Progress Towards a Hybrid Monte Carlo-Deterministic Method for Gray Thermal Radiative Transfer with Fully-Implicit Emission-Absorption Physics

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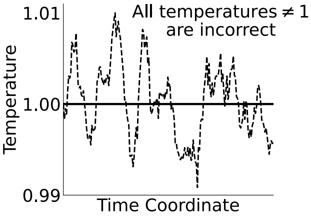
Can Monte Carlo radiative transfer preserve a maximum principle?

An infinite medium has a constant temperature for all time.

Numerical Method

Numerical Results

1) **Infinite Medium**



An inflow problem temperature cannot exceed the boundary value.

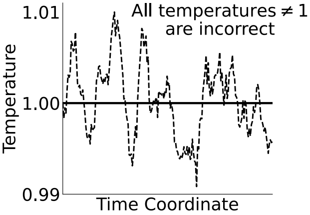
Numerical Method

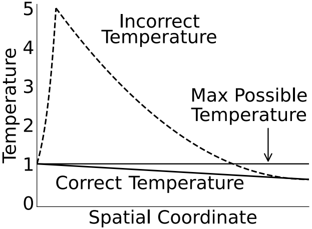
Numerical Results

1) **Infinite Medium**

2) **Inflow Problem**

Conclusion





We want to solve the thermal radiative transfer (TRT) equations.

Find I_ν and T satisfying:

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mathbf{\Omega} \cdot \nabla I_\nu + \sigma I_\nu = \sigma B \,,$$

$$C_v \frac{\partial T}{\partial t} = \int_0^\infty \int_{\mathbb{S}^2} \sigma (I_\nu - B) \, \mathrm{d}\nu \, \mathrm{d}\Omega \,.$$

For simplicity, we consider the “gray” TRT equations.

Find I and T satisfying:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{\Omega}\cdot\nabla I + \sigma I = \frac{c\sigma}{4\pi}U(T)\,, \tag{1a}$$

$$C_v\frac{\partial T}{\partial t} = c\sigma E - c\sigma U(T)\,, \tag{1b}$$

where $E = \frac{1}{c}\int_{\mathbb{S}^2} I\,\mathrm{d}\Omega,$ $U(T) = aT^4,$ and $a = \frac{8\pi^4 k^4}{15h^3c^3}\,.$

The second moment system [1] is an equivalent reformulation.

Find E, $\boldsymbol{F}$, and T satisfying:

$$\frac{\partial E}{\partial t} + \nabla \cdot \boldsymbol{F} + c\sigma E = c\sigma U(T)\,, \quad \mathbf{x} \in \mathcal{D}\,, \tag{2a}$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}}{\partial t} + \frac{c}{3}\nabla E + \sigma \boldsymbol{F} = -\nabla \cdot \mathbf{R}\,, \quad \mathbf{x} \in \mathcal{D}\,, \tag{2b}$$

$$C_v \frac{\partial T}{\partial t} = c\sigma E - c\sigma U(T)\,, \quad \mathbf{x} \in \mathcal{D}\,, \tag{2c}$$

where $\mathbf{R} = \int_{\mathbb{S}^2} \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} I \,\mathrm{d}\Omega - \frac{1}{3}\mathbb{I} \int_{\mathbb{S}^2} I \,\mathrm{d}\Omega$.

[1] Lewis and Miller, Trans. Am. Nucl. Soc. 23 (1976)

Discretize the emission implicitly in time.

$$\frac{I^{k+1} - I^{k}}{c\Delta t} + \boldsymbol{\Omega} \cdot \nabla I^{k+1} + \sigma I^{k+1} = \frac{c\sigma}{4\pi} U(T^{k+1}) \,, \tag{3a}$$

$$\frac{E^{k+1} - E^{k}}{\Delta t} + \nabla \cdot \boldsymbol{F}^{k+1} + c\sigma E^{k+1} = c\sigma U(T^{k+1}) \,, \quad \mathbf{x} \in \mathcal{D} \,, \tag{3b}$$

$$\frac{\boldsymbol{F}^{k+1} - \boldsymbol{F}^{k}}{c\Delta t} + \frac{c}{3} \nabla E^{k+1} + \sigma \boldsymbol{F}^{k+1} = -\nabla \cdot \mathbf{R}^{k+1} \,, \quad \mathbf{x} \in \mathcal{D} \,, \tag{3c}$$

$$\frac{C_v}{\Delta t} (T^{k+1} - T^{k}) = c\sigma E^{k+1} - c\sigma U(T^{k+1}) \,, \quad \mathbf{x} \in \mathcal{D} \,. \tag{3d}$$

Drop the superscript $(\cdot)^{k+1}$ and replace $(\cdot)^k$ with $(\cdot)^*$.

$$\nabla \cdot \boldsymbol{F} + c\tilde{\sigma} E = c\sigma U(T) + \frac{1}{\Delta t} E^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \tag{4a}$$

$$\frac{c}{3} \nabla E + \tilde{\sigma} \boldsymbol{F} = -\nabla \cdot \mathbf{R} + \frac{1}{c \Delta t} \boldsymbol{F}^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \tag{4b}$$

$$\left(\frac{C_v}{\Delta t} + c\sigma U(\cdot) \right) T = c\sigma E + \frac{C_v}{\Delta t} T^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \tag{4c}$$

where $\tilde{\sigma} = \sigma + \frac{1}{c\Delta t}$.

Compute the emission using T from the moment system.

$$\mathbf{\Omega} \cdot \nabla I + \tilde{\sigma} I = \frac{c\sigma}{4\pi} U(T) + \frac{1}{c\Delta t} I^*$$

Estimate $\mathbb{R}$ using Monte Carlo.

$$\boldsymbol{\Omega} \cdot \nabla I + \tilde{\sigma} I = \frac{c\sigma}{4\pi} U(T) + \frac{1}{c\Delta t} I^*$$

$$\mathbf{R}(I) = \int_{\mathbb{S}^2} \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} \, I \, \mathrm{d}\Omega - \tfrac{1}{3} \mathbb{I} \int_{\mathbb{S}^2} I \, \mathrm{d}\Omega$$

Nonlinearly solve the low-order system.

$$\boldsymbol{\Omega} \cdot \nabla I + \tilde{\sigma} I = \frac{c\sigma}{4\pi} U(T) + \tfrac{1}{c\Delta t} I^*$$

$$\begin{aligned}
\nabla \cdot \boldsymbol{F} + c\tilde{\sigma} E &= c\sigma U(T) + \tfrac{1}{\Delta t} E^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \\
\tfrac{c}{3} \nabla E + \tilde{\sigma} \boldsymbol{F} &= -\nabla \cdot \mathbf{R} + \tfrac{1}{c\Delta t} \boldsymbol{F}^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \\
\left(\tfrac{C_v}{\Delta t} + c\sigma U(\cdot) \right) T &= c\sigma E + \tfrac{C_v}{\Delta t} T^* \,, \quad \mathbf{x} \in \mathcal{D} \,.
\end{aligned}$$

$$\mathbf{R}(I) = \int_{\mathbb{S}^2} \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} \, I \, \mathrm{d}\Omega - \tfrac{1}{3} \mathbb{I} \int_{\mathbb{S}^2} I \, \mathrm{d}\Omega$$

Iterate to converge the emission source.

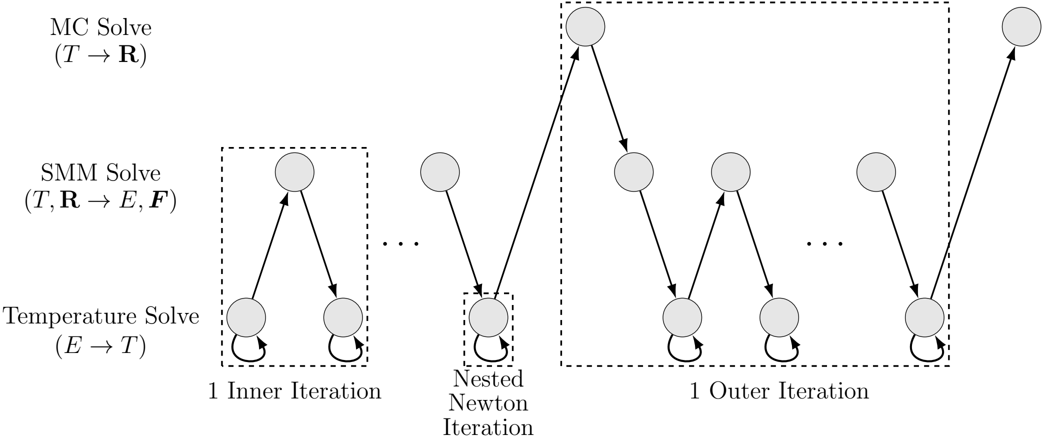
T

$$\boldsymbol{\Omega} \cdot \nabla I + \tilde{\sigma} I = \frac{c\sigma}{4\pi} U(T) + \tfrac{1}{c\Delta t} I^*$$

$$\begin{aligned}
\nabla \cdot \boldsymbol{F} + c\tilde{\sigma} E &= c\sigma U(T) + \tfrac{1}{\Delta t} E^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \\
\tfrac{c}{3} \nabla E + \tilde{\sigma} \boldsymbol{F} &= -\nabla \cdot \mathbf{R} + \tfrac{1}{c\Delta t} \boldsymbol{F}^* \,, \quad \mathbf{x} \in \mathcal{D} \,, \\
\left(\tfrac{C_v}{\Delta t} + c\sigma U(\cdot) \right) T &= c\sigma E + \tfrac{C_v}{\Delta t} T^* \,, \quad \mathbf{x} \in \mathcal{D} \,.
\end{aligned}$$

$$\mathbf{R}(I) = \int_{\mathbb{S}^2} \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} \, I \, \mathrm{d}\Omega - \tfrac{1}{3} \mathbb{I} \int_{\mathbb{S}^2} I \, \mathrm{d}\Omega$$

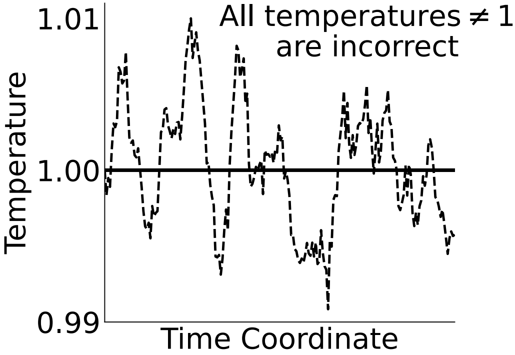
Nonlinearly solving the low-order system requires inner iterations.



An infinite medium has a constant temperature for all time.

Simulate infinite medium with,

- $T = 1$ keV,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- 20 ns $=$ 200 ps $\times$ 100 timesteps.



Plot material and radiation temperatures.

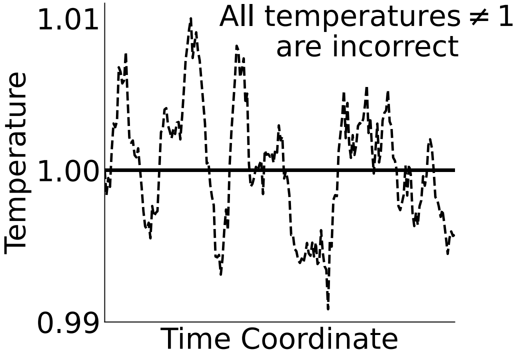
Simulate infinite medium with,

- $T = 1$ keV,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- 20 ns $=$ 200 ps $\times$ 100 timesteps.

Plot:

- $T_{\mathrm{mat}} = T$
- $T_{\mathrm{rad}} = (\hat{E}/a)^{1/4}$

where $\hat{E} = \frac{1}{c\Delta t}\frac{1}{V}\sum_i d_i w_i \approx \frac{1}{c}\int_{\mathbb{S}^2} I \,\mathrm{d}\Omega$.



Compare to Fleck & Cummings [2].

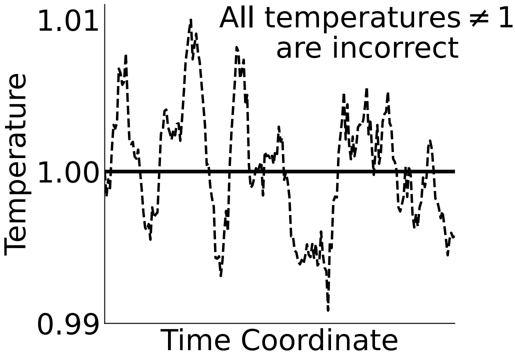
Simulate infinite medium with,

- $T = 1$ keV,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- 20 ns $=$ 200 ps $\times$ 100 timesteps.

Plot:

- $T_{\text{mat}} = T$
- $T_{\text{rad}} = (\hat{E}/a)^{1/4}$

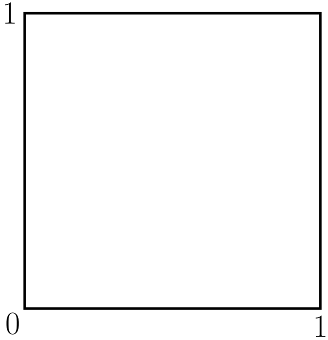
where $\hat{E} = \frac{1}{c\Delta t}\frac{1}{V}\sum_i d_i w_i \approx \frac{1}{c}\int_{\mathbb{S}^2} I \, \mathrm{d}\Omega$.



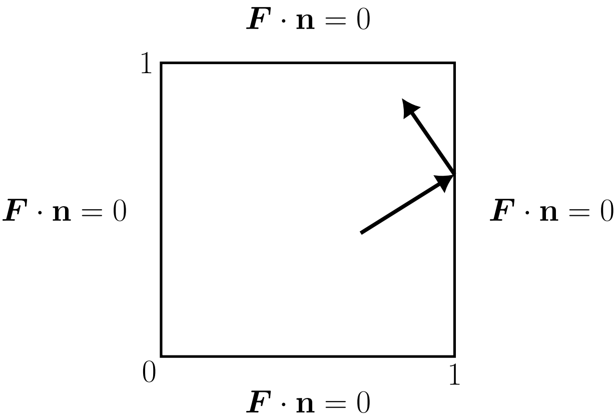
Compare to:

- [2] Fleck and Cummings, J. Comput. Phys. 8, 313-342 (1971)

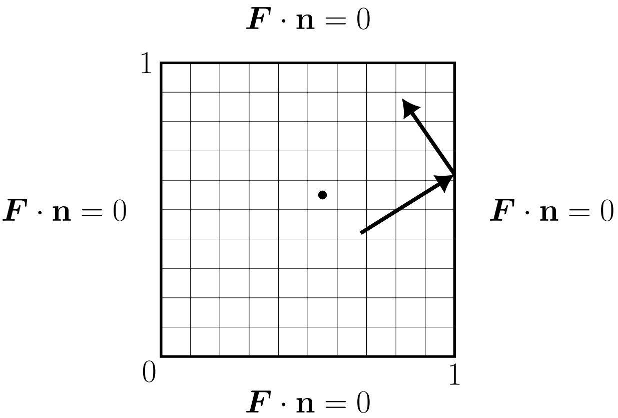
Model an infinite medium in the unit square.



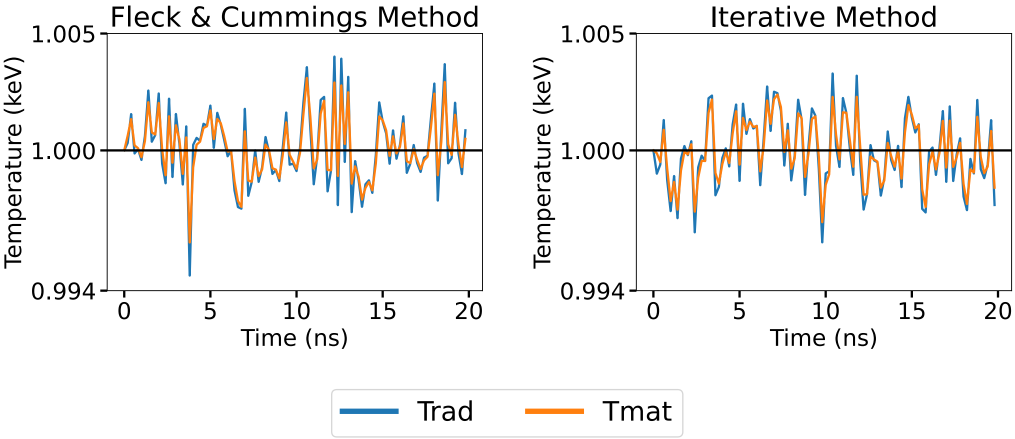
Reflecting boundary conditions emulate an infinite domain.



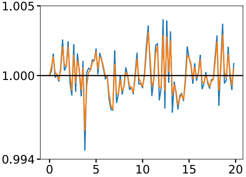
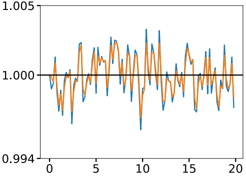
Use 10×10 mesh of squares and measure temperature at a point.



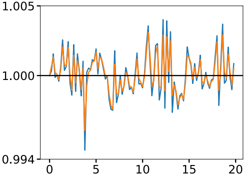
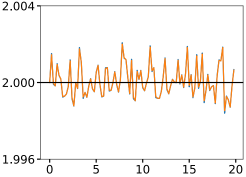
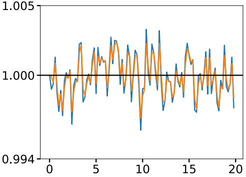
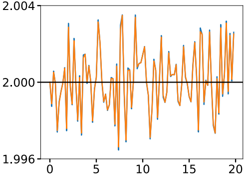
Fleck & Cummings and the iterative method give similar results.



These are the same plots from the previous slide.

	1 keV & 10^5 particles	2 keV & 10^6 particles	4 keV & 10^7 particles
Fleck & Cummings			
Iterative Method			

Increasing T^4 by 16x requires ~10x more particles to converge.

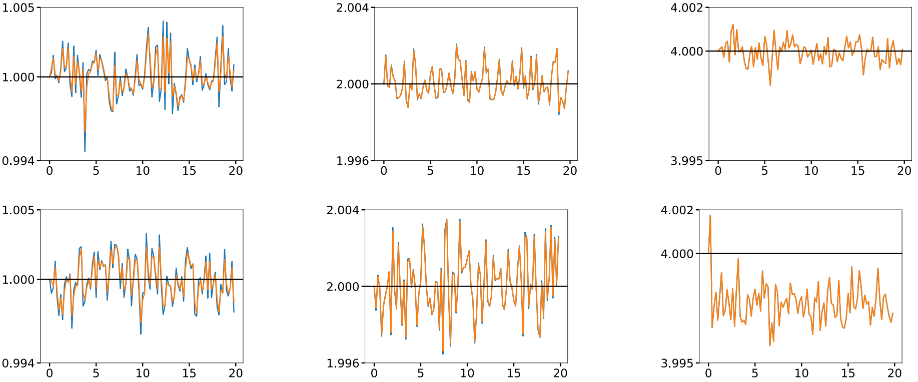
	1 keV & 10^5 particles	2 keV & 10^6 particles	4 keV & 10^7 particles
Fleck & Cummings			
Iterative Method			

Increasing T^4 by 256x requires ∼100x more particles to converge.

1 keV & 10^5 particles | 2 keV & 10^6 particles | 4 keV & 10^7 particles

Fleck & Cummings

Iterative Method



The emission source in Fleck & Cummings is attenuated by f.

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{\Omega}\cdot\nabla I + \sigma I = \frac{1-f}{4\pi}\sigma\int_{\mathbb{S}^2} I \,\mathrm{d}\Omega + \frac{f}{4\pi}c\sigma U(T)\,,$$

where $f = \frac{1}{1+\alpha\beta\sigma c\Delta t} \in (0,1]$ with $\alpha \in [0,1]$, $\beta = \frac{4aT^3}{C_v}$, and $\Delta t \in (0,\infty)$.

Un-attenuated emission leads to unbounded variance [3].

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega} \cdot \nabla I + \sigma I = \frac{1-f}{4\pi}\sigma \int_{\mathbb{S}^2} I \, \mathrm{d}\Omega + \frac{f}{4\pi} c\sigma U(T) \,,$$

where $f = \frac{1}{1+\alpha\beta\sigma c \Delta t} \in (0, 1]$ with $\alpha \in [0, 1]$, $\beta = \frac{4aT^3}{C_v}$, and $\Delta t \in (0, \infty)$.

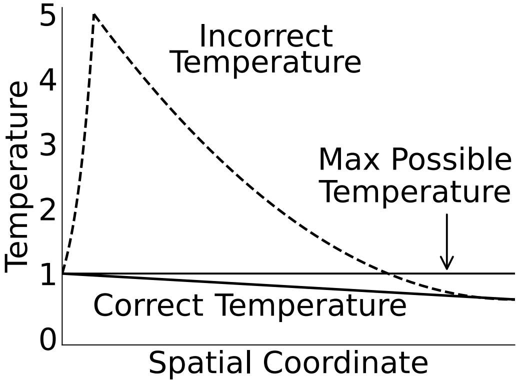
$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega} \cdot \nabla I + \sigma I = \frac{c\sigma}{4\pi} U(T)$$

[3] Pozulp and Haut, JCTT (2026) doi.org/10.1080/23324309.2026.2638245

An inflow problem temperature cannot exceed the boundary value.

Simulate inflow problem with,

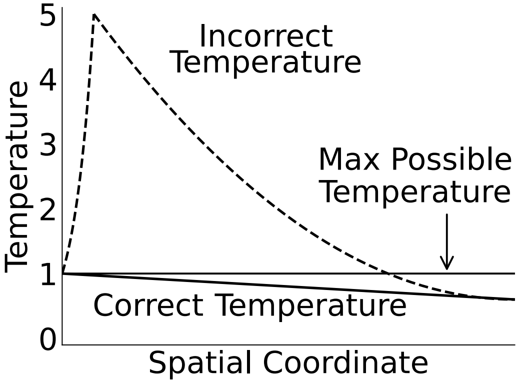
- $T_{\text{boundary}} = 1$ keV,
- $\Delta t = 4$ ns, 2 ns, 1 ns, $t_{\text{final}} = 8$ ns,



Model the inflow problem on the unit square.

Simulate inflow problem with,

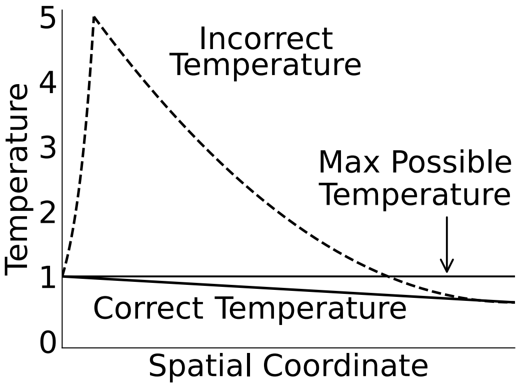
- $T_{\text{boundary}} = 1$ keV,
- $\Delta t = 4$ ns, 2 ns, 1 ns, $t_{\text{final}} = 8$ ns,
- $\mathcal{D} = [0, 1]^2$ and 1,000,000 particles,



The domain temperature is initially 10x colder than the inflow.

Simulate inflow problem with,

- $T_{\text{boundary}} = 1$ keV,
- $\Delta t = 4$ ns, 2 ns, 1 ns, $t_{\text{final}} = 8$ ns,
- $\mathcal{D} = [0, 1]^2$ and 1,000,000 particles,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- $T_{\text{initial}} = 0.1$ keV.



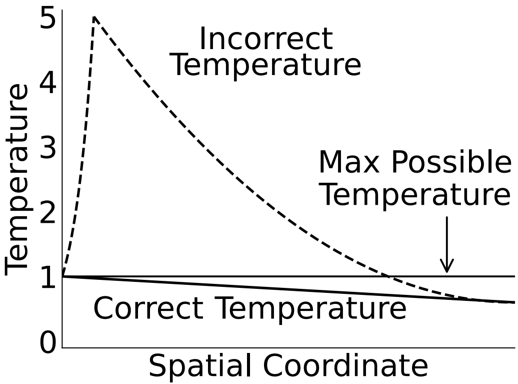
Plot a temperature lineout at $y = 0.5$.

Simulate inflow problem with,

- $T_{\text{boundary}} = 1$ keV,
- $\Delta t = 4$ ns, 2 ns, 1 ns, $t_{\text{final}} = 8$ ns,
- $\mathcal{D} = [0, 1]^2$ and 1,000,000 particles,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- $T_{\text{initial}} = 0.1$ keV.

Plot:

- T lineout at $y = 0.5$



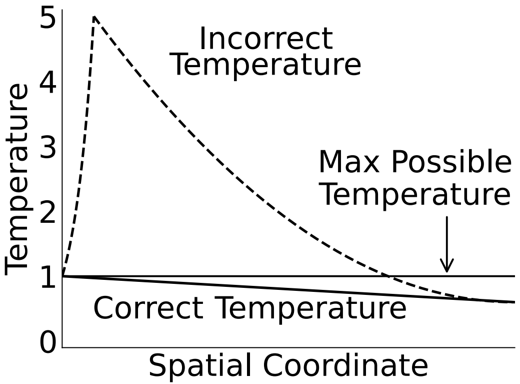
Compare to Fleck & Cummings [2].

Simulate inflow problem with,

- $T_{\text{boundary}} = 1$ keV,
- $\Delta t = 4$ ns, 2 ns, 1 ns, $t_{\text{final}} = 8$ ns,
- $\mathcal{D} = [0, 1]^2$ and 1,000,000 particles,
- $\sigma = 1$ cm^{-1}, $C_v = 0.1$ GJ / cm^3 keV,
- $T_{\text{initial}} = 0.1$ keV.

Plot:

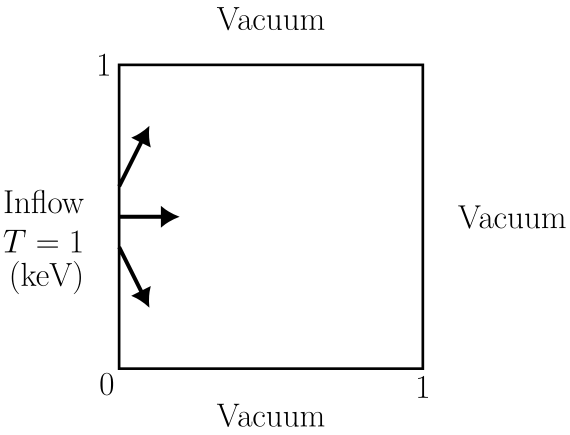
- T lineout at $y = 0.5$



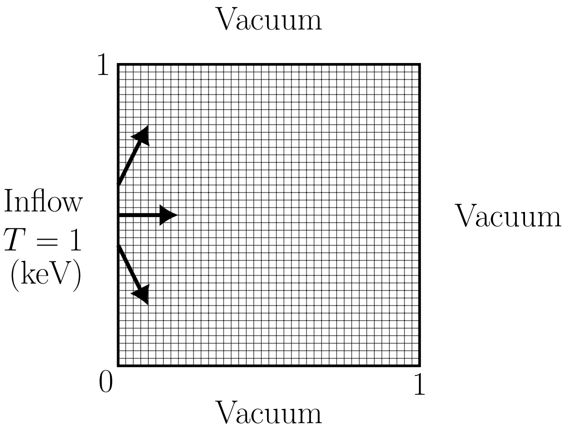
Compare to:

- [2] Fleck and Cummings, J. Comput. Phys. 8, 313-342 (1971)

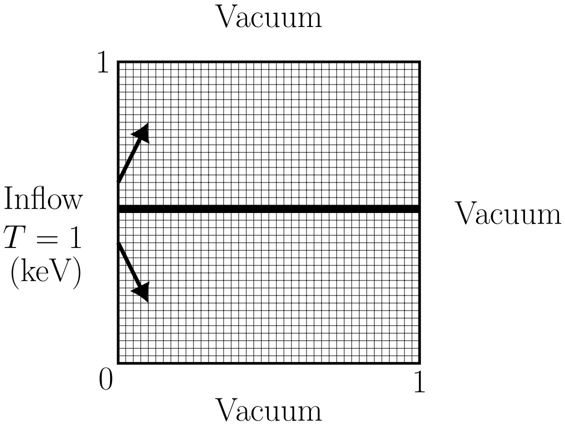
The inflow problem has one inflow and three vacuum boundaries.



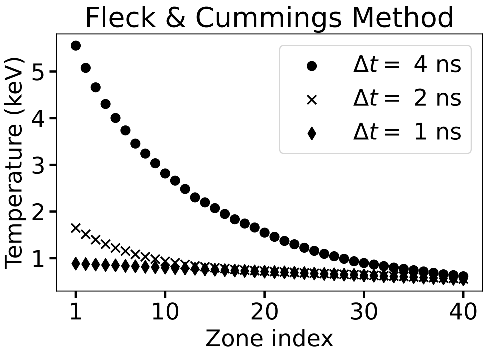
Use a 40×40 mesh of squares.



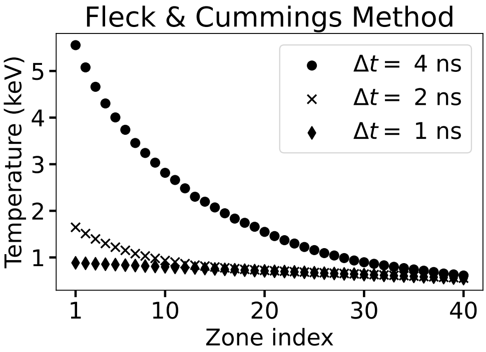
Measure temperature along the line $y = 0.5$.

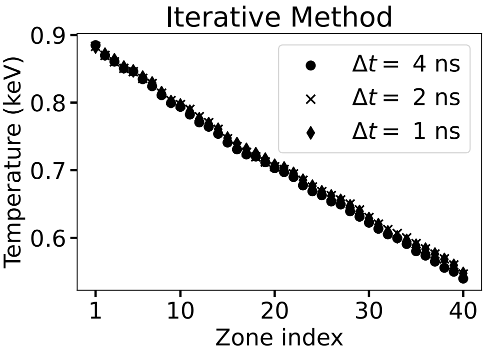


Fleck & Cummings' maximum principle violation worsens with Δt.



The iterative method does not violate the maximum principle.





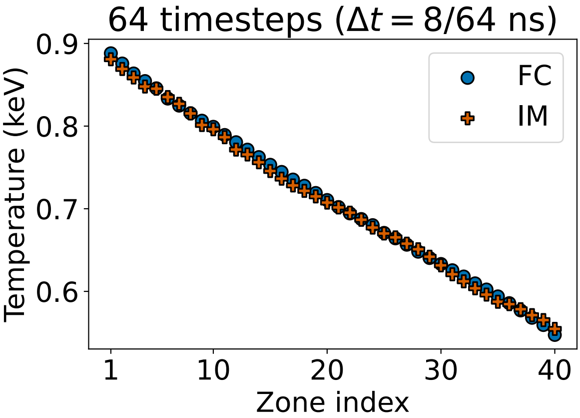
Note: explicit MC diverges unless timestep is refined by a factor of 4.

Iterations per timestep do not increase with timestep size.

	Δt (ns)		
	4	2	1
# of Timesteps	2	4	8
f (# Outer per Timestep)	3	3	3
f (# Inner per Outer)	2	2	2
f (# NN per Inner)	3	2	2

where $f(\cdot) = \text{floor}(\text{average}(\cdot))$.

Fleck & Cummings and iterative method agree for refined Δt.



We created & demonstrated a new iterative method for gray TRT.

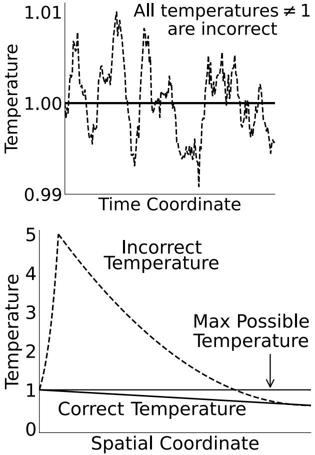
Numerical Method

Numerical Results

1) **Infinite Medium**

2) **Inflow Problem**

Conclusion



More research is required to improve the method.

Gray priorities:

- Variance reduction
- Linear temperatures

Multifrequency considerations:

- Gray collapse
- Scattering

Miscellaneous:

- Hybridization

References I

[1] E. Lewis and W. Miller. "A comparison of p1 synthetic acceleration techniques." Transactions of the American Nuclear Society, **volume 23** (1976).

[2] J. A. Fleck and J. D. Cummings. "An implicit Monte Carlo scheme for calculating time and frequency dependent nonlinear radiation transport." Journal of Computational Physics, **volume 8**, pp. 313–342 (1971).

[3] M. Pozulp and T. Haut. "A Proof of the Asymptotic Variance of Path Length Estimators for Single-Collision Monte Carlo Source Iteration in the Thick Diffusion Limit." Journal of Computational and Theoretical Transport (2026).

References II

[4] M. M. Pozulp, T. S. Haut, P. S. Brantley, and S. S. Olivier. "A Hybrid Monte Carlo-Deterministic Second Moment Method with Efficient Variance Reduction." Technical Report LLNL-JRNL-2010906-DRAFT, Lawrence Livermore National Laboratory. URL https://mike.pozulp.com/2026hsm_with_vr.pdf. Preprint.

Lawrence Livermore National Laboratory

Extra slides

Testing eqs. (4a) to (4c) with u and v gives a weak form.

Find $(\boldsymbol{F}, E, T) \in RT_0 \times Y_0 \times Y_0$ such that,

$$\int \tilde{\sigma} \boldsymbol{v} \cdot \boldsymbol{F} \, \mathrm{d}\mathbf{x} - \frac{c}{3} \int \nabla \cdot \boldsymbol{v} E \, \mathrm{d}\mathbf{x} = q_F \,, \qquad \forall \boldsymbol{v} \in RT_0 \,,$$

$$\int u \nabla \cdot \boldsymbol{F} \, \mathrm{d}\mathbf{x} + c \int u \tilde{\sigma} E \, \mathrm{d}\mathbf{x} - c \int u \sigma U(T) \, \mathrm{d}\mathbf{x} = q_E \,, \qquad \forall u \in Y_0 \,,$$

$$-c \int u \sigma E \, \mathrm{d}\mathbf{x} + \int u \left(\frac{C_v}{\Delta t} + c \sigma U(\cdot) \right) T \, \mathrm{d}\mathbf{x} = q_T \,, \qquad \forall u \in Y_0 \,.$$

The weak form can be written as a block system.

Find $(\boldsymbol{F}, E, T) \in RT_0 \times Y_0 \times Y_0$ such that,

$$\int \tilde{\sigma} \boldsymbol{v} \cdot \boldsymbol{F} \, \mathrm{d}\mathbf{x} - \frac{c}{3} \int \nabla \cdot \boldsymbol{v} E \, \mathrm{d}\mathbf{x} = q_F \,, \qquad \forall \boldsymbol{v} \in RT_0 \,,$$

$$\int u \nabla \cdot \boldsymbol{F} \, \mathrm{d}\mathbf{x} + c \int u \tilde{\sigma} E \, \mathrm{d}\mathbf{x} - c \int u \sigma U(T) \, \mathrm{d}\mathbf{x} = q_E \,, \qquad \forall u \in Y_0 \,,$$

$$-c \int u \sigma E \, \mathrm{d}\mathbf{x} + \int u \left(\frac{C_v}{\Delta t} + c \sigma U(\cdot) \right) T \, \mathrm{d}\mathbf{x} = q_T \,, \qquad \forall u \in Y_0 \,.$$

The block system is,

$$\begin{bmatrix} \mathbf{M}_F & -\frac{c}{3}\mathbf{D} & \\ \mathbf{D} & \mathbf{M}_E & -\mathbf{B}(\cdot) \\ & -\mathbf{M}_a & -\tilde{\mathbf{B}}(\cdot) \end{bmatrix} \begin{bmatrix} \boldsymbol{F} \\ E \\ T \end{bmatrix} = \begin{bmatrix} q_F \\ q_E \\ q_T \end{bmatrix} \,. \tag{5}$$

Apply Newton's method to the block system in eq. (5).

$$\begin{bmatrix} \mathbf{M}_F & -\frac{c}{3}\mathbf{D} & \\ \mathbf{D} & \mathbf{M}_E & -\delta\mathbf{B}(\cdot) \\ & -\mathbf{M}_a & -\delta\tilde{\mathbf{B}}(\cdot) \end{bmatrix} \begin{bmatrix} \boldsymbol{F} \\ E \\ T - T_0 \end{bmatrix} = \begin{bmatrix} q_F \\ q_E + \mathbf{B}(T_0) \\ q_T + \tilde{\mathbf{B}}(T_0) \end{bmatrix}$$

Eliminate temperature by "solving" the third row for $T - T_0$.

$$\begin{bmatrix} \mathbf{M}_F & -\frac{c}{3}\mathbf{D} & \\ \mathbf{D} & \mathbf{M}_E & -\delta\mathbf{B}(\cdot) \\ & -\mathbf{M}_a & -\delta\tilde{\mathbf{B}}(\cdot) \end{bmatrix} \begin{bmatrix} \boldsymbol{F} \\ E \\ T - T_0 \end{bmatrix} = \begin{bmatrix} q_F \\ q_E + \mathbf{B}(T_0) \\ q_T + \tilde{\mathbf{B}}(T_0) \end{bmatrix}$$

$$T - T_0 = (\delta\tilde{\mathbf{B}})^{-1}(q_T - \tilde{\mathbf{B}}(T_0) + \mathbf{M}_a E)$$

Substitute $T - T_0$ equation into second row to get 2×2 system.

$$\begin{bmatrix} \mathbf{M}_F & -\frac{c}{3}\mathbf{D} & \\ \mathbf{D} & \mathbf{M}_E & -\delta\mathbf{B}(\cdot) \\ & -\mathbf{M}_a & -\delta\tilde{\mathbf{B}}(\cdot) \end{bmatrix} \begin{bmatrix} \boldsymbol{F} \\ E \\ T - T_0 \end{bmatrix} = \begin{bmatrix} q_F \\ q_E + \mathbf{B}(T_0) \\ q_T + \tilde{\mathbf{B}}(T_0) \end{bmatrix}$$

$$T - T_0 = (\delta\tilde{\mathbf{B}})^{-1}(q_T - \tilde{\mathbf{B}}(T_0) + \mathbf{M}_a E)$$

$$\begin{bmatrix} \mathbf{M}_E - \delta\mathbf{B}(\delta\tilde{\mathbf{B}})^{-1}\mathbf{M}_a & \mathbf{D} \\ -\frac{c}{3}\mathbf{D}^T & \mathbf{M}_F \end{bmatrix} \begin{bmatrix} E \\ \boldsymbol{F} \end{bmatrix} = \begin{bmatrix} q_E + \mathbf{B}(T_0) + \delta\mathbf{B}(\delta\tilde{\mathbf{B}})^{-1}\left(q_T - \tilde{\mathbf{B}}(T_0)\right) \\ q_F \end{bmatrix}$$

We iterate to converge T for a fixed R from the last MC solve.

T

$$\begin{bmatrix} \mathbf{M}_E - \delta\mathbf{B}(\delta\tilde{\mathbf{B}})^{-1}\mathbf{M}_a & \mathbf{D} \\ -\frac{c}{3}\mathbf{D}^T & \mathbf{M}_F \end{bmatrix} \begin{bmatrix} E \\ \boldsymbol{F} \end{bmatrix} = \begin{bmatrix} q_E + \mathbf{B}(T) + \delta\mathbf{B}(\delta\tilde{\mathbf{B}})^{-1}(q_T - \tilde{\mathbf{B}}(T)) \\ q_F \end{bmatrix}$$

$$\tilde{\mathbf{B}}(T) = \mathbf{M}_a E + q_T$$

E

Fleck & Cummings [1] is equivalent to a single Newton step.

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{\Omega}\cdot\nabla I + \sigma I = \frac{1-f}{4\pi}\sigma\int_{\mathbb{S}^2} I\,\mathrm{d}\Omega + \frac{f}{4\pi}c\sigma U(T)\,,$$

$$C_v\frac{\partial T}{\partial t} = fc\sigma E - fc\sigma U(T)\,,$$

where $f = \frac{1}{1+\alpha\beta\sigma c\Delta t}$, $\beta = \frac{4aT^3}{C_v}$, $\alpha \in [0,1]$ and $\Delta t \in (0,\infty)$.

[1] Fleck and Cummings, J. Comput. Phys. 8, 313-342 (1971)