Efficient smoothed particle radiation hydrodynamics I: Thermal radiative transfer

Brody R. Bassett*, J. Michael Owena, Thomas A. Brunnera

bassett4@llnl.gov, owen8@llnl.gov, brunner6@llnl.gov

aLawrence Livermore National Laboratory
7000 East Avenue, Livermore, CA, 94550

*Corresponding author

Abstract

This work presents efficient solution techniques for radiative transfer in the smoothed particle hydrodynamics discretization. Two choices that impact efficiency are how the material and radiation energy are coupled, which determines the number of iterations needed to converge the emission source, and how the radiation diffusion equation is solved, which must be done in each iteration. The coupled material and radiation energy equations are solved using an inexact Newton iteration scheme based on nonlinear elimination, which reduces the number of Newton iterations needed to converge within each time step. During each Newton iteration, the radiation diffusion equation is solved using Krylov iterative methods with a multigrid preconditioner, which abstracts and optimizes much of the communication when running in parallel. The code is verified for an infinite medium problem, a one-dimensional Marshak wave, and a two and three-dimensional manufactured problem, and exhibits first-order convergence in time and second-order convergence in space. For these problems, the number of iterations needed to converge the inexact Newton scheme and the diffusion equation are independent of the number of spatial points and the number of processors.

Keywords: radiation hydrodynamics, smoothed particle hydrodynamics, radiative transfer, meshless method
1 Introduction

Smoothed particle hydrodynamics (SPH) is a meshless approach to solving the hydrodynamics equations, in which the fluid is separated into discrete masses that are used as interpolation points (for an overview, see Refs. [1, 2]). SPH has several good properties, such as automatic conservation of mass and enforced conservation of energy and momentum, flexible point topology, and Galilean invariance. Like mesh-based Lagrangian codes, the resolution of the problem follows the mass, but unlike mesh-based codes, SPH does not have issues with mesh tangling. Drawbacks of SPH include a lack of zeroth-order consistency (the interpolant cannot generally reproduce a constant exactly) [3], the use of a relatively low-order, unlimited artificial viscosity for shock hydrodynamics [4], and additional expense that comes from computing connectivity at each time step. There are extensions to SPH that correct some of these issues, such as moving least squares particle hydrodynamics [5, 6] and conservative reproducing kernel smoothed particle hydrodynamics [7].

The thermal radiative transfer equations have been solved using a smoothed particle hydrodynamics discretization previously. The most popular method is implicit, two-temperature, flux-limited diffusion, first implemented in Refs. [8, 9]. These papers assume an ideal gas equation of state. In the latter paper, the system is reduced to solving a quartic equation per point within a Gauss-Seidel iteration scheme. There are other implementations of flux-limited diffusion, most of which have been applied to astrophysical problems [10, 11]. The form of the second derivative used most often for the radiation diffusion second derivative was first applied to heat diffusion [12]. The optically-thin variable Eddington factor equations with Eddington factors determined by source information (as opposed to by a full transport calculation) have been applied to cosmological simulation [13]. Similar methods that have been studied include ray-tracing [14], Monte Carlo [15], and neutrino flux-limited diffusion [16].

Thermal radiative transfer couples the transport of photons with the hydrodynamic state. Common coupling techniques for the radiation and material equations include simple convergence of the residuals of both equations (including Newton-Krylov methods), using a single Newton iteration, lagging the nonlinear terms in the equation, predictor-corrector schemes, and linearization of the nonlinear emission source [17, 18]. The method used in this paper is based on nonlinear elimination methods, as described in Ref. [19] and applied to radiation diffusion in Ref. [20].

The radiation diffusion and transport equations have also been solved using meshless methods other than SPH, including for coupled radiative transport and conductive heat transfer [21, 22, 23], neutron transport [24], and neutron diffusion [25, 26]. Many of these discretizations involve either relatively flat meshless functions (which increases accuracy but makes the system ill-conditioned) or integration of the meshless functions. The advantage of using the SPH discretization directly is that the same functions that are used for hydrodynamics can be reused for the radiation, without recomputing the topology.

The goal of this research is to make SPH radiation diffusion more efficient. This is done by improving the solution of the diffusion problem using fast and accurate preconditioners and applying material-radiation coupling methods that speed up the convergence of the radiation emission and absorption. With appropriate time step constraints, the solver is stable and exhibits first-order convergence in time and second-order convergence in space to analytic solutions and manufactured problems. The methods used here scale well with the number of points and under domain decomposition due to the use of fast multigrid solvers [27], which also makes the method simple to implement on distributed architectures. The remainder of this paper is structured as follows. In Sec. 2, the SPH thermal radiative transfer equations are derived and discretized in time and space. In Sec. 3, the implementation of the equations is discussed. Finally, in Sec. 4, results for problems in one, two and three dimensions with known solutions are presented to verify the accuracy of the code. In Paper II, the full SPH radiation hydrodynamics equations are derived with appropriate radiation-material coupling terms, and results for full radiation hydrodynamics are presented.

2 Theory

The smoothed particle hydrodynamics method is used to discretize the thermal radiative transfer equations in space. The discretization in time reduces a coupled set of equations for the material and radiation energies to separate updates for the material and radiation energies in an iterative process. The resulting equations conserve energy.
2.1 The thermal radiative transfer equations

The thermal radiative transfer equations are

\[ \rho \frac{\partial e}{\partial t} = -c \sigma_a B + c \sigma_a E + Q_e, \]  
\[ \frac{\partial E}{\partial t} = -\partial_\alpha F_\alpha - c \sigma_a E + c \sigma_a B + Q_E, \]  
\[ \frac{1}{c} \frac{\partial F_\alpha}{\partial t} = -c \partial_\beta P_{\alpha \beta} - \sigma_t F_\alpha, \]

with the summation coefficients \( \alpha \) and \( \beta \) and the variables

- \( t \), time,
- \( x \), position,
- \( v_\alpha \), velocity,
- \( \rho \), mass density,
- \( e \), specific material energy,
- \( E \), radiation energy density,
- \( F_\alpha \), radiation flux,
- \( P_{\alpha \beta} \), radiation pressure,
- \( T \), material temperature,
- \( B \), integrated photon emission function,
- \( c \), speed of light in a vacuum,
- \( \sigma_t \), total opacity,
- \( \sigma_a \), absorption opacity,
- \( a \), black-body constant,
- \( Q_e \), nonhomogeneous material energy source,
- \( Q_E \), nonhomogeneous radiation energy source.

The radiation transport equation has been integrated over all energy frequencies (the grey approximation) and integrated over angle to produce the first two angular moments. For the derivation in Paper I, the material is assumed to be stationary. The emission term is defined as

\[ B = a T^4, \]

where the black body constant \( a \) is defined in terms of the Stefan-Boltzmann constant \( \sigma_{SB} \) and the speed of light \( c \) as \( a = 4 \sigma_{SB}/c \).

Assuming the specific intensity is linearly anisotropic in angle, the pressure term becomes

\[ P_{\alpha \beta} = \frac{1}{3} I_{\alpha \beta} E, \]

where \( I \) is the tensor identity. Assuming that the time derivatives are neglected, the first angular moment of the transport equation [Eq. (1b)] can be solved for the radiation flux to get Fick’s law,

\[ F_\alpha = -\frac{c}{3 \sigma_t} \partial_\alpha E. \]
Replacing the flux term in the zeroth angular moment equation [Eq. (1c)] with Fick’s law and replacing the pressure term by the linearly anisotropic value results in the diffusion equation,

\[
\frac{\partial E}{\partial t} = \partial_{\alpha} c_s \partial_{\alpha} E - \sigma_a E + c_s B + Q_E.
\]  

(5)

In the original radiation equations [Eqs. (1b) and (1c)], if the pressure were not isotropic, the radiation would propagate correctly at the speed of light. However, when the time derivative on the first moment equation is dropped, this adds an error that allows the radiation to propagate faster than the speed of light, \( |F| > cE \). This effect can be prevented by applying a flux limiter \( \lambda \) to the diffusion equation,

\[
\frac{\partial E}{\partial t} = \partial_{\alpha} c_s \lambda \sigma_t \partial_{\alpha} E - \sigma_a E + c_s B + Q_E.
\]  

(6)

With a constant \( \lambda = 1/3 \), the original equation is recovered. The flux limiter is usually written in terms of the constant \( R \),

\[
R = \sqrt{\frac{(\partial_{\alpha} E)(\partial_{\alpha} E)}{\sigma_t E}},
\]  

(7)

with examples such as the Levermore flux limiter [28],

\[
\lambda = \frac{2 + R}{6 + 3R + R^2},
\]  

(8)

and the Larsen flux limiter [29],

\[
\lambda = \frac{1}{(3^k + R^k)^{1/k}},
\]  

(9)

where \( k \) is a chosen constant. Both of these have the correct limits for diffusive regions \( (R \to 0) \), which is the diffusion equation, and optically thin regions \( (R \to \infty) \), which describes radiation propagating at the speed of light [30],

\[
F_\alpha \to \begin{cases} -\frac{c}{3\sigma_t} \partial_{\alpha} E, & R \to 0, \\ -\frac{\partial_{\alpha} E}{\sqrt{(\partial_{\beta} E)(\partial_{\beta} E)}} cE, & R \to \infty. \end{cases}
\]  

(10)

The Larsen flux limiter with \( k = 2 \) is used in most of the results in this paper.

### 2.2 Time discretization

The coupled material and radiation energy equations [Eqs. (1a) and (6)] are discretized fully implicitly in time, using the nonlinear elimination methodology described in Ref. [20]. The derivation begins with the coupled material and radiation diffusion equations discretized using backward Euler,

\[
G = \begin{bmatrix} m(e^n, E^n) \\ r(e^n, E^n) \end{bmatrix} = \begin{bmatrix} \rho \frac{\Delta t}{\Delta t} (e^n - e^{n-1}) + \sigma_a B^n - \sigma_a E^n - Q^n_e \\ \frac{1}{\Delta t} (E^n - E^{n-1}) - \partial_{\alpha} c_s \frac{c_s}{\sigma_t} \partial_{\alpha} E^n + \sigma_a E^n - \sigma_a B^n - Q^n_a \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},
\]  

(11)

where \( U = \begin{bmatrix} e & E \end{bmatrix}^T \). Newton’s method updates the state according to

\[
J^T \delta^t = -G^t,
\]  

(12a)

\[
U^{t+1} = U^t + \delta^t,
\]  

(12b)

where \( J \) is the Jacobian with respect to \( e \) and \( E \),

\[
J = \begin{bmatrix} J_{m,e} & J_{m,E} \\ J_{r,e} & J_{r,E} \end{bmatrix} = \begin{bmatrix} \rho \frac{\Delta t}{\Delta t} + \frac{c}{c_v} \sigma_a \partial_{\alpha} B \\ -\frac{c}{c_v} \sigma_a \partial_{\alpha} B \end{bmatrix},
\]  

(12c)

\[
\begin{bmatrix} -\sigma_a \\ 1 - \partial_{\alpha} \frac{c_s}{\sigma_t} \partial_{\alpha} + \sigma_a \end{bmatrix},
\]  

and \( \delta = [\delta_e, \delta_E]^T \) is the change in the state variables and \( c_v = \frac{\partial c}{\partial T} \) is the specific heat capacity.
To simplify the Newton iteration, the Schur compliment of the Jacobian is taken, resulting in the Jacobian system

\[
\begin{bmatrix}
J_{m,e} & J_{m,E} \\
0 & J_{r,E} - J_{r,e} J_{m,e}^{-1} J_{m,E}
\end{bmatrix}
\begin{bmatrix}
\delta_e \\
\delta_E
\end{bmatrix} =
\begin{bmatrix}
-F_e \\
-F_E + J_{r,e} J_{m,e}^{-1} F_e
\end{bmatrix}
\]  

(13)

can be solved first for \(\delta_E\) and then \(\delta_e\). This system of equations can be first solved for \(\delta_E\) and then \(\delta_e\). The solution in Eq. (13) combined with the update in Eq. (12b) is full Newton iteration without approximation. Noting that \(\partial_T B = 4aT^3\), the term \(J_{r,e} J_{m,e}^{-1}\) can be written in terms of the Fleck factor commonly used in implicit Monte Carlo [31],

\[
f = \left(1 + c\sigma_a \Delta t \frac{4aT^3}{\rho c_v}\right)^{-1},
\]

(14)

which is used to forward-predict the emission source, as

\[
J_{r,e} J_{m,e}^{-1} = f - 1.
\]

(15)

Finally, the temperature is held constant in \(f\) during each time step, which results in an inexact Newton iteration scheme,

\[
\frac{1}{\Delta t} E^{n+1} - \partial_{\alpha} \frac{c\lambda}{\sigma_t} \partial_{\alpha} E^{n+1} + c\sigma_a f E^{n+1} = \frac{1}{\Delta t} E^{n-1} + c\sigma_a B^{n-1} - (1 - f) c\sigma_a E^{n+1} + Q_n^n,
\]

(16)

with the time step index \(n\) and the iteration index \(\ell\). When \(E^{n}\) has converged, the terms involving \(f\) in the diffusion equation cancel out and the original, time-discretized diffusion equation is recovered.

Equations (12) represent the standard Newton solution method for the thermal radiative transfer equations. Here, a nonlinear acceleration technique from Ref. [20] is additionally applied. The following two functions are helpful in describing the iterative process of solving the equations,

\[
m(e^*, E) = \frac{\rho}{\Delta t} (e^* - e^{n-1}) + c\sigma_a B^* - c\sigma_a E - Q_n^e = 0,
\]

(17a)

\[
r^\dagger (e, E, E^*) = \frac{1}{\Delta t} E^* - \partial_{\alpha} \frac{c\lambda}{\sigma_t} \partial_{\alpha} E^* + c\sigma_a f E^* - \frac{1}{\Delta t} E^{n-1} - c\sigma_a B + (1 - f) c\sigma_a E - Q_n^e = 0
\]

(17b)

where \(e^*\) and \(E^*\) represent the values to be solved for. Note the use of \(r^\dagger\) to distinguish the diffusion equation from the starting equation \(r\). The solution of \(r^\dagger (e, E, E^*) = 0\) represents solving a spatially-coupled linear equation, as discussed in Sec. 3.1. Note that the value of the material energy in these equations is entirely dependent on the radiation energy, which means that a solution of \(r^\dagger\) represents an inexact Newton iteration of the full material and radiation energy system. After a solution of \(r^\dagger\) for the radiation energy, the material energy is updated by solving \(m(e^*, E) = 0\), which represents a nonlinear solve using Newton’s method,

\[
e^* \leftarrow e^* - (J_{m,e})^{-1} \left[ \frac{\rho}{\Delta t} (e^* - e^{n-1}) + c\sigma_a B^* - c\sigma_a E - Q_n^e \right],
\]

(18)

where \(\leftarrow\) represents an update to the value of \(e^*\). This update is performed until \(e^*\) is converged. This differs from standard Newton iteration, where the material energy update would be done simultaneously with the radiation energy update and without solving \(m(e^*, E) = 0\) until \(e^*\) is converged. The iterative solution procedure for these two equations is described in Alg. 1. The outer iterations, or the inexact Newton iteration of the material and radiation energy system, continue until the convergence criteria are met,

\[
\begin{align*}
\left| \frac{e^{n+1} - e^{n}}{e^{n+1}} \right| & < \epsilon_e, \\
\left| \frac{E^{n+1} - E^{n}}{E^{n+1}} \right| & < \epsilon_E.
\end{align*}
\]

(19a)

(19b)

The inner iterations, or the iterations required to converge \(m\) and \(r\) within an outer iteration, use similar equations for determining convergence. As the absorption term appears with both \(E^n\) and \(E^{n+1}\), convergence is required for energy conservation to be preserved (see Sec. 2.5).
2.3 Introduction to smoothed particle hydrodynamics

Smoothed particle hydrodynamics involves interpolation of fields using kernels, which are functions centered at interpolation points. The initial assumption needed is that SPH kernels approximate delta functions, or 
\[ W(x - x', h) \to \delta(x - x') \] as \( h \to 0 \), where \( h \) is the smoothing parameter that determines the width of the kernels.

\[
g(x) = \int_V \delta(x - x') g(x') dV' \\
\approx \int_V W(x - x', h) g(x') dV'.
\]

This also means that the integral of the kernel should be equal to one,
\[
\int_V W(x - x', h) dV' = 1. \tag{20}
\]

In practice, the \( h \) can depend on both \( x \) and \( x' \). The second assumption is that a set of kernels in space can be used to form a quadrature, with abscissas at the kernel centers \( x_i \) and weights equal to the kernel volume \( V_i \). With these two assumptions, the kernels can be used to interpolate a function,
\[
\langle g(x) \rangle = \int_V W(x - x', h) g(x') dV' \\
\approx \sum_j V_j W(x - x_j, h) g_j. \tag{21}
\]

Here \( g_j \) is the function evaluated at point \( j \), \( g_j = g(x_j) \), and \( \langle \cdot \rangle \) indicates an interpolated quantity. The interpolant is used to calculate derivatives of the field. This interpolant does not have the Kronecker delta property,
\[
\langle g(x) \rangle_i = \sum_j V_j W(x_i - x_j, h) g_j \neq g_i. \tag{22}
\]

To approximate a derivative in SPH, another three properties are needed from the kernel: that the kernel does not intersect a boundary, that the derivative of the kernel is antisymmetric in \( x \) and \( x' \), and that the integral of the derivative of the kernel is zero. With these approximations, the derivative of a function can be approximated as
\[
\langle \partial_{x,\alpha} g(x) \rangle = \int_V W(x - x', h) \partial_{x',\alpha} g(x') dV' \\
= - \int_V \partial_{x',\alpha} W(x - x', h) g(x') dV' \\
= \partial_{x,\alpha} \int_V W(x - x', h) g(x') dV' - g(x) \partial_{x,\alpha} \int_V W(x - x', h) dV' \\
\approx \sum_j V_j (g_j - g(x)) \partial_{x,\alpha} W(x - x_j, h). \tag{23}
\]

Note that because of the added \( g(x) \) term (which equals zero in integral form due to the derivative), this approximation of the derivative goes to zero for a constant function.

For a diffusion-like problem, a second-order series expansion for \( g(x) \) about \( x' \) and \( g(x') \) about \( x \),
\[
\partial_{x',\alpha} g(x') \approx \frac{x_\alpha - x'_\alpha}{(x_\beta - x'_\beta) (x_\beta - x'_\beta)} [g(x') - g(x)], \tag{24}
\]
can be used to produce a commonly-used second-order approximation to the second derivative [1],

\[
\langle \partial_{x,\alpha} [k(x) \partial_{x,\alpha} g(x)] \rangle = \int_V W(x-x',h) \partial_{x',\alpha} [k(x') \partial_{x',\alpha} g(x')] \, dV' \\
= - \int_V k(x') \partial_{x',\alpha} W(x-x',h) \partial_{x,\alpha} g(x') \, dV' \\
= \partial_{x,\alpha} \int_V k(x') W(x-x',h) \partial_{x,\alpha} g(x') \, dV' + k(x) \partial_{x,\alpha} g(x) \partial_{x,\alpha} \int_V W(x-x',h) \, dV' \\
= \int_V [k(x) \partial_{x,\alpha} g(x) + k(x') \partial_{x',\alpha} g(x')] \partial_{x,\alpha} W(x-x',h) \, dV' \\
\approx \int_V [k(x) + k(x')] \left[ g(x) - g(x') \right] \frac{x_{\alpha} - x'_{\alpha}}{(x_{\beta} - x'_{\beta})(x_{\beta} - x'_{\beta})} \partial_{x,\alpha} W(x-x',h) \, dV' \\
\approx \sum_j V_j(k(x) + k_j)(g(x) - g_j) \frac{x_{\alpha} - x_{\alpha,j}}{(x_{\beta} - x_{\beta,j})(x_{\beta} - x_{\beta,j})} \partial_{x,\alpha} W(x-x_j,h). \\
\tag{25}
\]

Like the first derivative approximation, the second derivative is zero for a constant function because the \( g \) terms cancel.

When discretizing an equation in SPH, the equation is first multiplied by the kernel \( W(x-x',h) \) and integrated, similar to the finite element method. The distinction is that the interpolant is only used to calculate derivatives. The terms without derivatives are approximated using the definition of the interpolant,

\[
\langle g(x) \rangle = \int_V W(x-x',h) g(x') \, dV' \approx g(x). \\
\tag{26}
\]

The terms with derivatives are approximated as derivatives of the interpolant, as in Eq. 23. The final step in an SPH discretization is to add constraints to match the free variables in the equations. This can be done by multiplying the equations by a delta function \( \delta(x-x_i) \) and integrating, or equivalently, evaluating the functions at \( x = x_i \). This results in the fully-discrete approximations to Eqs. (21), (23), and (25),

\[
\langle g(x) \rangle_i \approx \sum_j V_j W_{ij} g_j, \\
\tag{27a}
\langle \partial_{x,\alpha} g(x) \rangle_i \approx \sum_j V_j (g_j - g_i) \partial_{i,\alpha} W_{ij}, \\
\tag{27b}
\langle \partial_{x,\alpha} [k(x) \partial_{x,\alpha} g(x)] \rangle_i \approx \sum_j V_j (k_i + k_j)(g_i - g_j) \frac{x_{ij,\alpha}}{x_{ij,\beta}x_{ij,\beta}} \partial_{i,\alpha} W_{ij}, \\
\tag{27c}
\]

where

\[
x_{ij,\alpha} = x_{i,\alpha} - x_{j,\alpha}, \\
W_{ij} = W(x_{ij},h), \\
\partial_{i,\alpha} W_{ij} = \partial_{i,\alpha} W(x_{ij},h). \\
\tag{28}
\]

The smoothing length \( h \) connects the analytic kernel in Eq. (30c) with the SPH kernels,

\[
W(x-x',h) = \psi \left( \sqrt{\frac{(x_{\alpha} - x'_{\alpha})(x_{\alpha} - x'_{\alpha})}{h}} \right). \\
\tag{29}
\]

In practice, the smoothing length is not constant and instead has discrete values at the SPH nodes. To retain symmetry in the derivatives [such that \( \partial_{i,\alpha} W(x_i - x_j,h) = \partial_{j,\alpha} W(x_j - x_i,h) \)], the kernel values are taken to be an average of the evaluations using these two smoothing lengths,

\[
W_{ij} = \frac{1}{2} [W(x_{ij},h_i) + W(x_{ij},h_j)] \\
\tag{30a}
\partial_{i,\alpha} W_{ij} = \frac{1}{2} [\partial_{i,\alpha} W(x_{ij},h_i) + \partial_{i,\alpha} W(x_{ij},h_j)]. \\
\tag{30b}
\]
The Wendland functions [32] are one example of a kernel that can be used in SPH. The Wendland C4 kernel is used here,

\[
W_{\text{wendland}}(x_{ij}, h) = \begin{cases} 
 k (1 - r)^5 \big(8r^2 + 5r + 1\big), & r \equiv x_{ij}/h \leq 1, \\
 0, & \text{otherwise,}
\end{cases}
\]  

(30c)

with a dimensionally-dependent normalization constant \(k\) that is chosen such that Eq. (20) is satisfied.

### 2.4 Spatial discretization

To perform the spatial discretization, the material and radiation energy equations [Eqs. (17)] are multiplied by \(W(x_i - x', h)\) and integrated,

\[
\left\langle \frac{\rho_i}{\Delta t} \left( e_i^{n+1} - e_i^{n-1} \right) + c\sigma_a B_i^{n+1} - c\sigma_a E_i^{n+1} - Q_e \right\rangle_i = 0,
\]  

(31a)

\[
\left\langle \frac{1}{\Delta t} E_i^{n+1} - \partial_\alpha \frac{c_\lambda_i}{\sigma_i} \partial_\alpha E_i^{n+1} + c\sigma_a f E_i^{n+1} \right\rangle_i = \left\langle \frac{1}{\Delta t} E_i^{n-1} + c\sigma_a B_i^{n} - (1 - f) c\sigma_a E_i^{n} + Q^n_E \right\rangle_i,
\]  

(31b)

where \(\langle \cdot \rangle\) is the interpolant notation as defined in Sec. 2.3. The terms not involving derivatives can be approximated using Eq. (26), e.g.

\[
\left\langle \frac{\rho_i}{\Delta t} e_i^{n-1} \right\rangle \approx \rho_i e_i^{n-1},
\]  

(32)

\[
\langle c\sigma_a f E_i^{n+1} \rangle_i \approx c\sigma_a f e_i^{n+1}.
\]  

(33)

The second derivative in the radiation energy equation can be approximated using Eq. (25),

\[
\langle -\partial_\alpha D(x) \partial_\alpha E(x) \rangle \approx -\sum_j V_j (D_i + D_j) (E_i - E_j) \frac{x_{ij,\alpha}}{x_{ij,\beta}x_{ij,\beta}} \partial_\alpha W_{ij},
\]  

(34)

with the diffusion coefficient

\[
D_i = \frac{c\lambda_i}{\sigma_i,i}.
\]  

(35)

With these approximations, the material and radiation equations are

\[
\frac{\rho_i}{\Delta t} \left( e_i^{n+1} - e_i^{n-1} \right) + c\sigma_a,i B_i^{n+1} - c\sigma_a,i E_i^{n+1} - Q_e,i = 0,
\]  

(36a)

\[
\frac{1}{\Delta t} E_i^{n+1} - \sum_j V_j (D_i + D_j) \left( E_i^{n+1} - E_j^{n+1} \right) \frac{x_{ij,\alpha}}{x_{ij,\beta}x_{ij,\beta}} \partial_\alpha W_{ij} + c\sigma_a,f E_i^{n+1} = \frac{1}{\Delta t} E_i^{n-1} + c\sigma_a,B_i^{n} - (1 - f) c\sigma_a E_i^{n} + Q^n_E,i.
\]  

(36b)

The material energy equation is independent for each point \(i\), while the radiation energy equation for point \(i\) linearly couples to the radiation energy from nearby nodes. For more information on how these equations are solved, see Sec. 3.1.

### 2.5 Conservation

The coupled material and radiation equations [Eqs. (36)] are conservative in energy to the tolerance of the nonlinear iteration process once converged. The quantity that is conserved is the total energy over all points, which is the material energy plus the radiation energy,

\[
\sum_i (m_i e_i + V_i E_i) = \text{const.}
\]  

(37)

At convergence, \(e_i^{n+1} \approx e_i^{n}\) and \(E_i^{n+1} \approx E_i^{n}\), which results in the simplified equations

\[
\frac{\rho_i}{\Delta t} \left( e_i^n - e_i^{n-1} \right) + c\sigma_a,i B_i^n - c\sigma_a,i E_i^n = Q_e^n,i,
\]  

(38a)

\[
\frac{1}{\Delta t} (E_i^n - E_i^{n-1}) - \sum_j V_j (D_i + D_j) (E_i^n - E_j^n) \frac{x_{ij,\alpha}}{x_{ij,\beta}x_{ij,\beta}} \partial_\alpha W_{ij} + c\sigma_a,i E_i^n - c\sigma_a,i B_i^n = Q^n_E,i.
\]  

(38b)
Adding the two equations, multiplying by \( V_i \), and summing over \( i \) results in

\[
\sum_i \left[ m_i \left( e_i^n - e_i^{n-1} \right) + V_i \left( E_i^n - E_i^{n-1} \right) \right] = \Delta t \sum_i \left( Q_{e,i}^n + Q_{E,i}^n \right).
\]  \hspace{1cm} (39)

Because the diffusion spatial derivative is antisymmetric about \( i \) and \( j \), it disappears under summation over both \( i \) and \( j \). This final equation says that any gains or losses in the total energy are as a result of specified sources. At equilibrium and absence external sources, both the material and the radiation equations reduce to an equilibrium absorption-emission rate at every point \( x_i \), which is \( E_i = B_i \).

3 Methodology

The thermal radiative transfer methods described here are implemented within the open-source SPH code Spheral, described at \( \text{https://wci.llnl.gov/simulation/computer-codes/spheral} \) and publicly available at \( \text{https://github.com/jmikeowen/spheral} \), although the radiative transfer methods are not available in the open source version. For access to the full code, including thermal radiative transfer and input scripts for the problems presented in this paper, please contact the authors. Spheral is written in C++ with a Python interface, which allows for simple addition of new physics in either programming language. The opacities, flux limiters, and equations of state can be chosen arbitrarily for subsets of the SPH points as needed, allowing problems with any number of distinct materials to be studied.

In the succeeding examples Spheral’s default method \[33\] for computing the smoothing scale per point \( (h_i) \) is used with the C4 Wendland kernel \[Eq. (30c)\]. The target radius of support is 4 points, i.e., the local smoothing scale for each point is chosen to be 4 times the local particle spacing.

3.1 Material and radiation energy solve

The iterative process in Alg. 1 \[20\] can be written in terms of operator matrices as

\[
\begin{bmatrix}
  e_\ell+1 \\
  E_\ell+1
\end{bmatrix}
= \begin{bmatrix}
  M^{-1} & 0 \\
  0 & I
\end{bmatrix}
\begin{bmatrix}
  R & A \\
  0 & I
\end{bmatrix}
\begin{bmatrix}
  I & 0 \\
  0 & D^{-1}
\end{bmatrix}
\begin{bmatrix}
  I \\
  0
\end{bmatrix}
\begin{bmatrix}
  S & N \\
  0 & I
\end{bmatrix}
\begin{bmatrix}
  e_\ell \\
  E_\ell
\end{bmatrix},
\]  \hspace{1cm} (40)

with the operators defined by

\[
M^{-1}(P) \quad \text{Solve the nonlinear material equation, given a source } P_i,
\]

\[
\frac{\rho_i}{\Delta t} \left( e_i - e_i^{n-1} \right) + c\sigma_{a,i}aT_i^4 = P_i, \hspace{1cm} (41)
\]

for each \( e_i \),

\[
D^{-1}(P) \quad \text{Solve the diffusion equation, given a source } P_i,
\]

\[
\left( \frac{1}{\Delta t} + c\sigma_{a,i}f_i \right) E_i - \sum_j V_j \left( D_i + D_j \right) (E_i - E_j) \frac{x_{ij,\alpha}}{x_{ij,\alpha}x_{ij,\beta}} \partial_{i,\alpha}W_{ij} = P_i, \hspace{1cm} (42)
\]

for all \( E_i \),

\[
S(E) \quad \text{Calculate the radiation diffusion source, } \frac{1}{\Delta t} E_i^n - (1 - f_i) c\sigma_{a,i}E_i + Q_{E,i},
\]

\[
N(e) \quad \text{Calculate the emission of radiation from the material, } c\sigma_{a,i}aT_i^4,
\]

\[
A(E) \quad \text{Calculate the radiation energy absorption, } c\sigma_{a,i}E_i,
\]

\[
R(e) \quad \text{Set the material energy source, } Q_{e,i}^n,
\]

and the identity operator \( I \). This simplifies the addition of new physics, reduces code duplication, and allows testing of each operator independently. Note that \( M^{-1} \) and \( N \) are nonlinear operators, and should not be mistaken for matrices. The operators \( D^{-1}, S, \) and \( A \) are linear, but in practice, they are not explicitly formed into matrices. The
application of the combined operator in Eq. (40) is equivalent to a single outer iteration in Alg. 1. The opacities and other material data \((\sigma_a, \sigma_s, D, f, \lambda, \text{and } c_v)\) are calculated at the start of the time step and held constant within the time step.

The material energy solve in Eq. (41) is done independently for each point using Newton’s method, as shown in Eq. (18). Defining the function and Jacobian for the material energy solve as

\[ u(e_i) = \frac{\rho}{\Delta t} (e_i - e^{n-1}_i) + c \sigma_a a T^4 - P, \]  
\[ J_{m,e}(e) = \frac{\rho}{\Delta t} + \frac{4 c \sigma_a a T^3}{c_v}, \]

the material energy is solved iteratively as

\[ e^{k+1}_i = e^k_i - J_{m,e}^{-1}(e^k_i) u(e^k_i) \]

until converged, where \(k\) is the Newton iteration index. As the call to an external equation of state can be expensive, the temperature is updated for all points simultaneously, followed by an update of the material energy for each point independently. The iterative process in Eq. (43c) proceeds until convergence each time the \(M^{-1}\) operator is called.

The radiation energy solve in Eq. (42) is done using the Hypre BoomerAMG preconditioner with GMRES [27]. Because the material properties (opacities, specific heats, hydrodynamic variables) are held constant within a time step, the preconditioner can be initialized once at the start of each time step and then reused each time the \(D^{-1}\) operator is called within the time step. The radiation energy \(E^\ell\) is used as an initial guess for the GMRES solver when calculating \(E^{\ell+1}\), which reduces the number of GMRES iterations as the solution nears convergence, as is discussed in Sec. 4.3.

### 3.2 Time step choice

Due to the implicit solve, the time step is updated not based on the propagation speed of the radiation, but instead based on the observed change in radiation energy over a time step. This is a heuristic for the stability and accuracy of one Newton step. The idea is to limit the fractional change in the material and radiation energies to some finite value and increase or decrease the time step according to the change from the previous time step. For example, for the material energy, the fractional change in energy is calculated as

\[ \eta_e = \max_i \left( \frac{|e^n_i - e^{n-1}_i|}{\bar{e}^n_i + \eta_{e \text{target}} e^n_i} \right), \]

where \(\eta_{e \text{target}}\) is the target fractional change (\(\eta_{e \text{target}} = 0.05\) for the problems in this paper) and \(\bar{e}^n\) is the volume-averaged energy,

\[ \bar{e}^n = \frac{\sum_i e^n_i V_i}{\sum_i V_i}. \]

The \(\bar{e}^n\) in the denominator of the fractional change prevents points with very small radiation energy from dominating the time step when changing a small magnitude relative to the other points in the problem. Given the fractional change over the previous time step, a proposed time step is calculated as

\[ \Delta t^{n+1}_e = \Delta t^n \left( \frac{\eta_{e \text{target}}}{\eta_e} \right)^{1/2}. \]

The same is process is done for the radiation energy \(E\), and the time step is chosen to be the more restrictive of these, \(\Delta t^{n+1} = \min(\Delta t^{n+1}_e, \Delta t^{n+1}_E)\), within the minimum and maximum time steps specified by the user. For more information on time stepping strategies for thermal radiative transfer with diffusion, including the one used here, see Ref. [34].

### 4 Results

The results include three problems. The first is an infinite medium equilibrium test, which is designed to show that the material and radiation energies come to equilibrium at the correct rate, testing the time discretization,
emission, and absorption. The second is the Su-Olson Marshak wave, which simulates the diffusion of a planar radiation source into a vacuum, additionally testing the diffusion rate of the radiation. The final problem is a manufactured solution that extends the results to two and three dimensions. The tolerances used for each of these problems are listed in Table 1, with the inner tolerances referring to the convergence metric for ending the Newton solve for the material energy and the GMRES solve for the radiation energy and the outer tolerances used for ending the nonlinear elimination iteration process (see Sec. 3.1).

4.1 Infinite medium equilibrium test

The first problem involves a single material in an infinite medium in which the material and radiation energies are initially out of equilibrium. The units of length, time, temperature, and mass are chosen such that the absorption opacity $\sigma_z$, speed of light $c$, black body constant $a$, and ratio of proton mass to the Boltzmann constant, $m_p/k_B$, are all one. The equation of state is chosen to be an ideal gas, which in these units is defined as

$$ T = (\gamma - 1) \mu e = \alpha e, \quad (47) $$

where $\mu$ is the molecular mass and $\gamma$ is the heat capacity ratio. The problem can be written in the simplified unit system as a system of two ordinary differential equations,

$$ \rho \frac{\partial e}{\partial t} = E - (\alpha e)^4, \quad (48) $$
$$ \frac{\partial E}{\partial t} = -E + (\alpha e)^4. \quad (49) $$

These equations are solved using a fifth-order Radau IIA integrator [35] for comparison to the results given by the code.

The problem is run for two different cases, both of which have $\alpha = 1$ and a density of $\rho = 1$, and in each case, the simulation proceeds until $t_{end} = 10$, which allows the material and radiation energies to reach equilibrium. The first case starts with hot material and cold radiation, while the second starts with cold material and hot radiation, as shown in Table 2. The time step is allowed to increase by up to an order of magnitude per time step, up to the limit set by the changing material and radiation energies, with a hard cap of $\Delta t_{max} = 0.1$ (see Sec. 3.2).

The first and second cases take, respectively, 779 and 155 time steps to reach the goal time. The results are shown in Fig. 1. The reference and numeric solutions agree well for both problems. The $L_1$ relative error for this problem is calculated with an integral in time,

$$ L_1 \text{error} = \frac{\int_0^{t_{end}} |T_{ref} - T_{num}| dt}{\int_0^{t_{end}} T_{ref} dt}, \quad (50) $$

using Simpson’s rule evaluated at the time steps. The error between the reference and numeric solutions for the first case (with hot material) is $3.32 \times 10^{-4}$ for the material temperature and $2.55 \times 10^{-4}$ for the radiation temperature. The error calculated in the same way for the second case (with hot radiation) is $1.22 \times 10^{-3}$ for the material temperature and $6.21 \times 10^{-4}$ for the radiation temperature. For a fixed time step $\Delta t$, the error decreases linearly with $\Delta t$ as expected, as shown in Fig. 2.

The relative error between the initial and final energies ranges from $1.11 \times 10^{-15}$ (hot radiation) and $4.44 \times 10^{-16}$ (hot material) for $\Delta t = 0.1$ to $4.22 \times 10^{-13}$ (hot radiation) and $5.53 \times 10^{-13}$ (hot material) for $\Delta t = 0.0001$, which is of the correct order given the outer tolerance of $10^{-12}$ and inner tolerance of $10^{-14}$ (Table 1).

4.2 Su-Olson Marshak wave

The second problem is a Marshak planar wave as described in Ref. [36]. The problem consists of a reflecting plane at $x = 0$ and a radiation source from $0 \leq x \leq x_0$ that is turned on for $0 \leq \tau \leq \tau_0$, where $x$ is a scaled distance and $\tau$ is a scaled time ($z$ is used in the paper for physical distance). The problem is started with a material and radiation energy of $10^{-5}$ so the heat capacity (an analytic $c_e \propto T^3$) is nonzero. The units for the problem are chosen such that $\sigma_t = 1$, $cc = 1$, and $a = 1$, which makes the scaled units referenced in the paper equal to the physical units ($x = z$ and $\tau = t$). The solution to the problem is semianalytic, and involves evaluating integrals to
high precision over $\eta \in [0, 1]$ for each spatial point at each time. For these results, due to the complicated structure of the solution near $\eta = 1$, a quadrature is first generated in $\xi \in [-1, 1]$ and then transformed into $\eta$ via the relation

$$\eta = \frac{1}{\ell} \ln \left( \frac{1}{2} (1 - \xi + e^\ell (1 + \xi)) \right),$$

(51)

in which the transformation becomes linear as $\ell \to 0$ and concentrates more points near $\eta = 1$ as $\ell$ increases. A 5000-point Gauss-Legendre quadrature with $\ell = 3$ works well for the specific problem considered below. The numerical result at the end time is compared to this semianalytic result using an $L_1$ error,

$$L_1 \text{ error} = \frac{\sum |e_i - e^\text{semianalytic}_i|}{\sum e^\text{semianalytic}_i},$$

(52)

which differs from the standard approach of comparison to specific $x$ and $\tau$ values tabulated in the paper. The parameters used for these results include an absorption fraction of $c_a = 0.5$, a time scaling factor of $\epsilon = 1.0$, a radiation source extent of $x_0 = 0.5$, and a scaled time at which the source is turned off of $\tau_0 = 10.0$. The problem is run until $\tau = 100.0$. The spatial extent of the problem is $0 \leq x \leq 100$. The time evolution of the semianalytic and numeric solutions is shown in Fig. 3. The spatial convergence results are shown in Fig. 4 for three different time steps. The code converges to the semianalytic result with second-order accuracy spatially as the point spacing decreases and with first-order accuracy temporally as the time step decreases, as we expect based on SPH spatial interpolation and backward Euler time integration.

### 4.3 Manufactured solution for material-radiation coupling

This problem tests the material-radiation coupling using the method of manufactured solutions (MMS). To apply MMS to Eqs. (36), solutions for $e$ and $E$ are chosen for the equations,

$$e_m = e_0 \left[ 1.2 + \prod_{\alpha=1}^{\dim} \cos \left( \frac{2\pi x_\alpha - v_m t}{d_m} \right) \right],$$

(53a)

$$E_m = E_0 \left[ 1.2 + \prod_{\alpha=1}^{\dim} \cos \left( \frac{2\pi x_\alpha + v_m t}{d_m} - \omega_m \right) \right],$$

(53b)

with $e_0 = 10^{13}$ ergs$\cdot$g$^{-1}$, $E_0 = 7a (e_0/c_r)^4$ ergs$\cdot$cm$^{-3}$, $v_m = 5 \times 10^9$ cm$\cdot$s$^{-1}$, $d_m = 5$ cm, and $\omega_m = 1/16$. The opacities are set to constant values of $\sigma_a = 0.05$ cm$^{-1}$ and $\sigma_r = 0.95$ cm$^{-1}$. These solutions are inserted into the non-discretized equations [Eqs. (1a) and (6)] to calculate sources, $Q_e$ and $Q_E$. The solutions are chosen such that the magnitude of the individual terms in Eqs. (1a) and (6) is approximately equal, with the opposite time movement of the waves $\pm v$ allowing each individual piece of physics to dominate at certain times. The spatial extent of the problem is set to one full wavelength, or $d_m$ in each dimension (to allow for periodic boundary conditions), and the problem is run for one cycle, or until $t_{end} = d_m/v_m$, using a time step of $\Delta t = t_{end}/1000$. At $t_{end}$, the numerical solution is compared to the analytic solution in Eqs. (53) to calculate the $L_1$ relative error,

$$L_1 \text{ error} = \frac{\sum_i |e_i - e_{m,i}|}{\sum_i e_{m,i}}$$

(54)

(with a similar equation for $E$).

The solution for the problem with 128$^2$ points is shown in Fig. 5. At the end time, the solution should be equal to the initial condition. The relative error between the solution after one cycle (at $10^{-9}$ s) and the manufactured solution for the specific thermal energy and radiation energy density is shown in Fig. 6. The relative error is highest where the solution is lowest, with maxima of 0.006 for the specific material energy and 0.008 for the radiation energy. For much of the domain, the relative error is below 0.001 for both the material and radiation energy. At the end time, the relative difference between the starting and ending energy of the system is $1.67 \times 10^{-12}$, which indicates good energy conservation.

The $L_1$ error for the manufactured problem in 1D for several time step values is shown in Fig. 7. The numeric solution converges to the manufactured solution with second-order accuracy in space and first-order accuracy in time (again as expected). For a time step of $2 \times 10^{-13}$, the error in the radiation energy indicates second-order
convergence for all values of point spacing. The error in the material energy, which only has spatial coupling through the radiation, is much more dependent on the time step for this problem than the radiation energy. As in the previous problems, the error decreases linearly with the time step, when not limited by the spatial error.

Based on the results in 1D, a time step of $4 \times 10^{-13}$ is chosen for the comparison of 1D, 2D, and 3D results up to $128^d$ points (for the dimension $d$). The convergence results for 1D, 2D, and 3D are shown in Fig. 8. The 2D and 3D results have similar errors compared to the manufactured solution for similar spacing of points, although not identical due to differences in the interpolation functions for 2D and 3D, and also show second-order convergence when not limited by the time step.

While the number of processors used for each case was not chosen to show scaling with a constant number of points per processor or a constant number of total points, the performance results in Table 3 show some general scaling trends. In 2D, the small number of points per processor means that communication costs dominate, and adding more points per each processor helps reduce that cost. In 3D, the cases with 910 points per processor show around a 74 percent efficiency when the number of points and processors are quadrupled. With many more points per processor than the other cases, the 2,097,152-point problem on 576 processors runs with a similar efficiency to the 262,144-point problem in 288 processors. The number of outer iterations per time step is governed for this problem by the tolerance. For the tolerance given in Table 1, the solver needed two outer iterations to converge (and a third to check for convergence) in each time step. The number of GMRES iterations per outer iteration is around 3-4 on average. At the start of a time step, when the guess for the material and radiation energies is based on the values from the previous time step, the number is generally higher, around 6-8. On the last outer iteration, the number of GMRES solves is 1, indicating that the guess from the previous iteration satisfies the diffusion equation.

The solution to the problem is the same at the start and end times, so despite adding and subtracting energy in certain regions of the problem, the initial and final energies should be equal. The relative error between the initial and final energy in 2D ranges from $6.35 \times 10^{-14}$ for the 256 points to $1.69 \times 10^{-12}$ for 16,384 points. For 3D, the relative error ranges from $1.33 \times 10^{-13}$ for 4,096 points to $4.53 \times 10^{-12}$ for 2,097,152 points. In both cases, the relative error is on the order of the tolerance for the radiation solve of $10^{-12}$ and much lower than the tolerance of the coupled radiation and material energy solve of $10^{-8}$.

5 Conclusions and future work

The thermal radiative transfer equations with grey diffusion is discretized fully implicitly in time and solved using an efficient nonlinear elimination method that leads to fast convergence of the emission source. A standard SPH diffusion derivative is applied to the modified equations to form a fully discretized set of equations that are conservative in energy. The diffusion term is solved using optimized linear solvers, which permits good parallel efficiency.

The code is verified by comparison to three test problems with known solutions. The code gets the correct infinite medium behavior for either a hot material emitting radiation or a cold material absorbing radiation, with the expected first-order convergence in time. The results for a one-dimensional semianalytic Marshak wave problem are consistent with second-order spatial convergence. Finally, the code is run in 2D and 3D for a manufactured problem with sinusoidal radiation and material energy solutions traveling in opposite directions, which likewise exhibits second-order convergence in space and first-order convergence in time.

The diffusion discretization for SPH is stable and performs well, but lacks zeroth-order consistency. Other methods, such as reproducing kernel particle methods [37] and moving least squares particle hydrodynamics [5, 6], do not lack the zeroth-order consistency and perform better near boundaries. Conservative reproducing kernel smoothed particle hydrodynamics is implemented in the SPH code used for these results [7], and a similar diffusion discretization would make the hydrodynamics and radiation discretizations consistent. Other discretizations would also make the application of vacuum or incoming radiation boundary conditions more feasible.

Acknowledgements

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal
liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

References

[1] Joe J. Monaghan. Smoothed particle hydrodynamics. *Reports on progress in physics*, 68(8):1703, 2005.

[2] MB Liu and GR Liu. Smoothed particle hydrodynamics (SPH): an overview and recent developments. *Archives of computational methods in engineering*, 17(1):25–76, 2010.

[3] Joseph Peter Morris. A study of the stability properties of smooth particle hydrodynamics. *Publications of the Astronomical Society of Australia*, 13(1):97–102, 1996.

[4] Joseph J Monaghan and Robert A Gingold. Shock simulation by the particle method SPH. *Journal of computational physics*, 52(2):374–389, 1983.

[5] Gary A Dilts. Moving-least-squares-particle hydrodynamics I: Consistency and stability. *International Journal for Numerical Methods in Engineering*, 44(8):1115–1155, 1999.

[6] Gary A Dilts. Moving least-squares particle hydrodynamics II: conservation and boundaries. *International Journal for Numerical Methods in Engineering*, 48(10):1503–1524, 2000.

[7] Nicholas Frontiere, Cody D Raskin, and J Michael Owen. CRKSPH—a conservative reproducing kernel smoothed particle hydrodynamics scheme. *Journal of Computational Physics*, 332:160–209, 2017.

[8] Stuart C Whitehouse and Matthew R Bate. Smoothed particle hydrodynamics with radiative transfer in the flux-limited diffusion approximation. *Monthly Notices of the Royal Astronomical Society*, 353(4):1078–1094, 2004.

[9] Stuart C Whitehouse, Matthew R Bate, and Joe J Monaghan. A faster algorithm for smoothed particle hydrodynamics with radiative transfer in the flux-limited diffusion approximation. *Monthly Notices of the Royal Astronomical Society*, 364(4):1367–1377, 2005.

[10] Serge Vian, Pierre Bastien, and Seung-Hoon Cha. An implicit method for radiative transfer with the diffusion approximation in smooth particle hydrodynamics. *The Astrophysical Journal*, 639(1):559, 2006.

[11] Lucio Mayer, Graeme Lufkin, Thomas Quinn, and James Wadsley. Fragmentation of gravitationally unstable gaseous protoplanetary disks with radiative transfer. *The Astrophysical Journal Letters*, 661(1):L77, 2007.

[12] Leigh Brookshaw. A method of calculating radiative heat diffusion in particle simulations. *Publications of the Astronomical Society of Australia*, 6(2):207–210, 1985.

[13] Margarita Petkova and Volker Springel. An implementation of radiative transfer in the cosmological simulation code gadget. *Monthly Notices of the Royal Astronomical Society*, 396(3):1383–1403, 2009.

[14] Gabriel Altay, Rupert AC Croft, and Inti Pelupessy. Sphray: a smoothed particle hydrodynamics ray tracer for radiative transfer. *Monthly Notices of the Royal Astronomical Society*, 386(4):1931–1946, 2008.

[15] Sergei Nayakshin, Seung-Hoon Cha, and Alexander Hobbs. Dynamic monte carlo radiation transfer in SPH: radiation pressure force implementation. *Monthly Notices of the Royal Astronomical Society*, 397(3):1314–1325, 2009.

[16] Christopher L Fryer, Gabriel Rockefeller, and Michael S Warren. Snsph: a parallel three-dimensional smoothed particle radiation hydrodynamics code. *The Astrophysical Journal*, 643(1):292, 2006.

[17] Robert B Lowrie. A comparison of implicit time integration methods for nonlinear relaxation and diffusion. *Journal of Computational Physics*, 196(2):566–590, 2004.
[18] VA Mousseau, DA Knoll, and WJ Rider. Physics-based preconditioning and the newton–krylov method for non-equilibrium radiation diffusion. *Journal of computational physics*, 160(2):743–765, 2000.

[19] Paul J Lanzkron, Donald J Rose, and James T Wilkes. An analysis of approximate nonlinear elimination. *SIAM Journal on Scientific Computing*, 17(2):538–559, 1996.

[20] Tom Brunner and Paul Nowak. Nonlinear elimination applied to radiation transport. In *Proceedings of M&S C 2019*, 2019.

[21] Hamou Sadat. On the use of a meshless method for solving radiative transfer with the discrete ordinates formulations. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 101(2):263–268, 2006.

[22] LH Liu and JY Tan. Meshless local Petrov-Galerkin approach for coupled radiative and conductive heat transfer. *International journal of thermal sciences*, 46(7):672–681, 2007.

[23] Manuel Kindelan, Francisco Bernal, Pedro González-Rodríguez, and Miguel Moscoso. Application of the RBF meshless method to the solution of the radiative transport equation. *Journal of Computational Physics*, 229(5):1897–1908, 2010.

[24] Brody Bassett and Brian Kiedrowski. Meshless local Petrov–Galerkin solution of the neutron transport equation with streamline-upwind petrov–galerkin stabilization. *Journal of Computational Physics*, 377:1–59, 2019.

[25] B Rokrok, H Minuchehr, and A Zolfaghari. Element-free Galerkin modeling of neutron diffusion equation in x–y geometry. *Annals of Nuclear Energy*, 43:39–48, 2012.

[26] Tayfun Tanbay and Bilge Ozgener. Numerical solution of the multigroup neutron diffusion equation by the meshless RBF collocation method. *Mathematical and Computational Applications*, 18(3):399–407, 2013.

[27] Robert D Falgout and Ulrike Meier Yang. hypre: A library of high performance preconditioners. In *International Conference on Computational Science*, pages 632–641. Springer, 2002.

[28] CD Levermore. Relating eddington factors to flux limiters. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 31(2):149–160, 1984.

[29] JE Morel. Diffusion-limit asymptotics of the transport equation, the P1/3 equations, and two flux-limited diffusion theories. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 65(5):769–778, 2000.

[30] Dimitri Mihalas and Barbara Weibel Mihalas. *Foundations of radiation hydrodynamics*. Courier Corporation, 2013.

[31] JA Fleck Jr and JD Cummings Jr. An implicit monte carlo scheme for calculating time and frequency dependent nonlinear radiation transport. *Journal of Computational Physics*, 8(3):313–342, 1971.

[32] Holger Wendland. Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree. *Advances in computational Mathematics*, 4(1):389–396, 1995.

[33] J Michael Owen. ASPH modeling of material damage and failure. In *Proceedings of the 5th International SPHERIC Workshop*, pages 297–304, Manchester, UK, Jan 2010.

[34] William J Rider and Dana A Knoll. Time step size selection for radiation diffusion calculations. *Journal of Computational Physics*, 152(2):790–795, 1999.

[35] Ernst Hairer and Gerhard Wanner. Stiff differential equations solved by radau methods. *Journal of Computational and Applied Mathematics*, 111(1-2):93–111, 1999.

[36] Bingjing Su and Gordon L Olson. An analytical benchmark for non-equilibrium radiative transfer in an isotropically scattering medium. *Annals of Nuclear Energy*, 24(13):1035–1055, 1997.

[37] Wing Kam Liu, Sukky Jum, and Yi Fei Zhang. Reproducing kernel particle methods. *International journal for numerical methods in fluids*, 20(8-9):1081–1106, 1995.
| Problem              | Inner Material | Inner Radiation | Outer Material | Outer Radiation |
|----------------------|----------------|-----------------|----------------|-----------------|
| Infinite medium      | $10^{-14}$     | $10^{-14}$      | $10^{-12}$     | $10^{-12}$      |
| Marshak wave         | $10^{-12}$     | $10^{-12}$      | $10^{-8}$      | $10^{-8}$       |
| Manufactured problem | $10^{-12}$     | $10^{-12}$      | $10^{-8}$      | $10^{-8}$       |

Table 1: Convergence tolerances for the results. Then inner tolerance is for the independent radiation and material energy solves, while the outer tolerance is for the combined solve.

| Case               | $e_0$ | $E_0$ | $T_{r,0}$ | $T_{r,0}$ | $\Delta t_{init}$ |
|--------------------|-------|-------|-----------|-----------|-------------------|
| Hot material       | 1.0   | $10^{-16}$ | 1.0       | $10^{-4}$ | $10^{-20}$        |
| Hot radiation      | $10^{-4}$ | 1.0       | $10^{-4}$ | 1.0       | $10^{-7}$         |

Table 2: Initial conditions for infinite medium problem for two cases, one starting with a high thermal temperature and low radiation temperature and one with the temperatures reversed. See Sec. 4.1 for units.

**Algorithm 1** Material and radiation energy update, which is based on Ref. [20]. The material and radiation energy equations $m$ and $r^\dagger$ are defined in Eq. (17), while the Newton update for $m$ is described in Eq. (18). The convergence criteria are defined in Eqs. (19).

1: $\ell = 0$
2: set initial guesses to $e^{n,\ell} = e^{n-1}$ and $E^{n,\ell} = E^{n-1}$
3: solve $m(e^{n,\ell}, E^{n,\ell}) = 0$ for $e^{n,\ell}$
4: (perform Newton updates until converged to inner tolerance for $e$)
5: while $e^n$ and $E^n$ not converged to outer tolerances do
6: solve $r^\dagger(e^{n,\ell}, E^{n,\ell}, E^{n,\ell+1}) = 0$ for $E^{n,\ell+1}$
7: (if iterative solver is used, iterate until converged to inner tolerance for $E$)
8: solve $m(e^{n,\ell+1}, E^{n,\ell+1}) = 0$ for $e^{n,\ell+1}$
9: (perform Newton updates until converged to inner tolerance for $e$)
10: $\ell = \ell + 1$
11: end while
Figure 1: Comparison of reference and numerical results for the infinite medium problem. The time step is fixed at $\Delta t = 0.0001$.

Figure 2: Convergence of the numerical solution for the infinite medium problem to the reference solution with decreasing time step. The error is calculated using Eq. (50).

| Dimension | Points | Procs | Points/proc | GMRES/Outer | Outer/Step | Wall time (s) | Time×Proc/Point |
|-----------|--------|-------|-------------|-------------|------------|---------------|-----------------|
| 2         | 256    | 36    | 7           | 3.66        | 3          | 59            | 8.29            |
|           | 1,024  | 36    | 28          | 4.66        | 3          | 79            | 2.78            |
|           | 4,096  | 36    | 113         | 3.33        | 3          | 261           | 2.29            |
|           | 16,384 | 36    | 455         | 3.66        | 3          | 817           | 1.79            |
| 3         | 4096   | 36    | 113         | 3.66        | 3          | 815           | 7.21            |
|           | 32,768 | 36    | 910         | 4.66        | 3          | 5,610         | 6.20            |
|           | 262,144| 288   | 910         | 3.33        | 3          | 7,660         | 8.41            |
|           | 2,097,152| 576    | 3,640       | 3.66        | 3          | 31,975        | 8.78            |

Table 3: Timing for the manufactured problem in 3D.
Figure 3: The numeric and semianalytic solutions to the Marshak wave problem at $t = 10.0$. This figure is also available as a video.

Figure 4: Convergence of the numeric solution to the semianalytic solution for the Marshak wave with an increasing number of spatial points for three time step values. The error is calculated using Eq. (52).
Figure 5: The numeric solution to the manufactured problem in 2D for $128^2$ points after one cycle. This figure is also available as a video.

Figure 6: Pointwise relative error of the numeric solution to the manufactured problem at $10^{-9}$ s in 2D for $128^2$ points.
Figure 7: Convergence of the numeric solution to the manufactured problem for several time step values in 1D. The error is calculated using Eq. (54).

Figure 8: Convergence of the numeric solution to the manufactured problem in 1D, 2D, and 3D with a fixed time step of $\Delta t = 4 \times 10^{-13}$. The error is calculated using Eq. (54).