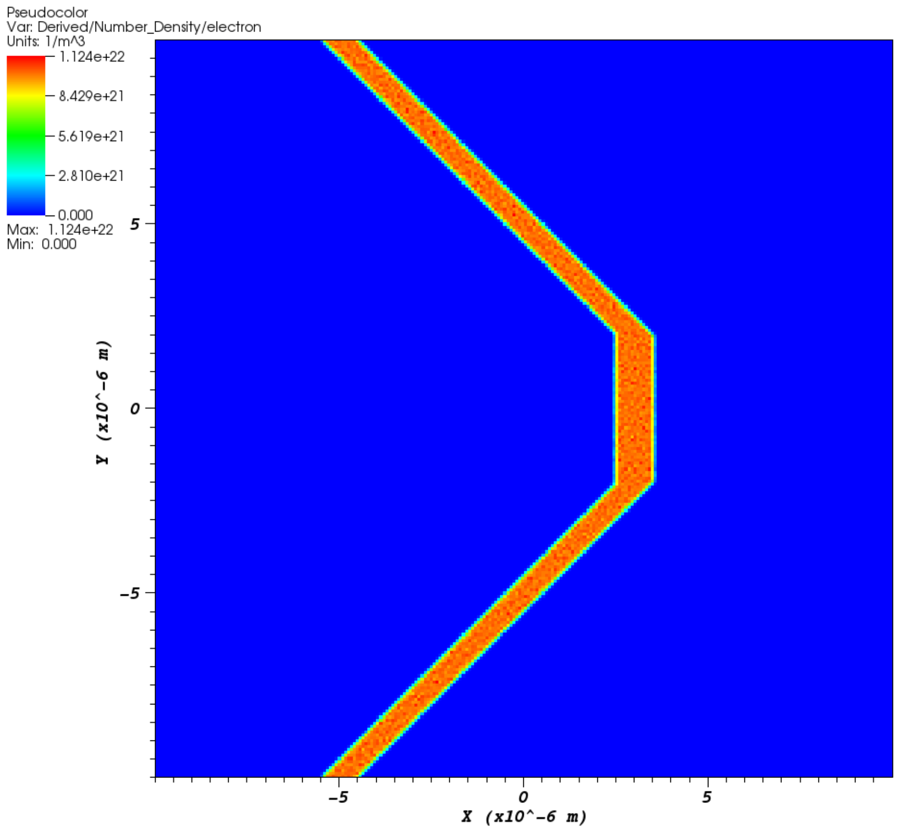


Figure 10: Cone initial conditions in 2D

This deck produces and initial condition which looks like Figure 9 and Figure 10 in 3D and 2D respectively.

The details presented above are a first rough guide to using EPOCH. To clearly understand EPOCH it is best to now try some simple examples. To view the results you will have to jump forward to "**6**" (Section 6).

6 Using IDL to visualise data

The EPOCH distribution comes with procedures for loading and inspecting SDF self-describing data files. The IDL routines are held in the `IDL/` directory for each of the `epoch*d/` directories. There is also a procedure named `Start.pro` in each of the `epoch*d/` directories which is used to set up the IDL environment.

To load data into IDL, navigate to one of the base directories (eg. `epoch/trunk/epoch2d/` where `epoch/` is the directory in which you have checked out the Subversion repository) and type the following:

```
$> idl Start
IDL Version 7.1.1, Mac OS X (darwin x86_64 m64). (c) 2009, ITT Visual Informat...
Installation number: .
Licensed for use by: STAR404570-32University of Warwick

% Compiled module: PARTICLEPHASEPLANE.
% Compiled module: TRACKEX_EVENT.
% Compiled module: ISOPLOT.
% Compiled module: READVAR.
% Compiled module: LOADCFDFILE.
% Compiled module: HANDLEBLOCK.
% Compiled module: GETMESH.
% Compiled module: GETMESHVAR.
% Compiled module: GETSNAPSHOT.
% Compiled module: READVAR.
% Compiled module: LOADSDFFILE.
% Compiled module: SDFHANDLEBLOCK.
% Compiled module: SDFGETPLAINMESH.
% Compiled module: SDFGETLAGRANMESH.
% Compiled module: SDFGETPOINTMESH.
% Compiled module: SDFGETPLAINVAR.
% Compiled module: SDFGETPOINTVAR.
% Compiled module: SDFGETCONSTANT.
% Compiled module: SDFCHECKNAME.
% Compiled module: INIT_SDFHELP.
% Compiled module: GETDATA.
% Compiled module: GETSTRUCT.
% Compiled module: EXPLORE_DATA.
% Compiled module: EXPLORE_STRUCT.
% Compiled module: LIST_VARIABLES.
% Compiled module: QUICK_VIEW.
% Compiled module: GET_WKDIR.
% Compiled module: SET_WKDIR.
% Compiled module: INIT_STARTPIC.
% Compiled module: SWAPCHR.
% Compiled module: CHECKNAME.
% Compiled module: RETURNIDLUSABLE.
% Compiled module: RETURNFRIENDLYTYPENAME.
% Compiled module: INIT_CFDHELP.
% Compiled module: INIT_WIDGET.
% Compiled module: GENERATE_FILENAME.
% Compiled module: COUNT_FILES.
% Compiled module: LOAD_RAW.
% Compiled module: GET_SDF_METATEXT.
% Compiled module: VIEWER_EVENT_HANDLER.
% Compiled module: EXPLORER_EVENT_HANDLER.
% Compiled module: XLOADCT_CALLBACK.
% Compiled module: LOAD_DATA.
% Compiled module: DRAW_IMAGE.
% Compiled module: LOAD_META_AND_POPULATE_SDF.
% Compiled module: CLEAR_DRAW_SURFACE.
% Compiled module: SDF_EXPLORER.
% Compiled module: EXPLORER_LOAD_NEW_FILE.
% Compiled module: CREATE_SDF_VISUALIZER.
% Compiled module: VIEWER_LOAD_NEW_FILE.
% Compiled module: LOADCT.
% Compiled module: FILEPATH.
% LOADCT: Loading table RED TEMPERATURE
IDL>
```

This starts up the IDL interpreter and loads in all of the libraries for loading and inspecting SDF files.

We begin by inspecting SDF file contents and finding out what variables it contains. To do this we execute the `list_variables` procedure call which is provided by the EPOCH IDL library.

At each timestep for which EPOCH is instructed to dump a set of variables a new data file is created. These files take the form `0000.sdf`. For each new dump the number is incremented. The procedure call accepts up to two arguments. The first argument is mandatory and specifies the number of the SDF file to be read in. This argument can be any integer from 0 to 9999. It is padded with zeros and the suffix '.sdf' appended to the end to give the name of the data file. eg. 99 ⇒ '0099.sdf'. The next arguments is optional. The keyword "`wkdir`" specifies the directory in which the data files are located. If this argument is omitted then the currently defined global default is used. Initially, this takes the value "`Data`" but this can be changed using the `set_wkdir` procedure and queried using the `get_wkdir()` function.

```
IDL> list_variables,0,"Data"
Available elements are
1) EX (ELECTRIC_FIELD) : 2D Plain variable
2) EY (ELECTRIC_FIELD) : 2D Plain variable
3) EZ (ELECTRIC_FIELD) : 2D Plain variable
4) BX (MAGNETIC_FIELD) : 2D Plain variable
5) BY (MAGNETIC_FIELD) : 2D Plain variable
6) BZ (MAGNETIC_FIELD) : 2D Plain variable
7) JX (CURRENT) : 2D Plain variable
8) JY (CURRENT) : 2D Plain variable
9) JZ (CURRENT) : 2D Plain variable
10) WEIGHT_ELECTRON (PARTICLES) : 1D Point variable
11) WEIGHT_PROTON (PARTICLES) : 1D Point variable
12) PX_ELECTRON (PARTICLES) : 1D Point variable
13) PX_PROTON (PARTICLES) : 1D Point variable
14) GRID_ELECTRON (GRID) : 2D Point mesh
15) GRID_PROTON (GRID) : 2D Point mesh
16) EKBAR (DERIVED) : 2D Plain variable
17) EKBAR_ELECTRON (DERIVED) : 2D Plain variable
18) EKBAR_PROTON (DERIVED) : 2D Plain variable
19) CHARGE_DENSITY (DERIVED) : 2D Plain variable
```

```
20) NUMBER_DENSITY (DERIVED) : 2D Plain variable
21) NUMBER_DENSITY_ELECTRON (DERIVED) : 2D Plain variable
22) NUMBER_DENSITY_PROTON (DERIVED) : 2D Plain variable
23) GRID (GRID) : 2D Plain mesh
24) GRID_EN_ELECTRON (GRID) : 1D Plain mesh
25) EN_ELECTRON (DIST_FN) : 3D Plain variable
26) GRID_X_EN_ELECTRON (GRID) : 2D Plain mesh
27) X_EN_ELECTRON (DIST_FN) : 3D Plain variable
28) GRID_X_PX_ELECTRON (GRID) : 2D Plain mesh
29) X_PX_ELECTRON (DIST_FN) : 3D Plain variable
IDL>
```

Each variable in the SDF self-describing file format is assigned a name and a class as well as being defined by a given variable type. The `list_variables` procedure prints out the variable name followed by the variable's class in parenthesis. Following the colon is a description of the variable type.

To retrieve the data, you must use the `getdata()` function call. The function must be passed a snapshot number, either as the first argument or as a keyword parameter "`snapshot`". It also accepts the wkdir as either the second argument or the keyword parameter "`wkdir`". If it is omitted alltogether, the current global default is used. Finally, it accepts a list of variables or class of variables to load. Since it is a function, the result must be assigned to a variable. The object returned is an IDL data structure containing a list of named variables.

To load either a specific variable or a class of variables, specify the name prefixed by a forward slash. It should be noted here that the IDL scripting language is not case sensitive so P_x can be specified as either "`/Px`" or "`/px`".

We will now load and inspect the "`Grid`" class, this time omitting the optional "`wkdir`" parameter. This time we will load from the third dump file generated by the EPOCH run, which is found in the file `0002.sdf` since the dump files are numbered starting from zero.

6.1 Inspecting Data

```
IDL> gridclass = getdata(1,/grid)

IDL> help,gridclass,/structures
** Structure <22806408>, 11 tags, length=536825024, data length=536825016, refs=1:
   FILENAME        STRING    'Data/0001.sdf'
   TIMESTEP        LONG                    43
   TIME            DOUBLE       5.0705572e-15
   GRID_ELECTRON   STRUCT    -> <Anonymous> Array[1]
   GRID_PROTON     STRUCT    -> <Anonymous> Array[1]
   GRID            STRUCT    -> <Anonymous> Array[1]
   X               DOUBLE    Array[1024]
   Y               DOUBLE    Array[512]
   GRID_EN_ELECTRON
                   STRUCT    -> <Anonymous> Array[1]
   GRID_X_EN_ELECTRON
                   STRUCT    -> <Anonymous> Array[1]
   GRID_X_PX_ELECTRON
                   STRUCT    -> <Anonymous> Array[1]
IDL> help,gridclass.grid,/structures
** Structure <1701168>, 5 tags, length=12376, data length=12376, refs=2:
   X               DOUBLE    Array[1025]
   Y               DOUBLE    Array[513]
   LABELS          STRING    Array[2]
   UNITS           STRING    Array[2]
   NPTS            LONG      Array[2]
```

Here we have used IDL's built in "`help`" routine and passed the "`/structures`" keyword which prints information about a structure's contents rather than just the structure itself.

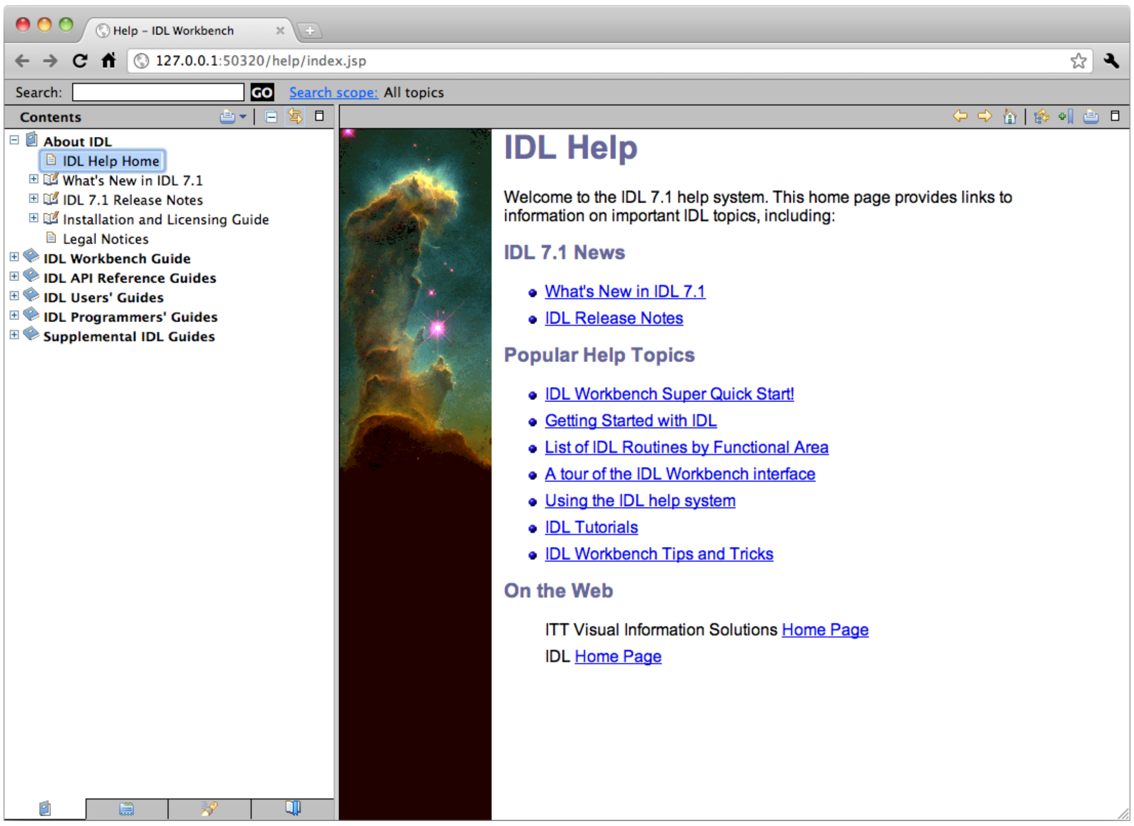
Since "`Grid`" is a class name, all variables of that class have been loaded into the returned data structure. It is a nested type so many of the variables returned are structures themselves and those variables may contain structures of their own.

The "`Grid`" variable itself contains "`x`" and "`y`" arrays containing the x and y coordinates of the 2D cartesian grid. The other variables in the "`Grid`" structure are metadata used to identify the type and properties of the variable. In order to access the "`Grid`" variable contained within the "`gridclass`" data structure we have used the "`.`" operator. In a similar way, we would access the "`x`" array contained within the "`Grid`" variable using the identifier "`gridclass.grid.x`".

6.2 Getting Help in IDL

IDL is a fairly sophisticated scripting environment with a large library of tools for manipulating data. Fortunately, it comes with a fairly comprehensive array of documentation. This can be accessed by typing `?` at the IDL prompt.

```
IDL> ?
% ONLINE_HELP: Starting the online help browser.
IDL>
```



- About IDL
  - IDL Help Home
  - What's New in IDL 7.1
  - IDL 7.1 Release Notes
  - Installation and Licensing Guide
  - Legal Notices
- IDL Workbench Guide
- IDL API Reference Guides
- IDL Users' Guides
- IDL Programmers' Guides
- Supplemental IDL Guides

IDL Help

Welcome to the IDL 7.1 help system. This home page provides links to information on important IDL topics, including:

IDL 7.1 News

- What's New in IDL 7.1
- IDL Release Notes

Popular Help Topics

- IDL Workbench Super Quick Start!
- Getting Started with IDL
- List of IDL Routines by Functional Area
- A tour of the IDL Workbench interface
- Using the IDL help system
- IDL Tutorials
- IDL Workbench Tips and Tricks

On the Web

ITT Visual Information Solutions Home Page
IDL Home Page

The documentation is divided into books aimed at users or developers and is fully searchable and cross indexed.

6.3 Manipulating And Plotting Data

Once the data has been loaded from the SDF file we will want to extract the specific data we wish to analyse, perhaps perform some mathematical operations on it and then plot the results.

To do this we must learn a few basic essentials about the IDL scripting language. Since we are all familiar with the basic concepts shared by all computer programming languages, I will just provide a brief overview of the essentials and leave other details to the excellent on-line documentation.

IDL supports multidimensional arrays similar to those found in the FORTRAN programming language. Whole array operations are supported such as "`5*array`" to multiply every element of "`array`" by 5. Also matrix operations such as addition and multiplication are supported.

The preferred method for indexing arrays is to use brackets. It is possible to use parenthesis instead but this usage is deprecated. Column ordering is the same as that used by FORTRAN, so to access the (i, j, k)th element of an array you would use "`array[i,j,k]`". IDL arrays also support ranges so "`array[5:10,3,4]`" will return a one dimensional array with five elements. "`array[5:*]`" specifies elements five to n of an n element array. "`array[*,3]`" picks out the third row of an array.

There are also a wide range of routines for querying and transforming arrays of data. For example, finding minimum and maximum values, performing FFTs, etc. These details can all be found by searching the on-line documentation.

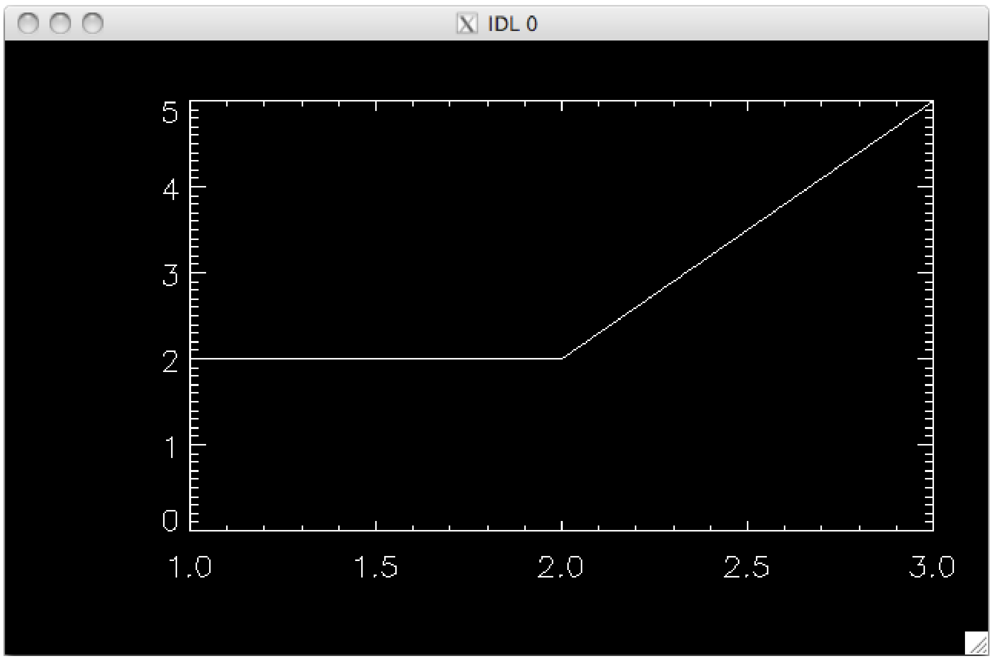
Finally, IDL is a full programming language so you can write your own functions and procedures for processing the data to suit your needs.

6.4 1D Plotting in IDL

The most commonly performed plot and perhaps the most useful data analysis tool is the 1D plot. In IDL, this is performed by issuing the command `plot,x,y` where "x" and "y" are one dimensional arrays of equal length. For each element "`x[i]`" plotted on the x-axis the corresponding value "`y[i]`" is plotted along the y-axis. As a simple example:

```
IDL> plot,[1,2,3],[2,2,5]
```

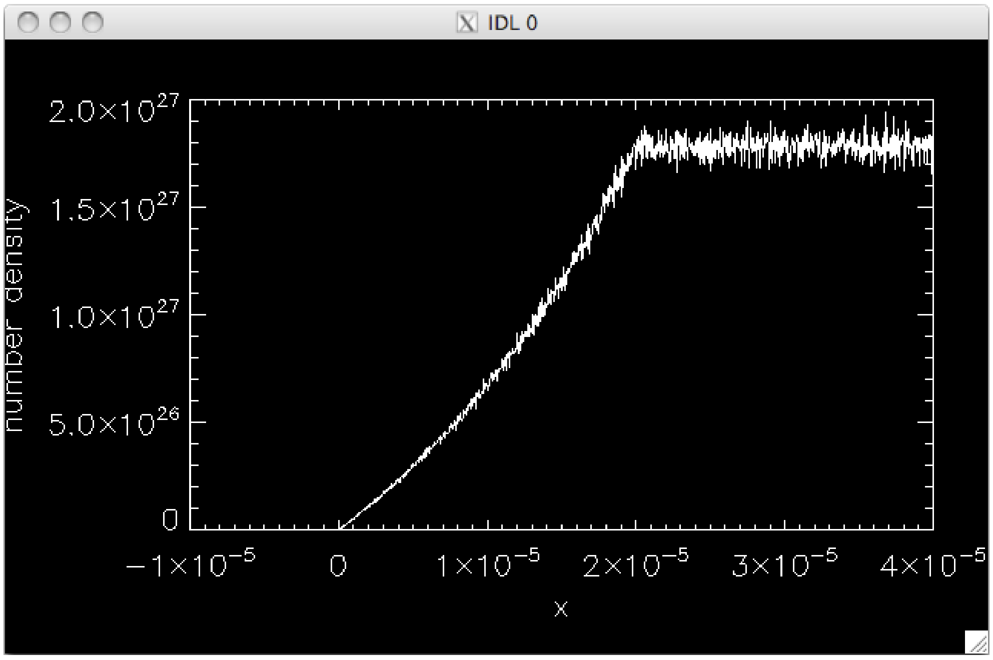
Gives rise to the following plot:



As a more concrete example, we will now take a one-dimensional slice through the 2D "`Number_Density`" array read in from our SDF data file. In this example we will give the x and y axes labels by passing extra parameters to the "`plot`" routine. A full list of parameters can be found in the on-line documentation. In this example we also make use of the "`$`" symbol which is IDL's line continuation character.

```
IDL> data = getdata(0)
IDL> plot,data.x,data.number_density[*,256],xtitle='x', $
IDL>    ytitle='number density'
```

This command generates the following plot:



6.5 Postscript Plots

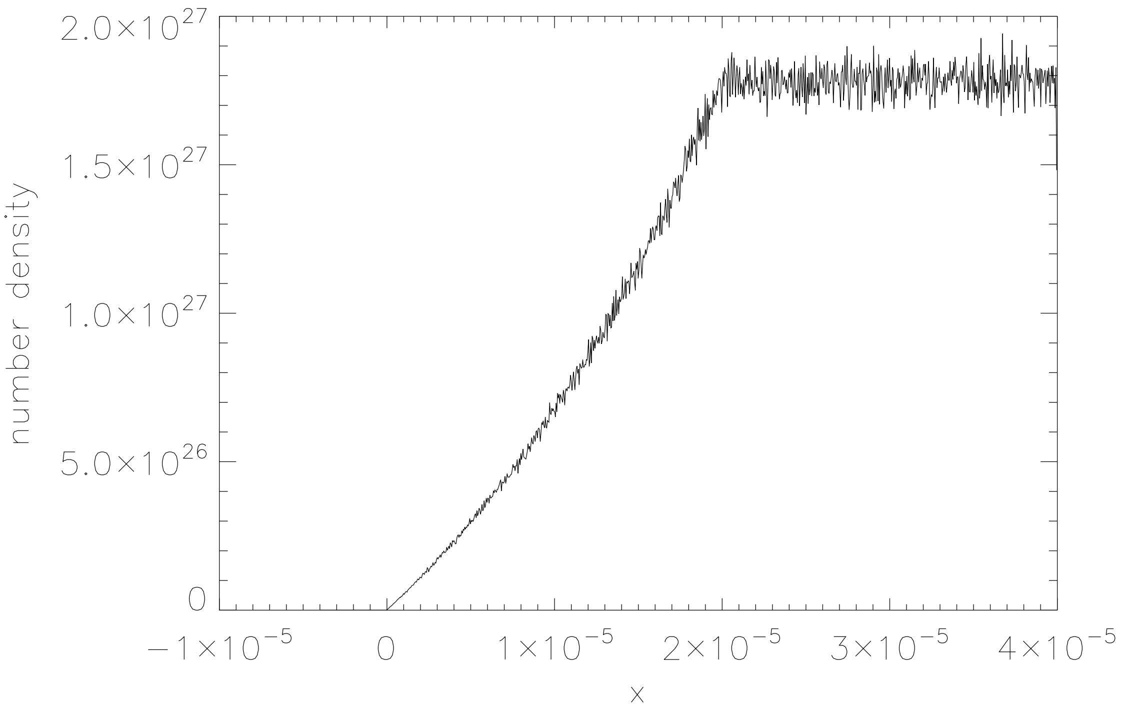
The plots shown so far have just been screen-shots of the interactive IDL plotting window. These are fairly low quality and could included as figures in a paper.

In order to generate publication quality plots, we must output to the postscript device. IDL maintains a graphics context which is set using the set_plot command. The two most commonly used output devices are "x" which denotes the X-server and "ps" which is the postscript device. Once the desired device has been selected, various attributes of its behaviour can be altered using the device procedure. For example, we can set the output file to use for the postscript plot. By default, a file with the name "idl.ps" is used.

Note that this file is not fully written until the postscript device is closed using the device,/close command. When we have finished our plot we can resume plotting to screen by setting the device back to "x".

```
IDL> set_plot,'ps'
IDL> device,filename='out.ps'
IDL> plot,data.x,data.number_density[*,256],xtitle='x', $
IDL>    ytitle='number density',charsize=1.5
IDL> device,/close
IDL> set_plot,'x'
```

This set of commands results in the following plot being written to a file named "out.ps".



By default, IDL draws its own set of fonts called "Hershey vector fonts". Much better looking results can be obtained by using a postscript font instead. These options are passed as parameters to the device procedure. More details can be found in the on-line documentation under "Reference Guides ⇒ IDL Reference Guide ⇒ Appendices ⇒ Fonts".

6.6 Contour Plots in IDL

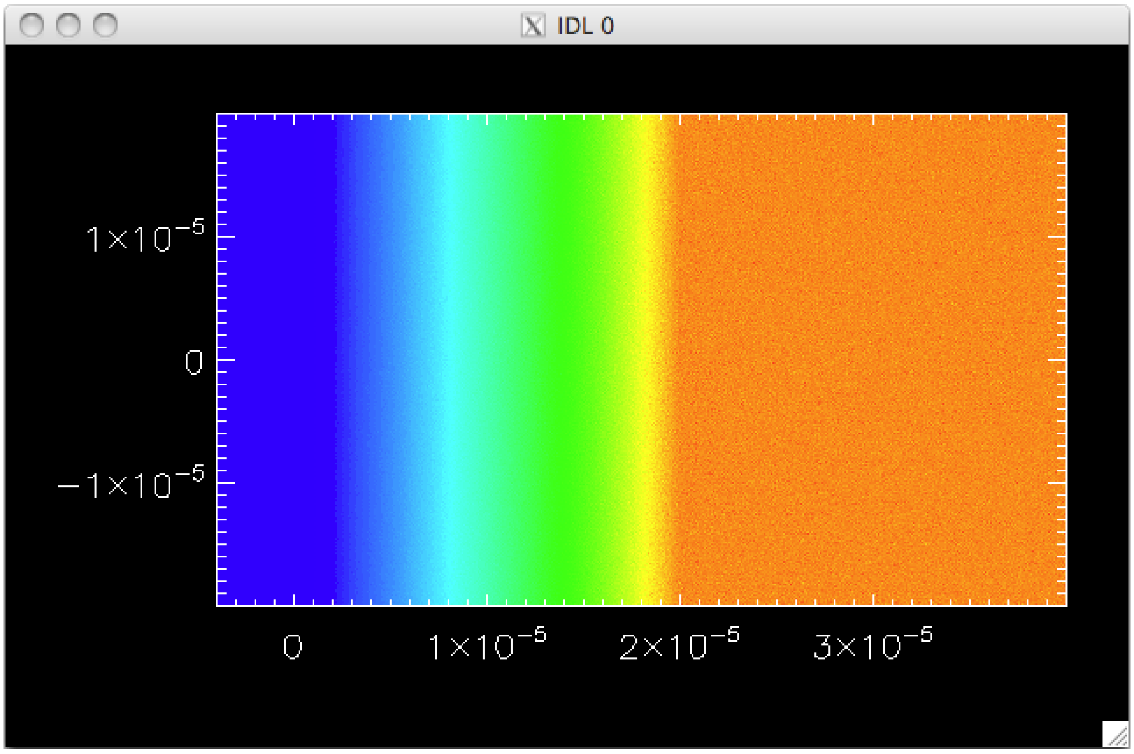
Whilst 1D plots are excellent tools for quantitive analysis of data, we can often get a better qualitative overview of the data using 2D or 3D plots.

One commonly used plot for 2D is the contour plot. The aptly named contour,z,x,y procedure takes a 2D array of data values, "z", and plots them against x and y axes which are specified in the 1D "x" and "y" arrays. The number of contour lines to plot is specified by the "`nlevels`" parameter. If the "`/fill`" parameter is used then IDL will fill each contour level with a solid colour rather than just drawing a line at the contour value.

The example given below plots a huge number of levels so that a smooth looking plot is produced. "`xstyle=1`" requests that the x axes drawn exactly matches the data in the "`x`" variable rather than just using a nearby rounded value and similarly for "`ystyle=1`".

```
IDL> n=100
IDL> levels=max(data.number_density)*findgen(n)/(n-1)
IDL> colors=253.*findgen(n)/(n-1)+1
IDL> contour,data.number_density,data.x,data.y,xstyle=1,ystyle=1, $
IDL>    levels=levels,/fill,c_colors=colors
```

Issuing these commands gives us the contour plot shown below. Note that the colour table used is not the default one but has been constructed to be similar to the one used by VisIt.

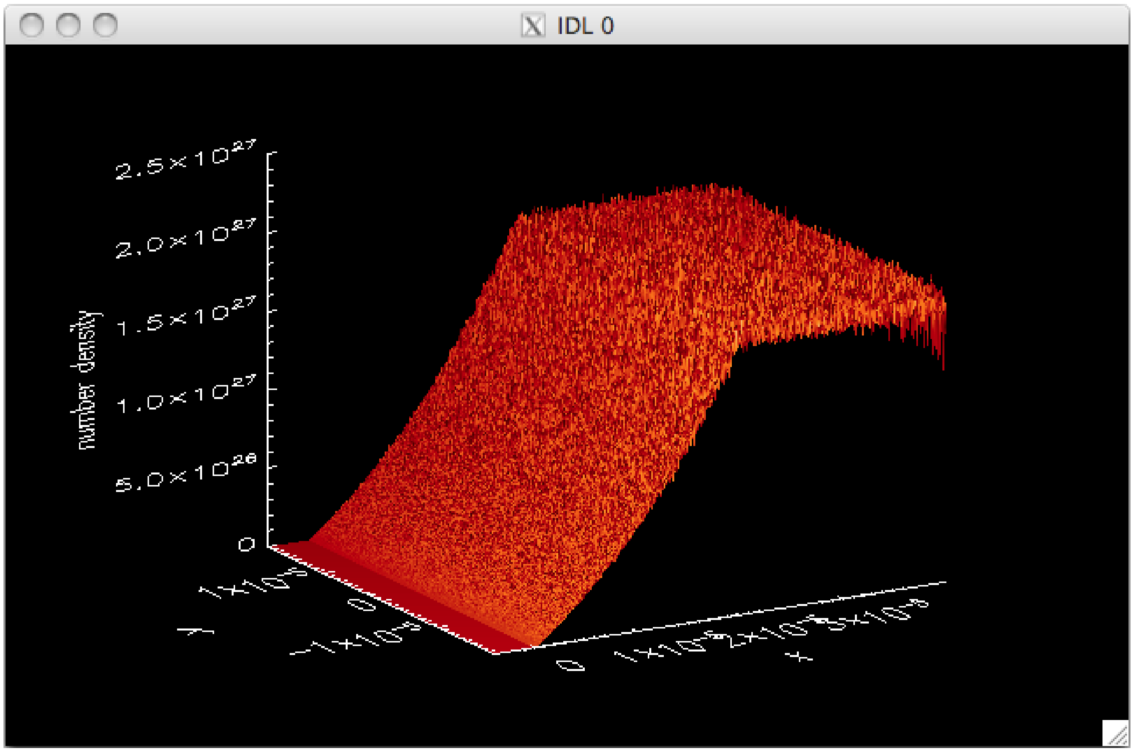


6.7 Shaded Surface Plots in IDL

Another method for visualising 2D datasets is to produce a 3D plot in which the data is elevated in the z direction by a height proportional to its value. IDL has two versions of the surface plot. `surface` produces a wireframe plot and `shade_surf` produces a filled and shaded one. As we can see from the following example, many of IDL's plotting routines accept the same parameters and keywords.

The first command shown here, `loadct,3`, asks IDL to load the third colour table which is "RED_TEMPERATURE".

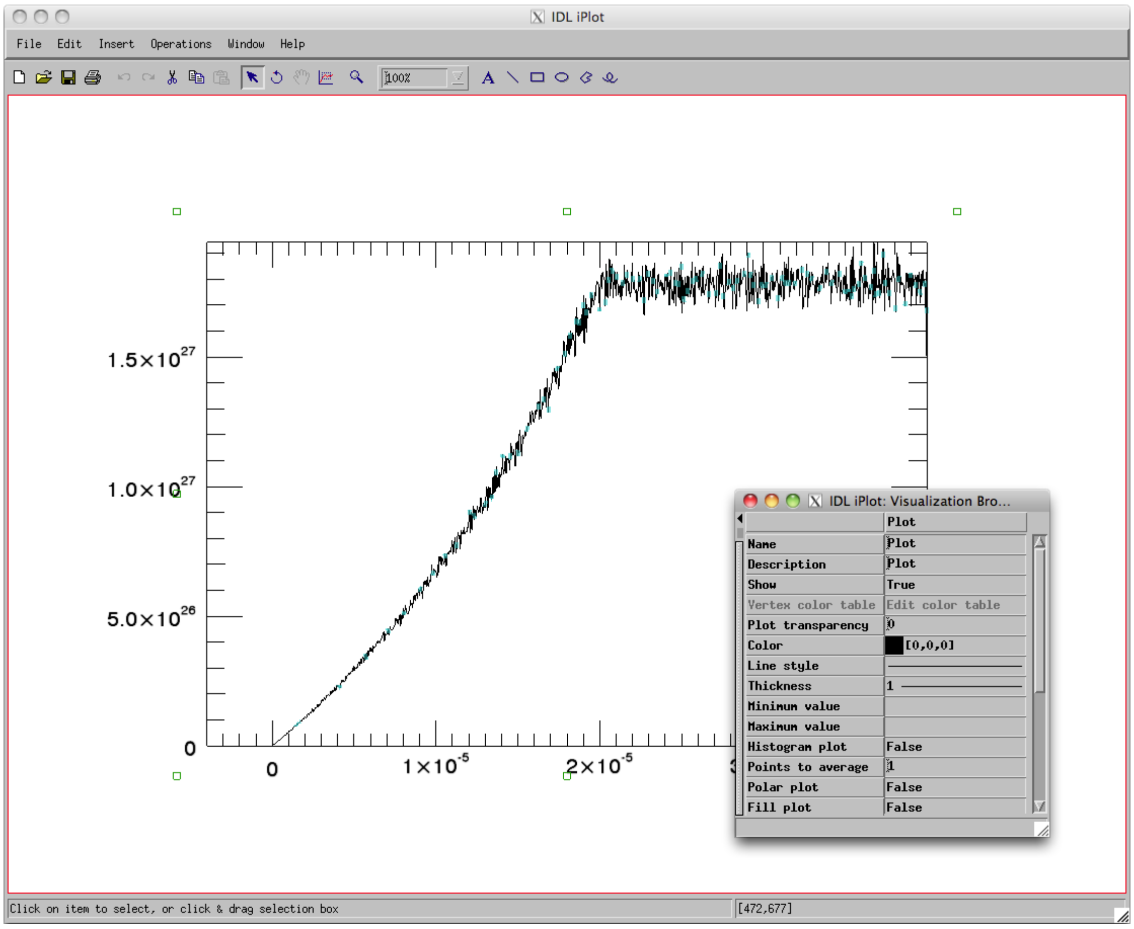
```
IDL> loadct,3
IDL> shade_surf,data.number_density,data.x,data.y,xstyle=1, $
IDL>    ystyle=1,xtitle='x',ytitle='y',ztitle='number density',charsize=3
```



6.8 Interactive Plotting

Finally, in recent versions of IDL it is now possible to perform all of these plot types in an interactive graphical user interface. The corresponding procedures are launched with the commands iplot, icontour and isurface.

```
IDL> iplot,data.x,data.number_density[*,256]
```



	Plot
Name	Plot
Description	Plot
Show	True
Vertex color table	Edit color table
Plot transparency	0
Color	■ [0,0,0]
Line style	———
Thickness	1 ———
Minimum value	
Maximum value	
Histogram plot	False
Points to average	1
Polar plot	False
Fill plot	False

Click on item to select, or click & drag selection box   [472,677]

IDL is an extremely useful tool but it also comes with a fairly hefty price tag. If you are not part of an organisation that will buy it for you then you may wish to look into a free alternative. It is also a proprietary tool and you may not wish to work within the restrictions that this imposes.

There are a number of free tools available which offer similar functionality to that of IDL, occasionally producing superior results.

For a simple drop-in replacement, the GDL project aims to be fully compatible and works with the existing EPOCH IDL libraries after a couple of small changes. Other tools worth investigating are “yorick” and “python” with the “SciPy” libraries. At present there is no SDF reader for either of these utilities but one may be developed if there is sufficient demand.

7 Using VisIt to visualise data

7.1 LLNL VisIt

LLNL’s VisIt software is a parallel data visualisation package (**`https://wci.llnl.gov/codes/visit/`**). EPOCH comes with source code for the plug-in needed to allow VisIt to load the SDF output files which are generated by EPOCH. There are full manuals for VisIt which can be downloaded from the above link so no further details will be given here. To build the plug-in, first ensure that the visit binary is in the $PATH environment variable. Then simply type “make visit” in one of the **`epoch{1,2,3}d`** directories. For more experienced users of VisIt, the xml file which is used to generate the plug-in is supplied in the VisIt subdirectory, called **`SDF2.xml`**.

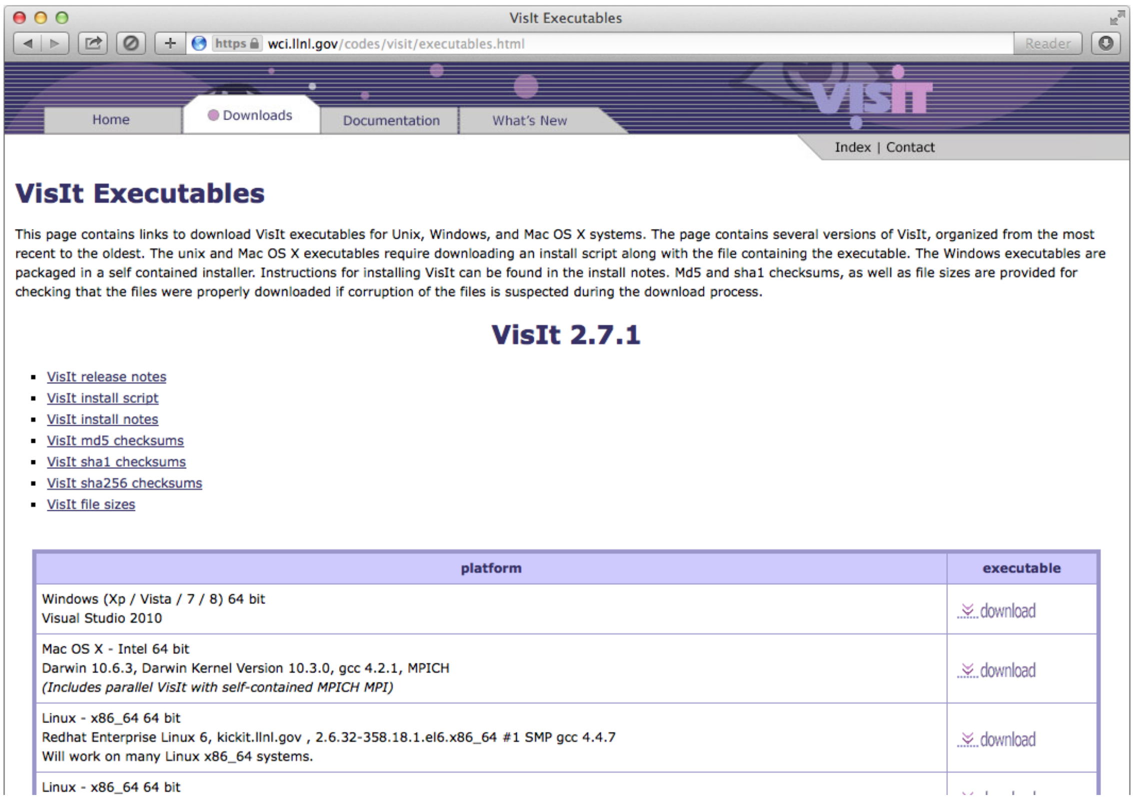
Whilst IDL is an excellent tool for visualising 1D and 2D datasets, it is extremely poor when it comes to dealing with 3D data. For this purpose, we recommend the use of the “VisIt” visualisation tool.

The other great advantage that VisIt has over IDL is the ability to render in parallel, enabling the visualisation of huge datasets which IDL would be incapable of dealing with.

- Initially developed by the Department of Energy (DOE) Advanced Simulation and Computing Initiative (ASCI)
- Now developed and maintained by the Lawrence Livermore National Laboratory along with a group of external contributors
- Written in C++ and supports python and Java interfaces
- Available for UNIX (Irix, Tru64, AIX, Linux, Solaris), Mac OS X (10.3 - 10.9), and Windows platforms
- Open source and freely available under the BSD license
- Plots, operators and database readers are implemented as plugins allowing the VisIt to be dynamically extended at run-time
- Powerful set of tools for manipulating, analysing and visualising 3D datasets
- Parallel and distributed architecture for visualising huge data sets

7.2 Obtaining And Installing VisIt

Both the source code and pre-compiled binaries are available for download from the projects web page which is found at the URL `https://wci.llnl.gov/codes/visit/home.html`



VisIt Executables

This page contains links to download VisIt executables for Unix, Windows, and Mac OS X systems. The page contains several versions of VisIt, organized from the most recent to the oldest. The unix and Mac OS X executables require downloading an install script along with the file containing the executable. The Windows executables are packaged in a self contained installer. Instructions for installing VisIt can be found in the install notes. Md5 and sha1 checksums, as well as file sizes are provided for checking that the files were properly downloaded if corruption of the files is suspected during the download process.

VisIt 2.7.1

- VisIt release notes
- VisIt install script
- VisIt install notes
- VisIt md5 checksums
- VisIt sha1 checksums
- VisIt sha256 checksums
- VisIt file sizes

platform	executable
Windows (Xp / Vista / 7 / 8) 64 bit Visual Studio 2010	download
Mac OS X - Intel 64 bit Darwin 10.6.3, Darwin Kernel Version 10.3.0, gcc 4.2.1, MPICH *(Includes parallel VisIt with self-contained MPICH MPI)*	download
Linux - x86_64 64 bit Redhat Enterprise Linux 6, kickit.llnl.gov , 2.6.32-358.18.1.el6.x86_64 #1 SMP gcc 4.4.7 Will work on many Linux x86_64 systems.	download
Linux - x86_64 64 bit	

There are full instructions for compiling the project from source code along with build scripts written to help ease the process. However, this is not recommended as it is an extremely large tool and the compilation takes hours to complete. It is usually far easier to download a pre-compiled binary which matches your system architecture.

However, occasionally compilation may be a necessary step. Linux in particular is a moving target and it is not always possible to find a binary which matches the particular combination of libraries installed on your system.

The easiest way to install the VisIt tool is to ask the system administrator to do it for you. However, this may not always be the best option. The system in question may be run by someone who is not concerned with your particular software needs or has insufficient skills to deal with the task. In any case, VisIt has a fairly rapid release schedule and you may find that some functionality you need is not present in the version installed on the machine.

Fortunately, for all these scenarios it is usually quite easy to install a copy in your own home directory. Just find a binary on the web page `https://wci.llnl.gov/codes/visit/executables.html` which closely matches your machine and download it. This can be unpacked into your home directory with the command `tar xzf visit2_7_1.linux-x86_64.tar.gz`. The actual name of the file will vary depending on which version you downloaded. This will unpack the VisIt binary into a subdirectory named `visit/`. Now all that is necessary is to add this to your search path. eg. `export PATH=$HOME/visit/bin:$PATH`

These instructions illustrate the steps required for installing your own copy of VisIt when you have no other choice. VisIt is an extremely large program, so if a version is already available then it is usually better to use the installed version.

The machines at Warwick have a recent version of VisIt installed which is available via the "`modules`" system. To make use of it you must first issue the command `module load visit`.

7.3 Compiling The Reader Plugin

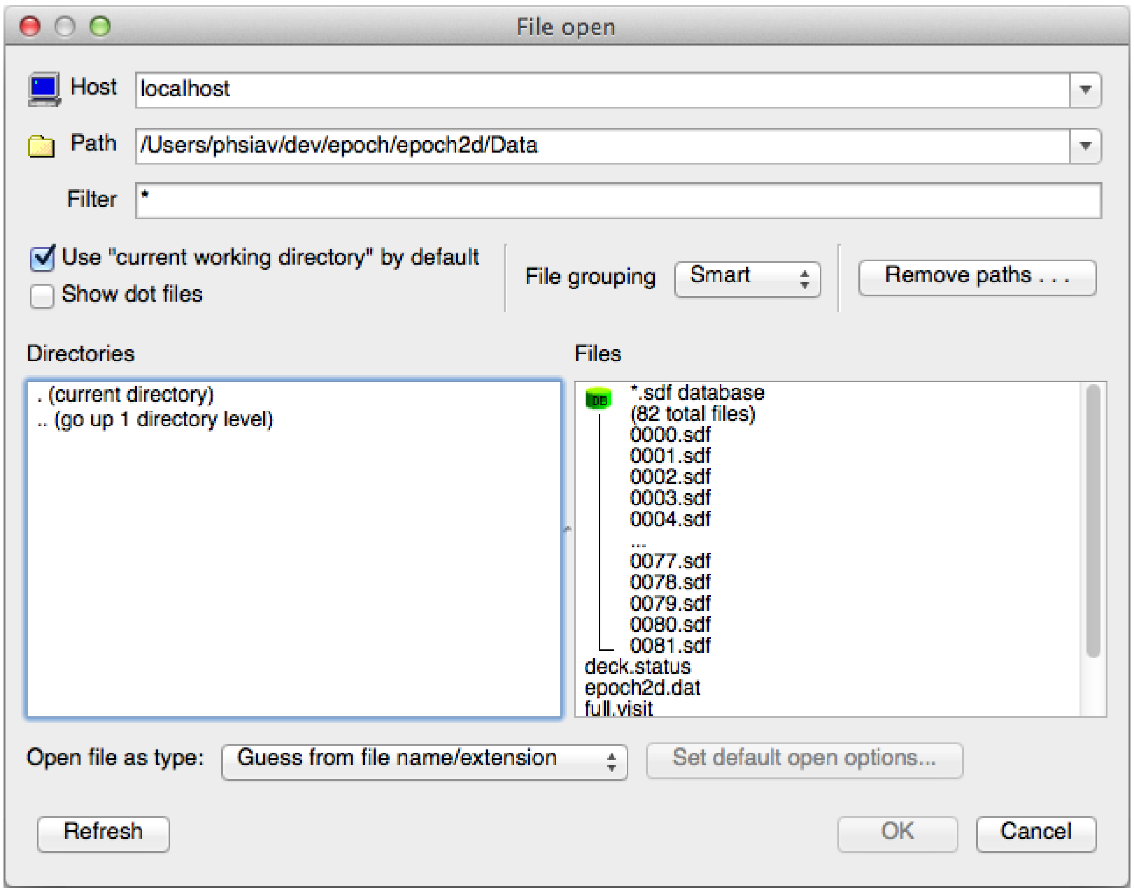
One piece of compilation which is almost always necessary is that of the SDF reader plugin. This is shipped as source code in a subdirectory of the EPOCH repository. It is located in the `VisIt/` subdirectory of the main `epoch/` directory. The reader will work for any SDF file generated by any code which uses the SDF I/O routines. You do not need a separate reader for each version of EPOCH.

To compile, first navigate to one of the `epoch*d/` directories in your EPOCH repository. Just type "make visit" and the build scripts should take care of the rest. The SDF reader plugin will be installed into the directory `$HOME/.visit/linux-intel/plugins/databases/` on your system. Note that the `linux-intel/` component will vary depending on your machine operating system and architecture.

Each time you install a new version of VisIt you must recompile the reader to match the new installation. It will also occasionally be necessary to recompile when changes occur to the SDF data format or the reader plugin itself. The developers will notify users if this is the case, although it does no harm to regularly recompile the reader as a matter of course.

We will see later that it is possible to do remote data visualisation with VisIt in which the GUI is launched and interacted with on one machine and the data files are located on a separate machine entirely. In this situation the reader must be installed on the remote machine and must match the setup there. The setup on the local machine is unimportant. In fact it is not even necessary to have the plugin installed on the local machine. This is particularly useful when using a Windows environment to analyse data located on a remote UNIX workstation.

7.4 Loading Data Into VisIt


File open

Host: localhost

Path: /Users/phsiav/dev/epoch/epoch2d/Data

Filter: *

☑ Use "current working directory" by default

☐ Show dot files

File grouping: Smart

Remove paths . . .

Directories

. (current directory)
.. (go up 1 directory level)

Files

```
*.sdf database
(82 total files)
  0000.sdf
  0001.sdf
  0002.sdf
  0003.sdf
  0004.sdf
  ...
  0077.sdf
  0078.sdf
  0079.sdf
  0080.sdf
  0081.sdf
deck.status
epoch2d.dat
full.visit
```

Open file as type: Guess from file name/extension

Set default open options...

Refresh

OK

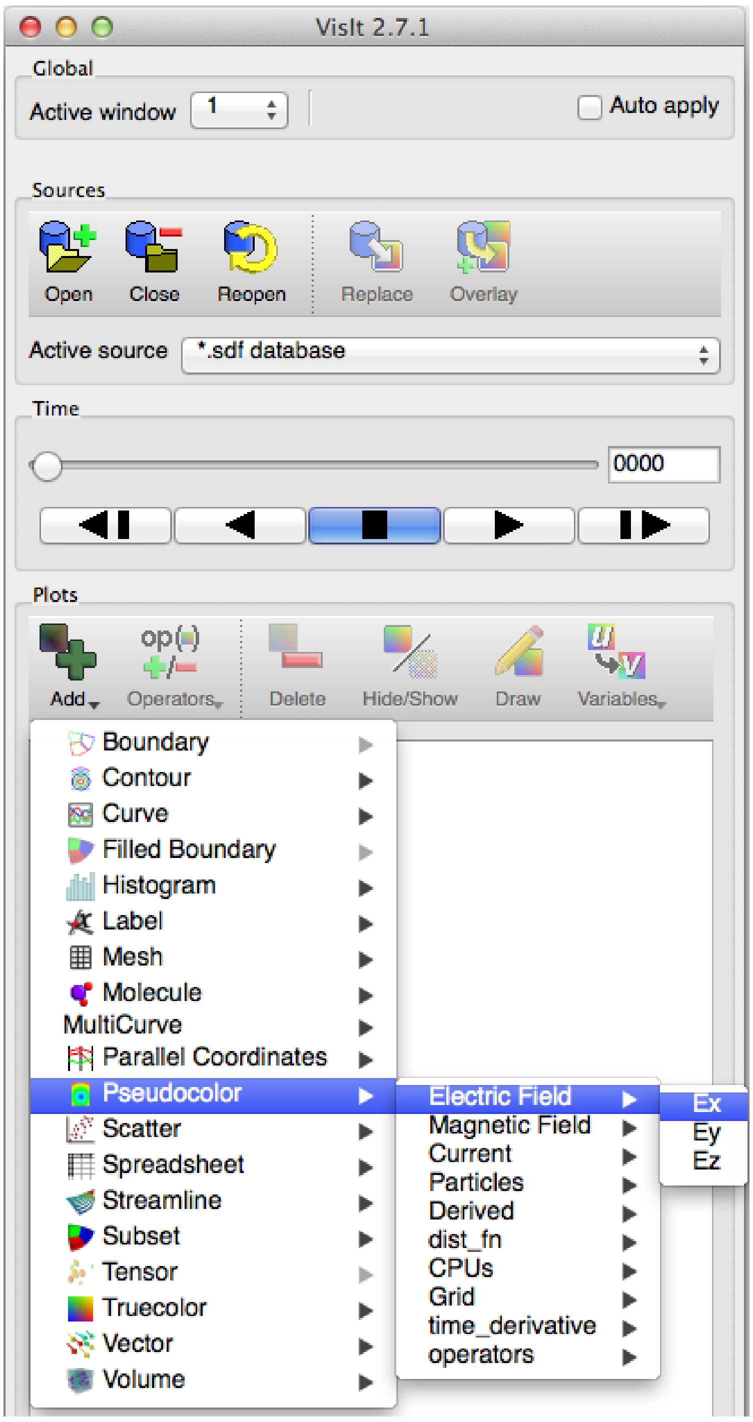
Cancel

The most straightforward method for loading data into VisIt is to start the application and then browse the filesystem for the dataset you are interested in. This is done by selecting "File ⇒ Open file" from the VisIt menu bar. A file selection dialogue will appear allowing you to browse directories along with the options to filter the results according to a given regular expression and grouping options. By default, VisIt will attempt to group all files containing the same suffix and some kind of numbering system into a sort of virtual database.

The right-hand pane of this window shows a list of selected files which will appear in the main VisIt window when you are finished.

An alternative method of specifying the data file to open is to pass a command line option when the tool is launched. An example of this method is `visit -o Data/0000.sdf`. When the file is specified in this manner the list of files shown in the VisIt window will also include the full list of files in the dataset's subdirectory and all the files in the current working directory. The other SDF files will be grouped together in a virtual database.

Yet another method for selecting the dataset to use is by opening a previously saved session file. We will discuss this further in a later section.


Active window 1
Auto apply
Active source *.sdf database
0000

Once an SDF file has been successfully loaded the "Add" menu item will become un-greyed and the cycle numbers for each file in the virtual database will be displayed. If we navigate to one of the plot types we are able to select the variable to plot from a drop-down list.

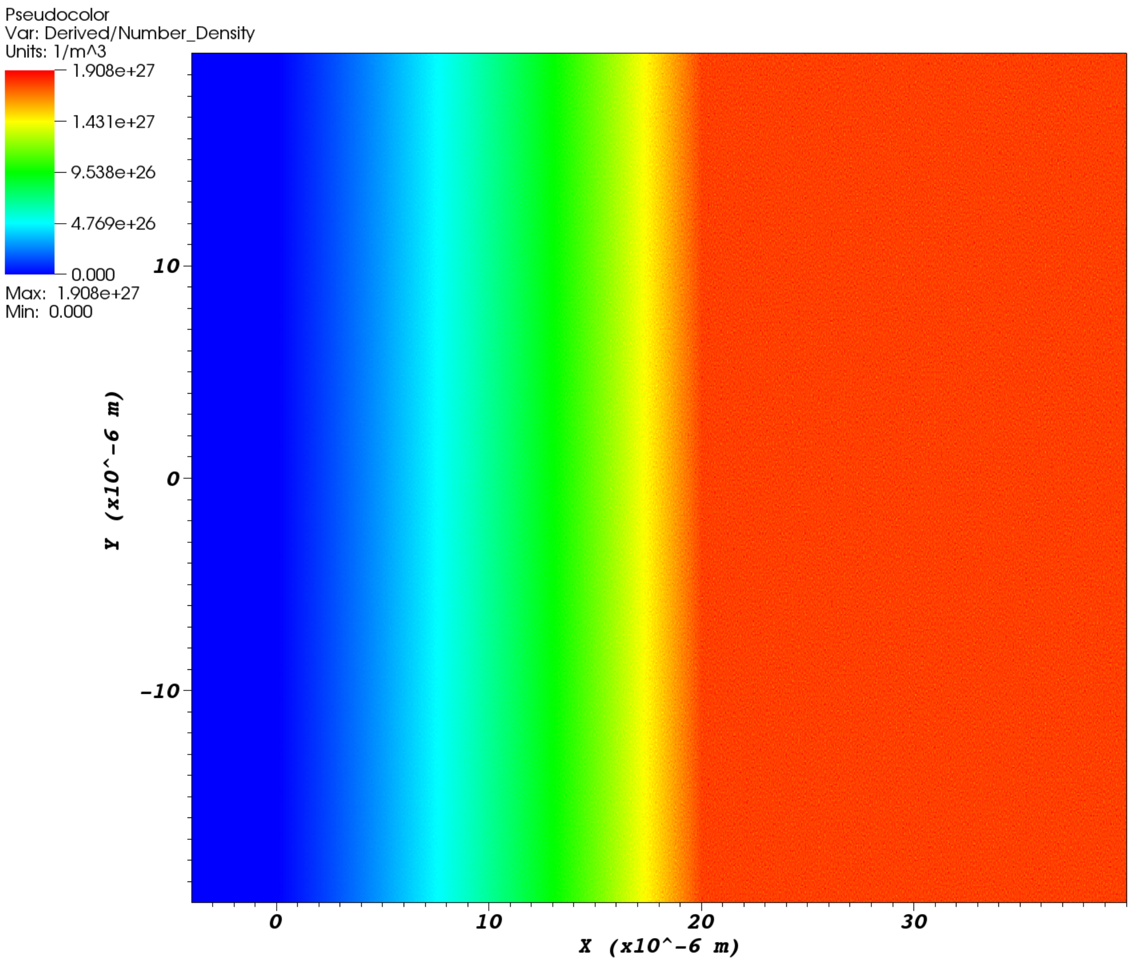
7.5 Contour Plots in VisIt

We will now replicate each of the plots which we generated using IDL in earlier sections. For reasons which will soon become clear we begin with the contour plot and move on to the 1D plot in the next section.

Having opened the same dataset we were using in the IDL discussion we now select the "Add" menu item. Notice that many of the plot types listed here are greyed out and cannot be selected. This is because many of the plots are dependent on the type or dimensionality of the variable to be plotted. If our dataset contains no variables which match the required properties for a plot, the plot menu will be disabled.

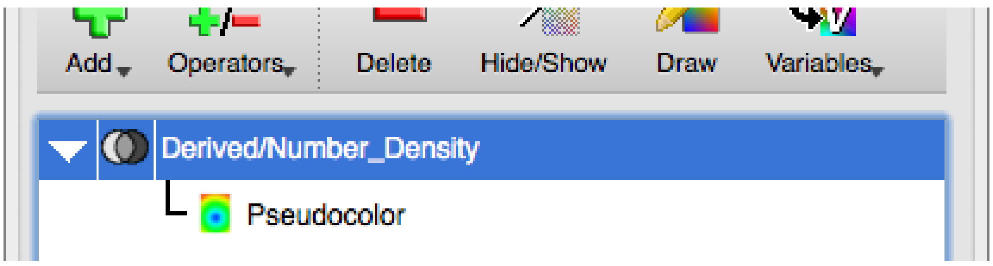
For the current dataset there is no "Boundary" plot available since this requires multi-material data and none of our variables meet that criteria.

The list contains a menu item for a "Contour" plot. We are not going to select this item since it only generates a contour plot with lines indicating each contour level and not a filled version. Instead we choose "Add ⇒ Pseudocolor ⇒ Derived ⇒ Number_Density" and then hit the "Draw" button.

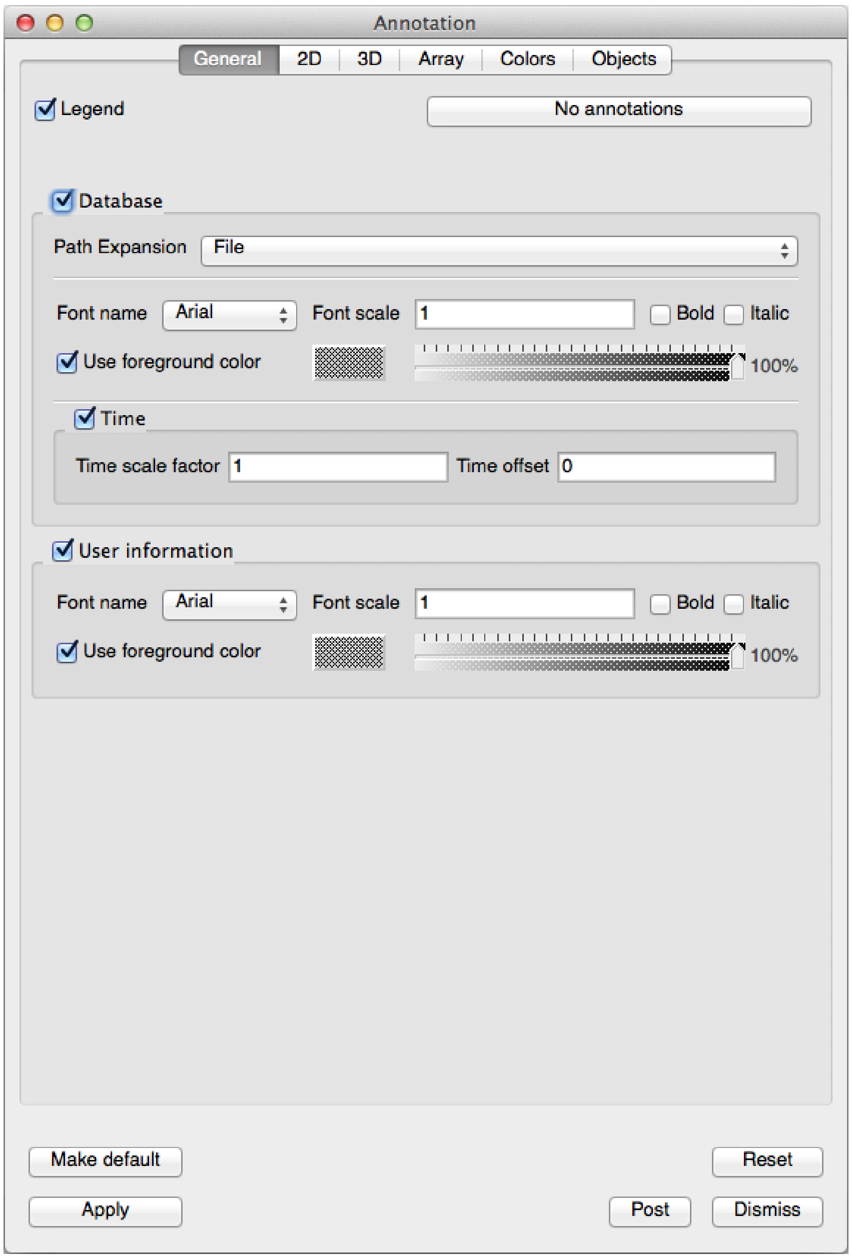


There are many settings which can alter the visual appearance of plots generated by VisIt. The first point of call is usually to open up the "Plot Attributes" or "Operator Attributes" dialogue corresponding to the plot in question. A simpler method for accomplishing this task is to double-click on the plot in the main VisIt menu pane which will launch the corresponding "Plot Attributes" dialogue.

If it is the operator attributes you wish to change, click on the white arrow on the left hand side of the plot in the main VisIt menu pane. This will drop down to reveal a list containing the plot and all operators acting on it. Double-clicking on an operator will launch the corresponding "Operator Attributes" dialogue.



Another important tool for controlling the appearance of plots can be found in "Controls ⇒ Annotation" from the VisIt menu bar. This allows all of the plot annotations to be modified such as the legend, title, axis labels, etc.


Annotation

General | 2D | 3D | Array | Colors | Objects

☑ Legend — No annotations

☑ Database
Path Expansion: File
Font name: Arial — Font scale: 1 — ☐ Bold ☐ Italic
☑ Use foreground color — 100%

☑ Time
Time scale factor: 1 — Time offset: 0

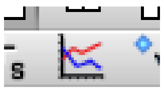
☑ User information
Font name: Arial — Font scale: 1 — ☐ Bold ☐ Italic
☑ Use foreground color — 100%

Make default | Reset
Apply | Post | Dismiss

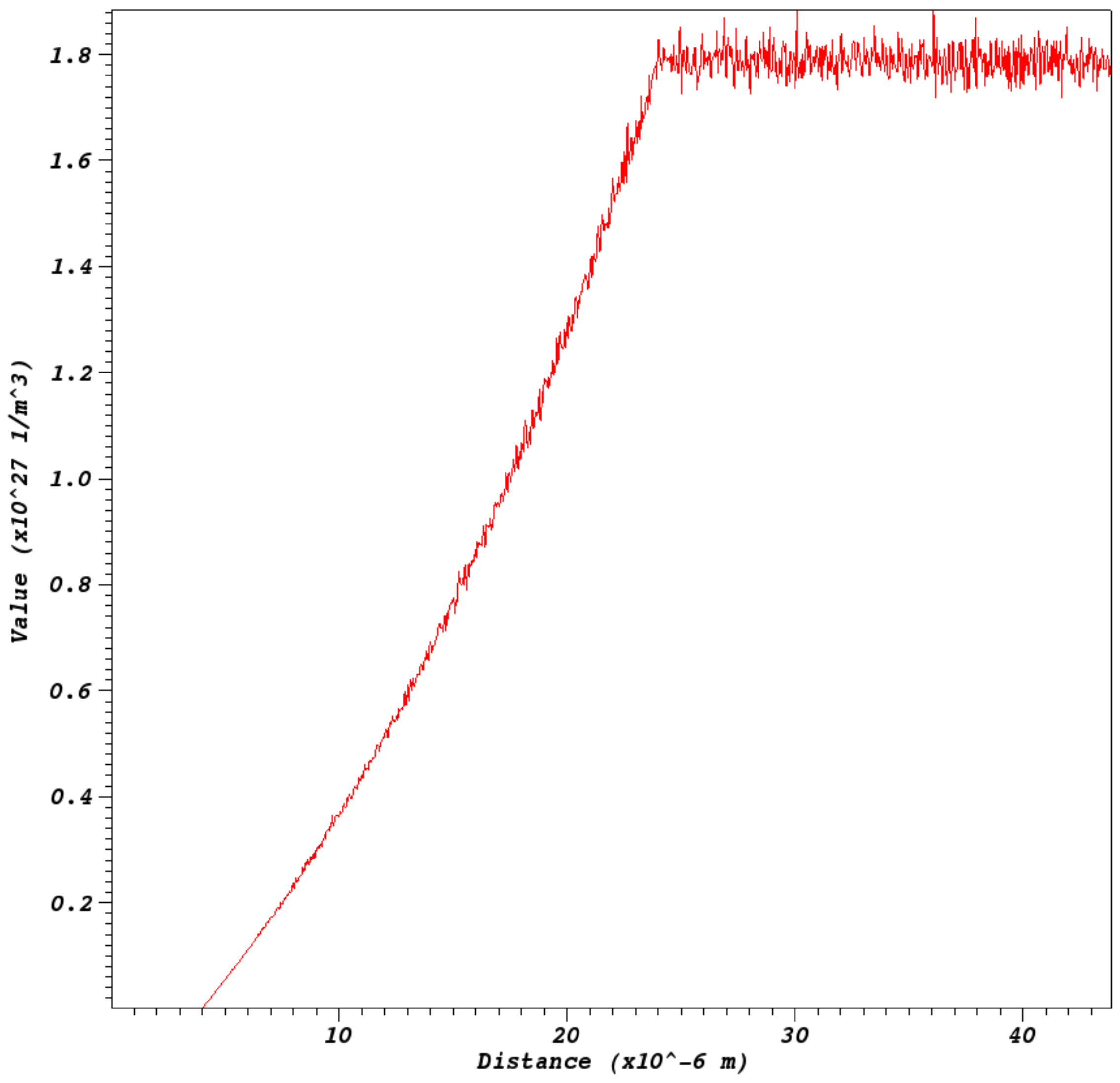
7.6 1D Plotting in VisIt

A 1D plot in VisIt is called a "Curve" plot. We already mentioned that this was greyed out because we have no one dimensional variables in our data file.

The solution to this dilemma is the lineout operator which extracts a one dimensional array from a 2D or 3D variable. This operator is selected by pressing the button with red and blue lines located at the top of the plot window.



Once the button has been pressed, we can click and drag anywhere in the "Pseudocolor" plot window. When we release the mouse button a new plot window pops up containing a "Curve" plot of the data just selected.

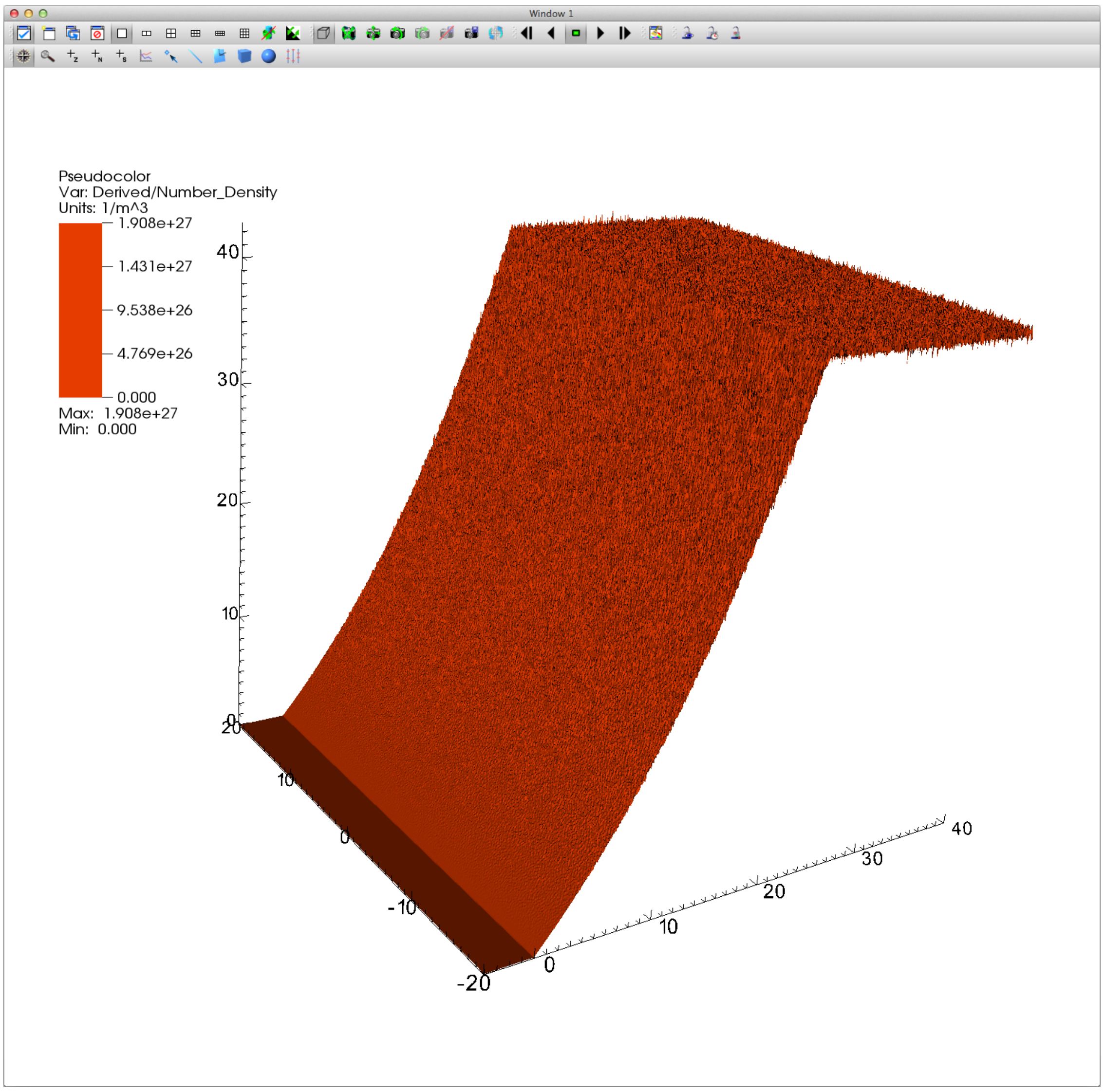


In order to change the attributes for this plot, we must first select "Active window" number 2 in the main VisIt pane.

7.7 Shaded Surface Plots in VisIt

Again, we will confusingly refuse to pick the obvious plot type for this task. There is "Surface" plot listed in the menu. However, most of the time the "Elevator" operator does what we want and also gives us more flexibility.

The first step is to do a "Pseudocolor" plot of "Number_Density" as we did before. Next select the "Operator Attributes ⇒ Transforms ⇒ Elevate" menu item. In the pop up dialogue click on the "Elevation height relative to XY limits?" and then "Apply". Click "Yes" when the warning dialogue pops up.

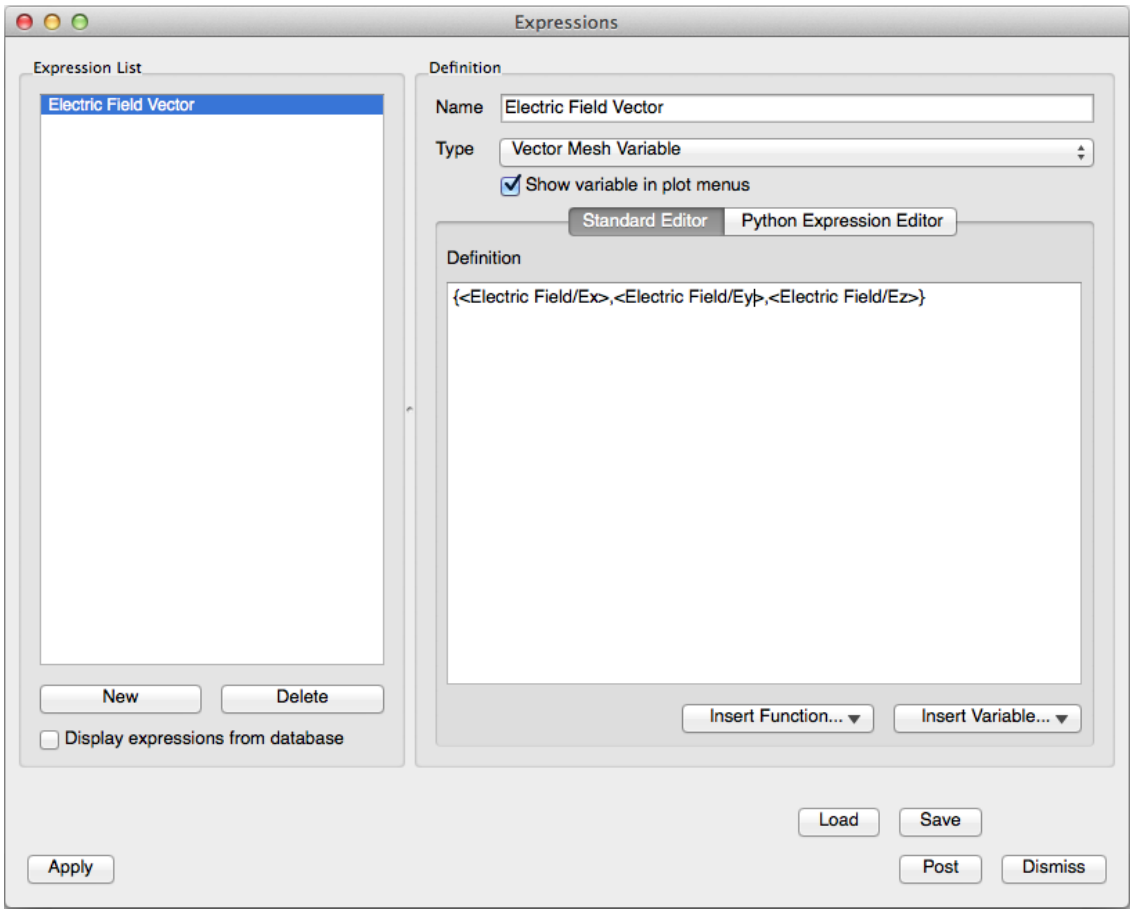


To make this plot look similar to the one generated by IDL, we have changed the colour table using "Controls ⇒ Color table". We also changed the axis appearance with the annotations menu discussed earlier and changed the height of the elevation using the min and max operator attributes.

7.8 Creating User-Defined Expressions

VisIt comes with an extremely powerful method of manipulating data before visualising the results. The basic idea is that an array is transformed by applying a set of mathematical functions on all its elements and then the result is defined as a new variable. Once defined, this variable behaves in exactly the same way as any of the variables read from the data file.

As an example, we can combine the three components of electric field to generate a single electric field vector.



Name: Electric Field Vector

Type: Vector Mesh Variable

☑ Show variable in plot menus

Definition: {<Electric Field/Ex>,<Electric Field/Ey>,<Electric Field/Ez>}

Now when we return to the “Add” menu we see that the “Vector” and “Streamline” plot types now have an entry for our newly defined vector.

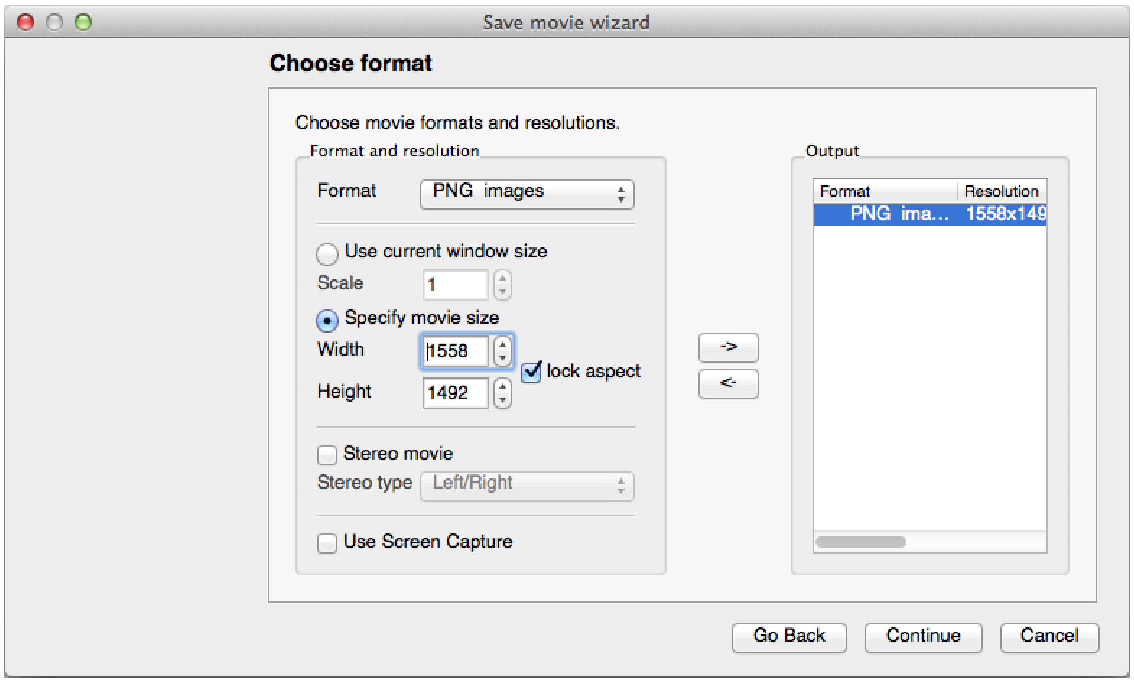
7.9 Creating Movies

A compelling visualisation of numerically generated data is often made by combining a series of images into a movie. This can be an invaluable method for illustrating the basic behaviour of a system as it changes over time. Alternatively rotating around a 3D scene can sometimes give a much better idea of the structure in the model being presented. There can also be much to gain by constructing visual fly-throughs of a scene, dynamically slicing through sets of data or combinations of all these techniques.

VisIt provides several facilities for generating movies from your data. The simplest of these is to select the “File ⇒ Save movie” menu item. This pops up a movie wizard which will walk you through the process of generating a simple linear movie based on the time-advancing snapshots represented by your virtual database of files. Alternatively you can select one of the pre-defined movie templates which manipulate the currently selected plot and create a movie from that.

Creating a simple time advancing movie is as simple as walking through the wizard dialogue and selecting from the self-explanatory options presented to you.

For many uses, the wizard will give exactly the desired results. However it is occasionally useful to have a little more control over how the movie is created. In such cases it can be useful to specify an image format such as “PNG” to save to rather than “MPEG”. VisIt will then generate one image per frame and number them consecutively. At the end of the process the images can be converted into a movie using whatever tool best accomplishes the task.


Save movie wizard

Choose format

Choose movie formats and resolutions.

Format and resolution

Format: PNG images

( ) Use current window size

Scale: 1

(●) Specify movie size

Width: 1558

Height: 1492

[✓] lock aspect

[ ] Stereo movie

Stereo type: Left/Right

[ ] Use Screen Capture

Output

Format	Resolution
PNG ima...	1558x149

Another useful tip is to select the “Later, tell me the command to run” radio button. This will output a long command which can run from a UNIX terminal screen. The advantage is that no X session is required so the command can be run in the background. It also becomes a simple task to interrupt the job at any point and resume it from where it left off at a later date. In a similar manner it is easy to resume a job which crashes half way through for any reason.

More complex movies can be created by using VisIt’s keyframing facility which allows you to change animation attributes such as view or plot attributes as the animation progresses. Further information about this somewhat complex task can be found in the on-line help.

Finally, you can use VisIt’s python scripting interface to programmatically describe the details of each frame as the movie progresses. This approach offers far more flexibility in what can be achieved but is also much more involved and time consuming than the previous two methods. Again, further information on this subject can be found in the on-line help system.

7.10 Remote Visualisation

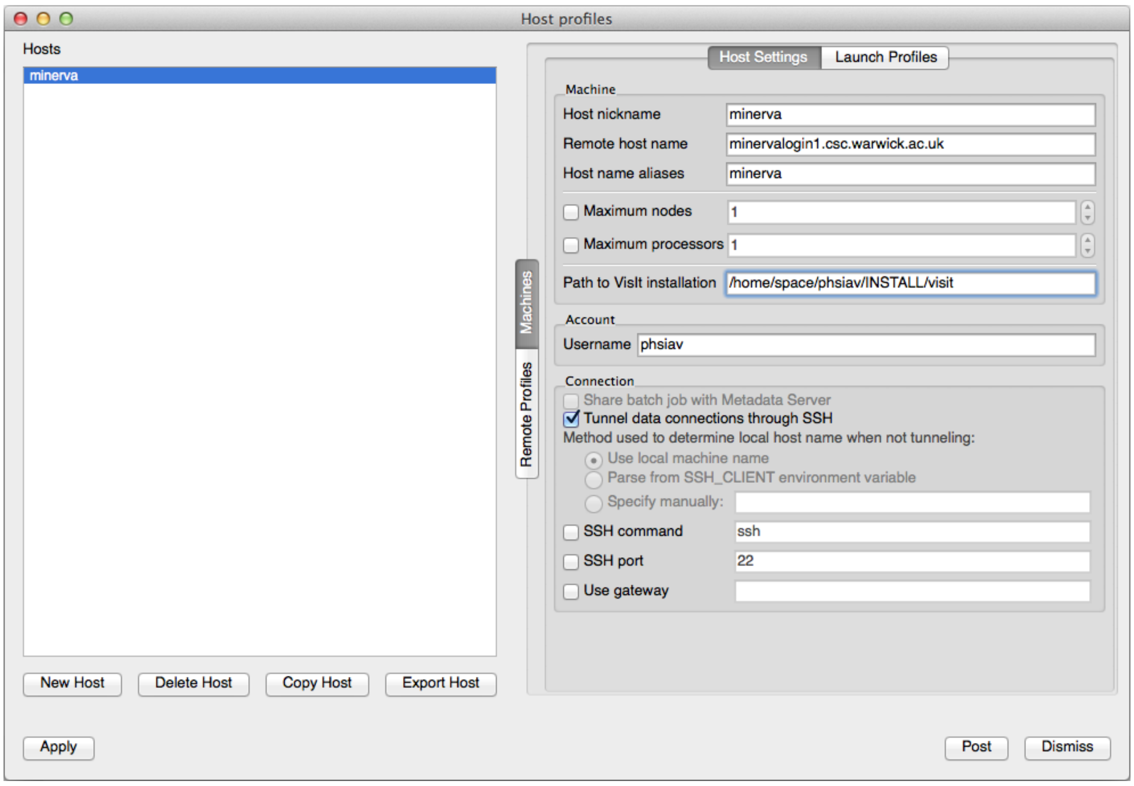
It was mentioned earlier that it is possible to perform remote visualisation using VisIt. This is a process in which the data files being interrogated reside on a different machine to the one on which the VisIt GUI runs and where the results are plotted.

This method of working can be extremely useful when the data is generated on a powerful machine located in an external environment such as a large cluster. Another common use is when EPOCH is executed on a UNIX machine and the desktop used for visualisation is running Windows.

It is sometimes possible to run a graphical tool on the remote machine and tunnel the X-server session through to the local machine but this can be quite slow and unstable. When connecting to a remote VisIt instance the only data which needs to be sent between machines is the pre-rendered image and a few simple plotting commands. Naturally, this can be a much faster approach.

Also, as mentioned before, it is possible to use a machine on which the reader plugin is difficult or impossible to compile for and connect to a machine on which the reader is already installed.

In order to use the remote visualisation facility, you must first set up a “Host profile” for the remote machine using the “Options ⇒ Host profiles” menu item. The pre-compiled binaries are shipped with a long list of pre-defined host profiles. These are unnecessary for anyone not affiliated and can safely be removed by deleting the directory `$HOME/visit/current/.visit/` (assuming you have unpacked the VisIt tarball into your home directory).


Host profiles

Hosts
minerva

Machines | Remote Profiles

Host Settings | Launch Profiles

Machine

Host nickname	minerva
Remote host name	minervalogin1.csc.warwick.ac.uk
Host name aliases	minerva
☐ Maximum nodes	1
☐ Maximum processors	1
Path to VisIt installation	/home/space/phsiav/INSTALL/visit

Account

Username	phsiav

Connection

☐ Share batch job with Metadata Server
✓ Tunnel data connections through SSH
Method used to determine local host name when not tunneling:
● Use local machine name
○ Parse from SSH_CLIENT environment variable
○ Specify manually:

☐ SSH command	ssh
☐ SSH port	22
☐ Use gateway	

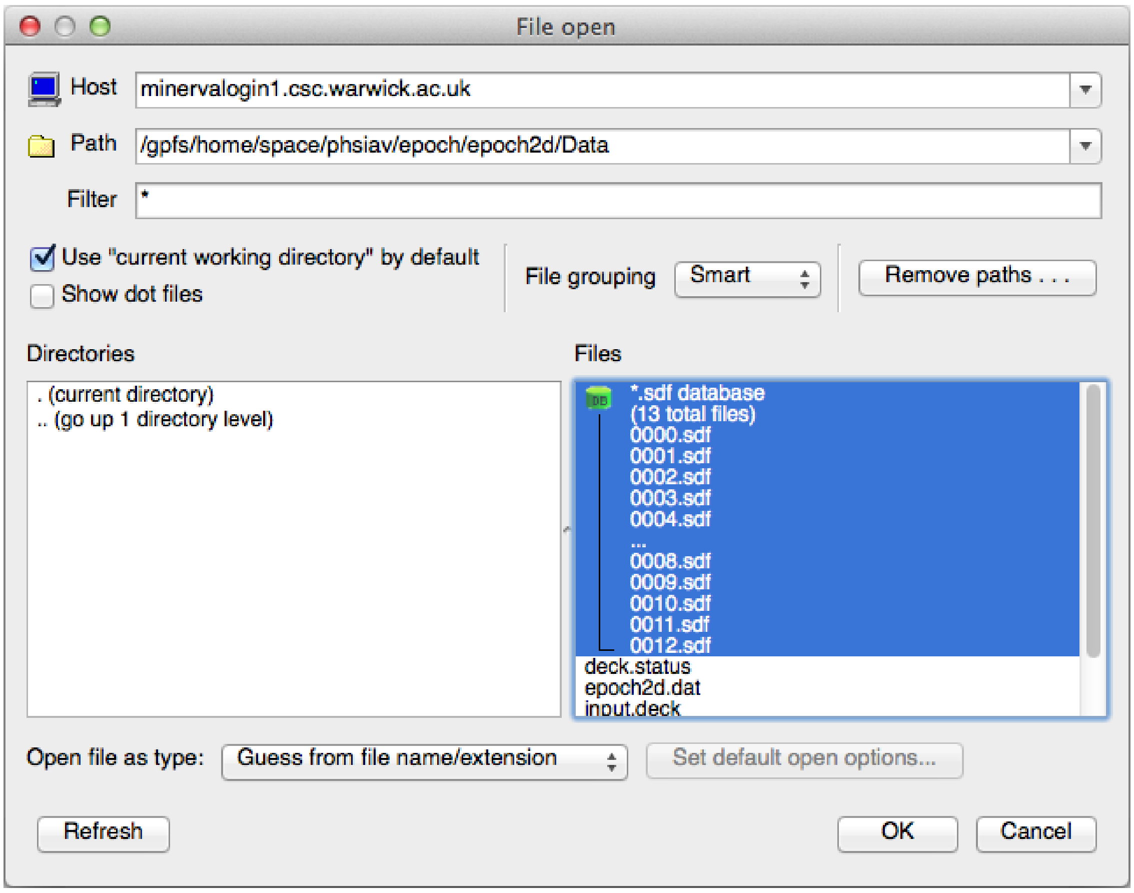
New Host | Delete Host | Copy Host | Export Host

Apply | Post | Dismiss

Create a new profile by clicking on the “New Host” button and filling out some of the form fields. The important ones to change are “Host nickname”, “Remote host name”, “Host name aliases” and “Username”. If the visit binary is not in your default search path on the remote machine then you must specify its location by filling in the “Path to VisIt installation” field.

Now click “Apply” and “Dismiss” followed by the “Options ⇒ Save Settings” menu item to ensure that the profile is saved for future sessions.

Data on the remote machine can now be loaded by selecting “File ⇒ Open file” and picking the desired host profile from the drop down list of “Hosts”. VisIt will wait for the remote process to launch and then continue with the file selection procedure but now displaying files located on the remote machine rather than the local one. From this point on everything should work as before except you should see the name of the remote machine in the “Selected files” dialogue.


File open

Host minervalogin1.csc.warwick.ac.uk

Path /gpfs/home/space/phsiav/epoch/epoch2d/Data

Filter *

[✓] Use "current working directory" by default

[ ] Show dot files

File grouping: Smart

Remove paths . . .

Directories
. (current directory)
.. (go up 1 directory level)

Files
*.sdf database
(13 total files)
0000.sdf
0001.sdf
0002.sdf
0003.sdf
0004.sdf
...
0008.sdf
0009.sdf
0010.sdf
0011.sdf
0012.sdf
deck.status
epoch2d.dat
input.deck

Open file as type: Guess from file name/extension

Set default open options...

Refresh OK Cancel

7.11 Parallel Visualisation

Parallel visualisation is performed in almost exactly the same manner as remote visualisation. Again, you must create a host profile for the purpose except this time you need to set up a parallel launch profile in the “Launch Profiles” tab pane. Click the “New Profile” button, give the profile a name and then set the required options in the “Parallel” tab on the bottom section of the page. Selecting the “Launch parallel engine” radio button will allow you to set the various launch options which relate to the cluster on which the job will run.

The major difference now is due to the fact that VisIt must be launched by an external job script which fits in with the queueing system used by the parallel machine. Usually you will need to consult with the system administrator of the cluster to confirm which launch method and arguments to use.

The details of job launch can be better understood by reading through the “User documentation” section provided at http://www.visitusers.org/. Of particular help here is the “Getting VisIt to run in parallel” section and the “How VisIt Launching works” entry in the “Developer documentation” section.

A Changes between version 3.1 and 4.0

A.1 Changes to the Makefile

Some changes have been made to the Makefile. These are documented in Section 2.4.

The following compile-time defines have been added to the Makefile:

- NO_IO
- PARTICLE_ID
- PARTICLE_ID4
- COLLISIONS_TEST
- PHOTONS
- TRIDENT_PHOTONS
- PREFETCH

The following compile-time defines have been removed from the Makefile:

- COLLISIONS
- SPLIT_PARTICLES_AFTER_PUSH
- PARTICLE_IONISE

A.2 Major features and new blocks added to the input deck

- CPML boundary conditions - See Section 3.2.1
- Thermal boundary conditions - See Section 3.2.2
- Collisions - See Section 3.11
- QED - See Section 3.12
- Subsets - See Section 3.13
- Ionisation - See Section 3.3.2
- Single-precision output - See Section 3.7.8
- Multiple output blocks - See Section 3.7.9
- Particle migration - See Section 3.3.1

A.3 Additional output block parameters

The following parameters have also been added to the "output" block (see Section 3.7.2):

- dump_first
- dump_last
- force_first_to_be_restartable
- ejected_particles
- absorption
- id
- name
- restartable

A.4 Other additions to the input deck

- npart_per_cell - See Section 3.3
- dir_{xy,yz,zx}_angle - See Section 3.9
- particle_tstart - See Section 3.1
- identify - See Section 3.3

Finally, the input deck now has a method for writing continuation lines. If the deck contains a "\" character then the rest of the line is ignored and the next line becomes a continuation of the current one.

B Changes between version 4.0 and 4.3

B.1 Changes to the Makefile

Some changes have been made to the Makefile. These are documented in Section 2.4.

The following compile-time define has been added to the Makefile:

- MPI_DEBUG

The following compile-time define has been removed from the Makefile:

- FIELD_DEBUG

B.2 Additions to the input deck

The following parameters have been added to the "control" block of the input deck (see Section 3.1):

- nproc{x,y,z}
- smooth_currents
- field_ionisation
- use_exact_restart
- allow_cpu_reduce
- check_stop_file_frequency
- stop_at_walltime
- stop_at_walltime_file
- simplify_deck
- print_constants
- The "restart_snapshot" parameter now accepts filenames

The following parameters have been added to the "output" block of the input deck (see Section 3.7):

- disabled
- time_start
- time_stop
- nstep_start
- nstep_stop
- dump_at_times
- dump_at_nsteps
- dump_cycle
- dump_cycle_first_index
- filesystem
- file_prefix
- rolling_restart
- particle_energy
- relativistic_mass
- gamma
- total_energy_sum
- optical_depth

- qed_energy
- trident_optical_depth
- The default value of "dump_first" is now "T"

The following parameter has been added to the "collisions" block of the input deck (see Section 3.11):

- collisional_ionisation

The following parameter has been added to the "qed" block of the input deck (see Section 3.12):

- use_radiation_reaction

The following parameter has been added to the "species" block of the input deck (see Section 3.3):

- immobile

The following parameters were changed in the "laser" block of the input deck (see Section 3.4):

- The "phase" parameter can now be time varying
- The "profile" parameter can now be time varying

The following parameters have been added to the list of pre-defined constants (see Section 3.15.1).

- nproc_{x,y,z}
- nsteps
- t_end
- cc

There has also been a new "output_global" block added to the input deck. This is documented in Section 3.8.

B.3 Changes in behaviour which are not due to changes in the input deck

- The species "drift" property is now applied to particles whilst the moving window model is active. In previous versions of the code, this property was ignored once the moving window began.
- Ionisation species now inherit their "dumpmask". See Section 3.3.2 for details.
- Default values for ignorable directions were added. This change allows submitting 3D or 2D input decks to a 1D version of EPOCH and 3D input decks to a 2D version of EPOCH. Any references to y/z will be set equal to zero unless overridden by a deck constant. Other y/z values also assume sensible defaults, eg. 1 grid cell, 1 metre thick, etc.
- Automatic byte swapping is carried out by the SDF library. The library now checks the endianness of the SDF file and byte-swaps the data if required.
- "qed" blocks may now be present even if the code was not compiled using the "-DPHOTONS" flag. The code will only halt if "use_qed=T" inside the "qed" block.
- The code now checks for the Data directory in a file named "USE_DATA_DIRECTORY" before prompting at the command-line. This allows the code to be run without waiting for input at the command-line.
- The field and particle grids are now automatically written to SDF output files if they are needed.
- The Data directory may now contain a '/' character.

C References

[1] T. D. Arber, K. Bennett, C. S. Brady, A. Lawrence-Douglas, M. G. Ramsay, N. J. Sircombe, P. Gillies, R. G. Evans, H. Schmitz, A. R. Bell, and C. P. Ridgers, "A particle-in-cell code for laser-plasma interactions: test problems, convergence and accuracy," J. Comput. Phys. (submitted), 2014.

[2] C. Ridgers, J. Kirk, R. Duclous, T. Blackburn, C. Brady, K. Bennett, T. Arber, and A. Bell, "Modelling gamma-ray photon emission and pair production in high-intensity lasermatter interactions," J. Comput. Phys., vol. 260, pp. 273 – 285, 2014.

[3] O. Buneman, "TRISTAN: The 3-D Electromagnetic Particle Code." in Computer Space Plasma Physics: Simulations Techniques and Software, 1993.

[4] A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method. Artech House, 2000.

[5] J. Roden and S. Gedney, "Convolution pml (cpml): An efficient fdtd implementation of the cfs-pml for arbitrary media," Microw. Opt. Technol. Lett., 2000.

[6] Y. Sentoku and A. J. Kemp, "Numerical methods for particle simulations at extreme densities and temperatures: Weighted particles, relativistic collisions and reduced currents," J. Comput. Phys., 2008.

[7] R. Duclous, J. G. Kirk, and A. R. Bell, "Monte carlo calculations of pair production in high-intensity laserplasma interactions," Plasma Phys. Contr. F., vol. 53, no. 1, p. 015009, 2011.