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Jayenne Physics Manual Revision 1.0

An Implicit Monte Carlo Code for Thermal Radiative Transfer

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Executive Summary

This physics manual is intended to document all of the methods used in version 8 of the Jayenne Implicit Monte Carlo solver library. The goal of this manual is to provide a general overview of the basic methods used, and provide a list of references that detail methods that have been implemented in to the Jayenne library.

1 Introduction

The Monte Carlo (MC) method was invented at Los Alamos in the immediate post-World- WarII era by Ulam and von Neumann to numerically simulate the complex transport of radiation through fissile material. It was the numerical basis for the first large scale scientific computation performed on the world's first electronic computer. It was also the only method at the time capable of the task. In the 1950's, Metropolis et al. invented the most widely used Monte Carlo method, the Metropolis algorithm, to study equations of states motivated by weapons research. The new algorithm was the only method at the time capable of the task. In between, Fermi, as a Laboratory consultant, offered that the Ulam-von- Neumann Monte Carlo strategy could solve Schrödinger's equation. It took until the dawn of the supercomputing age to realize Fermi's vision. Ulam and Metropolis offered that the method was particularly well suited for parallel computation, decades before a parallel computer existed. Unlike many numerical methods, the Monte Carlo technique is naturally parallel. These beginnings set the foundation not only for the legacy, still benefiting important portions of today's research at the Laboratory, but also for today's world-wide use of the Monte Carlo method for classical and quantum problems.

The enduring power of the Monte Carlo method lies in its unique ability to "break the curse of dimensionality." Many deterministic methods scale exponentially with the complexity of the problem, while (most) Monte Carlo methods scale independently of dimensionality. As the complexity of the mathematical, scientific, and engineering problems at the Laboratory keep increasing, Monte Carlo methods will remain the only viable simulation method for many tasks. As the ever-increasing size of supercomputers enables larger and more complex problems, Monte Carlo will remain in the Laboratory's code plan because it can do what other methods will be unable to do. Enabling Monte Carlo methods for exascale systems will likely unveil a new dimension to this fundamentally powerful numerical method.

The use and development of Monte Carlo methods are ubiquitous at Los Alamos. In addition to the efforts described in detail in this document, Monte Carlo is also being used and developed for modeling complex networks, social systems, classical kinetic theory, performance analysis, optimal estimation and more.

The Jayenne project [44] was original started in 1997 with the express goal of providing a Monte Carlo thermal radiation transport capability in the x-ray regime for high energy density physics applications such as supernova explosions, inertial confinement fusion, and radiation flow experiments at facilities such as Sandia's Z-Pinch, Omega Facility, and the National Ignition Facility. The Jayenne Project uses the Fleck and Cummings Implicit Monte Carlo (IMC) method. The Jayenne Project's software is powerful, robust, and massively parallel; it is multi-dimensional, runs on Adaptive Mesh Refinement (AMR) and unstructured meshes, and supports both domain-decomposed and particle-decomposed parallel topologies. These underlying components are used in the radiation-only code McGrid, which is also used as a testbed for advanced numerical methods research. The underlying components are also used in `IMC_API`, which is a high-level IMC component that hooks into multi-physics application codes and provides the transport capability for radiation-hydrodynamics simulations. The Jayenne Project libraries have run for countless millions of CPU-hours on the Department of Energy's supercomputers.

From its inception, the project has employed modern software development practices with emphasis on iterative, incremental tasking, configuration management, version control , design and

programming code reviews by peers, test driven development, design-by-contract testing and extensive unit and integrated testing and multi-platform development. The bulk of the software is written in C++ but also provides a Fortran API.

2 The Thermal Radiation Transport equations

The Jayenne library solves the standard thermal radiation transport (TRT) equations. We begin be defining the standard two-temperature radiation equation,

$$\frac{1}{c}\frac{dI(\vec{r},\hat{\Omega},\nu,t)}{dt} + \hat{\Omega}\cdot\nabla I + \sigma I = \sigma B(\nu,T), \tag{1}$$

where the photon intensity $I(\hat{\Omega},\vec{r},t,\nu)$ [GJ/cm^2/ns/sr/keV] is a function of solid angle direction $\hat{\Omega}$ [sr], position $\vec{r}$ [cm], frequency ν [keV], and time t [ns]. The remaining variables are the opacity $\sigma(\nu,\vec{r},t)$ [1/cm] and the Planck spectrum

$$B(\nu,T) = \frac{2hT^3}{c^3}\frac{(\nu/T)^3}{e^{\nu/T}-1}, \tag{2}$$

[Gj/cm^2/ns/sr/keV] with the constants are defined as c [cm/s] the speed of light, and h is the Planck constant [keV-ns]. The radiation equation above is coupled to the material energy balance equation

$$\frac{de}{dt} = \iint \sigma I d\hat{\Omega}d\nu - \iint \sigma B(\nu,T)d\hat{\Omega}d\nu. \tag{3}$$

where e is the material energy that is coupled to the material temperature via an equation of state

$$\frac{de}{dt} = C_v(\vec{r},T)\frac{dT}{dt}, \tag{4}$$

These equations are non-linearly coupled via the material temperature T. The tight non-linear coupling in high energy density physics regimes, with pressures greater than 1MBar and/or temperature on the order of 1×10^6 [45], make them unattractive to solve in there current form. In the next section we will outline the linearized form of the TRT equations that are solved via the Jayenne library.

2.1 The linearized TRT equations

The Jayenne libraries solve the linearized TRT equations original defined by Fleck and Cummings in 1971[23]. Wollaber provides an extensive derivation and analysis of this linearization procedure in his "Four Decades of Implicit Monte Carlo" review article [45]. For the purpose of this document we will only briefly cover this linearization to help motivate some of the improvements to the IMC method that will be discussed in later chapters. We begin the linearization by rewriting the original TRT equations in a more convent form

$$\frac{1}{c}\frac{dI}{dt} + \hat{\Omega}\cdot\nabla I + \sigma_n I = \frac{1}{4\pi}\sigma_n acT_{n+1}^4 b(\nu,T_n), \tag{5}$$

$$C_{v,n}\frac{dT}{dt} = \iint \sigma_n I d\hat{\Omega}d\nu - \sigma_p acT_{n+1}^4. \tag{6}$$

where we have substituted the material energy with a constant specific heat $C_{v,n}(\vec{r},T_n)\frac{dT}{dt}$ based on the initial material temperature T_n. Similarly we have chosen to lag the normalized material spectrum

$$b(\nu,T_n) = \frac{15}{\pi^4 T}\frac{(\nu/T)^3}{e^{\nu/T}-1}, \tag{7}$$

and the Planck opacity $\sigma_p(T_n) = \int \sigma_n b(\nu, T_n) d\nu$. Note that by directly specifying the time centering of these terms we have made an $O(\Delta t)$ approximation to the original system of equations. This form of the TRT equation illustrates the non-linear dependence of the material energy balance equation on temperature. We can now linearize the system by expanding the implicit temperature T_{n+1} using a Taylor series expansion

$$T_{n+1}^4 = T_n^4 + 4\Delta t T_n^3 \frac{dT}{dt} + O((\Delta t)^2). \tag{8}$$

Substituting this expansion into the TRT equation results in the classic Implicit Monte Carlo equations

$$\frac{1}{c}\frac{dI}{dt} + \hat{\Omega} \cdot \nabla I + \sigma_n I = \frac{1}{4\pi} f \sigma_n a c T_n^4 b(\nu, T_n) + \frac{\sigma b(\nu, T_n)}{\sigma_p 4\pi} \iint (1-f)\sigma_n I d\hat{\Omega} d\nu \tag{9}$$

$$C_{v,n}\frac{dT}{dt} = \iint f \sigma_n I d\hat{\Omega} d\nu - f \sigma_p a c T_{n+1}^4. \tag{10}$$

where the fleck factor

$$f = \frac{1}{1 + 4\frac{\sigma_p a c T_n^3 \Delta t}{c v_n}} \tag{11}$$

is used to approximate the absorption emission process over a single time step as an isotropic scattering event.

2.2 Limit Analysis

This section is not currently available.

2.3 Benefits and Deficiencies

To understand the benefits of the linearization we can examine the numerical absorption-emission time scales, this is the time it take for a particle to be re-emitted after being absorbed. The addition of the effective scattering term increases the numerical absorption emission time scale

$$t_{ae} = \frac{C_v}{4acT^3} + \frac{T_n^3}{T_{n+1}^3}\Delta t, \tag{12}$$

as compared to the absorption emission time scale of the standard TRT equations

$$t_{ae} = \frac{C_v}{4acT^3}. \tag{13}$$

This enables the MC solver to take large time steps when using the linearized system of equations. However, it should be noted that this is not a truly implicit system and that unphysical overheating can occur if a time step is taken such that it can not resolve this numerical time scale. Please see the chapter on "Iterative Multifrequency Corrected Implicit Monte Carlo" for more details on recent improvements to this methodology.

The linearized system also modifies the absorption time scale of the problem

$$t_a = \frac{1}{c\sigma f}, \tag{14}$$

while the collisional time scale remains unchanged

$$t_c = \frac{1}{c\sigma}, \tag{15}$$

As the fleck factor approaches zero, or the system because dominated by effective scattering, the absorption time scales can become excessively large. This can make the Monte Carlo histories extremely expensive to evaluate thus, the Jayenne library has two advanced moment based acceleration schemes to improve computational performance, which are outlined in the "IMC Acceleration" chapter.

Thus far in these definitions we have not discussed spatial discretization schemes. The material opacities are discretized as piece wise constant over a problem specific mesh. Using piece wise constant properties simplifies particle tracking. Densmore and others have shown that using a piece wise spatial discretization of the emission source term leads to nonphysically fast wave propagation speeds in optically thick diffusive materials [16]. Therefor, the Jayenne library has developed two different linear source shape options to mitigate this issue and details can be found in the "IMC Sources" chapter.

Finally we have also included additional chapters to discuss how other physics are coupled into the TRT equations. These chapters cover "Three Temperature Physics," "Physical Scattering," and "Radiation Hydrodynamics." Each of these chapters briefly covers the complexities of coupling multiphysics problems into the linearized TRT equations.

3 IMC Source

3.1 Radiation Sources

3.2 Tilt

The original IMC formulation of [23] assumes cell-centered, or piecewise-constant, material data. Assuming a piecewise-constant σacT^4 emissivity to sample new Monte Carlo particles implies uniform spatial position sampling in each cell. In 1D planar geometry, the source particle position would be

$$x = x_{i-1/2}(1-\xi) + x_{i+1/2}\xi \ ,$$

where x is the sampled particle coordinate, $x_{i\pm 1/2}$ are the edges of a cell indexed i, and $\xi \in (0,1)$ is a uniformly sampled random number. In contrast, since the Monte Carlo transport step in IMC is continuous, the distribution of spatial absorption positions are not necessarily uniform in each cell. For instance, assuming the emission inside a cell is negligible and there is an incident monodirectional flux at $x_{i-1/2}$, the average energy deposition position would be

$$\bar{x} = x_{i-1/2} + \frac{1}{\int_0^{\Delta x_i} e^{-\sigma_i s} ds} \int_0^{\Delta x_i} s e^{-\sigma_i s} ds = x_{i-1/2} + \frac{1}{\sigma_i}\left(1 - \frac{\tau_i e^{-\tau_i}}{(1-e^{-\tau_i})}\right) \ ,$$

where $\bar{x}$ is the expected absorption coordinate, σ_i is cell i absorption opacity, and τ_i is cell i absorption optical thickness. Since the expectation value of the position from source sampling is $\bar{x} = (x_{i-1/2} + x_{i+1/2})/2$, the expected absorption and emission locations do not have to agree.

In the limit of infinitesmal time step size, Δt, the IMC equations converge towards an explicit thermal radiative transfer solution, since the Fleck factor approaches 1. Consequently, effective scattering diminishes and effective absorption converges towards true absorption. Assuming non-zero absorption opacity, this implies that for sufficiently small Δt more energy will be emitted via source particle sampling. However, given the potential inconsistency in expected absorption and emission locations (see previous paragraph), substantial spatial error is incurred for cells of high optical depth (τ): this is the so-called "teleportation error" described by [39].

A clear illustration of the issue, and why it is sometimes called "teleportation error", is the following: consider a time step that is smaller than the light-crossing time of a cell,

$$\Delta t = \frac{1}{3}\frac{\Delta x_i}{c} \ ,$$

where $\Delta x_i = x_{i+1/2} - x_{i-1/2}$. If $\sigma_i = 1/\epsilon \Delta x_i$, where $\epsilon \ll 1$, the expectation value of an absorption position of a particle incident at $x_{i-1/2}$ is $\bar{x}_a \approx x_{i-1/2} + 1/\sigma_i$. In the subsequent time step, energy originating from the particle gets re-emitted at an expected position of $\bar{x}_e = x_{i-1/2} + \Delta x_i/2$. The implied energy propagation speed is

$$\frac{\bar{x}_e - \bar{x}_a}{\Delta t} = 3c\left(\frac{1}{2} - \epsilon\right) > c \ .$$

Teleportation error was first addressed by [24]; the authors provide a spatial probability distribution function (PDF) to sample source particles. This PDF is reconstructed from the cell-centered quantities used to calculate emissivity, $\sim \sigma T^4$. In IMC, the method is commonly referred to as

"source tilting". For instance, assuming a piecewise-constant cell opacity, a reconstruction of emission that is linear in T^4 will give the following PDF:

$$p(x) = \left(\frac{2}{T_{i,L}^4 + T_{i,R}^4}\right)\left(T_{i,L}^4 \frac{x_{i+1/2} - x}{\Delta x_i} + T_{i,R}^4 \frac{x - x_{i-1/2}}{\Delta x_i}\right) \quad ,$$

where $T_{i,(L,R)}^4$ are the left and right values of the linear profile. Note that σ_i is eliminated from the PDF through normalization. Regardless of the details of the PDF, $p(x)$, the sampling procedure follows the canonical procedure outlined by [35],

$$\xi = \int_{x_{i-1/2}}^{x} p(x')dx' \quad ,$$

where again ξ is a uniformly sampled random variable between 0 and 1. This integral equation is inverted to obtain x, the sampled location. For the linear T^4 sub-cell profiles, the inversion for x is analytic,

$$x = x_{i-1/2} + \Delta x_i \left(\frac{-T_{i,L}^4 + \sqrt{T_{i,L}^8 + (T_{i,R}^8 - T_{i,L}^8)\xi}}{T_{i,R}^4 - T_{i,L}^4}\right) \quad .$$

Alternatively, the PDF can be sampled first as a discrete distribution of "Left" (L) and "Right" (R),

$$P_{i,S} = \frac{T_{i,S}^4}{T_{i,L}^4 + T_{i,R}^4} \quad ,$$

where $S \in \{L, R\}$, then with

$$p(x|S) = 2\varphi_S(x) \quad ,$$

where $\varphi_{(L,R)}$ are the linear coefficients of $T_{i,(L,R)}^4$ in the original equation for $p(x)$. The sampled value of x would be

$$x = x_{i-1/2} + \Delta x_i \times \begin{cases} \sqrt{\xi} \ , & S = L \ , \\ 1 - \sqrt{1-\xi} \ , & S = R \ . \end{cases}$$

The question remains as to how to calculate $T_{i,(L,R)}$. In the standard IMC formulation[23], the update to the temperatures are at cell centers; in order to get values for $T_{i,(L,R)}$, a reconstruction (i.e. interpolation) must be used. The sub-cell profile has the linear form,

$$T(x)^4 = T_i^4 + m_i(x - x_i) \quad ,$$

which is cell-energy conservative,

$$\int_{x_{i-1/2}}^{x_{i+1/2}} T(x)^4 \, dx = T_i^4 \quad .$$

Thus $T_{i,L}^4 = T_i^4 - m_i \Delta x_i/2$ and $T_{i,R}^4 = T_i^4 + m_i \Delta x_i/2$. In the Jayenne package, the reconstruction is performed as follows.

1. Interpolate T^4 at edges of cell i,

$$T^4_{i\pm 1/2} = \frac{\Delta x_{i\pm 1} T^4_{i\pm 1} + \Delta x_i T^4_i}{\Delta x_{i\pm 1} + \Delta x_i} \quad .$$

2. Calculate the slope in cell i,

$$\tilde{m}_i = \frac{T^4_{i+1/2} - T^4_{i-1/2}}{\Delta x_i} \quad .$$

3. Limit the slope to prevent negative T^4,

$$m_i = \min(2T^4_i, \max(-2T^4_i, \tilde{m}_i)) \quad .$$

For 2D and 3D structured meshes, the reconstruction is performed along each dimension.

Sampling particles from a non-uniform profile at the sub-cell level indeed mitigates teleportation error, as demonstrated with asymptotic analysis by [16]. However, [16] shows that the degree to which source tilting mitigates teleportation error depends on the accuracy of the sub-cell profile. Similarly, [42] show that "jump terms", proportional to $T^4_{i,L} - T^4_{i-1,R}$, manifest to leading order. Several options exist to obtain the correct asymptotic discrete diffusion limit with IMC:

- [42] force the temperature profile to be continuous between cells, which affects the calculation of $T^4_{i,(L,R)}$, and the calculation of the emission and Fleck factor [48],
- [29] store probable absorption locations from the previous time step and use these as sites of emission in the next time step,
- [48] introduce a discontinuous galerkin finite element basis to the material energy equation, similar to what has been done for SIMC by [30] and [2].

In the subsequent section, we discuss the current implementation of a finite element form of the material energy equation, described by [48].

3.3 Linear-Discontinuous IMC

In the Jayenne package, the path chosen to obtain the correct discrete asymptotic diffusion limit involves a finite element formulation of the material energy equation. This is described by [48] and subsequently referred to as "LD IMC". The original form of LD IMC used non-uniform sub-cell opacity, which provides more accuracy, but is more expensive as well. In the Jayenne package, piecewise-constant opacities are used. In 1D planar geometry, the basis functions are

$$\varphi_{L,i}(x) = \frac{x_{i+1/2} - x}{\Delta x_i} \quad ,$$
$$\varphi_{R,i}(x) = \frac{x - x_{i-1/2}}{\Delta x_i} \quad .$$

It is assumed that the temperature can be represented by these functions,

$$T(x,t) = T_{L,i}(t)\varphi_{L,i}(x) + T_{R,i}(t)\varphi_{R,i}(x) \quad ,$$

where $T_{(L,R),i}$ are the vertex temperatures of cell i. The cell-centered temperature is the average of the vertex values.

$$T_i = \frac{T_{L,i} + T_{R,i}}{2} \quad .$$

Incorporating the temperature profile into the material energy equation, multiplying by the vector of φ functions and integrating over the cell gives

$$C_{v,n,i}\Delta x_i \begin{pmatrix} 1/3 & 1/6 \\ 1/6 & 1/3 \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} T_{L,i} \\ T_{R,i} \end{pmatrix} = \int_{x_{i-1/2}}^{x_{i+1/2}} f_{n,i}\sigma_{n,i} \begin{pmatrix} \varphi_{L,i} \\ \varphi_{R,i} \end{pmatrix} \int_{-1}^{1} I(x,\mu,t)d\mu dx - f_{n,i}\sigma_{n,i}T_{n,i}^3 ac\Delta x_i \begin{pmatrix} 1/3 & 1/6 \\ 1/6 & 1/3 \end{pmatrix} \begin{pmatrix} T_{L,n,i} \\ T_{R,n,i} \end{pmatrix} \quad ,$$

where subscript n implies the beginning of the time step, I is radiation intensity, $f_{n,i}$ is the cell-centered Fleck factor, $\sigma_{n,i}$ is the cell-centered opacity, and $C_{v,n,i}$ is the cell-centered heat capacity at constant volume. The first term on the right side of the above equation implies that the Monte Carlo tally of the energy deposition is weighted by the basis functions. The implementation can be outlined as follows. For the LD and BLD IMC methods, a summary of the algorithm is as follows:

1. Calculate sub-cell spatially dependent forms for $T(\vec{r},t)$ and emission, $\sigma T(\vec{r},t)^4$.

2. Sample source particle locations from the linear emission distribution.

3. For particle p, calculate the usual IMC distances.

4. Instead of tallying the standard Monte Carlo energy deposition, for particle weight E_p:

   - for analog absorption, for each cell i, for each basis function l, tally $\varphi_{l,i}(\vec{r})E_p$,
   - For non-analog absorption, the value $f_{n,i}\sigma_{n,i}\varphi_{l,i}(\vec{r})E_p e^{-\tau_{\rm ea}(\vec{r}_0,\vec{r})}$, where $\tau_{\rm ea}(\vec{r}_0,\vec{r}')$ is the effective absorption optical depth from $\vec{r}_0$ to $\vec{r}'$, must be integrated over the path length from $\vec{r}_0$ to the final location, $\vec{r}$.

5. Take the time integral of the finite element-integrated IMC material-energy equation to update the temperature.

The above enumeration is a specialization of the algorithm provided by [48].

The motivation for the LD IMC method follows from the asymptotic analysis provided by [48]. This analysis focuses on the worst manifestation of the jump terms [42] in the limit that Δt is asymptotically small. The typical scalings, given by [33] are applied,

$$\sigma \to \frac{\sigma}{\epsilon} \quad ,$$
$$c \to \frac{c}{\epsilon} \quad ,$$
$$C_v \to \epsilon C_v \quad ,$$

where $\epsilon \to 0$. Along with these scalings, expanding the dependent variables in ϵ,

$$I(x,\mu,t) = \sum_{k=0}^{\infty} I^{(k)}(x,\mu,t)\epsilon^k \quad ,$$

$$T_{(L,R),i}(t) = \sum_{k=0}^{\infty} T^{(k)}_{(L,R),i}(t)\epsilon^k \quad ,$$

will furnish an infinite system of equations relating lower-order coefficients of ϵ to higher-order. Further assuming $\Delta t \to 0$, integrating the transport equation in direction angle, multiplying by the basis function vector, integrating over the cell, and summing to the material energy equation gives

$$C_{v,i}\Delta x_i \begin{pmatrix} 1/3 & 1/6 \\ 1/6 & 1/3 \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} T_{L,i} \\ T_{R,i} \end{pmatrix} + \frac{1}{c}\frac{\partial}{\partial t} \int_{x_{i-1/2}}^{x_{i+1/2}} \begin{pmatrix} \varphi_{L,i} \\ \varphi_{R,i} \end{pmatrix} \phi(x,t)dx = \begin{pmatrix} F_{i-1/2} - F_i \\ F_i - F_{i+1/2} \end{pmatrix} \quad ,$$

where F_i and $F_{i\pm 1/2}$ are cell-average and cell-edge flux. Consequently, with the scalings, to leading order

$$0 = \begin{pmatrix} F^{(0)}_{j-1/2} - F^{(0)}_j \\ F^{(0)}_j - F^{(0)}_{j+1/2} \end{pmatrix} \quad .$$

The cell-interior fluxes can be shown to be 0 [48], and the cell-edge fluxes are proportional to the previously mentioned jump terms. Hence, the solution of the above equation is that the jump terms are 0, implying leading-order continuity.

4 IMC Acceleration

4.1 The zeroth angular moment of the TRT equations

The Jayenne library has two optional acceleration schemes that can be used; discrete diffusion Monte Carlo (DDMC), or Random Walk (RW). Both of these schemes accelerate the solution by decomposing it into transport (I_t) and diffusive ($\tilde{E}$) components. The diffusion domain is defined by series of heuristic diffusion criteria ($g(\nu, \overline{r}, t)$ outlined in a subsequent section), which is 1 for diffusion groups and 0 otherwise. Using this criteria, we can rewrite the linearized TRT equations as a function of diffusive energy density

$$\tilde{E} = \frac{1}{c} \iint g(\nu, \overline{r}, t) I d\nu d\Omega, \tag{19}$$

and the transport intensity

$$I_t = (1 - g(\nu, \overline{r}, t))I. \tag{20}$$

The linearized TRT equations are separated into a transport

$$\frac{1}{c}\frac{dI_t}{dt} + \overline{\Omega} \cdot \nabla I_t + \sigma_n I_t = S_t \tag{21}$$

and zeroth angular moment diffusion acceleration equation

$$\frac{1}{c}\frac{d\tilde{E}}{dt} + \frac{1}{c}\nabla \cdot \tilde{F}_j + (f\tilde{\sigma}_n + (1-f)(1-\gamma)\tilde{\sigma}_n)\tilde{E} = S_D. \tag{22}$$

The only assumption made at this point is that the diffusive energy density $\tilde{E}$ is described by the local Planck spectrum, which allows us to define the frequency averaged opacity as

$$\tilde{\sigma}_n = \int \sigma(\nu, \overline{r}, t_n) g(\nu, \overline{r}, t_n) b(\nu, T_n) d\nu \tag{23}$$

and the up-scattering ratio

$$\gamma = \frac{\int \sigma(\nu, \overline{r}, t_n) g(\nu, \overline{r}, t_n) b(\nu, T_n) d\nu}{\int \sigma(\nu, \overline{r}, t_n) b(\nu, T_n) d\nu}. \tag{24}$$

allowing us to define an average absorption opacity. These equations are solved simultaneously and coupled directly to the material energy balance equation

$$cv_n \frac{dT}{dt} = \tilde{\sigma}_n \tilde{E} + \iint f\sigma_n I_t d\overline{\Omega} d\nu - \iint f\sigma_p acT_{n+1}^4 d\overline{\Omega} d\nu. \tag{25}$$

The coupling between the transport intensity and the diffusive energy density is defined via boundary conditions that have been lumped into the diffusion and transport source terms (S_D and S_t). We have additionally left the closure relationship for the face (j) centered frequency integrated diffusive flux $\tilde{F}_j$ undefined. In the following sections we will describe how two different acceleration options are implemented by defining different closers and boundary conditions for the diffusion domain.

4.2 Discrete Diffusion Monte Carlo

The current default acceleration scheme is Discrete Diffusion Monte Carlo (DDMC) [25, 15, 20, 12, 7, 50, 49]. The fundamental concept of DDMC is to evaluate a discretized diffusion matrix via Monte Carlo. We close the frequency integrated diffusion flux by making the assumption that the flux is linearly anisotropic and therefore can be defined via Fick's Law

$$\tilde{F}_j = -c\frac{1}{3\tilde{\sigma}_{r,j}}\Delta\tilde{E}, \tag{26}$$

where the diffusion Roseland opacity is defined as

$$\tilde{\sigma}_{r,j\pm} = \frac{\int g(\nu,\overline{r_{j,j\pm}},t)\frac{dB(\nu,T_n)}{dT}d\nu}{\int g(\nu,\overline{r_{j,j\pm}},t)\frac{dB(\nu,T_{n,j})}{dT}\frac{1}{\sigma(\nu,T_{n,j})}d\nu} \tag{27}$$

this is the unique opacity for every cell face, $\pm$ cell on either side of face j, evaluated at the average face temperature

$$T_{n,j} = (0.5(T^4_{n,j-1/2} + T^4_{n,j+1/2}))^0.25. \tag{28}$$

For AMR faces the refined face uses an area weighted average temperature [18]. Given the face opacities we apply the standard Szilard-Pomraning [43] spatial discretization to the undefined streaming operator for all internal (diffusion-diffusion interface conditions between) cells and integrate over volume (ΔV)

$$\frac{1}{c}\frac{d\tilde{E}}{dt}\Delta V - \sum_j^J \overline{n}_j \cdot \frac{1}{3\tilde{\sigma}_{r,j}}\nabla\tilde{E}A_j + (f\tilde{\sigma}_n + (1-f)(1-\gamma)\tilde{\sigma}_n)\tilde{E} = S_D, \tag{29}$$

where the diffusion source

$$S_D = \gamma\sigma_p faT_n^4\Delta V + \frac{1}{c}\gamma\int\int\int(1-f)\sigma I_t d\nu d\overline{\Omega}dV + S_{t\to D,j}, \tag{30}$$

includes emission and effective scattering into the diffusion domain along with internal boundary source $S_{t\to D,j}$ for particles that move from the diffusion to the transport cells. The transport source

$$S_t = \xi(\nu,T)\gamma\sigma_p facT_n^4 + \xi(\nu,T)(1-\gamma)\int\int(1-f)\sigma I_t d\nu d\overline{\Omega} + \xi(\nu,T)(1-\gamma)(1-f)\tilde{\sigma}_n E + S_{D\to t,j}, \tag{31}$$

includes emission and effective scattering into the transport domain along with internal boundary source $S_{D\to t,j}$ for particles that move from the diffusion domain to the transport cells. We have defined an average face diffusion opacity

$$\tilde{\sigma}_{r,j} = \frac{\tilde{\sigma}_{r,j+}\tilde{\sigma}_{r,j-}\Delta x}{0.5(\tilde{\sigma}_{r,j-}\Delta x + \tilde{\sigma}_{r,j+}\Delta x)}, \tag{32}$$

and a normalized transport spectrum

$$\xi(\nu,T) = \frac{\int_0^\nu(1-g(\nu,\overline{r},t_n))\sigma(\nu,\overline{r},t_n)b(\nu,T_n)d\nu}{\int_0^\infty(1-g(\nu,\overline{r},t_n))\sigma(\nu,\overline{r},t_n)b(\nu,T_n)d\nu}. \tag{33}$$

In the next section will describe the spatial boundary conditions between diffusion and transport cells.

4.2.1 DDMC transport-diffusion interface boundary conditions

The transport-diffusion interfaces used by Jayenne are described in detailed by Cleveland et al. [11]. This interface condition is based on Densmore's emissivity preserving boundary condition [17]. We can define the diffusion to transport boundary condition as

$$S_{t\to D,j} = (1 - P(\mu_j))\mu_j I_t \tag{34}$$

where $\mu_j = \overline{\Omega} \cdot \overline{n}_j$ and the reflection probability is defined as

$$P(\mu) = (1 - P')2(1 + \frac{3}{2}\mu_j). \tag{35}$$

Here P' is defined such that we can preserve the emissivity limit as defined by Densmore [17]

$$P'_j = \frac{\epsilon'_j \beta_j}{\beta_j - \frac{4}{3}\epsilon'_j \tau_j} \tag{36}$$

The remaining variables are defined as:

$$\epsilon'_j = \frac{4}{3}\frac{\sqrt{3(1-\omega_j)}}{1 + \lambda\sqrt{3(1-\omega_j)}} \tag{37}$$

$$\beta = \frac{3}{2}(1-\omega_j)\tau_j^2 + \sqrt{3(1-\omega_j)\tau_j^2 + \frac{9}{4}(1-\omega_j)^2\tau_j^4} \tag{38}$$

$$\tau_j = \sigma_j \Delta_x \tag{39}$$

$$\omega_j = \frac{\tilde{\sigma}_r - \tilde{\sigma}_n f}{\tilde{\sigma}_r} \tag{40}$$

where the extrapolation distance has been modified to ensure positivity

$$\lambda = \frac{5}{3} + \frac{1}{\frac{3}{2}(1-\omega_j)\tau_j + \sqrt{3(1-\omega_j) + \frac{9}{4}(1-\omega_j)^2\tau^2}} - \frac{1}{\sqrt{(}3-\omega_j)} \tag{41}$$

Finally we can define the transport to diffusion source

$$S_{t\to D,j} = \frac{1}{2\pi}\frac{\mu_j}{\int_{-1}^{0}\mu d\mu} c\tilde{E}C_m + \frac{\mu_j}{\int_{-1}^{0}\mu d\mu}\int P(\mu_j)\mu_j I_j d\mu \tag{42}$$

as the amount of energy leaked from the diffusion domain and the transport particles reflected off of the diffusion cell. The diffusion leakage coefficient is defined as

$$C_m = \frac{P'_j}{4}. \tag{43}$$

4.3 Random Walk

The Jayenne project provides an additional diffusion acceleration scheme known as Random Walk [22]. This acceleration scheme uses the analytic solution of an impulse point source in the largest possible diffusive sphere that can be drawn in any given cell. Given that the random walk sphere is always contained in a single cell, we can apply Fick's Law and re-write the diffusion equation for the RW sphere as

$$\frac{1}{c}\frac{d\tilde{E}}{dt} - c\frac{1}{3\tilde{\sigma}_{r,j}}\nabla^2\tilde{E} + (f\tilde{\sigma}_n + (1-f)(1-\gamma)\tilde{\sigma}_n)\tilde{E} = \int\int \frac{I_0}{4\pi r^2}\delta(\nu-\nu')\delta r d\overline{\Omega} d\nu, \tag{44}$$

where I_0 is the initial photon intensity at the beginning of the random walk process. Here we are including the outscattering $(1-\gamma)$ term which demonstrates significant performance improvements over the original RW implemenation [31]. Integrating this equation over the homogenized sphere for radius R_0 and with a vacuum boundary condition applied at the outer surface results in an analytic solution

$$\begin{aligned} E(r,t) = \frac{I_0}{c}\exp(-c(1-f)(1-\gamma)\tilde{\sigma_n}t)\exp(-cf\sigma_n t) \\ \frac{1}{R_0^2}\sum_{n=1}^{\infty}(\frac{n}{r})\sin\left(\frac{n\pi}{R_0}r\right)\exp\left(-\left(\frac{n\pi}{R_0}\right)^2\frac{ct}{3\tilde{\sigma}_r}\right). \end{aligned} \tag{45}$$

We begin by sampling the time to leak from a given random walk sphere using pre-tabulated tables of the analytic solution

$$\xi = \int_0^{R_0} E(r, t_{leak})r^2 dr. \tag{46}$$

where ξ is a random number between 0 and 1. Assuming continuous energy deposition, where the absorbed energy is accounted for on a per track basis [35], we can sample the time to an upscattering event as

$$t_{up} = \frac{-\ln(\xi)}{(1-f)(1-\gamma)\tilde{\sigma}_n c}. \tag{47}$$

Given the particles time to census we can now select the next termination event as the smallest time to event. If the time to census or the time to upscattering is selected we need to determine the radial position of the event on the sphere

$$\xi = \frac{\int_0^{R_{event}} E(r, t_{event})r^2 dr}{\int_0^{R_0} E(r, t_{event})r^2 dr}. \tag{48}$$

The result of these integrals are sampled from the pre-tabulated analytic solution. We can uniformly sample the event location at the radial distance (R_{event}) from the middle of the random walk sphere. The outgoing direction is sampled from an isotropic cosine angle based on the sphere outward normal at the event location.

The Random Walk acceleration scheme is considerably less efficient than DDMC for most problems. However, Random Walk is currently the only acceleration scheme enabled on GPU hardware. It is also the only acceleration scheme currently available for unstructured mesh simulations.

4.4 Diffusion Criteria

In Jayenne both the RW and DDMC algorithm rely on a diffusion criteria to determine *a priori* which groups should be lumped into the diffusion domain. Random Walk uses a simple cutoff criteria

$$g_{rw}(\nu, \overline{r}, t) = \begin{cases} 1, & \text{if } \nu \leq \nu_c \\ 0, & \text{else} \end{cases}$$

where the cutoff criteria is the highest frequency group that has a mean free path $\tau = 2$. DDMC has a slightly more complex diffusion criteria because it allows the lumped diffusion groups to be non-contiguous

$$g_{ddmc}(\nu, \overline{r}, t) = \begin{cases} 0, & \text{if } c_s < 0.9 \\ 1, & \text{else if } \tau \geq 4.0 \ \&\& \ \xi > 0.0 \\ 0, & \text{else if } (1 - f_d) < 0.9 \\ 0, & \text{else if } \tau_r < 1.0 \\ 1, & \text{else if } \tau \geq 2.0 \ \&\& \ \xi > 1.0 \times 10^{-4} \\ 0, & \text{else .} \end{cases}$$

This conditional statement is non-contiguous in space, angle, and time [11]. This conditional statement introduces a few extra variables that need to be defined. The first is an alternative fleck factor f_d that is an approximate time-step independent fleck factor based on the ratio of the estimated particle residence time in the cell and the absorption re-emission timescale.

$$f_d = \frac{1}{1 + \frac{\Delta t_D}{\Delta t_{a\epsilon}}}, \tag{49}$$

where

$$\Delta t_D = \frac{\sigma R_0^2}{3c} \tag{50}$$

is the residence time, approximated by the average time to diffuse our of a sphere (with the radius R_0) approximately the size of the cell. The absorption re-emission time scale is defined by

$$\Delta t_{a\epsilon} = \frac{c_v}{\sigma 4 a T^3 c}. \tag{51}$$

We can rewrite the Fleck factor in terms of mean free paths $\tau = \sigma R_0$

$$f_D = \frac{1}{1 + \frac{\tau^2 a T^3}{3 c_v}} \tag{52}$$

5 Iterative Multifrequency Corrected Implicit Monte Carlo

The Jayenne library has a new advanced Iterative Multifrequency Implicit Monte Carlo (IMC^2) method that can be used to mitigate the unphysical overheating that occurs when using the standard IMC linearization [10]. This method uses a local, non-linear, zero-dimensional Newton iteration to accelerate an outer iteration of a standard IMC simulation.

5.1 The IMC^2 derivation

This derivation begins by defining a linearization around the current iteration, which is constrained by setting it equal to the most recent estimate of the fully-implicit emission temperature.

$$T_{i+1}^4 \Delta t \equiv \int_{t_n}^{t_{i+1}} \left(T_n^4 + 4T_{c,i+1}^3 \frac{dT}{dt} \Delta t \right) dt. \tag{53}$$

where T_{i+1} is the implicit temperature for the current iteration i. Given this integration we obtain the definition of $T_{c,i}$ defined by Cleveland and Wollaber [8],

$$T_{c,i+1}^3 \equiv \left(\frac{1}{4} \frac{(T_{i+1}^4 - T_n^4)}{(T_{i+1} - T_n)} \right). \tag{54}$$

The expansion (Eqs. 53 and 54) of the implicit emission term can be substituted back into the original TRT equations, as was done by Fleck and Cummings [23], to yield a new "IMC like" set of TRT equations. If we define a correction $\epsilon_{i+1} = f_{c,i+1} - f_{c,i}$, as was done by Cleveland and Wollaber [8], we can operator split the implicit ϵ_i term to form a set of non-linear TRT equations for a single iteration i,

$$\begin{aligned} \frac{1}{c}(I_i - I_n) + \overline{\Omega \cdot \nabla I_i} + \overline{\sigma(\nu, T_n) I_i} &= f_{c,i} \frac{\sigma(\nu, T_n) b(\nu, T_i)}{4\pi} acT_n^4 \Delta t \\ &+ \frac{\sigma(\nu, T_n) b(\nu, T_i)}{4\pi \sigma_{p,i}} \int \int \overline{(1 - f_{c,i}) \sigma(\nu, T_n) I_i} d\nu d\Omega, \end{aligned} \tag{55}$$

$$\rho c_v (T_{i+1} - T_n) = \frac{f_{c,i+1}}{f_{c,i}} S_{c,i}, \tag{56}$$

and

$$\frac{1}{c}(I_{n+1} - I_i) \quad = \quad -\frac{\sigma(\nu, T_n) b(\nu, T_i,)}{4\pi \sigma_{p,i}} \frac{\epsilon_{i+1}}{f_{c,i}} S_{c,i}, \tag{57}$$

where T_i is the current iterate's guess for the implicit material temperature (or the T_{i+1} from the previous iteration),

$$S_{c,i} = \left(\int \int \overline{f_{c,i} \sigma(\nu, T_n) I_i} d\nu d\Omega - f_{c,i} ac \sigma_{p,i} T_n^4 \Delta t \right), \tag{58}$$

$$f_{c,i+1} = \frac{1}{1 + \frac{\sigma_{p,i} 4acT_{c,i+1}^3 \Delta t}{\rho c_v}}, \tag{59}$$

$$f_{c,i} = \frac{1}{1 + \frac{\sigma_{p,i} 4acT_{c,i}^3 \Delta t}{\rho c_v}}, \tag{60}$$

and,

$$T_{c,i}^3 \equiv \left(\frac{1}{4} \frac{(T_i^4 - T_n^4)}{(T_i - T_n)} \right). \tag{61}$$

Note that this form is slightly different than what was previously presented by Cleveland and Wollaeger where the iteration scheme was not properly carried through the linearization [9]. As our initial guess in the iteration scheme we use $T_{i+1} = T_i = T_n$, where T_n is the initial material temperature for the current time step. Then we evaluate Eq. 55 using Monte Carlo. Given the energy deposition information for the current iteration (i) we perform a Newton solve on Eq 56, making use of Eqs. 54, 59, 60 and 61, until we converge on a new T_{i+1}. Then we check if the intensity correction (Eq. 57) will adhere to the maximum principle. We can define an inequality for correction source (ϵS_c) that will guarantee that the maximum principle ($I_{n+1} \leq B(\nu, T_u)$) is satisfied for the correction [34] (T_u denotes the maximum temperature in the problem including any sources). We already know from the analysis performed by Cleveland and Wollaber that the LCIMC equations guarantee that $T_{i+1} \leq T_u$ [8] for any given iteration. The following inequality ensures that the photon intensity will adhere to the maximum principle in each cell.

$$\left(1 + \frac{\left(\frac{1}{c} \int \int I_i d\nu d\Omega + \epsilon_i S_{c,i} - aT_u^4 \right)}{aT_u^4} \right)^{-1} \geq 1 \tag{62}$$

Note that it is possible to satisfy this inequality after a single iteration if the energy exchange is well approximated by the original Fleck and Cummings expansion. If this inequality is not satisfied for all cells we update $T_{c,i}^3$ and f_i based on the new T_{i+1}, then set $T_i = T_{i+1}$, and continue to iterate. After Eq. 62 is satisfied in all cells we update the final photon intensity (I_{n+1}) using Eq. 57 and set the final material temperature $T_{n+1} = T_{i+1}$. Note that IMC^2 can produce negative corrections to the intensity for Eq. 57. Rather than reducing the current census energy we simply set the correction $\epsilon S_c = 0$. The negativity is an indication that the linearization in the current iteration will not overheat or excessively cool the cell, therefore we can accept it without fear of violating the maximum principle. This is equivalent to taking a semi-implicit IMC step, that will not violate the maximum principle, without a correction.

5.2 Time step controller

Jayenne also provides a time step controller associated with the iterative solver[10]. Although IMC^2 will adhear to the maximum principle, upon iteration convergence, a time step controller can still be valuable to both ensure accuracy and computational efficiency. If the coupling in a problem is sufficiently stiff it could take many transporter iterations per time step to converge. Additionally, because we are currently lagging the opacity, wave stagnation can occur for large time steps. Therefore we wish to define a time step control that attempts to maximise the correction for a single iteration. This can be achieved making Eq. 62 an equality and multiplying both sides by Δt such that

$$\Delta t_c = \Delta t_n \left(1 + \frac{\left(\frac{1}{c} \int \int I_i d\nu d\Omega + \epsilon_i S_{c,i} - aT_u^4 \right)}{aT_u^4} \right)^{-1} \tag{63}$$

This represents an assumed first order relationship between the overheating and the time step size. To prevent us from taking too large of a time step we set a max increase in the time step as $\Delta t_{max} = 1.5\Delta t_n$. Using this max change in time step size the final time step controller can be defined as

$$\Delta t_{n+1} = \min(\Delta t_c, \Delta t_{max}) \tag{64}$$

where Δt_c is the most restrictive time step for all cells.

6 Three Temperature Physics

Currently the Jayenne library is natively two temperatures, only accounting for separate electron and radiation temperature, assuming that ion and electrons are in equilibrium. Evans and Densmore developed a three temperature operator split that mimics the two-temperature equations using a linearization of the electron temperature [21]. In the following section we will present the standard three temperature split that can be used the Jayenne IMC library.

6.1 The Evans and Densmore 3T split

The three-temperature (3T) radiation transport equations are commonly used in high energy density physics applications such as inertial confinement fusion. Evans and Densmore [21] demonstrated how the ion temperature equation can be eliminated, via substitution, and folded into the Fleck and Cummings [23] linearization. This creates a set of modified "two-temperature like" equation with a modified linearization,

$$\frac{1}{c}\frac{\partial I}{\partial t} + \overline{\Omega}\cdot\nabla I + \sigma I = \frac{1}{4\pi}\tilde{f}\sigma a c T_{e,n}^4 + \frac{1}{4\pi}\iint (1-\tilde{f})\sigma I d\nu d\overline{\Omega} + (1-\tilde{f})Q_+ + (1-\tilde{f})Q_e, \tag{65}$$

$$\tilde{c}_{v,e}\frac{\partial T_e}{\partial t} = \iint \sigma I d\nu d\overline{\Omega} - \tilde{f}\sigma a c T_{e,n}^4 + 4\pi\tilde{f}Q_+ + 4\pi\tilde{f}Q_e + 4\pi Q_-, \tag{66}$$

$$c_{v,i}\frac{\partial T}{\partial t} = Q_i - 4\pi\tilde{Q}, \tag{67}$$

$$\tilde{f} = \frac{1}{1+\tilde{\beta}\sigma c\Delta t} \tag{68}$$

$$\tilde{\beta} = \frac{4aT_{e,n}^3}{\tilde{c}_{v,e}}, \tag{69}$$

$$\tilde{c}_{v,e} = c_{v,e} + \tilde{\omega}\Delta t \tag{70}$$

$$\tilde{\omega} = \frac{c_{v,i}\omega}{c_{v,i}+\omega\Delta t}, \tag{71}$$

$$\tilde{Q} = \frac{1}{4\pi}\tilde{\omega}(T_{i,n} - T_{e,n}) \tag{72}$$

$$Q_+ = \frac{1}{2}(\tilde{Q} + |\tilde{Q}|), \tag{73}$$

$$Q_- = \frac{1}{2}(\tilde{Q} - |\tilde{Q}|). \tag{74}$$

Note the addition of the positive and negative source terms (Q_+ and Q_-) are added to account for the possibility of a negative electron ion coupling source ($(\tilde{Q}) < 0$). This is used because the linearization bring the electron ion coupling into the radiation equation and a negative source would produce

negative weighted particles. Negative weighted Monte Carlo particles can significantly increase the variance in calculations and can eventually create negative temperatures. This additional positive and negative source terms are not used in deterministic methods that can treat negative radiation source directly.

7 Physical Scattering

The original Fleck and Cummings derivation of the IMC equations neglects physical scattering , focusing instead on the regime where absorption-emission is dominant. As a result, most physical scattering processes are simply applied to the IMC equations independent of the original Fleck and Cummings linearization. The Jayenne package offers several options for physical scattering, but only one may be selected for any simulation. Thus, the impetus is on the user to decide which physical scattering option is appropriate for their temperature/frequency regime.

7.1 Isotropic Coherent ("Thomson-esque") Scattering

The simplest option for physical scattering in Jayenne is the straightforward addition of isotropic coherent scattering, a scattering process which does not change the frequency of the particle. The outgoing photon direction is chosen isotropically, as the name suggests. This option is somewhat analogous to Thomson scattering (a coherent process), but does not accurately treat the non-isotropic Thomson angular distribution.

Thomson scattering occurs when very low-energy photons scatter off of free electrons. It is the low-frequency limit of Compton scattering. No energy is exchanged between radiation and matter in Thomson interactions; the only quantity that changes is the outgoing direction of the photon. As previously mentioned, the coherent scattering option in Jayenne does not produce the correct angular distribution for Thomson scatters, instead using an isotropic outgoing angular distribution.

7.2 Compton Scattering

Compton scattering involves the incoherent scattering of photons off of free electrons, and can dominate radiation-matter coupling when the material temperature is hotter than $\sim \mathcal{O}(1\text{ keV})$. Because photons are bosons, the Compton scattering process is subject to stimulated effects. In essence, the probability of a photon Compton-scattering from some initial state to some final state is enhanced by the population of photons at the final state. When stimulated effects are included, the in-scattering term of the TRT radiation equation takes the form:

$$\int_0^\infty d\nu' \int_{4\pi} d\Omega' \frac{\nu}{\nu'} \sigma_s(\nu' \to \nu, \Omega' \cdot \Omega) I(\nu', \Omega') [1 + c^2 I(\nu, \Omega)/2h\nu^3]$$

The bracketed term in red represents the stimulated contribution to the in-scattering term. From a Monte Carlo perspective, accurate treatment of the stimulated Compton effect is exceedingly difficult, as it requires estimation of the full time- and frequency-dependent photon spectrum before each scattering event. **To avoid this complication, we neglect the stimulated term in all Jayenne Compton implementations**. While this greatly simplifies numerical treatment of the Compton process, it also modifies the equilibrium photon distribution from a Planck distribution to a Wien. Simulations with both absorption-emission and Compton scattering will equilibrate to a distribution that is neither purely Planckian nor purely Wien, but some superposition of the two. Improved treatments for stimulated emission are an active area of research.

Even with the simplifying assumption of no stimulated emission, the Compton kernel is by itself a complicated function of temperature, frequency, and angle. When treated probabilistically, it is very difficult to sample the detailed phase space of the scattering kernel adequately. When

treated deterministically (e.g. numerically integrated to form scattering matrices or simplified energy exchange terms), issues arise with underflow / overflow errors and other numerical sensitivities. Methods representing both approaches are implemented in Jayenne.

In the following subsubsections, we describe the primary Compton treatments available in the Jayenne package – the Bowers-Wilson method, explicit Compton, linearized Compton, and the average energy exchange. Some of these treatments may be combined in a single simulation.

7.2.1 The Bowers-Wilson correction

The Bowers-Wilson (BW) correction [1] is the most robust and, conversely, least accurate method available for simulating effects of Compton scattering. The BW correction does not capture any of the spectral effects of Compton; it only approximates the bulk material heating (or cooling) rate from Compton scattering. In addition, the BW correction was derived for a gray (frequency-independent) system, but is often applied to multigroup systems in an ad hoc fashion. We omit the full derivation of the BW correction here for brevity, but note that the correction term is applied to the groupwise absorption opacity, and takes the form:

$$\kappa_C = \frac{4\sigma_T n_e c k a T_R^4}{m_e c^2} \frac{1}{T^3 + T^2 T_R + T T_R^2 + T_R^3} \,, \tag{75}$$

where T is the material temperature, T_R the radiation temperature, n_e the electron density, $(m_e c^2)$ the electron rest mass, and k and a the Boltzmann and radiation constants, respectively. A more complete description and derivation can be found in Chapter 7 of [1]. We expect the BW correction to be accurate in near-equilibrium conditions, when the radiation spectrum is nearly Planckian. Even in these conditions, the BW correction will only estimate the bulk rate of energy transfer, and will not capture Compton effects in the radiation spectrum.

7.2.2 Explicit Compton

The explicit Compton methodology in Jayenne is an analog representation of Compton scattering in the absence of induced effects. While the total groupwise Compton scattering rate is provided via an opacity library, the specifics of the scattering event (colliding electron speed and angle, outgoing photon frequency, direction, and angle) are sampled from governing distribution functions for the physical process. The rejection sampling procedure used to accomplish this is expensive, but the resulting photon distributions are accurate. Unfortunately, the high dimensional Compton phase space must be adequately sampled to ensure a reasonable estimate of the total energy transfer between radiation and matter. In some cases, this requires tens of thousands of scattering events per cell, per timestep.

In addition, the explicit-in-time evaluation of the total scattering rate can lead to onerous timestep restrictions in problems where Compton is dominant and the energy exchange timescale is very short.

The explicit Compton procedure involves the following steps:

1. Sample an appropriate electron from a relativistic Maxwellian distribution at the material temperature, T. This involves sampling an electron speed and an angle (relative to the incoming photon) [3].

2. Boost the photon into the electron rest frame
3. Using the Klein-Nishina formula for Compton scattering off of a free electron, sample the outgoing photon frequency ν' and direction Ω' in the electron rest frame
4. Un-boost the photon back to the lab frame
5. Deposit the difference between the photon's initial and final energy-weight, $N(\nu' - \nu)$, to the material

7.2.3 Average energy exchange

The average energy exchange technique replaces the (noisy) explicit Compton energy exchange with an average value (integrated over all possible outgoing frequencies). For consistency, the scattering opacity is set to a numerically-consistent value when the average treatment is enabled.

This implementation uses Compton opacities and relative energy exchange data from the CSK project [36]. The CSK project calculates the Compton opacity using:

$$\sigma_c(\nu, T) = \int_0^\infty \int_{4\pi} \sigma_c(\nu \to \nu', \Omega \cdot \Omega', T) d\Omega' d\nu \ , \tag{76}$$

where $\sigma_c(\nu \to \nu', \Omega \cdot \Omega', T)$ is the Compton scattering kernel [32]. The expected relative energy change for a photon with frequency ν scattering in a material with temperature T is then calculated using:

$$\frac{\langle \nu' - \nu \rangle}{\nu} = \frac{\int_0^\infty \left(\frac{\nu'}{\nu} - 1 \right) \int_{4\pi} \sigma_c(\nu \to \nu', \Omega \cdot \Omega', T) d\Omega' d\nu'}{\sigma_c(\nu, T)} \tag{77}$$

The average energy exchange methodology can be enabled with both the explicit Compton treatment and the linearized Compton treatment.

8 Radiation Hydrodynamics

As carriers of electromagnetic force, photons impart momentum to matter via interaction with charged particles (e.g. free electrons or electrons bound to an atomic orbital). The cumulative effect of photon-matter interactions on the energy and momentum of a fluid is a topic of radiation hydrodynamics. More generally, radiation hydrodynamics is the study of the interaction between particles with dynamics that can be described with a transport or diffusion equation (radiation) with particles that behave hydrodyamically (fluid/material). The origin of both the transport equation and hydrodynamics equations is the Boltzmann equation,

$$\frac{d\psi}{ds} = \frac{\partial \psi}{\partial t} + \vec{v} \cdot \nabla \psi + \vec{a} \cdot \nabla_v \psi = \mathcal{C}[\psi] + \frac{q}{4\pi} \quad ,$$

where ψ is a particle distribution, s is the characteristic particle path (in units of time) over independent variables (sometimes referred to as an affine parameter), t is time, $\vec{v}$ is velocity, ∇ is the gradient operator, $\vec{a}$ is acceleration from external (long-distance) forces, ∇_v is the gradient operator in velocity space, and $\mathcal{C}$ is a functional of the distribution that describes scattering. The photon transport equation is straightforward to derive from the Boltzmann equation: $\vec{v} = c\hat{\Omega}$ (speed of light times the unit direction), $\vec{a} = 0$ (photons travel at c in all reference frames), and

$$\mathcal{C}[\psi] = c \int_{4\pi} \int_0^\infty R(\nu' \to \nu, \hat{\Omega}' \to \hat{\Omega}) \psi' d\nu' d\Omega' - c\sigma_t \psi \quad ,$$

where ν is frequency, R is the redistribution or scattering kernel, and $\sigma_t = \sigma_a + \sigma_s$ is the total opacity. The substitutions give

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \nabla \psi = \int_{4\pi} \int_0^\infty R(\nu' \to \nu, \hat{\Omega}' \to \hat{\Omega}) \psi' d\nu' d\Omega' - \sigma_t \psi + \frac{q}{4\pi} \quad .$$

The linear form of the collision functional (a convolution minus a simple multiplication) sets the asymptotic particle behavior to be described by a diffusion equation. A diffusion equation can readily be obtained by introducing a scaling parameter, ϵ, (see, e.g., [28])

$$c \to \frac{c}{\epsilon} \quad ,$$
$$\sigma_t \to \frac{\sigma_t}{\epsilon} \quad ,$$
$$\sigma_a \to \epsilon \sigma_a \quad ,$$
$$q \to \epsilon q \quad ,$$

expanding ψ in terms of ϵ,

$$\psi = \sum_{k=0}^{\infty} \psi^{(k)} \epsilon^k \quad ,$$

assuming frequency independent, isotropic scattering, and matching terms by orders in ϵ,

$$\psi^{(0)} = \frac{\phi^{(0)}}{4\pi} \quad ,$$
$$\psi^{(1)} = \frac{\phi^{(1)}}{4\pi} - \frac{1}{4\pi\sigma_t} \hat{\Omega} \cdot \nabla \phi^{(0)} \quad ,$$
$$\frac{1}{c}\frac{\partial \psi^{(0)}}{\partial t} + \hat{\Omega} \cdot \nabla \psi^{(1)} + \sigma_s \psi^{(2)} + \sigma_a \psi^{(0)} = \frac{\sigma_s}{4\pi} \phi^{(2)} + \frac{q}{4\pi} \quad .$$

Integrating the second equation multiplying by $\hat{\Omega}$ over Ω, integrating the third equation over Ω, and solving the equations for $\phi^{(0)}$ gives the diffusion equation,

$$\frac{1}{c}\frac{\partial \phi^{(0)}}{\partial t} - \nabla \cdot \left(\frac{1}{3\sigma_t} \nabla \phi^{(0)} \right) + \sigma_a \phi^{(0)} = q \ .$$

Alternatively, for massive particles that interact by two-body collisions [27, 14],

$$\mathcal{C}[\psi] = \int d^3\vec{v}_* \int_{4\pi} d\Omega_s \, R(\vec{v} \leftrightarrow \vec{v}', \vec{v}_* \leftrightarrow \vec{v}'_*, \hat{\Omega}_s)(\psi'_* \psi' - \psi_* \psi) \ ,$$

where $\vec{v}_*$ is the velocity of the a particle that will collide with the particle moving at $\vec{v}$, ψ_* is the distribution evaluated at $\vec{v}_*$, $\hat{\Omega}_s$ is a unit vector that transforms pre- to post-collision velocity, and the $'$ denotes post-collision (or evaluation at post-collision velocities) [27]. This collision kernel poses unique challenges to solve for many-particle systems. For instance, in Monte Carlo, a particle's proximity to other particle's must be tracked in order to calculate collision interactions [41].

Neglecting external forces (long-distance interactions), and external sources, and incorporating the two-body collision kernel, the Boltzmann equation becomes,

$$\frac{\partial \psi}{\partial t} + \vec{v} \cdot \nabla \psi = \int d^3\vec{v}_* \int_{4\pi} d\Omega_s \, R(\vec{v} \leftrightarrow \vec{v}', \vec{v}_* \leftrightarrow \vec{v}'_*, \hat{\Omega}_s)(\psi'_* \psi' - \psi_* \psi) \ .$$

The scaling parameter is now the ratio of the mean free path for two-body collisions to the problem length. For the above equation, scaling

$$R \to \frac{R}{\epsilon}$$

and expanding $\psi_{(*)}$ and $\psi'_{(*)}$ in ϵ, the leading-order equations are

$$0 = \int d^3\vec{v}_* \int_{4\pi} d\Omega_s \, R(\vec{v} \leftrightarrow \vec{v}', \vec{v}_* \leftrightarrow \vec{v}'_*, \hat{\Omega}_s)(\psi'^{(0)}_* \psi'^{(0)} - \psi^{(0)}_* \psi^{(0)}) \ ,$$

$$\frac{\partial \psi^{(0)}}{\partial t} + \vec{v} \cdot \nabla \psi^{(0)} = \int d^3\vec{v}_* \int_{4\pi} d\Omega_s \, R(\vec{v} \leftrightarrow \vec{v}', \vec{v}_* \leftrightarrow \vec{v}'_*, \hat{\Omega}_s)(\psi'^{(0)}_* \psi'^{(1)} + \psi'^{(0)} \psi'^{(1)}_* - \psi^{(0)}_* \psi^{(1)} - \psi^{(0)} \psi^{(1)}_*) \ .$$

These equations are essentially the first two in the Chapman-Enskog hierarchy [26, 6]. The first equation implies a sufficient (not necessary) solution [14],

$$\ln(\psi'^{(0)}_*) + \ln(\psi'^{(0)}) = \ln(\psi^{(0)}_*) + \ln(\psi^{(0)}) \ .$$

This equation is a statment of pre- to post-collision conservation, and can be constructed from a linear sum of the particle conservation laws for mass, momentum, and kinentic energy, [14],

$$2\alpha m + \vec{\beta} \cdot m(\vec{v}'_* + \vec{v}') + \gamma \frac{1}{2} m(v'^2_* + v'^2) = 2\alpha m + \vec{\beta} \cdot m(\vec{v}_* + \vec{v}) + \gamma \frac{1}{2} m(v^2_* + v^2) \ ,$$

which holds for elastic collisions, for any constants α, $\vec{\beta}$, and γ. The above two equations imply a Maxwellian/Gaussian distribution for the solution,

$$\psi^{(0)} \sim e^{m(\alpha + \vec{\beta} \cdot \vec{v} + \gamma v^2/2)} \ .$$

After properly normalizing $\psi^{(0)}$, the solution for $\psi^{(1)}$ can be obtained from the $\psi^{(1)}$ equation, following the detailed derivation given by, for instance, [14]. The Chapman-Enskog restriction on α, $\vec{\beta}$, and γ [6] forces $\psi = \psi^{(0)}$ and $\psi^{(1)} = 0$ in equilibrium. Consequently, setting

$$\rho = m \int \psi d^3\vec{v} \ ,$$
$$\rho\vec{U} = m \int \vec{v}\psi d^3\vec{v} \ ,$$
$$(\mathbf{P})_{i,j} = m \int (\vec{v}_i - \vec{U}_i)(\vec{v}_j - \vec{U}_j)\psi d^3\vec{v} \ ,$$
$$\rho e = \frac{1}{2} m \int |\vec{v} - \vec{U}|^2 \psi d^3\vec{v} \ ,$$
$$\vec{Q} = \frac{1}{2} m \int (\vec{v} - \vec{U})|\vec{v} - \vec{U}|^2 \psi d^3\vec{v} \ ,$$

multiplying the Boltzmann equation by m, $m\vec{v}$, and $m|\vec{v}|^2/2$, and integrating over velocity space,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\vec{U}) = 0 \ ,$$
$$\frac{\partial (\rho\vec{U})}{\partial t} + \nabla \cdot \left(\mathbf{P} + \rho\vec{U}\vec{U}\right) = 0 \ ,$$
$$\frac{\partial}{\partial t}\left(\rho e + \frac{1}{2}\rho U^2\right) + \nabla \cdot \left(\vec{Q} + \vec{U}\rho e + \vec{U}\rho\frac{U^2}{2} + \mathbf{P} \cdot \vec{U}\right) = 0 \ .$$

These are the hydrodynamic (Euler) equations without external sources (i.e. no long-distance forces, which would manifest from integrating the $\vec{a} \cdot \nabla_v$ term). The above equations require a closure relationship; if one is supplied, then the above equations can be solved for ρ, $\vec{U}$, and e to obtain a macroscopic description of the hydrodynamic state.

To summarize, the origin of the hydrodynamics/fluid equations or the transport/radiation equation is the Boltzmann equation with a quadratic or linear collision functional, respectively.

- For radiation, the linearity of the scattering kernel causes the asymptotic (short mean free path) behavior to be described by a diffusion equation.
- For the fluid, the quadratic scattering kernal, along with the Chapman-Enskog equilibrium restriction, causes the asymptotic (short two-body mean free path) behavior to be described by the hydrodynamics equations.
- The difference in the scattering kernel implies different algorithmic requirements, but the asyptotic limit of either version of the Boltzmann equation permits optimization of the solution procedure in high-scattering regions (e.g. DDMC).

The opacities, which mediate the interaction of radiation with a material, must set the degree to which massive particles are accelerated, and hence must manifest as source terms in the Euler equations. Equivalently, these terms introduce emissivity (a source) into the transport equation. The resulting system of equations is nonlinear, even when the material is static. The following sections describe how the Jayenne library's IMC solution is coupled to the hydrodynamic solution from a host code.

Radiation Hydrodynamics

8.1 The radiation hydrodynamics equations

In conservative form, the inviscid Euler equations are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{U}) = 0 \ ,$$
$$\frac{\partial (\rho \vec{U})}{\partial t} + \nabla \cdot \left(\rho \vec{U}\vec{U}\right) + \nabla P = \frac{1}{c}\vec{q} \ ,$$
$$\frac{\partial (\rho \mathcal{E})}{\partial t} + \nabla \cdot \left(\vec{U}(\rho \mathcal{E} + P)\right) = q_0 + \frac{\vec{U}}{c} \cdot \vec{q} \ ,$$

where $\vec{q}$ and q_0 are the external source terms, and $\mathcal{E} = e + U^2/2$. Differing from the previous section, the heat conduction flux term $\vec{Q}$ has been dropped, and the pressure tensure has been assumed to have no shear terms, so $\mathbf{P} = P\mathbf{I}$, where $\mathbf{I}$ is the identity tensor. Using the Lagrangian time derivative,

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{U} \cdot \nabla \ ,$$

the above equations can be cast in the Lagrangian form,

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{U} = 0 \ ,$$
$$\rho \frac{D\vec{U}}{Dt} + \nabla P = \frac{1}{c}\vec{q} \ ,$$
$$\rho \frac{De}{Dt} + P \nabla \cdot \vec{U} = q_0 \ .$$

The second equation can be derived by utilizing the Product Rule on the derivatives in the momentum-conservation equation and eliminating terms that form the mass-conservation equation. Likewise, the third equation can be obtained by the Product Rule and eliminating terms that form the mass-conservation equation (multiplying e and $U = |\vec{U}|$) and substituting $\vec{q}/c$ for the terms dotting $\vec{U}$ that form the left side of the momentum-conservation equation. It is worth noting that the change from $q_0 + \vec{U} \cdot \vec{q}/c$ to q_0 in the transformation of the energy-conservation equation is not of relativistic origin, despite its appearance; q_0 and $\vec{q}$ are defined in one inertial, or "lab", frame.

Assuming the equation of state is known for the material (for instance, the gamma-law $P \sim \rho e$), more information is needed for q_0 and $\vec{q}$ to close the system of equations. If q_0 and $\vec{q}$ are sources due to a radiation field, then the additional information is the transport equation, which in local thermodynamic equilibrium is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I = \int_{4\pi} \int_0^\infty \frac{\nu}{\nu'} R(\nu' \to \nu, \hat{\Omega}' \to \hat{\Omega}) I' d\nu' d\Omega' - (\sigma_s + \sigma_a) I + \sigma_a B \ ,$$

where B is the Planck function transformed into the lab frame, and $I = \nu\psi$. The only difference with the previous section is that $q/4\pi$ has been replaced with $\sigma_a B$. Having been integrated over the space of all single-particle velocities, the Euler equations are lower-dimensional than the transport equation. This suggests that equivalently, integrals of the transport equation have to be taken over

frequency and direction, to couple with hydrodynamics,

$$\frac{\partial E}{\partial t} + \nabla \cdot \vec{F} = \tilde{q}_0 \ ,$$
$$\frac{\partial \vec{F}}{\partial t} + c\nabla \cdot \mathbb{P} = \tilde{\vec{q}} \ ,$$

where

$$E = \frac{1}{c}\int_{4\pi}\int_0^\infty I d\nu d\Omega \ ,$$
$$\vec{F} = \int_{4\pi}\int_0^\infty \hat{\Omega} I d\nu d\Omega \ ,$$
$$\mathbb{P} = \frac{1}{c}\int_{4\pi}\int_0^\infty \hat{\Omega}\hat{\Omega} I d\nu d\Omega \ ,$$

and $\tilde{q}_0$ and $\tilde{\vec{q}}$ follow from the transport equation. Assuming the total available momentum and energy is in either the fluid or the radiation field,

$$\tilde{q}_0 = -q_0 \ ,$$
$$\tilde{\vec{q}} = -\vec{q} \ .$$

In Monte Carlo, the energy and momentum absorbed into the material from the radiation can be tallied, which in turn permits calculation of q_0 and $\vec{q}$.

The Jayenne library assumes the radiation transport will be operator-split from the hydrodynamics: during the Monte Carlo phase, the state of the material will be a snapshot. The simplest operator split is as follows:

1. solve the Euler equations without sources,
2. with the updated hydrodynamic state, solve the radiation transport equations, accounting for (sub-)relativistic effects of photons changing reference frames between fluid parcels,
3. with energy and momentum deposition tallies, calculate sources and update the hydrodynamic state again.

The question remains as to how to treat relativistic corrections. In Monte Carlo, Lorentz transformations to energy, frequency, and direction can be performed for each particle to boost into and out of the comoving frame of the fluid (see, e.g. [14, 4]),

$$E_p = E_p^{(0)}\gamma\left(1 + \frac{\vec{U}}{c}\cdot\hat{\Omega}_p^{(0)}\right) \ ,$$
$$\hat{\Omega}_p = \frac{\hat{\Omega}_p^{(0)} + \gamma\vec{U}/c + (\gamma-1)\hat{\Omega}_p^{(0)}\vec{U}\vec{U}/U^2}{\gamma(1+\vec{U}\cdot\hat{\Omega}_p^{(0)}/c)} \ ,$$
$$\nu_p = \nu_p^{(0)}\gamma\left(1 + \frac{\vec{U}}{c}\cdot\hat{\Omega}_p^{(0)}\right) \ ,$$

where subscript (0) denotes the comoving frame here, E_p is particle energy weight, and here $\gamma = 1/\sqrt{1-U^2/c^2}$. In the comoving frame, it is often simpler to treat scattering and absorption (where the material can be treated as though it isn't moving after the particle's Lorentz transformation). Alternatively, when the fluid motion is sub-relativistic, or $U/c \ll 1$ everywhere, it's possible to post-process the radiation and fluid fields after a transport step that threats the fluid as though it is a frozen snapshot in time [38, 46]. In the next section, the sub-relativistic material motion corrections, as they are implemented in the Jayenne library, are discussed.

8.2 Material Motion Corrections

The material motion corrections in the Jayenne library can be seen as an approximate comoving formulation that preserves lab-frame energy and momentum conservation [38]. As particles stream through a fluid, their frequency and direction change between the reference frames of the fluid parcels they pass, according to the Lorentz transformations written in the previous section. This implies that the expansion of the Lorentz-invariant intensity, I/ν^3 [14, 5], from the characteristic includes more terms (see beginning of this chapter),

$$(\nu^{(0)})^3 \frac{d}{ds}\left(\frac{I^{(0)}}{(\nu^{(0)})^3}\right) = \frac{\partial I^{(0)}}{\partial t}\frac{dt}{ds} + \frac{d\vec{r}}{ds}\cdot\nabla I^{(0)} + \left(\frac{\partial I^{(0)}}{\partial \nu^{(0)}} - 3\frac{I^{(0)}}{\nu^{(0)}}\right)\frac{d\nu^{(0)}}{ds} + \frac{d\hat{\Omega}^{(0)}}{ds}\cdot\frac{\partial I^{(0)}}{\partial \hat{\Omega}^{(0)}} \quad ,$$

where (0) superscripts imply the comoving, or fluid, frame. the method of characteristics applies in the usual way to the time and space derivatives (which are in the lab frame). For the third term, the Doppler shift formula from the previous section may be used; to $\mathrm{O}(\vec{U}/c)$,

$$\Delta\nu^{(0)} = -\frac{\nu^{(0)}}{c}\Delta\vec{U}\cdot\left(\hat{\Omega}^{(0)} + \frac{\vec{U}}{c}\right) \quad ,$$

where use has been made of the $\mathrm{O}(U/c)$ Lorentz transform from the lab frame to the comoving frame, and $\nu\hat{\Omega} \approx \nu^{(0)}(\hat{\Omega}^{(0)} + \vec{U}/c)$. Dividing by $\Delta s \to 0$, using the Chain Rule, $d\vec{U}/ds = \nabla\vec{U}\cdot\vec{\Omega}$, and keeping only $\mathrm{O}(U/c)$ terms,

$$\frac{d\nu^{(0)}}{ds} = -\frac{\nu^{(0)}}{c}\hat{\Omega}^{(0)}\cdot\nabla\vec{U}\cdot\hat{\Omega}^{(0)} \quad .$$

Following the same procedure for $d\hat{\Omega}/ds$,

$$\Delta\hat{\Omega}^{(0)} = -\frac{\Delta\vec{U}}{c}\cdot\left(\mathbf{I} - \hat{\Omega}\hat{\Omega}\right) \quad ,$$

and, since $\vec{U}\cdot\hat{\Omega}\hat{\Omega}/c \approx \vec{U}\cdot\hat{\Omega}^{(0)}\hat{\Omega}^{(0)}/c$,

$$\frac{d\hat{\Omega}^{(0)}}{ds} = -\frac{\hat{\Omega}^{(0)}\cdot\nabla\vec{U}}{c}\cdot\left(\mathbf{I} - \hat{\Omega}^{(0)}\hat{\Omega}^{(0)}\right) \quad .$$

Streaming is balanced by comoving absorption and emission, $j^{(0)} - \sigma_t^{(0)} I^{(0)}$. Thus, to $\mathrm{O}(U/c)$, the comoving transport equation is

$$\frac{1}{c}\frac{DI^{(0)}}{Dt} + \left(1 - \hat{\Omega}^{(0)}\frac{\vec{U}}{c}\right)\hat{\Omega}^{(0)} \cdot \nabla I^{(0)} - \frac{\nu^{(0)}}{c}\hat{\Omega}^{(0)} \cdot \nabla\vec{U} \cdot \hat{\Omega}^{(0)}\frac{\partial I^{(0)}}{\partial \nu^{(0)}} + \frac{3}{c}\hat{\Omega}^{(0)} \cdot \nabla\vec{U} \cdot \hat{\Omega}^{(0)} I^{(0)}$$
$$- \frac{\hat{\Omega}^{(0)} \cdot \nabla\vec{U}}{c} \cdot \left(\mathbf{I} - \hat{\Omega}^{(0)}\hat{\Omega}^{(0)}\right)\frac{\partial I^{(0)}}{\partial \hat{\Omega}^{(0)}} = j^{(0)} - \sigma_t^{(0)} I^{(0)} \quad .$$

This is the comoving transport equation given by [5]. Integrating this in comoving frequency and direction, the first two moment equations are (dropping some terms found unimportant by [5]),

$$\frac{DE^{(0)}}{Dt} + \nabla \cdot \vec{F}^{(0)} + 4\nabla\vec{U} : \mathbb{P}^{(0)} = -q_0^{(0)} \quad ,$$
$$\frac{D\vec{F}^{(0)}}{Dt} + c\nabla \cdot \mathbb{P}^{(0)} + 4\nabla\vec{U} : \mathbb{Q}^{(0)} = -\vec{q}^{(0)} \quad ,$$

where $\mathbf{V} : \mathbf{W}$ is the trace of the matrix product $\mathbf{V}\mathbf{W}^T$, and $\mathbb{Q}$ is the radiative flux tensor (analogous to the heat flux vector for matter, derived at the beginning of the chapter). The factor of 4 in the third terms on the left side arises from using integration by parts when integrating over frequency. Assuming the Lagrangian time derivative of the comoving flux and the high-order heat flux tensor are negligible, and assuming isotropric in the comoving frame, the above equations become

$$\frac{\partial E^{(0)}}{\partial t} + \nabla \cdot \left(\frac{4}{3}\vec{U}E^{(0)}\right) + \nabla \cdot \vec{F}^{(0)} = -q_0^{(0)} + \frac{\vec{U}}{c} \cdot \frac{c\nabla E^{(0)}}{3} \quad ,$$
$$\frac{c}{3}\nabla E^{(0)} = -\vec{q}^{(0)} \quad .$$

It is straightforward to show that $(q_0, \vec{q})$ is a four-vector that obeys Lorentz transformation [4], so to $\mathrm{O}(U/c)$ incorporating the second equation into the first and dropping (0) superscripts gives

$$\frac{\partial E}{\partial t} + \nabla \cdot \left(\frac{4}{3}\vec{U}E\right) + \nabla \cdot \vec{F} = -\left(q_0 + \frac{\vec{U}}{c} \cdot \vec{q}\right) \quad .$$

At the sub-relativistic limit, $U/c \ll 1$, the distinction between lab and comoving frame values of E and $\vec{F}$ vanish, so the frame superscripts can be dropped. This equation has been arrived at asymptotically as well [37, 40, 38] (as apposed to truncating harmonic moments in $\hat{\Omega}^{(0)}$). This equation has two additional terms, compared to the original lab-frame zeroth-moment equation given in the previous section. In the Jayenne library, the form of the transport equation preserves this integral moment,

$$\frac{1}{c}\frac{\partial I}{\partial t} + \nabla \cdot \left(\frac{4}{3}\frac{\vec{U}}{c}I\right) + \hat{\Omega} \cdot \nabla I = \int_{4\pi}\int_0^\infty \frac{\nu}{\nu'}R(\nu' \to \nu, \hat{\Omega}' \to \hat{\Omega})I' d\nu' d\Omega' - (\sigma_s + \sigma_a)I + \sigma_a B - \frac{\vec{U}}{c} \cdot \frac{\vec{q}}{4\pi} \quad ,$$

which is essentially the form given by [47], the static-material transport equation with two additional terms. It turns out that leading-order angular/directional moments of the above equation preserve global energy and momentum conservation, when coupled with the Euler equations (the coupling

term merely has a work contribution but it still cancels with the conservative energy equation, and there are new $4\vec{U}/3$ advection terms). These modest additions to the static-material radiation transport equation permit a straightforward operator split with the hydrodynamic equations.

Here the outline of the operator split from the previous section is expanded upon to provide details for the sub-relativistic material motion corrections (see, e.g. [38, 47]).

1. Have the host code solve an uncoupled hydrodynamic step,

$$\frac{\rho_{n+1}-\rho_n}{\Delta t_n} + [\nabla\cdot(\rho\vec{U})]_* = 0 \ ,$$
$$\frac{\rho_{n+1}\vec{U}_h-\rho_n\vec{U}_n}{\Delta t_n} + [\nabla\cdot(\rho\vec{U}\vec{U})+\nabla P]_* = 0 \ ,$$
$$\frac{\rho_{n+1}\mathcal{E}_h-\rho_n\mathcal{E}_n}{\Delta t_n} + [\nabla\cdot\Big(\vec{U}(\rho\mathcal{E}+P)\Big)]_* = 0 \ ,$$

   where the subscript n is the time step index, h denotes the value at the end of the pure hydrodynamic step, and $*$ denotes an arbitrary time-centering evaluation.

2. The next step is to solve radiation transport using the updated hydrodynamic state. The material-motion correction approach adopted by the Jayenne package is discussed in the next section. For clarity, they are written here,

$$\frac{I_h-I_n}{\Delta t_n} + \nabla\cdot\left(\frac{4}{3}\vec{U}_h I_n\right) = 0 \ ,$$
$$\frac{I_r-I_h}{c\Delta t_n} + \hat{\Omega}\cdot\nabla I_* = \int_{4\pi}\int_0^\infty \frac{\nu}{\nu'}R(\nu'\to\nu,\hat{\Omega}'\to\hat{\Omega})I'_* d\nu' d\Omega' - (\sigma_{s,h}+\sigma_{a,h})I_* \tag{92a}$$
$$+(1-f_h)\frac{\sigma_{a,h}b_h}{4\pi\sigma_{P,h}}\int_{4\pi}\int_0^\infty \sigma_{a,h}I'_* d\Omega' d\nu' + f_h\sigma_{a,h}b_h\frac{acT_h^4}{4\pi} \ ,$$
$$\frac{I_{n+1}-I_r}{\Delta t_n} = -\left[\vec{U}\cdot\frac{\vec{q}}{4\pi}\right]_* \ ,$$

   where subscript r denotes the end of the Monte Carlo step, f_h is the Fleck factor, $\sigma_{P,h}$ is the Planck opacity, and b_h is the normalized Planck function [23]. Algorithmically,

   (a) the first equation corresponds to advecting the initial census particles by $4\vec{U}_h/3$,
   (b) the second equation involves the standard IMC method,
   (c) and the third equation involves post-processing the particles by scaling their energy weights, to account for work done by the radiation to the fluid.

3. Update the hydrodynamic state again, using the Monte Carlo tallies of energy and momentum deposition from the previous step,

$$\rho_{n+1}\frac{\vec{U}_{n+1}-\vec{U}_h}{\Delta t_n} = \left[\frac{\vec{q}}{c}\right]_* \ ,$$
$$\rho_{n+1}\frac{e_{n+1}-e_h}{\Delta t_n} = f_h[q_0]_{a,*} + [q_0]_{s,*} \ ,$$
$$\rho_{n+1}\frac{U_{n+1}^2/2-U_h^2/2}{\Delta t_n} = \left[\frac{\vec{U}}{c}\cdot\vec{q}\right]_* \ ,$$

where $[q_0]_{a,*}$ is the internal energy coupling due to absorption included in the IMC linearization and $[q_0]_{s,*}$ is the inelastic scattering coupling excluded from the IMC linearization. $\vec{U}_*$ is obtained by requiring consistency between the first and third equation, so

$$\vec{U}_* = \frac{\vec{U}_{n+1} + \vec{U}_h}{2} \quad .$$

Since this part involves updating the fluid variables, it must be done by the host code.

In the following section, we discuss the remaining piece needed to solve the radiation hydrodynamics equations with the Jayenne library: energy and momentum tallies. These tallies permit the calculation of q_0 and $\vec{q}$ needed in the above operator split outline.

8.3 Momentum Deposition

In the Jayenne package, both energy and momentum deposition are tallied via implicit capture (see, e.g. [35]). For absorption, the tally formulae follow from

$$\Delta I = I_0 \int_0^d \sigma_a e^{-\sigma_a s} ds \quad ,$$
$$\Delta(\hat{\Omega} I) = I_0 \int_0^d \hat{\Omega} \sigma_a e^{-\sigma_a s} ds \quad ,$$

where I is the final intensity after streaming distance d and I_0 is the initial intensity. In Cartesian coordinates the direction $\hat{\Omega}$ will be constant along path, but in curvilinear coordinates (e.g. cylindrical or spherical) the direction will change along the path. Since the intensity of a particle is merely a product of Dirac-delta functions multiplied by the energy weight, the above formulae are quivalent to

$$\Delta E_p = E_{p,0} \int_0^d \sigma_a e^{-\sigma_a s} ds \quad ,$$
$$\frac{1}{c}\Delta(\hat{\Omega}_p E_p) = \Delta P_p = \frac{1}{c} E_{p,0} \int_0^d \hat{\Omega} \sigma_a e^{-\sigma_a s} ds \quad .$$

The above formulae, together with instantaneous changes in energy and momentum from scattering (effective or physical),

$$\Delta E_p = E_p - E_{p,0} \quad ,$$
$$\frac{1}{c}\Delta(\hat{\Omega}_p E_p) = \Delta P_p = \frac{1}{c}(E_p \hat{\Omega}_p - E_{p,0}\hat{\Omega}_{p,0}) \quad ,$$

give a history of values for each particle that are summed in each spatial cell, over particles that cross or scatter in the cell.

In curvilinear coordinates, the momentum absorption implicit capture has to be done numerically along particle paths, described by [13]. For cylindrical geometry, if the radially-projected path is short with respect to the initial radius and the projected optical depth is small over the path, or [13]

$$\frac{\sigma_a(1-\xi_p^2)d^2}{\sigma_a(1-\xi_p^2)d^2 + r_{p,0}} < \epsilon_t \quad ,$$

where ξ is the axial (z-axis) projection of the particle direction and ϵ_t is some acceptable tolerance level, the integral can be approximated as [13]

$$\Delta P_p = \frac{1}{c} E_{p,0} \hat{\Omega}_* \int_0^d \sigma_a e^{-\sigma_a s} ds \quad ,$$

where $\hat{\Omega}_*$ is an average direction of the path. This is now an analytic integral. Otherwise, the full numerical integral is performed with the Midpoint Rule on up to twelve integration points on the path, with seven of the points resulting from an equipartition of the energy attenuation,

$$\Delta\varepsilon = \frac{\Delta E_p}{6E_{p,0}} = \frac{1 - e^{-\sigma_a d}}{6} \quad ,$$
$$s_k = -\frac{\ln(1 - k\Delta\varepsilon)}{\sigma_a} \quad , \tag{97a}$$

where s_k are a subset of points along the integration path. If the particle is travelling inward in radius, it may have an "inflection point", where the radial projection of the direction goes from negative to positive (the particle travels outward again). In this instance, an additional five integration points are added: the inflection point and two points geometrically spaced on either side of the inflection point in the path,

$$\tilde{s}_0 = -\frac{\mu_{p,0} r_{p,0}}{1 - \xi_p^2} = \tilde{\mu}_{p,0} r_{p,0} \quad ,$$
$$\tilde{s}_{\pm j} = \tilde{s}_0 \pm \left(\left. \frac{d\tilde{\mu}}{ds} \right|_{s_0} \right)^{-j} \quad .$$

The set of $\tilde{s}_j$ points are then added to the s_k set.

It is noteworthy that going to fully special relativistic transport would complicate the numerical integral of the momentum deposition further. For instance, tracking particles in the lab frame would require an angularly anisotropic opacity, since the Lorentz-invariant form of the opacity is actually $\nu\sigma_a$ [5]. The Jayenne library currently only supports sub-relativistic (or, as it is called in the literature, non-relativistic) transport, so the lab and comoving frame opacities are not distinguishable.

The above discussion on momentum deposition only applies to pure transport, so a separate treatment is needed for the diffusion optimization, DDMC [20, 19, 11]. The approach to tallying momentum is discussed in the following subsubsection.

8.3.1 DDMC Momentum Deposition

DDMC particles do not possess direction or position at the sub-cell level [25, 20, 19, 11]. Consequently, direction cannot be used in the tally of momentum for DDMC particles and an alternate method must be applied. However, the momentum deposition is an integral over direction solid angle, which in the diffusion limit can be estimated as at cell i, face j as [20]

$$A_{i,j} \Delta\vec{P}_{i,j} = A_{i,j} \sigma_{i,j} \sum_p \vec{F}_{p,i,j} \quad ,$$

where $\sigma_{i,j}$ is the opacity at face j evaluated in cell i, $A_{i,j}$ is the area of face j, and $\vec{F}_{p,i,j}$ is the contribution of particle p to the net flux across face j. In interior DDMC cells,

$$\hat{z} \cdot \sum_p \vec{F}_{p,i,j} = \hat{z} \cdot \vec{F}_{i,j} = (\vec{n}_{i,j} \cdot \hat{z})\sigma_{j,i\to i'} c E_i V_i - (\vec{n}_{i,j} \cdot \hat{z})\sigma_{j,i'\to i} c E_i' V_i' \ ,$$

where V_i is the volume of cell i. This is the expected net leakage to cell i' across face j, along dimension z. At an IMC-DDMC (hybrid) interfaces, one of the terms on the right side of the previous equation is replaced with the diffusion-limit boundary condition [20],

$$\hat{z} \cdot \sum_p \vec{F}_{p,i,j} = \hat{z} \cdot \vec{F}_{i,j} = (\vec{n}_{i,j} \cdot \hat{z})\sigma_{j,i\to i'} c E_i V_i - (\vec{n}_{i,j} \cdot \hat{z}) \int_0^1 P(\mu)\mu I' d\mu \ ,$$

where $\mu = |\hat{\Omega} \cdot \vec{n}_{i,j}| = |\hat{\Omega} \cdot \hat{z}|$. Transport particles from cell i' that sample transmission into cell i contribute the net flux in cell i, in other words. The cell average net momentum in cell i is

$$\Delta \vec{P}_i = \frac{1}{A_i} \sum_j A_{i,j} \Delta \vec{P}_{i,j} \ ,$$

where $A_i = \sum_j A_{i,j}$ is the surface area of cell i. This formula reduces to an arithmetic average in planar/Cartesian coordinates.

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