Monte Carlo Charged Particle Tracking Algorithm For Lagrangian RZ Meshes

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Abstract

ICF target ignition and burn sensitively depend upon the details of alpha particle deposition and boot-strap heating. A time dependent Monte Carlo algorithm for charge particle transport has been developed and implemented in DRACO, a 2-D Lagrangian radiation hydrodynamics code. Details of the algorithm, including: particle tracking on distorted meshes and detecting zone boundaries, "lost particle" fix-ups, dE/dx calculations and energy deposition, data structures for saving time dependence information, check-point and restart methods, decomposition for parallel execution, parallel performance and dependence of statistic fluctuations on number of histories will be presented.

Outline

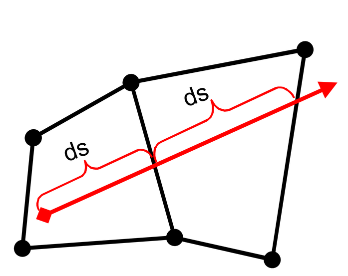
I. Monte Carlo particle tracking algorithm
   1. Random sampling of particles in a cell
   2. Readjustment particle cell index
   3. Intersection with a quadrilateral
   4. Particle travel history
   5. Moving mesh, rezoning and restart

II. Simulation example for a NIF target
   1. The Monte Carlo method predicts earlier ignition and higher gain than predicted by the diffusion method.
   2. Almost linear speed up

III. Future work

Monte Carlo Particle Tracking

In the Monte Carlo particle tracking method, a bunch of particles is followed from random generation to termination. Particle trajectories are approximated by straight lines. Energy loss to the plasma is calculated from the travel distance to each cell edge, and the amount of lost energy is governed by the stopping power.



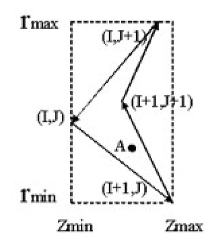
For the RZ two-dimensional geometry, it is actually a 3D problem. The position of generated particle is represented by a point (x,y,z) in a volume enclosed by four hyperbolas defined by the quadrilateral edges

Tracking Algorithm

The Monte Carlo particle transport algorithm has to fulfill the basic tasks:

(1) to generate particles randomly in the source cells,
(2) to determine the intersection with a quadrilateral and get the particle information updated.
(3) Other tasks, such as the treatment of boundary conditions and tally, are also required.
(4) Since the algorithm is coupled with Lagrangian hydro, moving mesh must be considered.
(5) Rezoning and remapping.
(6) Restart.

Random Sampling of Particles in a Cell



Rejection sampling method is used for the random particle generation.

The random selection of radius r in the rectangle is given by

$$r^2 = r_{min}^2 + \xi(r_{max}^2 - r_{min}^2)$$

The x and y coordinates of the particle position are sampled from a random polar angle as

$$x = r\cos(\vartheta) \qquad y = r\sin(\vartheta)$$

The z coordinate of the particle position is given by

$$z = z_{min} + \xi(z_{max} - z_{min})$$

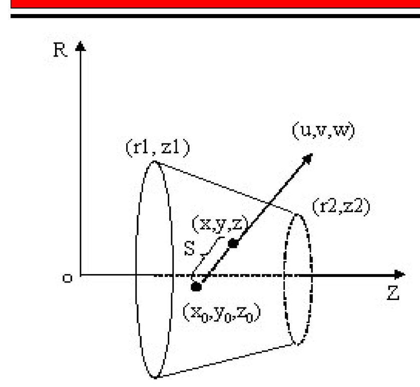
Readjust Particle Cell Index if it is on the Edge

1) Determine the inward normal direction vector of the edge. A reference point inside of the quadrilateral is needed.

2) Choose the inward normal direction vector if the cosine of the angle between the normal line vector and the vector from the particle position to the reference point is less than zero.

3) The assigned index needs to be adjusted according to the location of the edge if the cosine of the angle between the inward normal direction vector and the particle direction is less than zero.

Intersection With a Quadrilateral



The distance to intersection, which is the work horse for the Monte Carlo particle tracking, is calculated from the following equation. Special cases need to be handled.

$$S^2(1 - w^2 - k^2w^2) + S(2x_0u + 2y_0v - 2kw(r_1 + k(z_0 - z_1)) + r_0^2 - (r_1 + k(z_0 - z_1))^2 = 0$$

Particle Travel History

Once a particle is launched in a cell its trajectory is constructed by a straight line which encounters the cells' edges. The particle trajectory is terminated under one of the following three circumstances,

- the particle travels out of the region of interest,
- the particle energy falls below the preset cut-off energy,
- the particle travel time is larger than the hydro time step if the time dependent tracking is applied.

The alternative tracking approach is time independent or adiabatic, in which the particle continues to propagate until the above first two conditions are met.

Moving Mesh, Rezoning and Restart (1)

- Rezoning is included in DRACO to keep the computational mesh from severe distortion, and material interfaces are tracked in the mixed material cells.
- For the time independent tracking method, the particle transport separates from the hydrodynamics, which means the particle loses its energy by propagating to the end in the current hydro time step. Thus, no action is necessary
- For the time dependent tracking method, the Monte Carlo transport is coupled with hydrodynamics in terms that the hydro time serves as a clock for the particle traveling.

Moving Mesh, Rezoning and Restart (2)

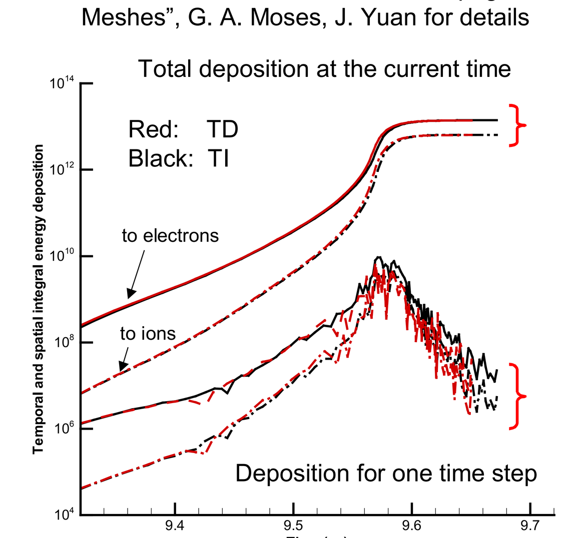
- At the beginning of next time step or after mesh rezoning, the cell index of particle location needs to be readjusted according to the changed mesh.
- The numeric stability requires that the CFL condition holds which restricts a cell to move for a distance less than one cell length. This is also true for mesh rezoning which relocates the cell vertices to reconstruct a smoother mesh while it restricts the relocation beyond one cell to minimize the re-flux diffusion associated with the rezoning. This restriction greatly simplified the cell index search algorithm and reduces the computing time, since only the four neighbor cells need to be searched .

Two Approaches for Restart (3)

- One approach is to force all live particles to deposit their remained energy by propagating until either they are out of the region or their energies drop below the cut-off energy right before the operation to write data at the check point is taken.
- Another approach is to build an energy distribution function and a direction distribution function statistically from the data structures of live particles, and write these distribution functions to disk storage instead. When the program resumes from the previous run, the Monte Carlo particles are dynamically sampled from these distribution functions.

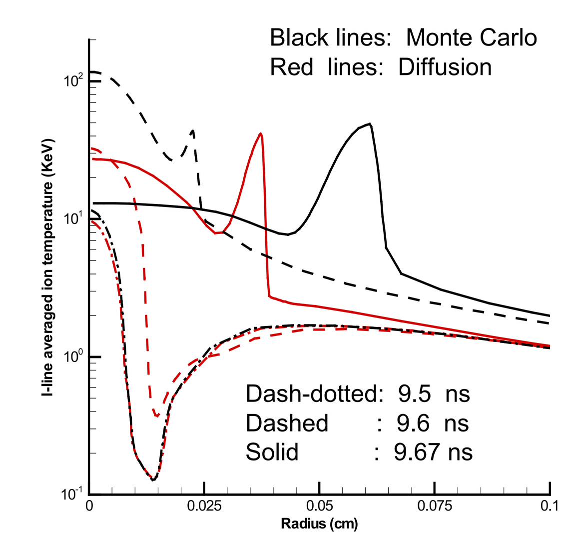
MC Time Dependent and Independent Tracking

See " Simulation of Burn Wave Propagation on Two Dimensional Distorted Meshes", G. A. Moses, J. Yuan for details



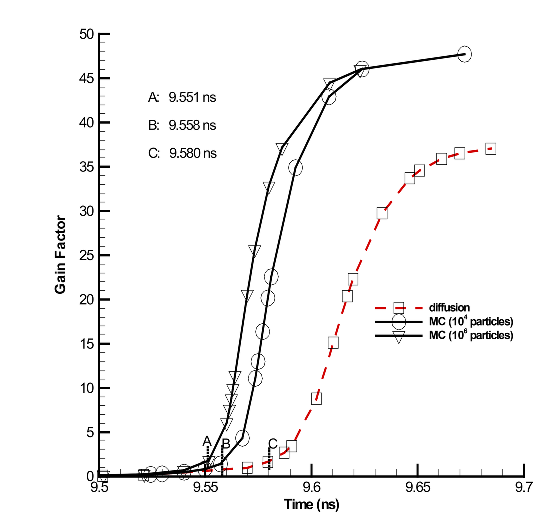
In the hydro-time dependent method, the hydro time step acts as a clock for particles to march, while in the independent method the particles deposit all their energies in the current time interval. The results are similar.

MC Predicts Earlier Ignition than Diffusion



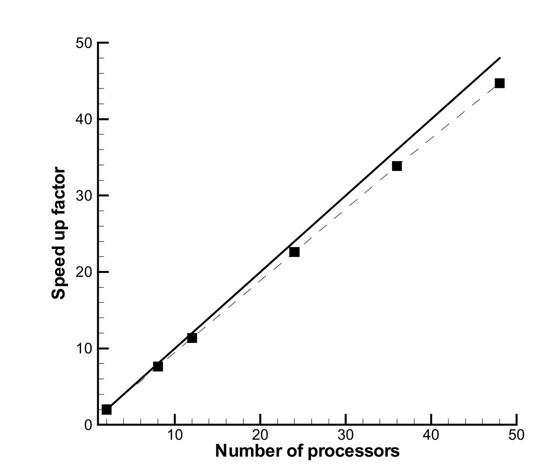
The resulting burn waves from energy deposition show that the ignition predicted by the Monte Carlo method is earlier than predicted by the diffusion method.

Effects of Particle Number Used in Simulations



Fewer particles (10^4) are used to study the statistical effect. It can be seen that the calculation with few particles gives 7 ps delay for the ignition but generates similar total gain. It also shows the burn dynamics is very sensitive to the energy deposition. The total gain from the diffusion method is 20 percent lower than using the Monte Carlo method.

Speed up Factor Measurement



The greatest advantage of the Monte Carlo particle transport is that the program is "embarrassingly" parallelizable. With negligible communication cost, the program can achieve linear speed-up.

Summary and Future Work

- A Monte Carlo particle tracking algorithm for charged particle transport has been implemented in the multi-dimensional hydrodynamic code DRACO.
- The particle trajectory is followed cell-by-cell in three dimensional real space.
- Comparison shows that the Monte Carlo method predicts earlier ignition and higher gain than predicted by the diffusion method.
- In the future, we will apply this tracking framework to the Implicit Monte Carlo (IMC) transport for radiation.