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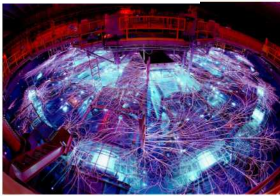

Hybrid Defect Correction Methods for Time-dependent Radiation Transport Simulations

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General form of transport equation

$$\frac{1}{v}\partial_t\psi(\boldsymbol{x},\boldsymbol{\Omega},E,t)+\boldsymbol{\Omega}\cdot\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},\boldsymbol{\Omega},E,t)=\mathcal{C}\left[\psi\right]$$

$\psi\left(\boldsymbol{x},\boldsymbol{\Omega},E,t\right)$ is the angular flux

- at the point $\boldsymbol{x}\in X\subset\mathbb{R}^3$,
- with energy $E>0$,
- in the direction $\boldsymbol{\Omega}\in\mathbb{S}^2$,
- at time $t\geq 0$.

$\mathcal{C}$ is the collision operator that describes radiation-material interactions.

Sources of difficulty:

- 7 dimensional.
- Wide range of timescales.
- Strong material coupling.
- Nonlinearity.

Gray equation with isotropic scattering

Assumptions:

- Background material is fixed.
- Cross sections are known.
- Source is known.
- Scattering is isotropic.
- Neglect energy dependence and normalize to unit speed.

This yields the following gray equation:

$$\partial_t \psi + \boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{x}} \psi + \sigma_{\mathrm{t}} \psi = \frac{\sigma_{\mathrm{s}}}{4\pi} \int_{\mathbb{S}^2} \psi(\boldsymbol{\Omega}') \, d\boldsymbol{\Omega}' + q.$$

Diffusive scaling

Scale for:

- Large time and length scales.
- Strong scattering.
- Small absorption.

$$\varepsilon \partial_t \psi + \mathbf{\Omega} \cdot \nabla_{\boldsymbol{x}} \psi + \frac{\sigma_{\mathsf{t}}}{\varepsilon} \psi = \frac{1}{4\pi} \left(\frac{\sigma_{\mathsf{t}}}{\varepsilon} - \varepsilon \sigma_{\mathsf{a}} \right) \phi + \varepsilon q, \qquad \phi = \int_{\mathbb{S}^2} \psi(\mathbf{\Omega})\, d\mathbf{\Omega}.$$

Up to $O(\varepsilon)$, the scalar flux ϕ satisfies

$$\partial_t \phi - \nabla_{\boldsymbol{x}} \cdot \left(\frac{1}{3\sigma_{\mathsf{t}}} \nabla_{\boldsymbol{x}} \phi \right) + \sigma_{\mathsf{a}} \phi = \langle q \rangle,$$

with $\psi = \frac{1}{4\pi} \phi$.

Discrete ordinates method (DOM)

Approximate the integral over angle using a quadrature $\{(\mathbf{\Omega}_k, \omega_k)\}_{k=1}^{K} \subset \mathbb{S}^2 \times \mathbb{R}$ and evaluate the resulting equation at each quadrature node:

$$\partial_t \psi_k + \mathbf{\Omega}_k \cdot \nabla_{\boldsymbol{x}} \psi_k + \sigma_{\mathrm{t}} \psi_k = \frac{\sigma_{\mathrm{s}}}{4\pi} \sum_{\ell=1}^{K} \omega_\ell \psi_\ell + q_k, \qquad (k = 1, \ldots, K).$$

This can be written in the compact form

$$\partial_t \Psi = -\left(\mathcal{L} - \mathcal{S}\mathcal{P}\right) \Psi + Q,$$

where $\mathcal{L}_k = \mathbf{\Omega}_k \cdot \nabla_{\boldsymbol{x}} + \sigma_{\mathrm{t}}$,

$$\Psi = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_K \end{bmatrix}, \quad Q = \begin{bmatrix} q_1 \\ \vdots \\ q_K \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} \mathcal{L}_1 & & 0 \\ & \ddots & \\ 0 & & \mathcal{L}_K \end{bmatrix}, \quad \mathcal{S}\mathcal{P} = \begin{bmatrix} \frac{\sigma_{\mathrm{s}}}{4\pi} \\ \vdots \\ \frac{\sigma_{\mathrm{s}}}{4\pi} \end{bmatrix} \left[\omega_1, \ldots, \omega_K\right].$$

Implicit Euler approximation

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An implicit Euler approximation of the discrete ordinates system

$$\frac{1}{\Delta t}\left(\Psi^{n} - \Psi^{n-1}\right) = -\left(\mathcal{L} - \mathcal{S}\mathcal{P}\right)\Psi^{n} + Q^{n}$$

yields the following linear system to be solved for each timestep update:

$$\left(\mathcal{L} + \frac{1}{\Delta t} - \mathcal{S}\mathcal{P}\right)\Psi^{n} = \frac{1}{\Delta t}\Psi^{n-1} + Q^{n}.$$

- System is solved using iterative techniques (source iteration, GMRES).
- Solves are built around the direct inversion of $\mathcal{L}$ through "transport sweeps".

Two options to reduce cost of linear solve:

1. Reduce the number of iterations.
2. Reduce the cost of each iteration.

Accuracy and efficiency of DOM

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The accuracy and computational cost of discrete ordinates methods depends strongly on collisionality:

Regime:	free-streaming	diffusive	multiscale
Ordinates required:	many[1,2]	few	many
Solver iterations:	few	many[3]	many

Motivation for hybrid:

Isolate streaming and diffusive regimes and choose a different number of ordinates for each case.

[1] K. D. Lathrop (1968). "Ray Effects in Discrete Ordinates Equations". In: *Nucl. Sci. & Eng.* 32, pp. 357–369.

[2] K. D. Lathrop (1971). "Remedies for Ray Effects". In: *Nucl. Sci. & Eng.* 45, pp. 255–268.

[3] J. S. Warsa, T. A. Wareing, and J. E. Morel (2004). "Krylov Iterative Methods and the Degraded Effectiveness of Diffusion Synthetic Acceleration for Multidimensional S_N Calculations in Problems with Material Discontinuities". In: *Nucl. Sci. & Eng.* 147, pp. 218–248.

A first-collision splitting

Split the angular flux as $\psi = \psi_{\mathsf{u}} + \psi_{\mathsf{c}}$ where[4,5],

ψ_{u} is the flux of uncollided particles,

ψ_{c} is the flux of collided particles.

The split densities satisfy

$$\partial_t \psi_{\mathsf{u}} + \boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{x}} \psi_{\mathsf{u}} + \sigma_{\mathsf{t}} \psi_{\mathsf{u}} = q,$$

$$\partial_t \psi_{\mathsf{c}} + \boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{x}} \psi_{\mathsf{c}} + \sigma_{\mathsf{t}} \psi_{\mathsf{c}} = \frac{\sigma_{\mathsf{s}}}{4\pi} \Big[\langle \psi_{\mathsf{u}} \rangle + \langle \psi_{\mathsf{c}} \rangle \Big], \qquad \langle \cdot \rangle = \int_{\mathbb{S}^2} (\,\cdot\,)\, d\boldsymbol{\Omega}.$$

Apply discrete ordinates approximations with different quadratures:

$$\partial_t \Psi_{\mathsf{u}} = -\mathcal{L}_{\mathsf{u}} \Psi_{\mathsf{u}} + Q,$$

$$\partial_t \Psi_{\mathsf{c}} = -\left(\mathcal{L}_{\mathsf{c}} - \mathcal{S}_{\mathsf{c}} \mathcal{P}_{\mathsf{c}} \right) \Psi_{\mathsf{c}} + \mathcal{S}_{\mathsf{c}} \mathcal{P}_{\mathsf{u}} \Psi_{\mathsf{u}}.$$

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[4] C. D. Hauck and R. G. McClarren (2013). "A collision-based hybrid method for time dependent, linear, kinetic transport equations". In: *Multiscale Modeling and Simulation* 11.4, pp. 1197–1227.

[5] R. E. Alcouffe, R. D. O'Dell, and F. W. Brinkley, Jr. (1990). "A First-Collision Source Method That Satisfies Discrete S_n Transport Balance". In: *Nucl. Sci. & Eng.* 105, pp. 198–203.

First-order hybrid method

An implicit Euler approximation yields two systems to be solved at each timestep:

$$\left(\mathcal{L}_{\mathsf{u}} + \frac{1}{\Delta t}\right)\Psi_{\mathsf{u}}^{n} = \frac{1}{\Delta t}\Psi_{\mathsf{u}}^{n-1} + Q^{n},$$

$$\left(\mathcal{L}_{\mathsf{c}} + \frac{1}{\Delta t} - \mathcal{S}_{\mathsf{c}}\mathcal{P}_{\mathsf{c}}\right)\Psi_{\mathsf{c}}^{n} = \frac{1}{\Delta t}\Psi_{\mathsf{c}}^{n-1} + \mathcal{S}_{\mathsf{c}}\mathcal{P}_{\mathsf{u}}\Psi_{\mathsf{u}}^{n}.$$

Uncollided:
- Can be solved using a single transport sweep.
- Use a large number of ordinates to reduce ray effects.

Collided:
- Requires a full iterative solve.
- Use fewer ordinates to reduce computational cost.

Problem:
- Once collided, particles stay collided.
- Accuracy is reduced due to the low number of collided ordinates.

“Relabeling” the collided flux

Introduce an operator $\mathcal{R}_\mathsf{c}^\mathsf{u}$ to map from the collided quadrature set to the uncollided quadrature[6]. Apply this operator to relabel the collided particles as uncollided after each timestep:

$$\left(\mathcal{L}_\mathsf{u} + \frac{1}{\Delta t}\right)\Psi_\mathsf{u}^n = \frac{1}{\Delta t}\Psi_*^{n-1} + Q^n$$

$$\left(\mathcal{L}_\mathsf{c} + \frac{1}{\Delta t} - \mathcal{S}_\mathsf{c}\mathcal{P}_\mathsf{c}\right)\Psi_\mathsf{c}^n = \mathcal{S}_\mathsf{c}\mathcal{P}_\mathsf{u}\Psi_\mathsf{u}^n$$

A timestep of the hybrid method with relabeling is composed of three steps:

- Solve uncollided system for Ψ_u^n.
- Solve collided system for Ψ_c^n.
- Reconstruct $\Psi_*^n = \mathcal{R}_\mathsf{c}^\mathsf{u}\left(\Psi_\mathsf{u}^n, \Psi_\mathsf{c}^n\right)$.

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[6] C. D. Hauck and R. G. McClarren (2013). “A collision-based hybrid method for time dependent, linear, kinetic transport equations”. In: *Multiscale Modeling and Simulation* 11.4, pp. 1197–1227.

How to define $\mathcal{R}_{\mathsf{c}}^{\mathsf{u}}$?

Initial approach: $\Psi_*^n = \mathcal{R}_{\mathsf{c}}^{\mathsf{u}}\left(\Psi_{\mathsf{u}}^n, \Psi_{\mathsf{c}}^n\right) = \Psi_{\mathsf{u}}^n + \mathcal{R}_{\mathsf{c}}^{\mathsf{u}}\Psi_{\mathsf{u}}^n$

- Given values at each collided quadrature node.
- Extend to a function on all of $\mathbb{S}^2$.
- Evaluate this function at each of the uncollided quadrature nodes.

Desired properties:

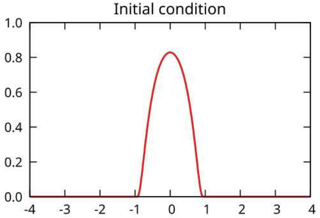
- Computationally inexpensive.
- Parallelizable.
- Guarantee positivity of reconstructed values.
- Preserve physical quantities, etc. (e.g., angular moments).
- Applicable to a wide range of angular quadratures.

Slab-geometry convergence

Gray equation in slab geometry with diffusive scaling:

$$\varepsilon \partial_t \psi + \mu \partial_z \psi + \frac{\sigma_\mathrm{t}}{\varepsilon} \psi = \frac{\sigma_\mathrm{t}}{2\varepsilon} \int_{-1}^{1} \psi\left(\mu'\right)\, d\mu'$$

where $\psi = \psi(z, \mu, t)$ and $\mu \in [-1, 1]$.



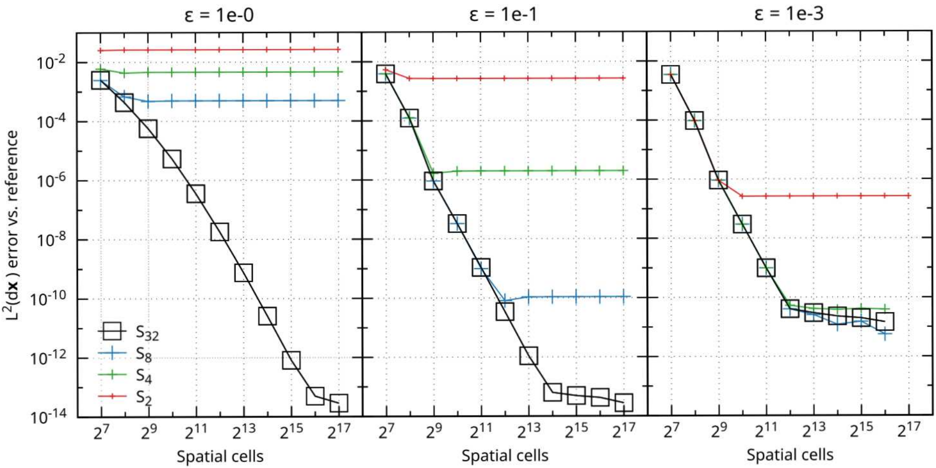
Run convergence tests with

$$\sigma_\mathrm{t} = 1/\varepsilon$$
$$t_\mathrm{final} = 1/2\varepsilon$$
$$\mathrm{CFL} = 8/\varepsilon$$

using $\varepsilon = 1\text{e-}0, 1\text{e-}1, 1\text{e-}3$.

- Uncollided Angles: 32
- Collided Angles: $2, 4, 8$
- Relabel by interpolation.

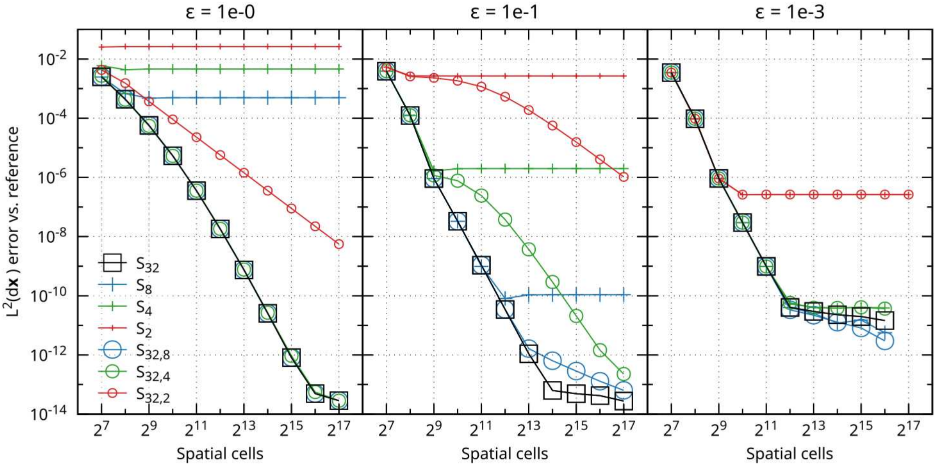
Slab-geometry convergence



Low-resolution discrete ordinates methods:

- Saturate due to error of angular discretization.
- Saturation error depends on collisionality regime.

Slab-geometry convergence



Hybrid methods show:

- Order reduction in low- to moderately-collisional regimes.
- Saturation in highly-collisional regimes.

Nyström reconstruction (implicit Euler)

For each implicit Euler step, the hybrid fluxes satisfy:

$$\left(\mathcal{L}_{\mathsf{u}} + \tfrac{1}{\Delta t}\right) \Psi_{\mathsf{u}}^{n} = \tfrac{1}{\Delta t} \Psi_{*}^{n-1} + Q^{n}$$
$$\left(\mathcal{L}_{\mathsf{c}} + \tfrac{1}{\Delta t} - \mathcal{S}_{\mathsf{c}} \mathcal{P}_{\mathsf{c}}\right) \Psi_{\mathsf{c}}^{n} = \mathcal{S}_{\mathsf{c}} \mathcal{P}_{\mathsf{u}} \Psi_{\mathsf{u}}^{n}$$

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We want to solve the non-hybrid system:

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Instead, use the hybrid components to approximate the scattering source:

$$\left(\mathcal{L}_{\mathsf{u}} + \tfrac{1}{\Delta t}\right) \Psi_{*}^{n} = \tfrac{1}{\Delta t} \Psi_{*}^{n-1} + Q^{n} + \mathcal{S}_{\mathsf{u}} \left(\mathcal{P}_{\mathsf{u}} \Psi_{\mathsf{u}}^{n} + \mathcal{P}_{\mathsf{c}} \Psi_{\mathsf{c}}^{n}\right)$$

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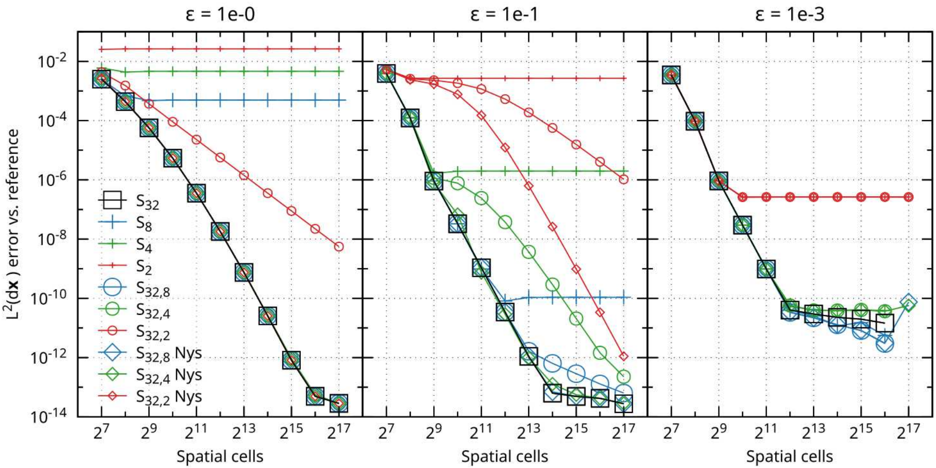
Pros:

- Quadrature agnostic.
- Uses standard procedures found in existing discrete ordinates implementations.
- Preserves positivity.

Cons:

- Requires additional high-resolution sweep(s) (expensive).

Nyström reconstruction convergence



- Nyström reconstruction improves order reduction.
- Saturation in highly-collisional regimes remains.

Basics of defect correction

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System: $$Ax = b$$

Solution: $$x = A^{-1}b$$

Basics of defect correction

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Residual: $r^{(1)} = b - A\xi^{(1)}$

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Error equation: $Ae^{(1)} = b - A\xi^{(1)}$

Approximate Error: $\epsilon^{(1)} = \tilde{H}\left(b - A\xi^{(1)}\right)$

Updated solution: $\xi^{(2)} = \xi^{(1)} + \epsilon^{(1)}$

Basics of defect correction

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System: $$Ax = b$$

Solution: $$x = A^{-1}b$$

Approximate solution: $$\xi^{(1)} = \tilde{H}b$$

Error: $$e^{(k)} = x - \xi^{(k)}$$

Residual: $$r^{(k)} = b - A\xi^{(k)}$$

Error equation: $$Ae^{(k)} = b - A\xi^{(k)}$$

Approximate Error: $$\epsilon^{(k)} = \tilde{H}\left(b - A\xi^{(k)}\right)$$

Updated solution: $$\xi^{(k+1)} = \xi^{(k)} + \epsilon^{(k)}$$

Basics of defect correction

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System:	$Ax = b$
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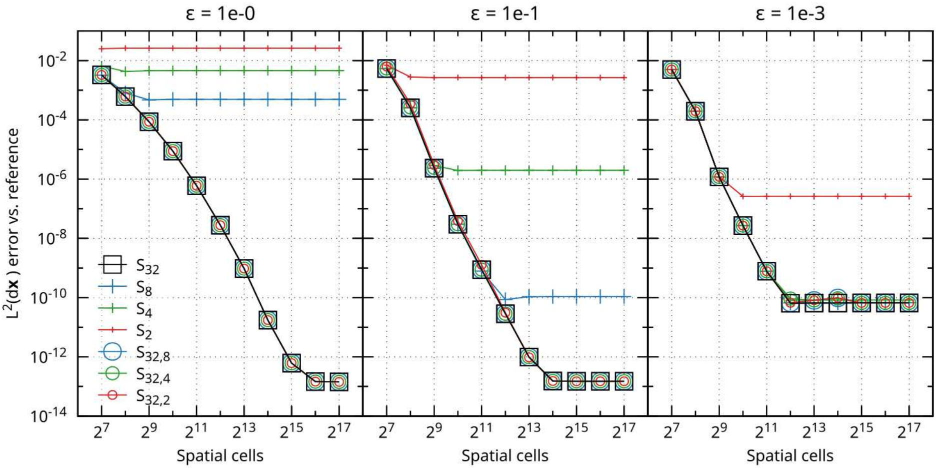
Approximate solution:	$\xi^{(1)} = \tilde{H}b$
Approximate Error:	$\epsilon^{(k)} = \tilde{H}\left(b - A\xi^{(k)}\right)$
Updated solution:	$\xi^{(k+1)} = \xi^{(k)} + \epsilon^{(k)}$

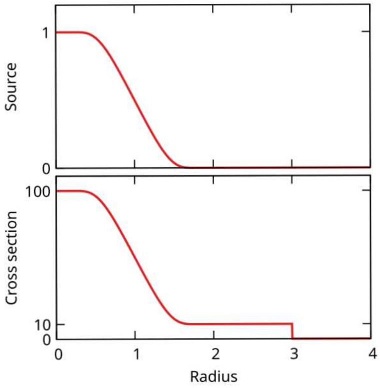
- Integral deferred correction (IDC):
  - High-order accuracy using low-order method.
  - Increase order of accuracy by one at each iteration.
  - Extended to correct other errors; e.g., operator splitting.
- Wrap hybrid into IDC defect correction iteration.
- Effectively a two-grid collocation method in angle.

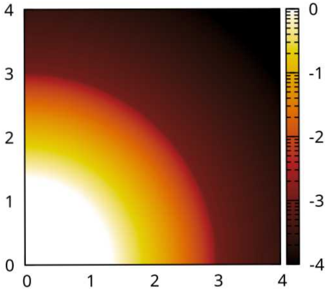
Defect correction convergence



- Hybrid + Nyström reconstruction + defect correction virtually eliminates splitting error.

Inhomogeneous sphere test problem



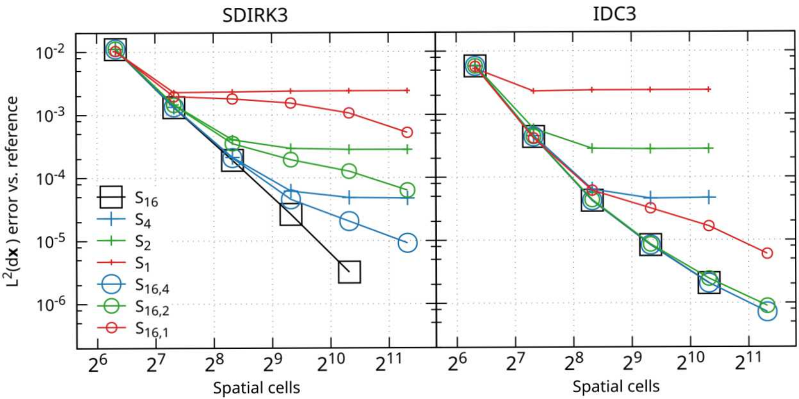


Order:	3
Final time:	8
CFL:	160

T_N angular quadratures[7].

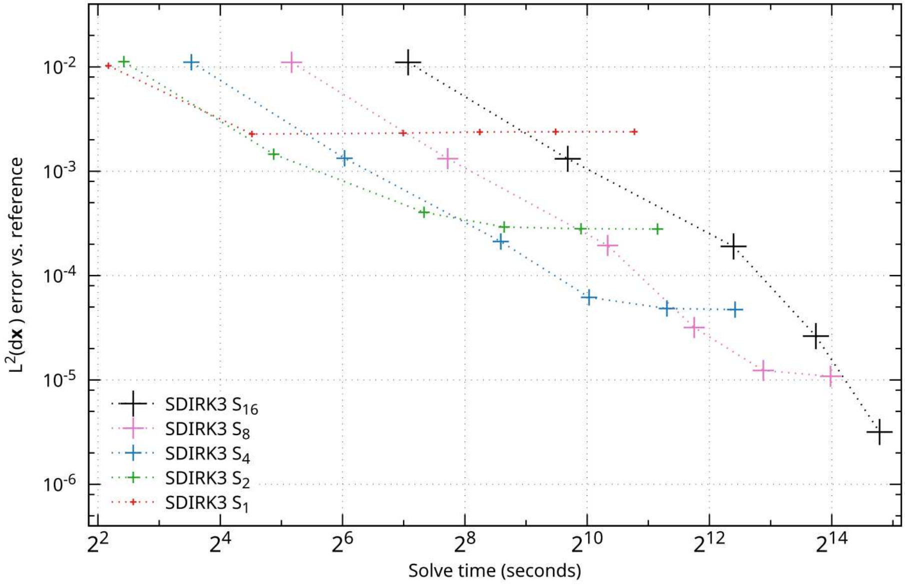
[7] C. P. Thurgood, A. Pollard, and H. A. Becker (1995). "The T_N Quadrature Set for the Discrete Ordinates Method". In: *Journal of Heat Transfer* 117.4, p. 1068. doi: 10.1115/1.2836285.

Inhomogeneous sphere convergence

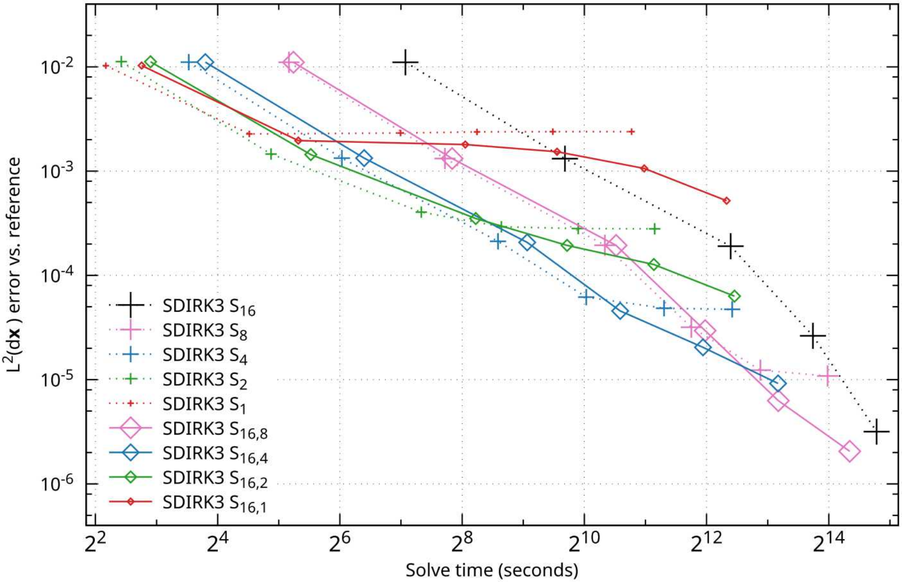


- Don't iterate two-grid/hybrid IDC method to convergence.
- $16^2 = 256$ vs $1^2 = 1$ ordinates/octant for $S_{16,1}$ method.

Inhomogeneous sphere efficiency



Inhomogeneous sphere efficiency



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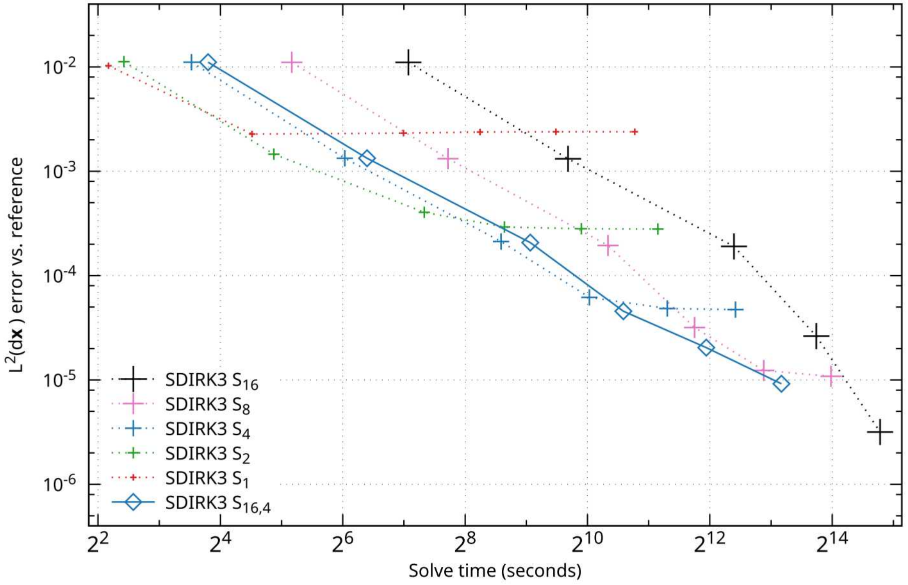

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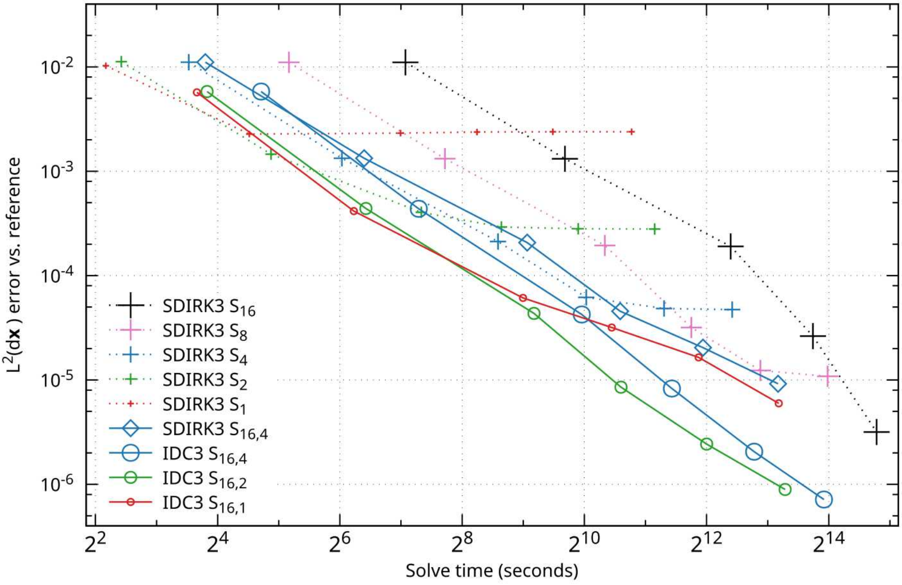

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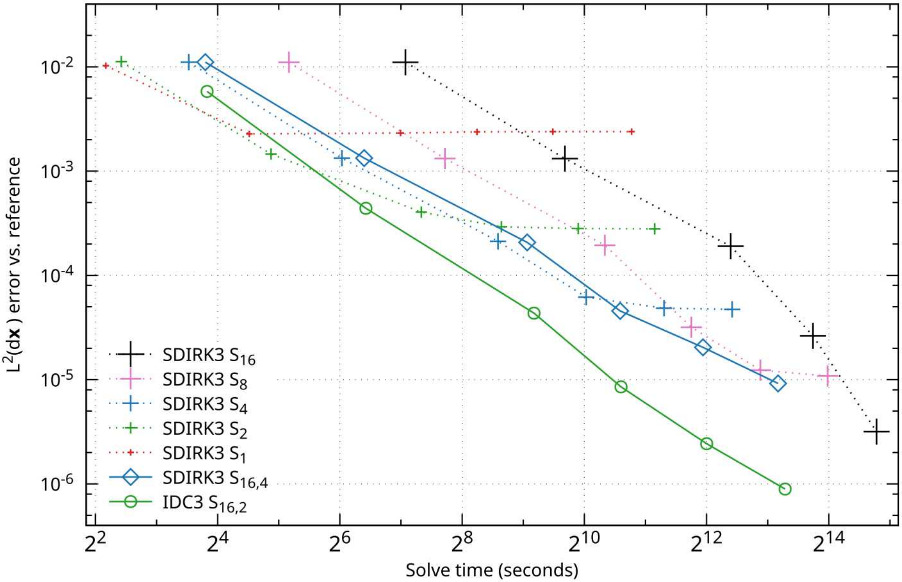

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Thank you.

Questions?