A New Neutrino Transport Module Available in FLASH-X

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Number-Conservative Spectral $\mathcal{O}(v/c)$ Two-Moment Model[1]

- **Number equation**

$$\partial_t\big(\,\mathcal{D}+v^i\mathcal{I}_i\,\big)+\partial_i\big(\,\mathcal{I}^i+v^i\mathcal{D}\,\big)-\frac{1}{\varepsilon^2}\partial_\varepsilon\big(\,\varepsilon^3\,\mathcal{K}^i{}_k\partial_i v^k\,\big)=\frac{1}{4\pi}\int_{\mathbb{S}^2}\mathcal{C}[f]\,d\omega$$

- **Number flux equation**

$$\partial_t\big(\,\mathcal{I}_j+v^i\mathcal{K}_{ij}\,\big)+\partial_i\big(\,\mathcal{K}^i{}_j+v^i\mathcal{I}_j\,\big)-\frac{1}{\varepsilon^2}\partial_\varepsilon\big(\,\varepsilon^3\,\mathcal{L}^i{}_{kj}\partial_i v^k\,\big)$$
$$+\big(\,\mathcal{I}^i\partial_i v_j-\mathcal{L}^i{}_{kj}\partial_i v^k\,\big)=\frac{1}{4\pi}\int_{\mathbb{S}^2}\mathcal{C}[f]\,\ell_j\,d\omega$$

- Angular moments of kinetic distribution f

$$\big\{\mathcal{D},\mathcal{I}^i,\mathcal{K}^{ij},\mathcal{L}^{ijk}\big\}(\varepsilon,\boldsymbol{x},t)=\frac{1}{4\pi}\int_{\mathbb{S}^2}f(\omega,\varepsilon,\boldsymbol{x},t)\big\{1,\ell^i,\ell^i\ell^j,\ell^i\ell^j\ell^k\big\}d\omega$$

- Closed by specifying $\mathcal{K}^{ij}$ and $\mathcal{L}^{ijk}$ in terms of $\mathcal{D}$ and $\mathcal{I}^i$
- Components of fluid three-velocity v^i
- Comoving-frame spherical-polar momentum coordinates (ω,ε)

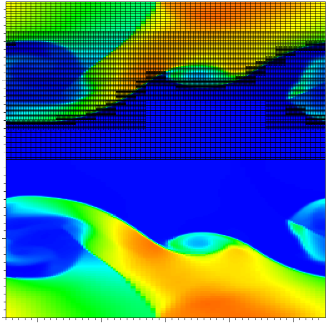
[1] Liau, E, Harris, Zelledge, Mezzacappa arXiv:2309.04429

Collision Term

$$
\begin{aligned}
\mathcal{C}[f,\bar{f}](\boldsymbol{p}) = {} & (1 - f(\boldsymbol{p}))\,\eta(\boldsymbol{p}) - \chi(\boldsymbol{p})\,f(\boldsymbol{p}) && \text{(Emission/absorption)} \\
& + (1 - f(\boldsymbol{p}))\int_{V_{\boldsymbol{p}}} R^{\mathrm{IN}}(\boldsymbol{p},\boldsymbol{p}')\,f(\boldsymbol{p}')\,dV_{\boldsymbol{p}'} && \text{(Scattering)} \\
& - f(\boldsymbol{p})\int_{V_{\boldsymbol{p}}} R^{\mathrm{OUT}}(\boldsymbol{p},\boldsymbol{p}')\,(1 - f(\boldsymbol{p}'))\,dV_{\boldsymbol{p}'} && \\
& + (1 - f(\boldsymbol{p}))\int_{V_{\boldsymbol{p}}} R^{\mathrm{PRO}}(\boldsymbol{p},\boldsymbol{p}')\,(1 - \bar{f}(\boldsymbol{p}'))\,dV_{\boldsymbol{p}'} && \text{(Pair processes)} \\
& - f(\boldsymbol{p})\int_{V_{\boldsymbol{p}}} R^{\mathrm{ANN}}(\boldsymbol{p},\boldsymbol{p}')\,\bar{f}(\boldsymbol{p}')\,d\boldsymbol{p}' &&
\end{aligned}
$$

- Opacities depend nonlinearly on matter state (e.g., ρ, T, and Y_e)
- Pauli blocking factors: $(1 - f)$
- Scattering and pair processes couple in momentum space: $\mathcal{O}(N_{\boldsymbol{p}}^2)$
- Pair processes couple neutrinos and antineutrinos

Toolkit for High-Order Neutrino Rad-Hydro (THORNADO[4])



- Discontinuous Galerkin (DG) methods
  - Hydrodynamics[2]
  - **Spectral, two-moment neutrino transport[3]**
- Tabulated microphysics (WEAKLIB)
  - Equations of State
  - Neutrino opacities
- GPU offloading with OpenMP or OpenACC
- Distributed parallelism and AMR through AMREX or FLASH-X

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[2] Pochik et al. (2021), ApJS, 253:21; Dunham et al. (arXiv:2307.10904)

[3] Chu et al. (2019), JCP, 389, 62; Laiu et al. (2021), ApJS, 253:52; Laiu et al. (arXiv:2309.04429)

[4] github.com/endeve/thornado

WEAKLIB[5]

- Library for tabulated microphysics (EoS and weak interactions)
  - Tabulation in terms of matter states (e.g., ρ, T, and Y_{e}) and neutrino energy (ε)
- Basic functionality for hydrodynamics and neutrino transport algorithms
  - Interpolation on shared grids (EoS and weak interactions)
  - EoS inversions (e.g., $\epsilon \to T$ and $s \to T$)
- GPU offloading with OpenMP or OpenACC

	Process	original WeakLib	updated WeakLib
I	$e^- + p \rightleftharpoons n + \nu_{\mathrm{e}}$	Bruenn (1985)	Reddy et al. (1998); Horowitz (2002)
II	$e^+ + n \rightleftharpoons p + \bar{\nu}_{\mathrm{e}}$	Bruenn (1985)	Reddy et al. (1998); Horowitz (2002)
III	$e^- + A(Z,N) \rightleftharpoons A(Z-1,N+1) + \nu_{\mathrm{e}}$	Fuller et al. (1982)	Langanke et al. (2003); Hix et al. (2003)
IV	$\nu + \{n,p,A\} \rightleftharpoons \nu + \{n,p,A\}$	Bruenn (1985)	Bruenn & Mezzacappa (1997); Horowitz (1997, 2002)
V	$\nu + e^{\pm} \rightleftharpoons \nu' + e^{\pm\,\prime}$	Bruenn (1985)	Bruenn (1985)
VI	$e^- + e^+ \rightleftharpoons \nu + \bar{\nu}$	Bruenn (1985)	Bruenn (1985)
VII	$N + N \rightleftharpoons N' + N' + \nu + \bar{\nu}$	X	Hannestad & Raffelt (1998)

[5] github.com/starkiller-astro/weaklib

Self-Gravitating Neutrino Radiation Hydrodynamics

- **Hydrodynamics** (Euler equations with nuclear EoS)

$$d_t \boldsymbol{u} = \boldsymbol{T}_{\boldsymbol{u}}(\boldsymbol{u}, \Phi) + \boldsymbol{C}_{\boldsymbol{u}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u})$$

  Hyperbolic system with sources — $\boldsymbol{u} \in \mathbb{R}^6$ per spacetime point

- **Neutrino transport** (spectral two-moment model)

$$d_t \boldsymbol{\mathcal{U}} = \boldsymbol{T}_{\boldsymbol{\mathcal{U}}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u}) + \boldsymbol{C}_{\boldsymbol{\mathcal{U}}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u})$$

  Hyperbolic system with sources — $\boldsymbol{\mathcal{U}} \in \mathbb{R}^{6\times 4\times 32=768}$ per spacetime point

- **Gravity** (Poisson equation)

$$F(\Phi, \boldsymbol{u}) = 0$$

  Elliptic equation for scalar potential Φ

Coupling Thornado with Flash-X

- First-order Lie–Trotter splitting
- Flash-X: Euler–Poisson system with finite-volume and RK methods

$$d_t \boldsymbol{u} = \boldsymbol{T}_{\boldsymbol{u}}(\boldsymbol{u}, \Phi)$$
$$F(\Phi, \boldsymbol{u}) = 0$$

- Thornado: Two-moment model with DG and IMEX-RK methods
  - Phase-space advection (explicit)

$$d_t \boldsymbol{\mathcal{U}} = \boldsymbol{T}_{\boldsymbol{\mathcal{U}}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u})$$

  - **Collisions (implicit)**

$$d_t \boldsymbol{u} = \boldsymbol{C}_{\boldsymbol{u}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u})$$
$$d_t \boldsymbol{\mathcal{U}} = \boldsymbol{C}_{\boldsymbol{\mathcal{U}}}(\boldsymbol{\mathcal{U}}, \boldsymbol{u})$$

- Fluid fields $\boldsymbol{u}$ require finite-volume *and* DG representations

Neutrino-Matter Solver: Moment Update

- Implicit update on primitive moments $\boldsymbol{\mathcal{M}} = (\,\mathcal{D},\, \mathcal{I}_j\,)^{\intercal}$

$$\begin{aligned}(\,\mathcal{D} + v^i \mathcal{I}_i\,) &= \mathcal{N}^n + \Delta t(\,\eta - \chi\,\mathcal{D}\,)\\ (\,\mathcal{I}_j + v^i \mathcal{K}_{ij}\,) &= \mathcal{G}_j^n - \Delta t\,\kappa\,\mathcal{I}_j\end{aligned}$$

  η, χ, and κ depend on $\boldsymbol{\mathcal{M}}$, $\bar{\boldsymbol{\mathcal{M}}}$, and $\boldsymbol{u}$

- Modified Richardson iteration with step size $\lambda = 1/(1+|\boldsymbol{v}|)$

$$\begin{aligned}\mathcal{D}^{[k+1]} &= \mathcal{D}^{[k]} + \lambda\,\frac{\left[\,\mathcal{N}^n - (\,\mathcal{D}^{[k]} + v^i \mathcal{I}_{s,i}^{[k]}\,) + \Delta t\,(\,\eta^{[k]} - \chi^{[k]}\,\mathcal{D}^{[k]}\,)\;\right]}{(\,1 + \Delta t\,\chi^{[k]}\,)}\\ \mathcal{I}_j^{[k+1]} &= \mathcal{I}_j^{[k]} + \lambda\,\frac{\left[\,\mathcal{G}_j^n - (\,\mathcal{I}_j^{[k]} + v^i \mathcal{K}_{s,ij}^{[k]}\,) - \Delta t\,\kappa^{[k]}\,\mathcal{I}_j^{[k]}\,\right]}{(\,1 + \Delta t\,\kappa^{[k]}\,)}\end{aligned}$$

  Realizability-preserving with guaranteed convergence*

- Write as fixed-point map

$$\boldsymbol{\mathcal{M}}^{[k+1]} = \boldsymbol{\mathcal{G}}(\boldsymbol{\mathcal{M}}^{[k]}, \boldsymbol{u})$$

Neutrino-Matter Solver: Fluid Update

- Fluid system for $\boldsymbol{u} = (\,\rho,\, \rho v_j,\, \rho\epsilon_{\mathrm{f}},\, \rho Y_{\mathrm{e}}\,)^{\intercal}$: Enforce conservation laws

$$
\begin{aligned}
\rho &= \rho^{n} \\
\rho v_j &= \rho v_j^{n} - \big(\, \mathsf{S}_j - \mathsf{S}_j^{n}\,\big) \\
\rho\epsilon_{\mathrm{f}} &= \rho\epsilon_{\mathrm{f}}^{n} - \big(\, \mathsf{E} - \mathsf{E}^{n}\,\big) \\
\rho Y_{\mathrm{e}} &= \rho Y_{\mathrm{e}}^{n} - m_{\mathrm{b}}\big(\, \mathsf{N} - \mathsf{N}^{n}\,\big)
\end{aligned}
$$

  S_j, E, and N: **neutrino momentum, energy, and number densities**

- Write as fixed-point map

$$\boldsymbol{u} = \boldsymbol{g}(\boldsymbol{\mathcal{M}}, \boldsymbol{u})$$

Neutrino-Matter Solver: Nested Algorithm[6]

- Coupled nonlinear system

$$\boldsymbol{u} = \boldsymbol{g}(\boldsymbol{\mathcal{M}}, \boldsymbol{u}) \quad \text{and} \quad \boldsymbol{\mathcal{M}} = \boldsymbol{\mathcal{G}}(\boldsymbol{\mathcal{M}}, \boldsymbol{u})$$

- **Solved in nested manner**

$$\boldsymbol{u}^{[k+1]} = \boldsymbol{g}\big(\widehat{\boldsymbol{\mathcal{M}}}^{[k]}, \boldsymbol{u}^{[k]}\big) \quad (k = 1, \dots, k_{\text{max}}),$$

where $\widehat{\boldsymbol{\mathcal{M}}}^{[k]}$ is limit point of inner iteration sequence

$$\boldsymbol{\mathcal{M}}^{[k,\ell+1]} = \boldsymbol{\mathcal{G}}\big(\boldsymbol{\mathcal{M}}^{[k,\ell]}, \boldsymbol{u}^{[k]}\big) \quad (\ell = 1, \dots, \ell_{\text{max}}).$$

  - Opacities only evaluated in outer loop
  - Fixed-point iteration avoids Jacobian and solution of dense linear system
  - Easy to implement and extend for additional opacities
  - Anderson acceleration can be applied separately to outer and inner loops

[6] Laiu, E, Chu, Harris, Messer, ApJS, 253:52

Anderson Accelerated Fixed-Point Method[7]: $\boldsymbol{u} = \boldsymbol{g}(\boldsymbol{u})$

$\boldsymbol{u}^{[1]} = \boldsymbol{g}(\boldsymbol{u}^{[0]})$; $\boldsymbol{F}^{[0]} = \boldsymbol{u}^{[0]} - \boldsymbol{g}(\boldsymbol{u}^{[0]})$;
for $k = 1, \ldots, k_{\max}$ **do**
  $m_k = \min(k, M)$;
  $\boldsymbol{F}^{[k]} = \boldsymbol{u}^{[k]} - \boldsymbol{g}(\boldsymbol{u}^{[k]})$;
  Solve

$$\min_{\alpha_j} \left|\left| \sum_{j=0}^{m_k} \alpha_j \, \boldsymbol{F}^{[k-m_k+j]} \right|\right| \quad \text{subject to} \quad \sum_{j=0}^{m_k} \alpha_j = 1$$

  Update

$$\boldsymbol{u}^{[k+1]} = \sum_{j=0}^{m_k} \alpha_j \, \boldsymbol{g}(\boldsymbol{u}^{[k-m_k+j]})$$

end

Algorithm 1: Anderson Accelerated Fixed-Point Iteration

- Uses information from previous iterates to improve convergence rate
- Memory M typically small. We use $M = 2$ or 3 ($M = 1$ is Picard iteration)

[7] Toth & Kelley (2015), SIAM J. Numer. Anal, **53**, 805

Collisional Relaxation

- Space homogeneous, $\nu_{\rm e} + \bar{\nu}_{\rm e}$, tabulated Bruenn 85 opacities
  - Emission/Absorption, Iso-energetic scattering, NES, and Pairs
- **Goals:** (i) Relaxation to equilibrium, (ii) iteration counts, and (iii) GPU timings

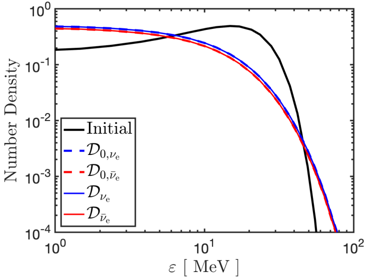
Problem Specifications

- $\Omega^{\varepsilon} = [\varepsilon_{\text{min}}, \varepsilon_{\text{max}}] = [0, 300]$ MeV
- Gaussian initial spectrum

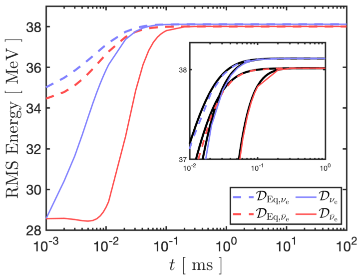
$$\mathcal{D}_0(\varepsilon) = \frac{1}{2} \times \exp\Big[-\frac{(\varepsilon - 2k_{\rm B}T)^2}{200 \text{ MeV}} \Big]$$

  Forward-isotropic distribution with $|\boldsymbol{\mathcal{I}}_0|/\mathcal{D}_0 = 0.5$
- Initial matter states with low and high collisionality
  - $\rho_0 = 10^{12}$ g cm^{-3}, $\boldsymbol{v}_0 = (0.1\text{ c}, 0, 0)^{\intercal}$, $T_0 = 7.6$ MeV, $Y_{\rm e,0} = 0.14$
  - $\rho_0 = 10^{14}$ g cm^{-3}, $\boldsymbol{v}_0 = (0.1\text{ c}, 0, 0)^{\intercal}$, $T_0 = 15$ MeV, $Y_{\rm e,0} = 0.27$
- $N^{\varepsilon} = 16$ (geometric; $\Delta\varepsilon_1 = 1.9$ MeV)
- Evolve to equilibrium: $t = 100$ ms. $\Delta t = 10^{-3}$ ms (low) and $t = 1$ ms (high). $\Delta t = 10^{-3}$ ms

Collisional Relaxation

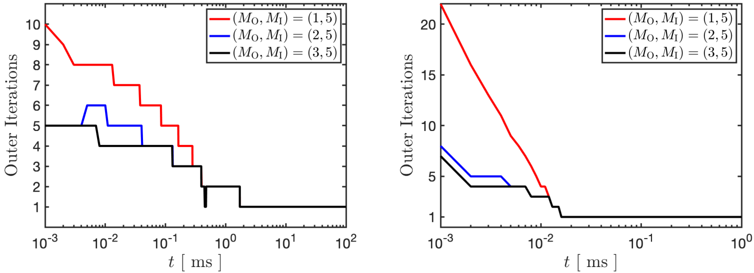


(a) Initial and Final Spectra



(b) Evolution of RMS Energies

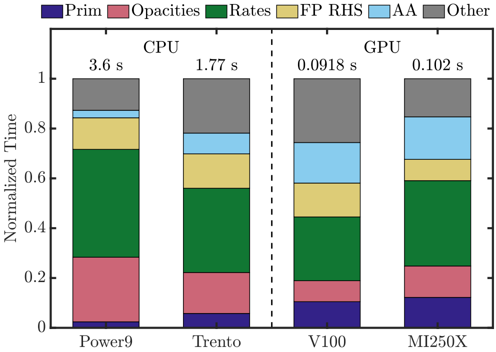
Collisional Relaxation: Iteration Counts



(a) Outer Iterations (**Low Collisionality**)

(b) Outer Iterations (**High Collisionality**)

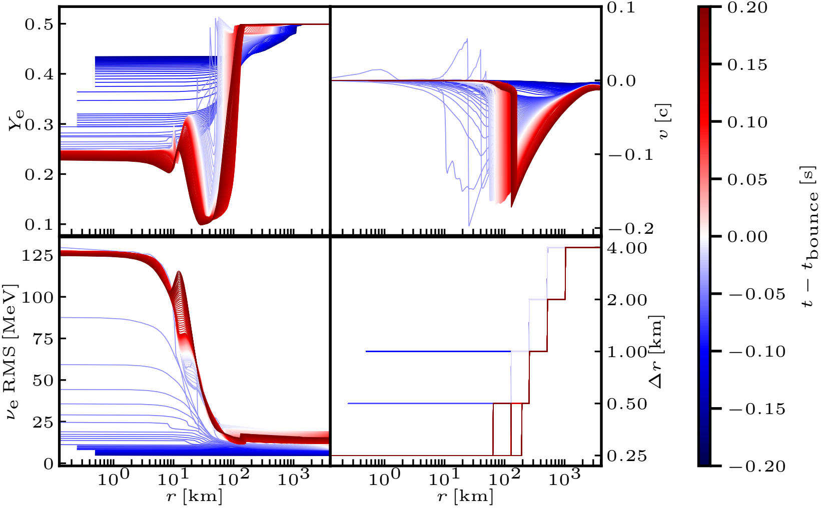
Collisional Relaxation: GPU Timings



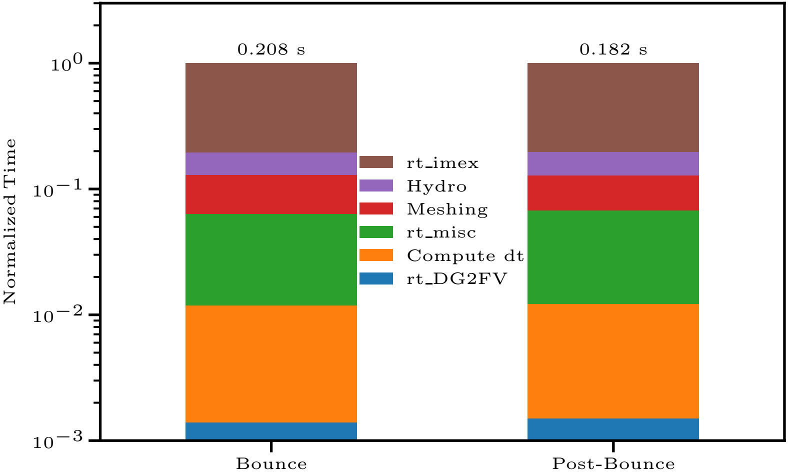
- One $8^3 \times 16$ grid block, 2 nodes per phase-space dimension
- Bruenn 85 + Bremsstrahlung (HR98), six neutrino species
- **CPU:**
  - Summit: 7 OpenMP threads on 7 Power9 cores; NVIDIA compiler (22.5), ESSL libs
  - Frontier: 7 OpenMP threads on 7 AMD Trento; CCE compiler (15.0.1), Cray LibSci
- **GPU:**
  - Summit: NVIDIA V100 with OpenACC; NVIDIA compiler (22.5) and libs
  - Frontier: AMD MI250X with OpenMP OL; CCE compiler (15.0.1), ROCm libs (5.4.0)

Collapse and Post-Bounce Evolution with FLASH-X+THORNADO

- 15 $M_\odot$ progenitor from Woosley & Heger (2007)
- Spark hydrodynamics from FLASH-X
- Spectral, two-moment neutrino transport from THORNADO
  - Six species, 16 linear elements in $\varepsilon \in [0, 300]$ MeV
  - Updated WEAKLIB opacities
- SFHo EoS tabulated with WEAKLIB
- Five AMR levels $\Delta r = 4 - 0.25$ km



0.5
0.4
0.3
0.2
0.1
Y_e
0.1
0.0
−0.1
−0.2
v [c]
125
100
75
50
25
0
ν_e RMS [MeV]
4.00
2.00
1.00
0.50
0.25
Δr [km]
10^0
10^1
10^2
10^3
r [km]
10^0
10^1
10^2
10^3
r [km]
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
$t - t_{\rm bounce}$ [s]



- $T_{\mathrm{Trans}}/T_{\mathrm{HD}} \sim 12$
- Collisions about 3 times more expensive than advection in rt-imex

Summary

- DG-IMEX method for $\mathcal{O}(v/c)$ two-moment model in THORNADO
  - Neutrino-matter coupling algorithm
  - Ported to use GPUs with OpenMP or OpenACC
- Interface to multi-physics simulation framework FLASH-X
  - Simulate neutrino transport in CCSN models with DG methods
- Ongoing
  - Multi-dimensional simulations
  - General relativistic model
  - Improvements to neutrino weak interaction physics
    (e.g., muons, inelastic scattering on nucleons)