Multigroup smoothed particle radiation hydrodynamics

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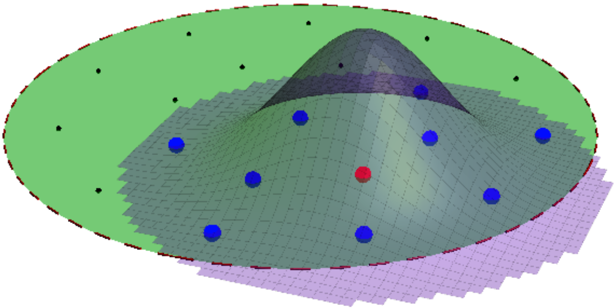
Introduction

The goal: multigroup radiative transfer compatible with SPH

- Smoothed particle hydrodynamics (SPH) uses no mesh
  - This means no mesh tangling
  - The derivatives are based on a set of nearest neighbors
- The goal is to discretize the radiative transfer equations using the same meshless points
  - This consistent discretization simplifies the coupling

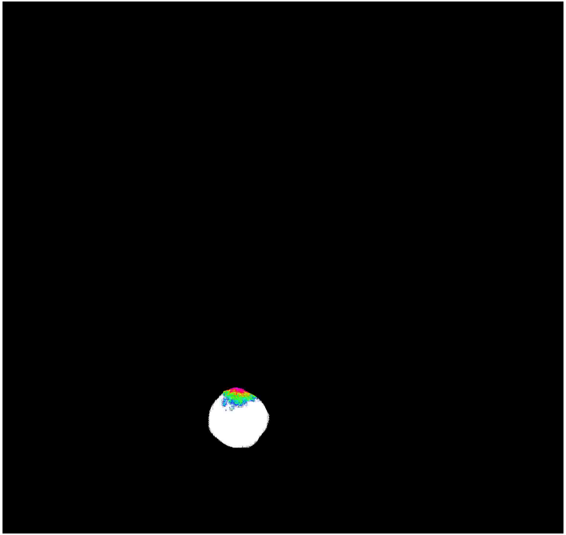


Rad-hydro with SPH has numerous applications

The applications of meshfree radiation hydrodynamics include:

- Simulating fluid instabilities in laser experiments
- Ablation of an asteroid in planetary defense
- Astrophysics, including supernovae, accretion disks, star formation, and large scale cosmological structure formation

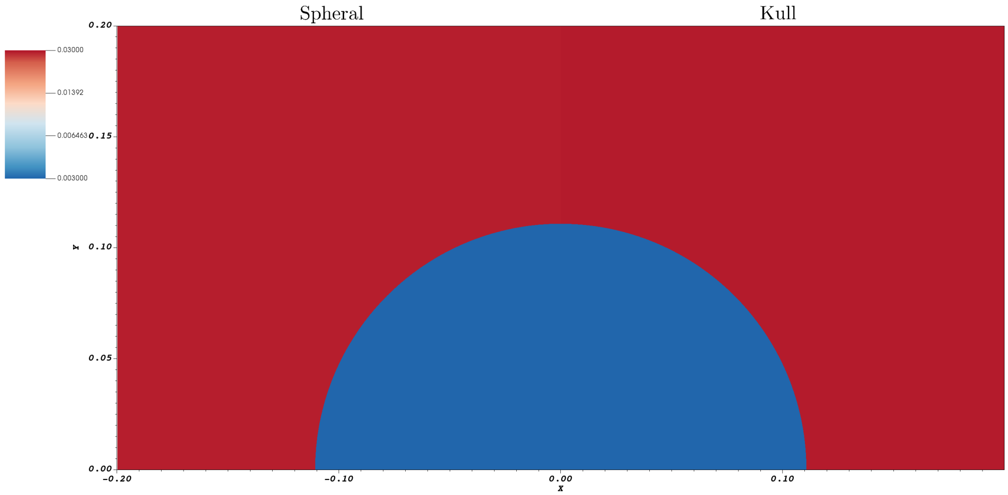
Spheral excels at simulating complicated flows with instabilities. A consistent, robust radiation treatment allows us to consider high energy density problems that may be difficult to run in other codes.



Nuclear disruption of an asteroid. Video courtesy of Megan Syal.

This work extends the previous gray SPH rad hydro to multigroup

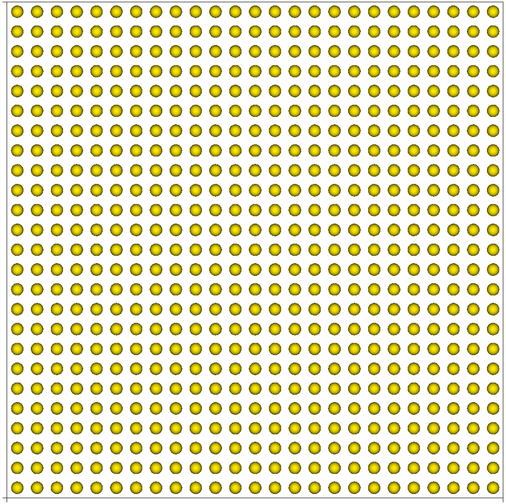
- This is an ICF-inspired ablation problem with gray diffusion
- A multigroup version will be presented later



The hydrodynamic fields move with the SPH particles

- The points represent the locations of the SPH nodes
- The color represents the magnitude of the pressure
- The method is completely Lagrangian
- The hydrodynamic properties move with the particles

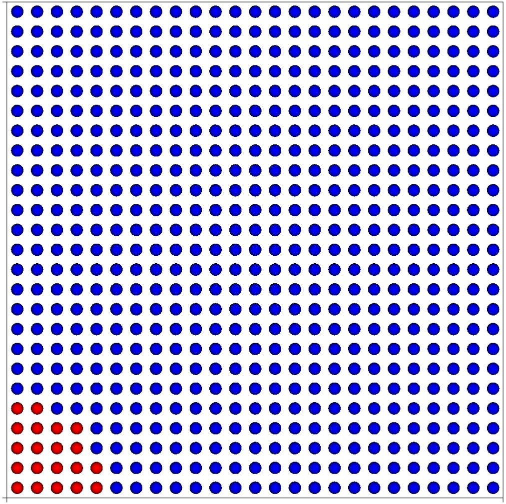
Pressure for a quarter-geometry blast wave



Radiation moves through the SPH particles

- Radiation works on much smaller time scales than hydrodynamics
  - This means we need to do an implicit solve
- The coupling between the radiation and hydrodynamics needs to be done correctly
  - As particles squish together, there is work done on radiation pressure
  - As particles move, radiation is dragged along with the fluid
  - The radiation transfers momentum to the fluid
  - The radiation heats up the fluid

Radiation energy for a quarter-geometry blast wave



Theory

The radiation and hydrodynamics equations are closely coupled

The important terms for coupling of radiation and hydrodynamics include radiation momentum, emission, absorption, entrainment, and work.

$$
\begin{aligned}
\text{mass} \qquad & \frac{D\rho}{Dt} = -\rho \partial_x^\alpha v^\alpha, \\
\text{momentum} \qquad & \rho \frac{Dv^\alpha}{Dt} = -\partial_x^\alpha p - \sum_g \lambda_g \partial_x^\alpha E_g, \\
\text{material energy} \qquad & \rho \frac{De}{Dt} = -\partial_x^\alpha p v^\alpha - \sum_g \left(c\sigma_{a,g} B_g + c\sigma_{a,g} E_g \right) + Q_e, \\
\text{radiation energy} \qquad & \frac{DE_g}{Dt} = -\frac{4}{3} E_g \partial_x^\alpha v^\alpha + \partial_x^\alpha \frac{c\lambda_g}{\sigma_{t,g}} \partial_x^\beta E - c\sigma_{a,g} E_g + c\sigma_{a,g} B_g + Q_{E,g},
\end{aligned}
$$

The diffusion and multigroup approximations have been applied here.

Radiation hydrodynamics operator split

The equations are operator split into hydrodynamics, radiation, and radiation work.

- Radiation
  - Implicit time discretization
  - SPH-like spatial discretization

$$\rho \frac{De}{Dt} = -c\sigma_a B + c\sigma_a E + Q_e,$$

$$\frac{DE_g}{Dt} = -\frac{4}{3}E_g \partial_x^\alpha v^\alpha + \partial_x^\alpha \frac{c\lambda_g}{\sigma_{t,g}} \partial_x^\beta E - c\sigma_{a,g} E_g + c\sigma_{a,g} B_g + Q_{E,g}.$$

- Hydrodynamics
  - Explicit time discretization
  - SPH spatial discretization
  - Radiation momentum lagged

$$\frac{D\rho}{Dt} = -\rho \partial_\alpha v_\alpha,$$

$$\rho \frac{Dv_\alpha}{Dt} = -\partial_\alpha p - \sum_g \lambda_g \partial_x^\alpha E_g,$$

$$\rho \frac{De}{Dt} = -\partial_\alpha p v_\alpha.$$

- Radiation work
  - Updated after the hydro step but before the radiation

$$\frac{DE_g}{Dt} = -\frac{4}{3}E_g \partial_\alpha v_\alpha.$$

The time discretization is performed using nonlinear elimination[†]

- This method contains $G+1$ diffusion solves per TRT iteration, which represent much of the computational cost:
  - G solves for uncollided photons
  - 1 solve for the gray corrections
- Most equations are 0D, or spatially independent
- Differs from Brunner et al.[†]
  - There, ζ_g calculated based on first-flight photons, which adds G diffusion solves
  - Here, ζ_g calculated using infinite medium solution, as in Morel et al.[‡]

$t = 0$
set initial conditions
while $t <$ end time **do**
  material initialization: evaluate $\sigma_{a,g}, \sigma_{s,g}, \lambda_g$
  hydrodynamics update: explicit update to $\rho^n, v^n, e^n_{\text{hydro}}$
    calculate radiation momentum
  radiation work: update radiation energy density
  material update: update $\sigma_a, \sigma_s, \lambda, c_v, f$
  repeat (iteration for **thermal radiative transfer**)
    solve for uncollided photons, $E_g^\star$
    calculate spectral term, ζ_g
    solve for gray corrections, $E^\dagger$
    combine these for inner update to E_g
    solve for e with source from hydrodynamics update
  until converged
  $t = t + \Delta t^n$
end while

[†] Brunner et. al, "Nonlinear Elimination Applied to Radiation Diffusion," NSE (2020)

[‡] Morel et. al, "Linear Multifrequency-Grey Acceleration Recast for Preconditioned Krylov Iterations," JCP (2007)

This is straightforward to add to an SPH code

Hydrodynamics

- Add radiation momentum to RHS of velocity equation
- Track energy gained/lost in specific thermal energy

Thermal energy solve

- Use the gained/lost energy in RHS of material solve
- Solve the material energy equation using Newton iteration

Radiation energy solve

- Update radiation energy from radiation work term once hydrodynamics solve is complete
- Solve diffusion system using linear solver, e.g. Hypre with AMG preconditioning
- Iterate on scattering and emission sources until convergence

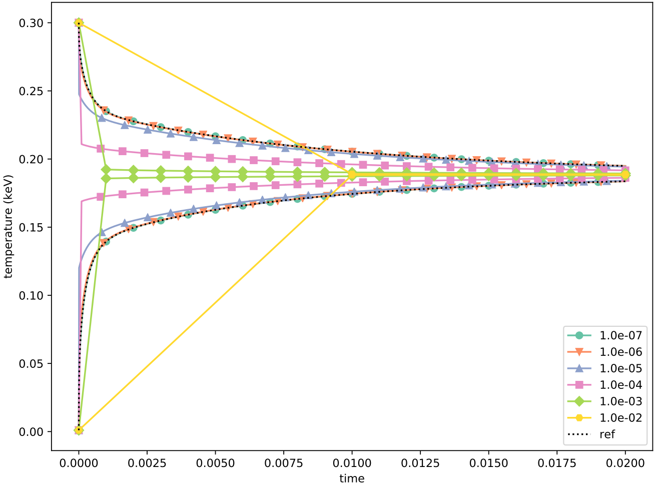
Results

Material and radiation temperatures equilibrate at the correct rates

- Opacities of the form

$$\rho 10 T^{-1} \nu_g^{-3},$$

  where v_g are group-averaged energies
- Initial conditions:
  - Material T: 0.001 keV
  - Radiation T: 0.3 keV
- Let material and radiation temperatures come into equilibration
- Compare different time steps to reference solution (provided by Tom Brunner)



The manufactured solution tests the coupling terms

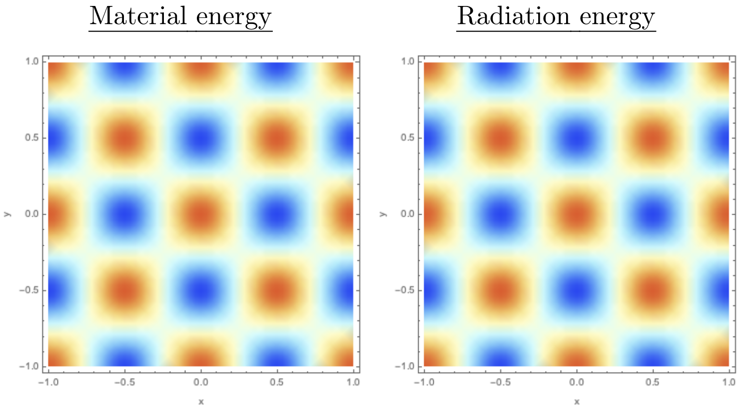
Process of verification:

- Insert the solution into non-discretized equations to calculate sources
- Use these sources in the discretized equation and calculate e and E
- Calculate error of numeric solution using the original manufactured solutions

The manufactured solutions are of the form

$$k_0\left(1.2 + \cos\left(k_1\left(x+t\right)\right)\cos\left(k_2\left(y+t\right)\right)\right)$$

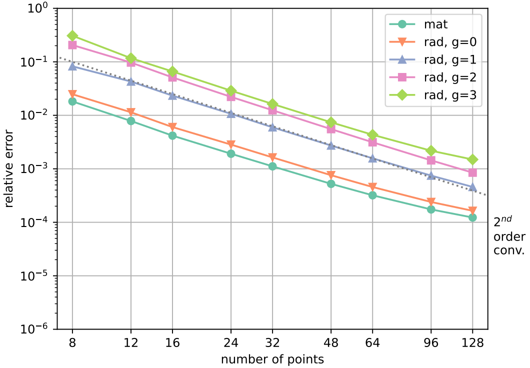
for the internal and radiation energies.



The SPH and RK results converge at the expected rates

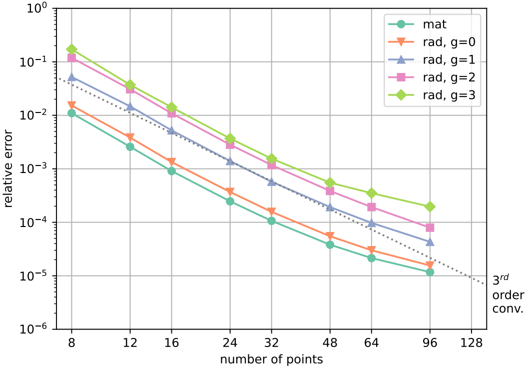
Standard SPH kernels

- The convergence agrees with the expected second-order convergence.
- The convergence plot for 2D/3D is nearly



Reproducing kernels

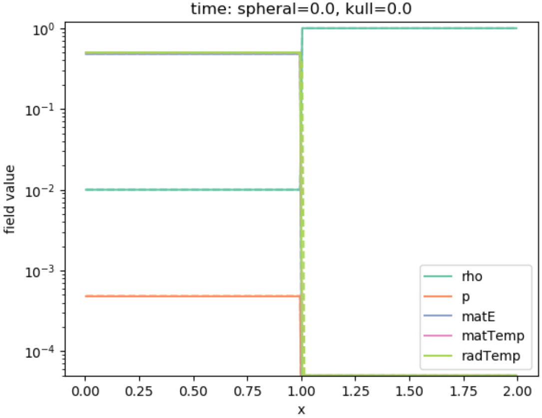
- Using quadratic kernels, the convergence is third-order.
- The RK diffusion solver struggles with 2D/3D



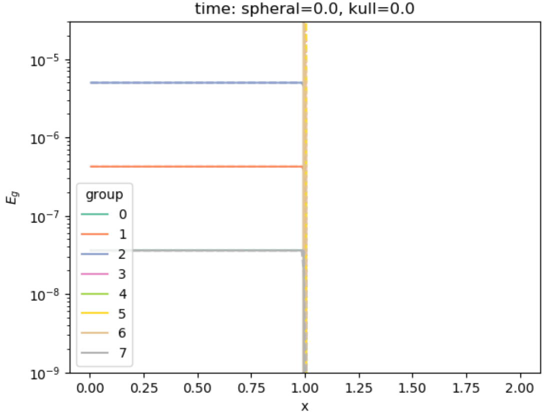
This two-region problem tests shock propagation

- This is a shock tube problem with significant radiation coupling
- The results are compared to an ALE rad-hydro code, Kull

Hydro fields



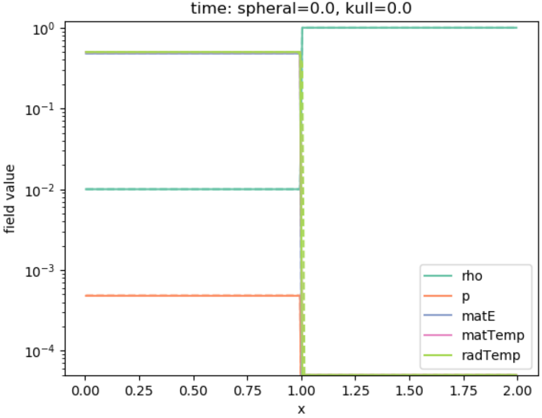
Radiation energy



The results agree well with the reference solution

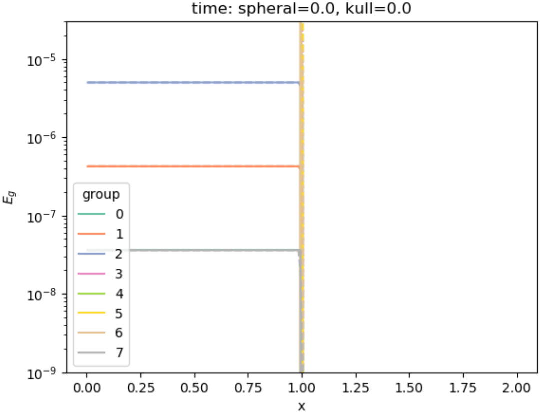
Hydro fields

- Note the overshoots near the shock front due to low resolution



Radiation energy

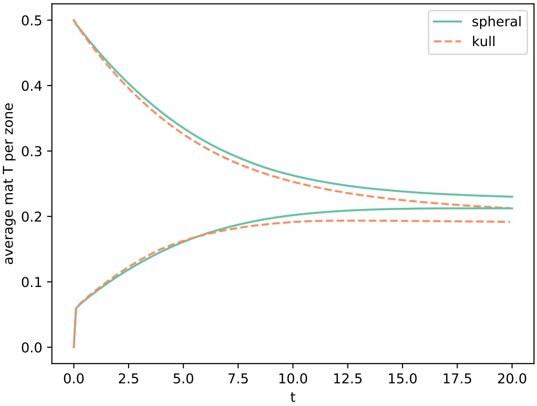
- There are small energy differences in a few groups



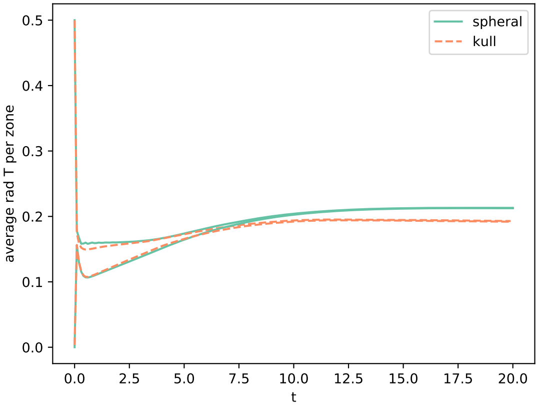
The temperatures are somewhat higher in Spheral than in Kull

- May need to reduce time step for this problem to get better agreement

Material temperature



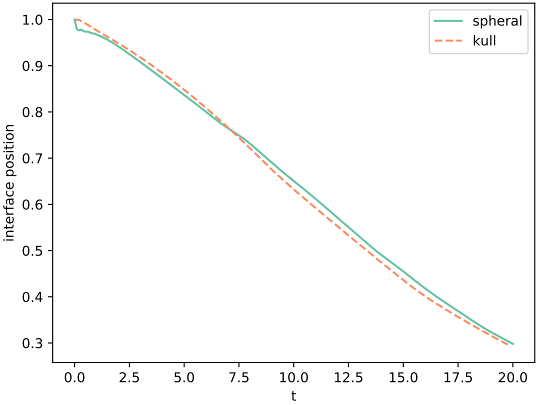
Radiation temperature



The position of the interface agrees reasonably well

The plot shows the position of the interface between the two materials.

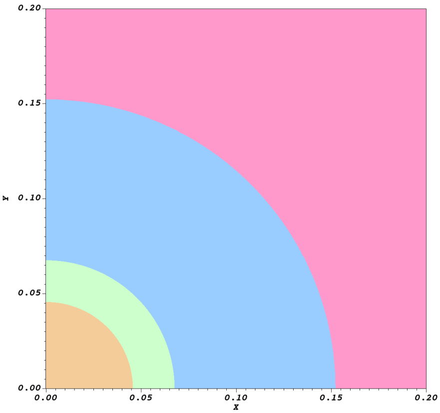
- The radiation leads to ablation as the right material heats up, which accelerates the interface to the left
- Comparing these rates ensures that the radiation travels through the material at the correct speeds



This ICF-like ablation problem tests multi-material coupling

- The ablation problem is a simplified version of an inertial confinement fusion (ICF) capsule†
  - Instead of using a specified boundary source, the helium is set to a high initial temperature
  - Increased gas densities to make mass matching easier
- Number of energy groups: 4
- The results are in cylindrical geometry

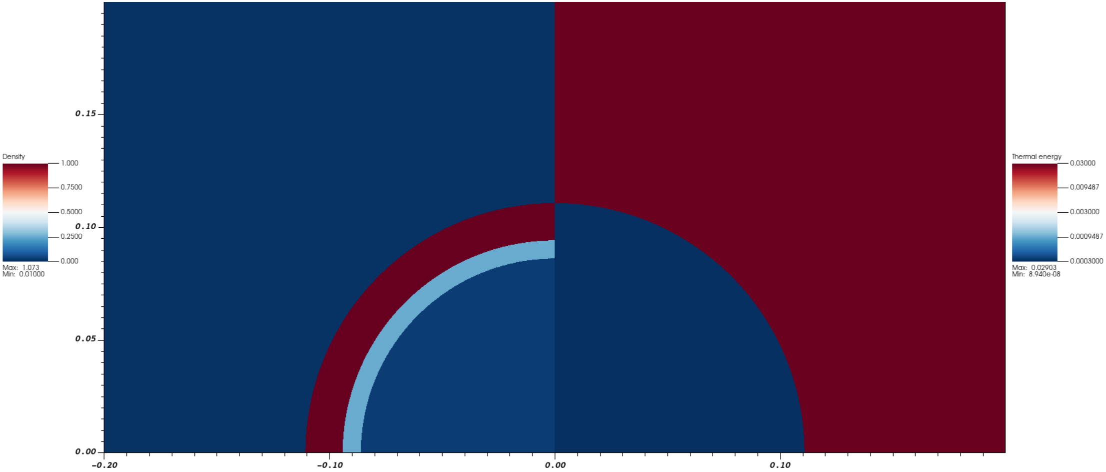
Material	Outer radius (cm)	Initial ρ $(\mathrm{g \cdot cm^{-3}})$	Initial T (keV)	γ	μ
DT Gas	0.08628	3.0×10^{-2}	1.7×10^{-6}	1.45	1.0
DT Ice	0.0943	0.25	4.2×10^{-7}	1.45	1.0
CH 1% Si	0.1108	1.073	8.6×10^{-6}	1.3	13.0
Helium	0.2	1.0×10^{-2}	0.4	1.66	2.0



†Robert Tipton, "An ICF test problem for single group radiation-hydrodynamics codes" (2016)

Initial results for the ablation problem look promising

Future work: Compare these to another rad-hydro code.



Conclusions

Multigroup radiation hydrodynamics with SPH works

Conclusions

- Multigroup radiation hydrodynamics works well for smoothed particle hydrodynamics
  - Equilibration at correct rates
  - Shocks propagate at expected velocities
- This runs for complicated problems with multiple materials
  - Need to verify this by comparison to other codes

Future work

- The second derivative for reproducing kernels does not work well with our diffusion solvers
- Try extra solves for spectrum from Brunner et. al
- Work on SPH-compatible S_N transport
  - Gray is working, but solvers for the "sweep" remain an issue
  - Multigroup transport can use a similar rad-hydro algorithm to the diffusion presented here

Backup slides

SPH interpolation

SPH is so named because the kernels, $W(x, h)$, smooth out values of the function throughout some smoothing length, h.

1. Start with the definition of the delta function
2. Insert a kernel that approximates the delta function
3. Convert the integral to a summation with the centers as quadrature points

$$
\begin{aligned}
f(x) &= \int_V \delta(x - x') f(x') \, dV' \\
&\approx \int_V W(x - x', h) f(x') \, dV' \\
&\approx \sum_j V_j W(x - x_j, h) f_j
\end{aligned}
$$

SPH derivatives

In SPH, derivatives are approximated by using this interpolant

1. Use the smoothing function approximation on the derivative
2. Integrate by parts and discard the surface integral
3. Add a term that is equal to zero for symmetry
4. Convert to a summation

$$
\begin{aligned}
\partial_{x,\alpha} f(\boldsymbol{x}) &\approx \int_V W(x - x', h)\, \partial^{\alpha}_{x'} f(\boldsymbol{x}')\, dV' \\
&= -\int_V \partial^{\alpha}_{x'} W(x - x', h)\, f(x')\, dV' \\
&= \partial^{\alpha}_{x} \int_V W(x - x', h)\, f(x')\, dV' \\
&\quad - f(x)\, \partial^{\alpha}_{x} \int_V W(x - x', h)\, dV' \\
&\approx \sum_j V_j \left(f_j - f(x)\right) \partial^{\alpha}_{x} W(x - x_j, h)\,.
\end{aligned}
$$

Note if this is evaluated at x_i, the derivative is antisymmetric for i and j, and disappears when $i = j$.

SPH diffusion derivative

To avoid mixed first and second derivatives in the diffusion derivative, $\partial^\alpha \left(g\partial^\alpha f\right)$, we add together the following two identities,

$$\partial^\alpha \left(g\partial^\gamma f\right) = g\partial^{\alpha\alpha} f + \partial^\alpha g\partial^\alpha f,$$
$$\partial^\alpha \left(g\partial^\alpha f\right) = \partial^{\alpha\alpha} \left(gf\right) - f\partial^{\alpha\alpha} g - \partial^\alpha g\partial^\alpha f,$$

which results in

$$\partial^\alpha \left(g\partial^\gamma f\right) = \frac{1}{2}\left[\partial^{\alpha\alpha} \left(gf\right) + g\partial^{\alpha\alpha} f - f\partial^{\alpha\alpha} g\right].$$

Since SPH doesn't do second derivatives well, the $\partial^{\alpha\alpha} W_{ij}$ term is replaced by a Taylor expansion of the kernel. The SPH approximation of this is

$$\partial^\gamma \left(g\partial^\gamma f\right)\Big|_{x=x_i} \approx \frac{1}{2}\sum_j V_j \left(D_i + D_j\right)\left(E_j - E_i\right)\partial^{\gamma\gamma} W_{ij} \approx \sum_j V_j \left(D_i + D_j\right)\left(E_j - E_i\right)\frac{x_{ij}^\alpha}{x_{ij}^\beta x_{ij}^\beta}\partial^\alpha W_{ij}$$

Spatial discretization

The material energy equation is 0D and can be solved independently for each point,

$$\frac{\rho_i}{\Delta t}\left(e_i^{n,\ell+1} - e_i^{n-1}\right) + c\sigma_{a,i}B_i^{n,\ell+1} - c\sigma_{a,i}E_i^{n,\ell+1} - Q_{e,i}^n = 0.$$

Given some $Q_{e,i}^n$ and $E_i^{n,\ell+1}$, this equation is solved for $e_i^{n,\ell+1}$ [with $B\left(T\left(e\right)\right)$] using Newton iteration.

The radiation energy equation with the diffusion derivative we just introduced,

$$\frac{1}{\Delta t}E_i^{n,\ell+1} - \sum_j V_j\left(\frac{c\lambda_i}{\sigma_{t,i}} + \frac{c\lambda_j}{\sigma_{t,j}}\right)\left(E_i^{n,\ell+1} - E_j^{n,\ell+1}\right)\frac{x_{ij}^\alpha}{x_{ij}^\beta x_{ij}^\beta}\partial_i^\alpha W_{ij} + c\sigma_{a,i}f_iE_i^{n,\ell+1}$$
$$= \frac{1}{\Delta t}E_i^{n-1} + c\sigma_{a,i}B_i^{n,\ell} - \left(1 - f_i\right)c\sigma_{a,i}E_i^{n,\ell} + Q_{E,i}^n.$$

is solved using an iterative linear solver (Hypre or Trilinos).

Reproducing kernels

The standard SPH kernels cannot reproduce even a constant solution exactly. One way to enhance the SPH kernels so that they can reproduce up to a chosen polynomial order exactly is reproducing kernels.

The P_{ij} is a set of polynomials, e.g. $P_{ij} = [1, x_{ij}, y_{ij}, z_{ij}]$ for linear corrections. The C_i is corrections for the point i.

The corrections are imposed by ensuring that the kernel exactly reproduces a polynomial.

- Enhance the kernels:

$$W_{ij} \to W_{ij}^R = P_{ij}^\top C_i W_{ij}$$

- Calculate the corrections:

$$\left[\sum_j V_j P_{ij} P_{ij}^\top C_i W_{ij}\right] C_i = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

- For zeroth order:

$$\sum V_j W_{ij}^R C_i = 1$$

$$\Downarrow$$

$$C_i = \left(\sum V_j W_{ij}^R\right)^{-1}$$