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Basic structure of MIGRAINe

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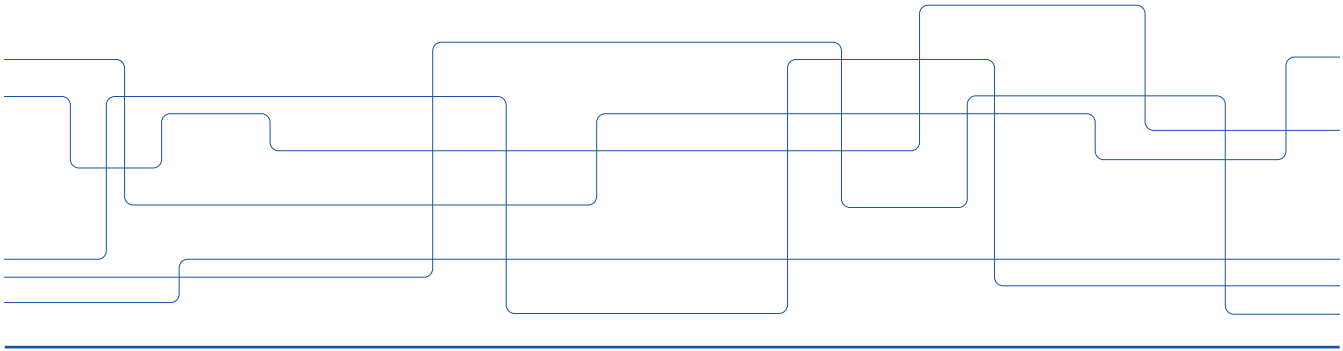

Overview

- Serial ODE/DAE Fortran solver simulating dust trajectories
- 1 trajectory = 1 initial value problem for a state vector $S(t)$ (dust position, velocity, mass, etc) dependent on "external" input (plasma profiles, wall geometry, numerical tables for physical models, etc)
- "Internal" input consists in a list of initial values for S
- 1 single-trajectory simulation = 1 loop over time steps
- 1 MIGRAINe run = 1 loop over N single-trajectory simulations (currently $N \sim 10^5$ but might need to go up by 1 or 2 orders of magnitude)
- Data corresponding to the external input (e.g. tables) is loaded at the start of a run and kept in memory for the entire run
- $S(t)$ is updated in place at the end of every time step: prints to file are used to keep track of time evolution

File and I-O structure

- External input files are opened, read and closed before the first single-trajectory simulation starts
- Internal input files and output files are kept open for the entire run
- A new line of the internal input file is read before each single-trajectory simulation
- New lines are printed to output files whenever a print condition is met
  - Record the evolution of $S(t)$ → multiple prints per single-trajectory simulation
  - Record information on final state values ($S(t_f)$ + some details on how the trajectory was terminated) → one print at each step of the main loop
  - Record aggregated data → one print at the end of the run

Possible issues for parallelization

- Assume parallelization is achieved by distributing single-trajectory simulations across different cores
- Should external input data be copied locally on each core?
- The computational time of a single-trajectory simulation can vary enormously depending on initial conditions → possible to distribute the single-trajectory simulations in real time?
- How to handle output (especially aggregated output)?
  - Have each core produce its own output files and post-treat it externally?
  - Output file merging at end of run?
  - Something else?
- Minimal output consists in ~ 10 floats per trajectory