An Overview of Numerical Radiation Transport Techniques in Asteroid Deflection Modeling

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Nicholas A. Gentile

Lawrence Livermore National Laboratory

P. O. Box 808, Livermore, CA 94551

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Photon transport is necessary to accurately model deflection scenarios using x-ray deposition

- Inertial confinement fusion (ICF) and asteroid simulations share some commonalities and challenges
  - Both have large length, density, and opacity scales

> - Both model round things suspended in vacuum hit by x-rays
> - We can use the same code for both

- ICF codes discretize in space and time
  - Zones have ρ, T, P, radiation intensity, etc.
  - Energy deposition done by a radiation transport method
  - Hydrodynamic motion and shocks handled by a hydro method
  - Radiation and matter are coupled by thermal emission from material and electron and ion conduction
- Transport dominates the simulation run time
  - We face tradeoffs in the radiation methods between speed and accuracy

The transport equation describes the motion of photons including interactions with moving matter

$$\frac{1}{c}\frac{\partial I(\nu,\Omega)}{\partial t} + \Omega\cdot\nabla I(\nu,\Omega) = -\,\gamma D\sigma_a I(\nu,\Omega) + \sigma_a \frac{B[\nu,T]}{[\gamma D(\Omega)]^2}$$

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

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

Absorption (Doppler-shifted)

Thermal emission Doppler-shifted

Photons move in straight lines at speed c

In-scattering

Out-scattering

Stimulated scattering

with $\gamma \equiv \left(1-\frac{v^2}{c^2}\right)^{-\frac{1}{2}}$ and $D \equiv 1-\Omega\cdot\frac{v}{c}$ arising from material motion and $B(\nu,T)=\frac{2h\nu^3}{c^2}\left[\exp\left(\frac{h\nu}{kT}\right)-1\right]^{-1}$ the Planck function describing thermal emission in Local Thermodynamic Equilibrium

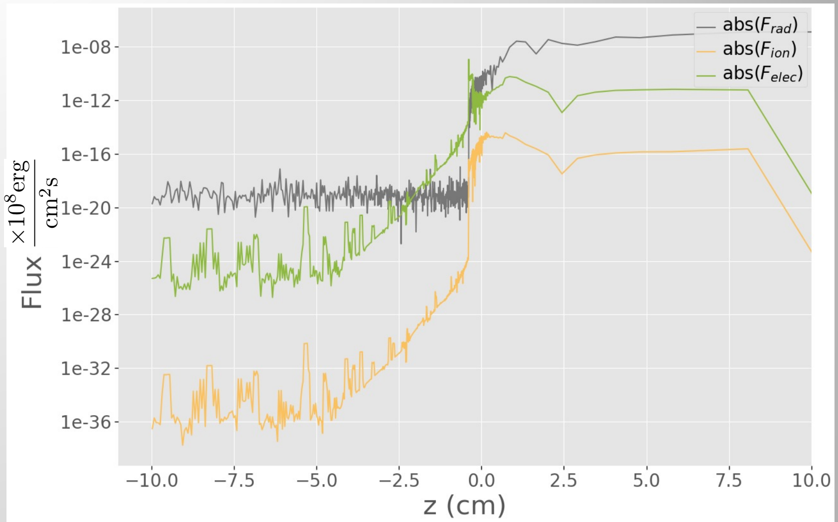
- This is the Boltzmann equation written in terms of Intensity
  - I has units of Energy/(Length^2-Time-Steradian)
- Material motion corrections (MMC) need to be included
  - Emission isn't isotropic, absorption is angle dependent
  - There are many O(v/c) MMC approximations; also many numerical simplifications are employed, some inaccurate
- Radiation exchanges energy and momentum with matter

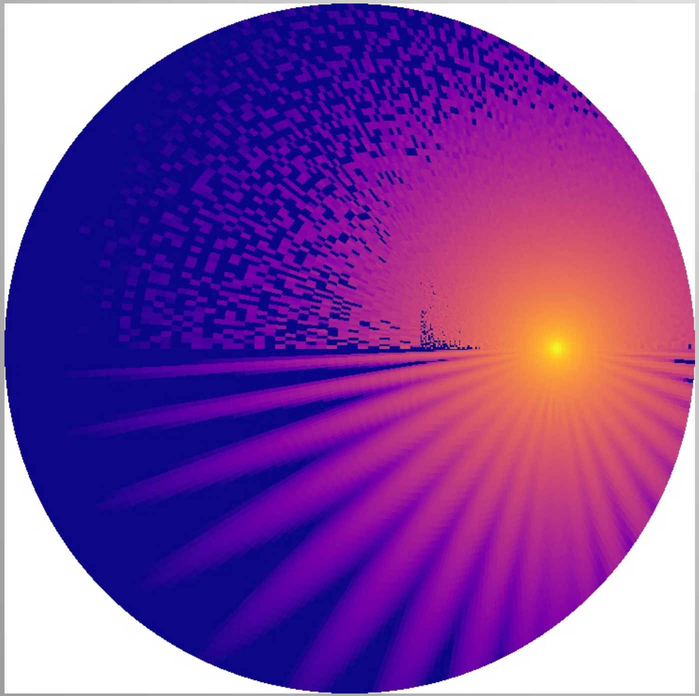
The two common numerical methods for transport simulations are IMC and S_N

- Implicit Monte Carlo (IMC) simulates radiation by computational particles with randomly selected emission positions and directions
  - Emit, scatter, track, and absorb "fake" photons
  - "implicit" refers to a numerical extrapolation in time of the matter temperature used in emission
  - Allows accurate simulation of scattering and Doppler shifts
    - Energy-angle correlation in Compton scattering can be simulated
  - Use of random numbers causes statistical noise ~ $N_{particles}^{-1/2}$ in the results
    - Reducing the slowly-declining noise leads to long simulation times
    - Discretization errors in thermal emission, both temperature and emission location, require small Δx and Δt
    - Stimulated Compton is approximated or ignored
- S_N or Discrete Ordinates represents I at fixed angles using finite element basis functions in each zone
  - The discrete angles are selected to enable Gauss integration of spherical harmonics
  - Faster than IMC (>10x in opaque problems)
  - Fully implicit in emission temperature; smaller spatial discretization error
  - Can simulate stimulated Compton
  - The use of discrete angles makes anisotropic scattering approximate and can lead to simulation artifacts

Computational artifacts of IMC and S_N

- IMC simulation of radiation flux in an illuminated asteroid shows statistical noise
- The electron and ion conduction flux also shows noise, seeded by the IMC through its effect on the electron temperature





Simulation with an isotropic point source in an absorbing non-scattering medium

- IMC simulation (top) shows statistical noise
- S_N simulation shows ray effects

Flux-limited Diffusion is a quick but very approximate transport simulation technique

- Averaging the transport equation over angle plus an ansatz for the flux results in diffusion equation

Material motion correction terms

$$\frac{\partial E}{\partial t} + \nabla \cdot [-\mathcal{L} F] + \frac{4}{3} \nabla \cdot (E v) + \frac{1}{3} v \cdot \nabla E = c \sigma a T^4 - c \sigma_a E$$

Here $E = -\frac{1}{c} \int_{4\pi} \mathrm{d}\Omega I$ is the radiation energy density (Energy/Length^3) and

$$F = -\frac{c}{3(\sigma_a + \sigma_s)} \nabla E$$

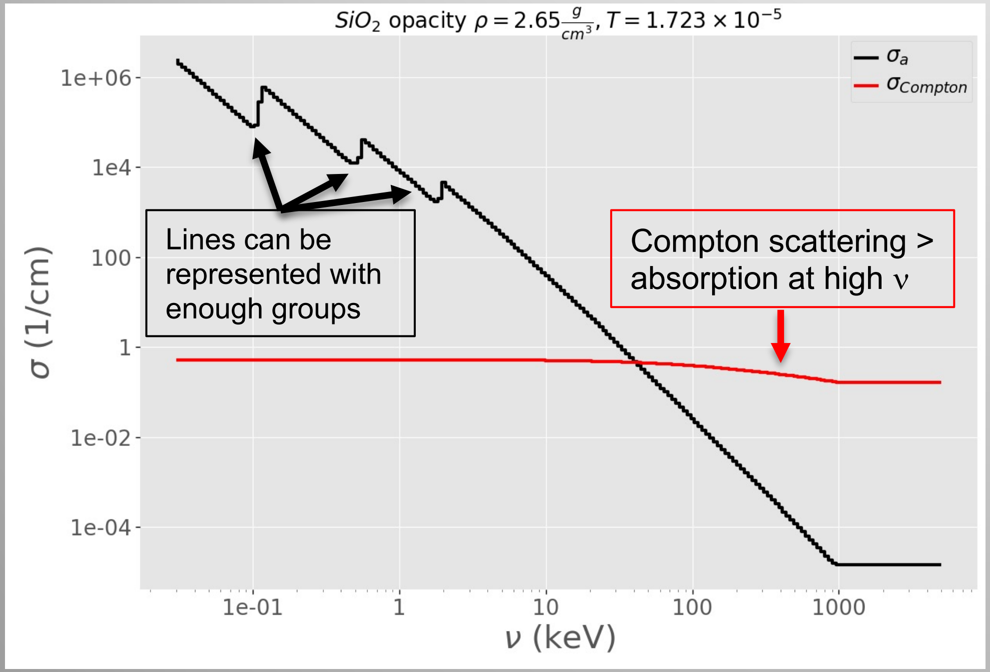
is the radiation flux (Energy/Length^2-Time)

- This expression for F is <u>an approximation</u>

- Diffusion can't model angular information – no shadows
- Diffusion is accurate when radiation is isotropic AND gradients in E are small
  - Ad hoc flux limiter $\mathcal{L}$ in [0,1] needed to suppress superluminal energy flow ($F > c\, \Delta E$) when σ is small
- For heat conduction in electrons and ions, which typically have small flux, a similar diffusion approximation is accurate

The Multigroup approximation is used to express frequency dependence of σ and $\mathbf{I}$ (or $\mathbf{E}$)

- We pick O(10)-(100) fixed values of ν; each range is called a “group”
  - Group bounds are constant in time and space in a simulation
  - We solve one transport or diffusion equation per group
  - Scattering and absorption-reemission couple the groups and the per-group equations
    - This requires iteration in S_N and FLD



- Opacities are constant in each group during a time step
  - Recalculated in each group at the beginning of the time step to account for changes in ρ and T

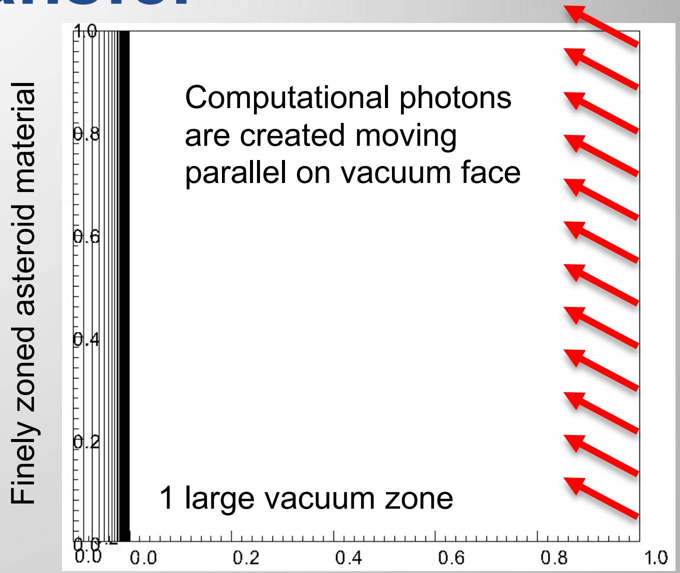
We are using IMC in our deflection calculations because they contain vacuum and point sources

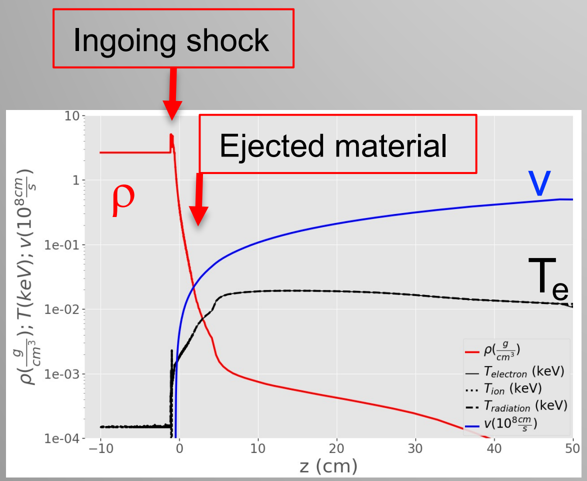
- Diffusion has poor accuracy in vacuum
  - It also can't simulate the directionality of a point source
- S_N suffers from ray effects in vacuum
  - Can't accurately model strongly peaked scattering like Compton
- IMC can simulate point and ray sources
  - We have to incur and mitigate the drawbacks:
    - Statistical noise
    - Long runtimes
    - Use lots of zones and time steps

We must use lots of particles and processors

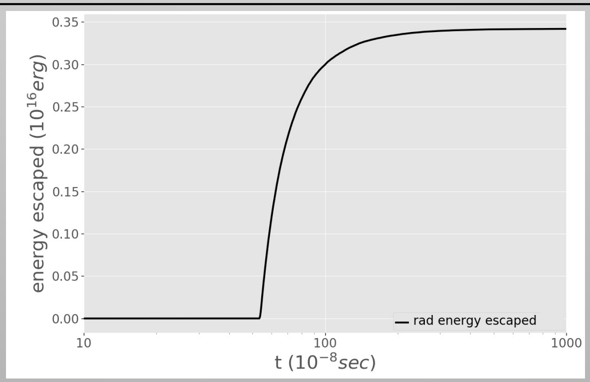
1D simulations simulate surface absorption, reemission, and momentum transfer

- 1 sq. cm chunk ~ 60 cm deep
- Source equivalent to 1 kiloton 85 m away
  - Spectrum = 1 keV Planckian
- 200 groups in [3 x 10^{-3}, 1000] keV log-spaced
- Run to ~ 1e-4 sec
  - Δt in [10^{-16}, 10^{-9}] sec
- 2000 zones with Δx in [10^{-5},.4] cm
- 10^6 computational photons
- Materials = SiO2, Fe, H_2O, Fosterite
- Simulations take ~ 1 Day on 144 2.1 MHz procs
- Hydrodynamics is Lagrangian
  - Mesh moves with the material

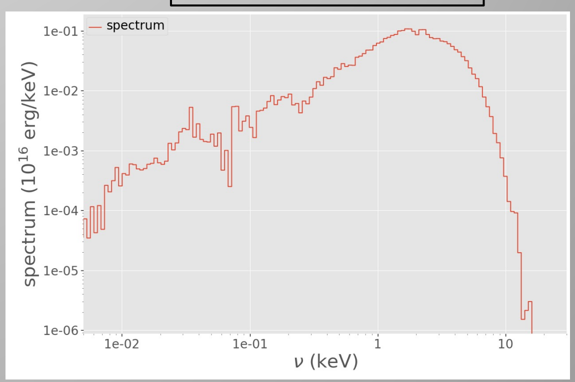




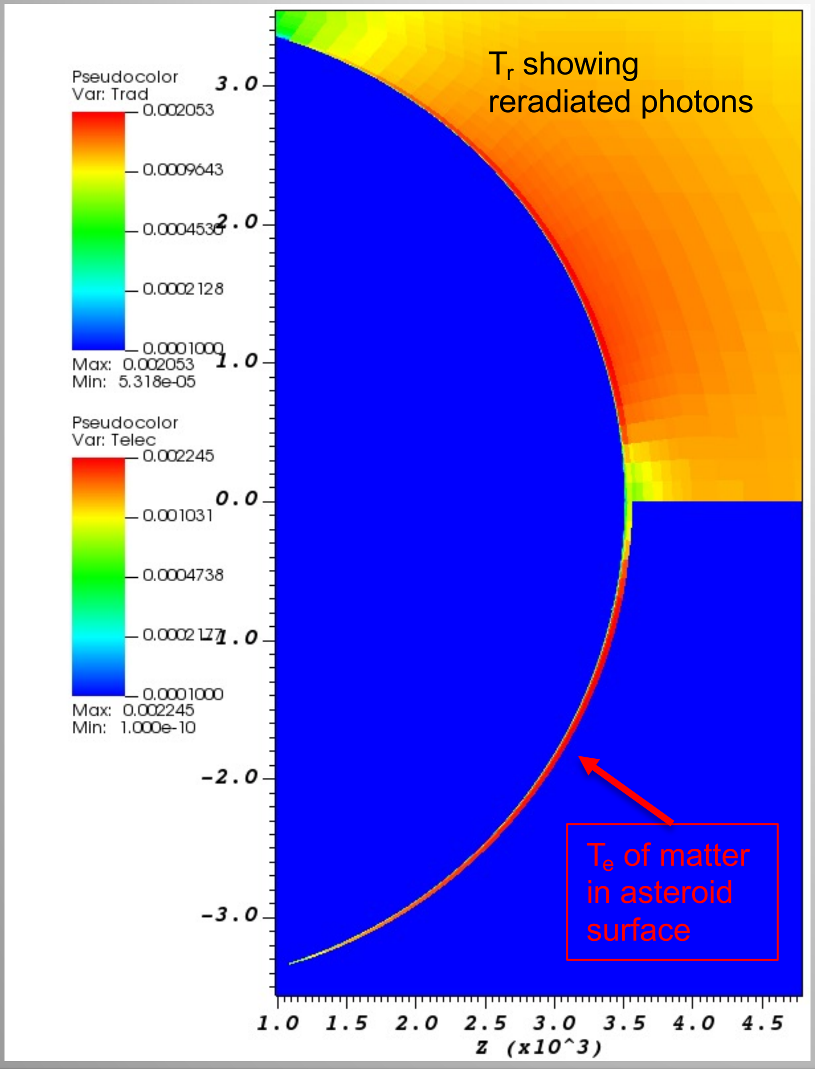
Energy escaping through asteroid surface



Escaping spectrum

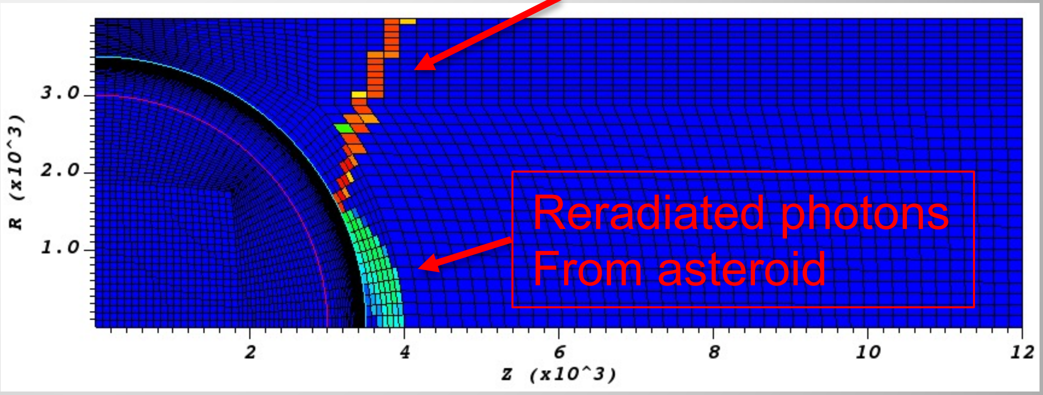


2D simulations provide more realistic exploration of deposition as a function of angle



Source photons

- The computational photons have exact positions on a spherical shell
- The jaggedness is an artifact of the coarse vacuum zoning



- ½ of 35 m asteroid on an axisymmetric mesh
- Source is 1 kiloton, 85 m from surface
  - Spectrum = 1 keV Planckian
- 200 groups in [3 x 10^{-3}, 1000] keV log-spaced
- 20719 zones; sizes in [10^{-6}, 100] cm
- 10^8 computational photons
- Materials = SiO2, Fe, H_2O, Forsterite
- Simulations take ~ 1 Week on 144 2.1 MHz procs
- Hydrodynamics is Lagrangian
  - Mesh moves with the material

Radiation hydrodynamics simulations using IMC will contribute to asteroid deflection modeling

- We are currently running radiation hydrodynamics calculations in 1 and 2D
  - These expensive calculations model absorption and reemission, shock physics, and asteroid momentum
- These simulations allow us to characterize energy deposition with relevant physics
- We are investigating whether we can use that deposition in hydro-only calculations and still obtain accurate results for momentum coupling
  - These simulations ignore radiation transport but are much faster

A derivation of FLD with MMC

1) $$\frac{\partial E_L}{\partial t} + \frac{\partial F_{L,i}}{\partial x_i} = c\sigma_a a T^4 - c\sigma_a E_F - \sigma_t \frac{v_i}{c} F_{F,i}$$

Energy conservation in lab frame: $\nabla_a T^{a0}_{rad} = g^0_L$ with $g^0_L = g^0_F + v_i g^i_F$, $g^0_F = c\sigma_a a T^4 - c\sigma_a E_F$ and $g^i_F = -\frac{1}{c}\sigma_t F^i_F$ [See [2], Eqs.(6.31)—(6.38)]

2) $$E_L = E_F + 2\frac{v_i}{c^2} F_{F,i} \approx E_F$$ since we will drop $\frac{1}{c}\frac{\partial F_F}{\partial t}$

$$F_{L,i} = F_{F,i} + v_i E_F + v_j P_{F,ij} + O(\frac{v}{c})$$

Express lab frame radiation quantities in fluid frame to O(v/c) via Lorentz transformation [2] Eq.(6.30)

3) $$P_{F\ ij} \equiv \frac{1}{c}\int_{4\pi} I_F \Omega_i \Omega_j \, d\Omega \approx \frac{1}{3} E_F \delta_{ij}$$ assuming $I_F = \frac{1}{4\pi}(cE_F + \Omega_F \cdot F_F)$ I_F is weakly anisotropic

4) $$F_F = -\mathcal{L}c\frac{1}{3\sigma_t}\frac{\partial E_F}{\partial x_{F,i}} \approx -\mathcal{L}c\frac{1}{3\sigma_t}\frac{\partial E_F}{\partial x_i}$$

Flux ansatz in fluid frame and $\frac{\partial}{\partial x_{F,i}} = \frac{\partial}{\partial x_i} + \frac{v_i}{c^2}\frac{\partial}{\partial t}$ with $\mathcal{L} \in [0,1]$ the flux limiter, used in $\frac{\partial F_{L,i}}{\partial x_i}$ term

5) $$F_{F,i} = -c\frac{1}{3\sigma}\frac{\partial E}{\partial x_i}$$

Inconsistent !

Flux ansatz in fluid frame without the flux limiter, used in $\sigma_t \frac{v_i}{c} F_{F,i}$ term

Steps 1-5 finally yield the standard form of the diffusion equation with MMC

$$\frac{DE}{Dt} - \frac{\partial}{\partial x_i}\mathcal{L}\frac{1}{3\sigma_t}\frac{\partial E}{\partial x_i} + \frac{4}{3}E\frac{\partial v_i}{\partial x_i} = c\sigma a T^4 - c\sigma_a E$$

Eq.(11.9) in [2], Eq.(7.18) in [6]

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