closures-2d Design Documentation

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1 Purpose

This software that implements various numerical methods for approximating the angular variable in kinetic transport in order to study performance, accuracy, and robustness on common test problems. Whereas fluid equations describe a vector of quantities dependent on space, kinetic transport equations describe a scalar density of particles depending on both space and velocity. Such numerical methods occur frequently in production codes modeling certain physical systems, such as neutron transport inside a reactor, neutrino transport in supernova simulations, photon transport, and rarefied gas dynamics. Rather than simulating a specific physical system, this software solves toy problems that capture issues commonly encountered in full simulations. Comparing the performance of these numerical methods on our simplified problems can give researchers insight into the behavior of similar methods in more complicated implementations.

In addition to evaluating the methods themselves, this software is written to allow study of performance with modern high-performance computing resources. This software optionally uses OpenMP and Message Passing Interface (MPI) to carry out parallel and concurrent computations. Studying the behavior of numerical methods with such acceleration techniques provides reference for implementations on large-scale problems.

This software also supports profiling measurements such as timings, flop rates, memory rates, and cache misses. Using statistics about runtime performance, we examined code optimizations, bottlenecks, etc. that occur in our implementations.

2 Problem

This software simulates particles with unit speed that scatter isotropically from an infinite background medium according to a simple kinetic equation. External sources are not included, but could be added in the future. The equation governing particle behavior takes the form

$$\partial_t f + \Omega \cdot \nabla_x f + \sigma_T f = \frac{\sigma_S}{4\pi} \langle f \rangle$$
 (1)

where $x \in \mathbb{R}^3$ is position, $\Omega \in \mathbb{S}^2$ (the unit sphere) is the direction of travel, $\sigma = \sigma(x)$ is the scattering cross section, and $\langle \cdot \rangle$ is shorthand for integration over \mathbb{S}^2 .

The kinetic solver directly computes solutions to Equation 1, while the moment solver calculates solutions based on the spherical harmonic basis functions. The momopt solver includes additional optimizations and experimental features. This program explicitly computes approximate solutions to Equation 1 as the system evolves from one of several initial conditions, defined in Section ??.

2.1 Initial Conditions

At the beginning of simulation, the grid is initialized according to one of several configurations. First, σ on the whole grid is set to the value from the configuration file and the initial grid is set to the given floor value at all points. Further changes to the initial grid are dependent on the choice of initial condition.

2.1.1 Gaussian Initial Condition

In the Gaussian initial condition, a two dimensional Gaussian function is placed with its peak at the center of the grid. The σ value is provided as a configuration option to the program. Each point on the initial grid is set to

$$\frac{1}{2\pi\sigma^2}e^{-(x^2+y^2)/(2\sigma^2)}. (2)$$

 σ_S and σ_T are uniformly set to the configured value for sigma.

2.1.2 Delta Initial Condition

The limiting case, as $\sigma \to 0$, is the Delta initial condition. For this condition, the centermost cell is set to $\frac{1}{\Delta x \Delta y}$ where Δx and Δy are the cell dimensions. σ_S and σ_T are uniformly set to the configured value for sigma.

2.1.3 Lattice Initial Condition

The Lattice initial condition corresponds to a checker board pattern of highly scattering and highly absorbing regions. This configuration is reminiscent of a small section of a nuclear reactor core. The Lattice initial condition leaves the grid initially empty, but has the most complicated scattering pattern of the initial conditions. σ_S and σ_T are set to 1 at all positions, except for several blocks arranged throughout the grid at which $\sigma_S = 0$ and $\sigma_T = 10$.

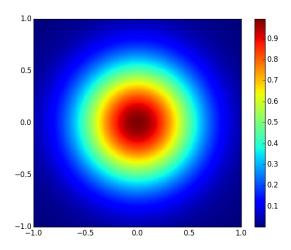


Figure 1: Gaussian Initial Condition

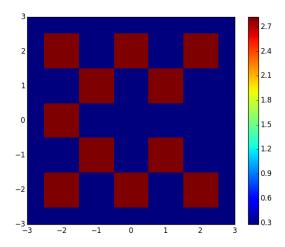


Figure 2: σ_T for Lattice Initial Condition

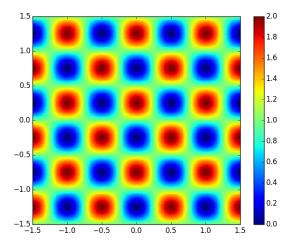


Figure 3: Smooth Initial Condition

2.1.4 Smooth Initial Condition

The Smooth initial condition is primarily intended for testing convergence. This configuration initializes the grid points with a periodic boundary. Each point in the initial grid is set to

$$1 + \sin(2\pi x)\cos(2\pi y). \tag{3}$$

 σ_S and σ_T are uniformly set to the configured value for sigma.

2.2 kinetic Solver

The kinetic solver is an implementation of the discrete ordinates method, also known as S_N . Our implementation uses a Chebyshev-Legendre quadrature on the unit sphere. A Lebedev quadrature is also implemented for this solver, but is considered experimental. Details of the quadratures are given in Section 3.1. Let $\{\Omega_1,\ldots,\Omega_Q\}\in\mathbb{S}^2$ be be a set of nodes with corresponding weights $\{w_1,\ldots,w_Q\}$. Then from Equation 1

$$\partial_t f_q + \Omega_q \cdot \nabla_x f_q + \sigma_t f_q = \frac{\sigma_s}{4\pi} \sum_{q'=1}^Q w_{q'} f_{q'}, \tag{4}$$

where $f_q(x,t) \approx f(x,\Omega_q,t)$ for $q=1,\ldots,Q$.

This implementation uses Heun's method to achieve second order convergence. Edge values are computed via upwinding. For approximate slopes, the double minmod limiter is used.

2.3 moment Solver

The moment solver uses standard spectral methods with Equation 1. The real spherical harmonics serve as an orthonormal basis of L^2 with respect to \mathbb{S}^2 for the expansion of the moments. Let $\mathbf{m}(\Omega) = (Y_{0,0}, Y_{1,-1}, Y_{1,0}, Y_{1,1}, \dots, Y_{N,-N}, \dots, Y_{N,N})^T$ be a vector of spherical harmonics up to and including degree N. The the moments with respect to \mathbf{m} are given by

$$\mathbf{u}(\mathbf{x},t) = \langle \mathbf{m}(\Omega) f(\mathbf{x}, \Omega, t) \rangle \tag{5}$$

since $u_{\ell,m} = f_{\ell,m}$ and the collision operator is diagonalized. The exact moment system is given by

$$\partial_t \mathbf{u} + \nabla_x \cdot \langle \Omega \mathbf{m} f \rangle = D \mathbf{u}, \tag{6}$$

but this formulation is not closed. Thus f is replaced with a P_N moment closure $\mathcal{E}(\mathbf{u})$ such that $\langle \mathbf{m}\mathcal{E}(\mathbf{u}) \rangle = \mathbf{u}$. In this case,

$$\mathcal{E}(\mathbf{u}) = \sum_{k} u_k m_k = \mathbf{u}^T \mathbf{m} \tag{7}$$

yielding the closed moment system

$$\partial_t \mathbf{u} + \nabla_x \cdot \langle \Omega \mathbf{m} \mathcal{E}(\mathbf{u}) \rangle = D \mathbf{u}.$$
 (8)

It is only necessary to use the spherical harmonics $Y_{\ell,m}$ such that $\ell+m$ is even. Various filters can also be applied to suppress oscillations in spherical harmonics. These filters use a scale factor on each cell and timestep to compute a perturbed differential equation with minimal added computation.

• The Hauck filter is described in (insert citation). Let N be the moment order and ω be the filter tune, and define

$$\alpha = \frac{\omega}{N^2 (\sigma_T L + N)^2}. (9)$$

Scale each moment by

$$\frac{1}{1 + \alpha n^2 (n+1)^2} \tag{10}$$

for the $n^{\rm th}$ moment.

• The Spline filter is given in (insert citation). With moment order N and filter tune σ_e , let

$$s = \frac{-\sigma_e \Delta t}{\log F(N/(N+1))} \tag{11}$$

where $F(x) = 1/(1+x^4)$. The scale factor is given by

$$F(n/(N+1))^s. (12)$$

• The Lanczos filter is taken from (insert citation). Again with moment order N and filter tune σ_e , let

$$s = \frac{-\sigma_e \Delta t}{\log L(N/(N+1))} \tag{13}$$

where

$$L(x) = \begin{cases} 1 & \text{when } x = 0\\ \frac{\sin x}{x} & \text{otherwise.} \end{cases}$$
 (14)

Now the moment scale factor is

$$L(n/(N+1))^s. (15)$$

2.4 momopt Solver

One serious drawback of the moment solver is the possibility of non-realizable solutions with negative densities, oscillatory approximations of nonsmooth solutions. Nonlinear approaches can ensure positivity, but come with increased complexity and computational cost. In general, entropy-based moment closures, like the momopt solver, can be cast in the framework of the following minimization problem

$$\mathcal{E}(\mathbf{u}) = \underset{g \in L^1}{\operatorname{arg min}} \langle \eta(g) \rangle$$
 subject to $\langle \mathbf{m}g \rangle = \mathbf{u}$ (16)

where η is a smooth, strictly convex, coercive¹ function. For the momopt solver, $\eta(\mathbf{r}) = \mathbf{r} \log \mathbf{r} - \mathbf{r}$ and its Legendre dual² $\eta * (\mathbf{s}) = \mathbf{e}^{\mathbf{s}}$.

The solution to Equation 16, if it exists, is given by

$$\mathcal{E}(\mathbf{u}) = \eta_*'(\hat{\alpha}(\mathbf{u})^T \mathbf{m}) \tag{17}$$

where η_* is the Legendre dual of η and $\hat{\alpha}(\mathbf{u})$ solves the dual problem

$$\hat{\alpha}(\mathbf{u}) = \operatorname*{arg\,min}_{\alpha \in \mathbb{R}^n} \left\{ \langle \eta_*(\alpha^T \mathbf{m}) \rangle - \alpha^T \mathbf{u} \right\}$$
 (18)

3 Implementation

3.1 Quadratures

The Chebyshev-Legendre quadrature is used for numerical integration over \mathbb{S}^2 in all of the solvers. This quadrature is constructed from an n point Gauss-Legendre rule, which exactly integrates smooth functions of order less than

The Legendre dual of η to be coercive if $\lim_{r\to\infty}\frac{\eta(r)}{|r|}=\infty$ The Legendre dual of η is given by $\eta_*(s)=rs-\eta(r)$ where $s=\eta'(r)$. By differentiating this relation, one can show that $r=\eta'_*(s)$. Thus η' and η'_* are inverses of each other.

2n-1. Since this is a 2D code, it is only necessary to integrate over the upper half of \mathbb{S}^2 , which is divided into n layers along the z axis. Abscissae and weights from GSL are arranged in a circle around \mathbb{S}^2 at each layer, giving n^2 points on the upper half of \mathbb{S}^2 . The Chebyshev-Legendre quadrature is not optimal with respect to number of points, but is simple to implement. The Lebedev quadrature, for example, is optimal in number of points, and an experimental implementation is available for the kinetic solver. This quadrature, however, uses a more complicated arrangement of points, making exploiting symmetries in the integral more difficult. In addition, the points of the Chebyshev-Legendre quadrature are simply the Cartesian product of n angles spaced around a circle and n values of z. This structure could allow the evaluation of integrals via the Chebyshev-Legendre quadrature to be optimized more easily than the Lebedev quadrature, which is arranged nontrivially and becomes denser with increasing order.

3.2 Time

Time steps are carried out via Heun's method to achieve second order. Heun's method is a two-stage Runge-Kutta method that improves on the basic Euler method. To compute the value at the next time step, the solver first records the current state, then runs two Euler steps, then takes the average of the new state and the initial state. Since Heun's method is a strong stability preserving (SSP) method, the stability properties of the forward Euler method are preserved in a higher order setting.

3.3 Space

Space is discretized using the finite volume method. The problem domain is decomposed into a regular grid of cells with an additional halo of ghost cells to enforce the boundary condition and allow synchronization with other nodes. At each update, the program first computes the flux at each cell, then updates the cell values according to the kinetic transport equation. Several of the solvers guarantee positivity on the grid.

For the kinetic solver (implementing S_N), the timestep Δt is chosen with respect to the cell size so as not to violate the CFL condition. To eliminate the possibility of negative density due to scattering, an additional term is included in the CFL check.

The momopt solver also ensures positivity as part of the flux calculations. The flux is based on an ansatz grid with strictly positive values. For M_N , the ansatz grid value a at each cell and direction is given by

$$a = \exp(\alpha^T m). \tag{19}$$

For PP_N ,

$$a = \begin{cases} \frac{1}{2}k + \frac{1}{2}\sqrt{k^2 + 4\delta} & \text{if } k > 0\\ \frac{-\delta}{\frac{1}{2}k - \frac{1}{2}\sqrt{k^2 + 4\delta}} & \text{if } k \le 0 \end{cases}$$
 (20)

where $k = \alpha^T m$.

3.4 Optimization Procedure

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4 Program Layout

All options controlling the runtime operation of the program reside in input.deck. Comments prefixed with # are allowed, and options not used by the selected solver are ignored. Available options are listed in Section ??, and example options for the various solvers are included in the examples/ directory. The outputs are binary files with extensions .sn, .pn, and .opt, depending on the solver. Python code for reading and working with these files is provided in util/formats.py.

The common functionality is split up among the files in src/.

- main.cpp Entry point of program
- comm.cpp Controls MPI communication
- utils.cpp Helper functions used throughout the code

The solver code has an approximately common layout, e.g. in src/moment/

- moment_init.cpp Read config, set up quadrature and filters, etc.
- moment_boundaries.cpp Communicate boundary data with other nodes
- moment_update.cpp Solve flux, update the grid with time, etc.
- moment_output.cpp Write out results

5 Results

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A Gritty Details

A.1 main.cpp

The main entry point for the program, main.cpp, is responsible for reading the input files dictating runtime behavior, setting up MPI, and running the chosen solver. In addition, the grid initialization used by all solvers is defined here, so main.cpp controls the grid geometry and initial configuration. Program flow is as follows

- 1. Determine the current node and total number of nodes. If MPI support is not compiled in, fall back to default values corresponding to the primary and only node.
- 2. Read in the configuration stored in input.deck. This format is described in Section C.1.
- 3. Configure the solver. Solvers are described in Section B.
- 4. Set the domain of the current node.
- 5. Initialize the grid.
- 6. Run the solver over the specified time interval.
- 7. Output data.

The default grid initialization, Solver::initializeGrid, also resides in main.cpp. At present, all solvers use this method. The grid is represented as a two dimensional array of floating point values. The grids used in the program are larger than configured in input.deck; a border of a specified width of ghost cells is added outside the grid described in the configuration. The center points of the cells are used for calculation of initial conditions. Figure 4 illustrates this layout. There are two other arrays of identical size storing σ_S and σ_T values. To initialize the grid, first set the border cells to the specified floor value, c_floor, and then calculate the initial values for the main cells.

A.1.1 Delta Initial Condition

When INITCOND_LINESOURCE is specified with Gaussian $\sigma=0$, the Delta Initial Condition applies. In this case, σ_S and σ_T for each cell are set to σ . The cells of the initial grid are set to c_floor, with the exception of the centermost cell, which is set to $1/\Delta x \Delta y$ where Δx and Δy denote the dimensions of each cell.

A.1.2 Gaussian Initial Condition

This condition is used when INITCOND_LINESOURCE is selected as the the initial condition and Gaussian $\sigma \neq 0$. Each cell's initial value is set to max{gaussianFactor, c_floor} where

gaussianFactor :=
$$\frac{1}{2\pi\sigma^2} \exp\left(-\frac{x_i^2 + y_j^2}{2\sigma^2}\right)$$
. (21)

 σ_S and σ_T for each cell is set to σ .

A.1.3 Lattice Initial Condition

When INITCOND_LATTICE is specified, each cell's initial value is set to c_floor, and $\sigma_S, \sigma_T := 1$. For any cell (x_i, y_i) with

$$\|(x_i, y_i) - (s_x, s_y)\|_{\infty} < 0.5 \tag{22}$$

for some $(s_x, s_y) \in \{ (2.0, 2.0), (2.0, 0.0), (2.0, -2.0), (1.0, 1.0), (1.0, -1.0), (0.0, -2.0), (-1.0, 1.0), (-1.0, -1.0), (-2.0, 2.0), (-2.0, 0.0), (-2.0, -2.0) \}, <math>\sigma_T$ is set to 10 and σ_S is set to 0.

A.1.4 Smooth Periodic Condition

When INITCOND_PERIODIC is selected, σ_S , σ_T are initialized to σ , and the initial value at each point (x_I, y_j) is set to

$$\sin(2\pi x_i)\cos(2\pi y_j) + 1. \tag{23}$$

A.2 comm.cpp

When using MPI, comm.cpp communicates boundary data between nodes. Solver::getInnerBoundaries is first called to obtain grid data on the boundaries of the current node's region of the domain. Next, each node trades boundary data with its neighbors to the north, south, east, then west via MPI_Sendrecv. Finally, the node calls Solver::setOuterBoundaries to update its grid with the data from neighboring nodes.

A.3 utils.cpp

utils.cpp is mostly comprised of IO-related utility functions. In addition, there are functions to compute the 1-norm of an arbitrary vector and to compute Gaussian weights and nodes using GSL.

A.4 timer.cpp

timer.cpp contains a timer class used in main.cpp to record the time taken by computations.

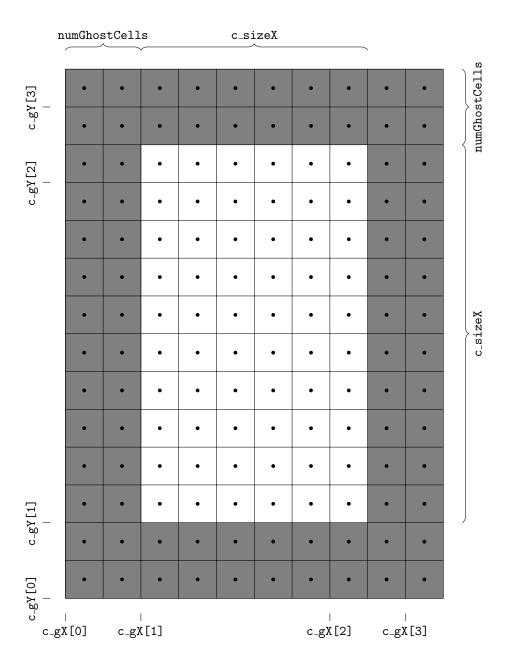


Figure 4: Grid layout

B Solvers

All solvers must store internal parameters and grid data, and implement methods to initialize, query grid parameters, update, and output data. See solver.h for more detail. Each solver is organized into a directory containing the necessary functionality split across several files. The solvers currently implemented are kinetic, moment, momopt, and dn.

B.1 kinetic

B.1.1 kinetic_init.cpp

kinetic reads its runtime configuration from the file kinetic.deck (see Section C.2). The maximum Δt value maxDt is calculated as

$$\text{maxDt} := \frac{1}{2} (\text{cflFactor}) \frac{\Delta x \Delta y}{\Delta x + \Delta y}. \tag{24}$$

The grid is initialized as described in Section A.1. In addition to the grid layers common to all solvers, kinetic uses two others, c_kinetic and c_flux. utils.cpp is used to get the quadrature as described in Section A.3. These fixed-order Gauss-Legendre integration points and weights returned will be referred to as μ_i , and w_i , respectively. Next, the azimuthal angles of quadrature, ϕ_k , are calculated as

$$\phi_k := \frac{(k+0.5)\pi}{\text{quadOrder}} \tag{25}$$

for $k \in \mathbb{Z}$ such that $0 \le k < 2$ (quadOrder), placing 2(quadOrder) points evenly around the unit circle. The quadrature weights are ultimately stored in c_quadWeights, and the points are mapped into cylindrical coordinates and stored in c_xi and c_eta.

For q_1,q_2 such that $0 \le q_1 < (\mathtt{quadOrder})/2$ and $0 \le q_2 < 2(\mathtt{quadOrder})$, define a quadrature counter $q := 2(\mathtt{quadOrder})q_1 + q_2$. Now

$$\mathtt{c_quadWeights}[\mathtt{q}] := \frac{2\pi w_{q_1}}{\mathtt{quadOrder}} \tag{26}$$

$$c_{xi}[q] := \sqrt{1 - \mu_{q_1}^2} \cos \phi_{q_2}$$
 (27)

$$\mathtt{c_eta}[\mathtt{q}] := \sqrt{1 - \mu_{q_1}^2} \sin \phi_{q_2} \tag{28}$$

${f B.1.2}$ kinetic_update.cpp

The core of the kinetic solver is the update method defined here. Each call to update one time step operates as follows:

- 1. Make a copy of the c_kinetic grid.
- 2. Carry out the first Euler step.

- 3. Carry out the second Euler step.
- 4. Average the initial grid with the results of the second iteration.

Some preliminary functions will be used in the discussion of the above steps. The minmod(double x, double y) function is designed to return

- 0 if xy < 1
- $\min\{x, y\}$ if x, y > 0
- $-\min\{|x|, |y|\}$ if x, y < 0

and implemented as follows.

$$\operatorname{minmod}(x, y) = \operatorname{sgn}'(x) \max \left(0, \min \left(|x|, y \operatorname{sgn}'(x)\right)\right) \tag{29}$$

where

$$\operatorname{sgn}'(x) = \begin{cases} 1 & \text{if } x \ge 0\\ -1 & \text{otherwise.} \end{cases}$$
 (30)

Additionally,

slopefit
$$(\ell, c, r, \theta) = \min \left((r - c)\theta, \min \left(\frac{1}{2}(r - \ell), (c - \ell)\theta \right) \right).$$
 (31)

To carry out each Euler step, the kinetic solver first communicates the current cell's boundaries with neighboring MPI cells (described in Section B.1.3) and then solves flux for the cell (described below). For each cell (i, j) in the main grid (excluding the ghost cells), the integral of F is calculated as

$$integral := \frac{\sigma_{S,(i,j)}}{4\pi} \sum_{q=0}^{n} w_q f_q(i,j)$$
 (32)

where w_q is the calculated quadrature weight for the q^{th} point of an n point Gauss-Legendre quadrature and $f_q(i,j)$ is the value of the c_kinetic grid at (i,j,q).

For each $0 \le q < n$, subtract from the value of c_kinetic at (i, j, q)

$$\Delta t \left(\sigma_{T,(i,j)}(\mathbf{c_kinetic})_{(i,j,q)} - \mathbf{integral} \right).$$
 (33)

Next, if using INITCOND_LATTICE, with the cell's bottom left point (x_i, y_j) add an additional Δt to c_kinetic at (i, j, q) if $\|(x_i, y_j)\|_{\infty} < 0.5$. Finally, subtract Δt (c_flux)_{i,j,q} from c_kinetic at (i, j, q).

Communicating boundaries, solving flux, and evaluating an Euler step are carried out again as above. Now for each (i,j) in the main grid, $0 \le q < n$, average c_kinetic at (i,j,q) with the corresponding cell from the copy made at the beginning of the procedure.

Solving for flux involves approximating the flux in each of four directions (north, south, east, west) using slopefit applied to the current cell and its neighbors. The overall flux for each cell is then calculated as

$$\frac{\xi_q}{\Delta x}({\tt eastFlux-westFlux}) + \frac{\eta_q}{\Delta y}({\tt northFlux-southFlux}). \eqno(34)$$

B.1.3 kinetic_boundaries.cpp

The kinetic solver uses the code in kinetic_boundaries.cpp in conjunction with Solver::communicateBoundaries() (see Section A.2) to coordinate the boundaries of different nodes when using MPI. The methods defined here take pointers to buffers from which and into which to copy grid data. These methods copy the north, south, east, and west parts of the gray area as shown in Figure 4.

B.1.4 kinetic_output.cpp

The kinetic solver exports data to files named out_%.3f_%d.sn formatted with the time under simulation and the node index. This file consists of a short header recording the dimensions of the grid, the domain bounds, and the number of quadrature points and weights. The rest of the file contains the floating point values of c_kinetic over the main grid (not including the ghost cells).

C Special Files

C.1 input.deck

input.deck is the primary input file which controls the basic operation of the program. input.deck is a line-based text file storing a set of runtime configuration options as an ordered listing of key-value pairs. An example file is included with the source code. The required options are discussed in Table 1.

C.2 kinetic.deck

kinetic.deck is a brief runtime configuration file controlling the behavior of the kinetic solver. This file uses the same format as input.deck (Section C.1). The required options are given in Table 2.

Table 1: Parameters for input.deck

Option	Type	Description
SOLVER	char[]	Solver to be used. Allowed values are
		kinetic, moment, momopt, and dn. The
		operation of each solver is discussed in
		Section B.
NUM_CELLS_X	int	Number of grid cells in the x direction
NUM_CELLS_Y	int	Number of grid cells in the y direction
NUM_MPI_PARTITIONS_X	int	Number of MPI partitions in the x
NUM_MPI_PARTITIONS_Y	int	direction Number of MPI partitions in the y
A_X	double	direction x coordinate of the bottom left corner
		of the grid
$B_{-}X$	double	x coordinate of the top right corner of
		the grid
$A_{-}Y$	double	y coordinate of the bottom left corner of
D. V	3	the grid
B_Y	double	y coordinate of the top right corner of
T_FINAL	double	the grid Duration of the simulation
OUT_DELTA_T	double	Temporal resolution of the output files
GAUSSIAN_SIGMA	double	σ used in the initial grid configurations
FLOOR	double	Minimum value that occurs in the grid
INIT_COND	int	How the initial grid values are
INII_COND	1116	~
		calculated. Allowed values are 0, 1, and
		2, corresponding to
		INITCOND_LINESOURCE,
		INITCOND_LATTICE, and
		INITCOND_PERIODIC, respectively. Grid
SIGMA	double	initialization is described in Section A.1. Default scattering used in the σ_S and
		σ_T grids. The scattering values for each
		grid position are determined based on
		the particular initial condition selected.

Table 2: Parameters for kinetic.deck

Option	Type	Description
QUAD_ORDER	int	Order of the Gaussian quadrature used for
CFL_FACTOR	double	integration Parameter used to choose the maximum Δt without violating the CFL Condition.