Efficient Transport

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Collaborators

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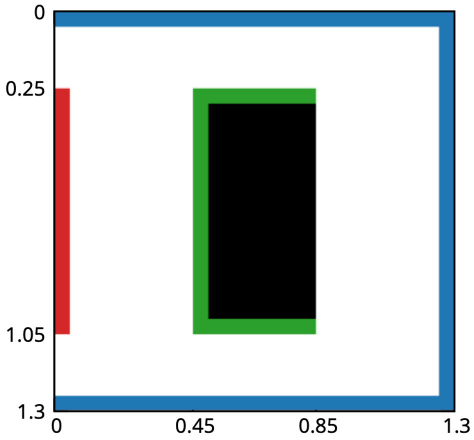
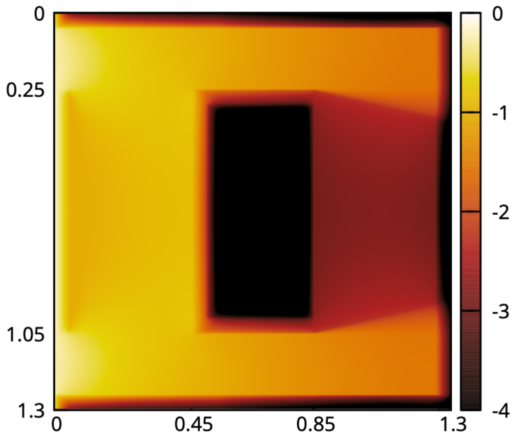
Note: Michael is my former PhD student who is now doing a post doc with John Shadid at Sandia. This work was Michael's thesis.

Outline of Talk

- Model – Gray equation
- Big Idea
- How it Works
- Examples
- Conclusion





Gray Equation

$$\partial_t \psi + \vec{\Omega} \cdot \nabla_{\vec{x}} \psi + \sigma_{\mathrm{t}} \psi = \frac{\sigma_{\mathrm{s}}}{4\pi} \langle \psi \rangle + q, \qquad \langle \cdot \rangle = \int_{\mathbb{S}^2} (\cdot)\, d\vec{\Omega},$$

$\psi = \psi(\vec{x}, \vec{\Omega}, t)$ is the flux of radiation

$\vec{x} \in X \subset \mathbb{R}^3$

$\vec{\Omega} \in \mathbb{S}^2$

$\sigma_{\mathrm{t}} = \sigma_{\mathrm{s}} + \sigma_{\mathrm{a}}$

σ_{s} scattering

σ_{a} absorption

$q = q(\vec{x}, \vec{\Omega}, t)$

$\psi_{\mathrm{B}} = \psi_{\mathrm{B}}(\vec{x}, \vec{\Omega}, t)$ inflow boundary

Notation

$$\partial_t \psi + \mathcal{L}\psi = \mathcal{S}\mathcal{P}\psi + q,$$

$$\mathcal{L} = \vec{\Omega} \cdot \nabla_{\vec{x}} + \sigma_{\mathrm{t}}, \qquad \mathcal{S} = \frac{\sigma_{\mathrm{s}}}{4\pi}, \qquad \text{and} \qquad \mathcal{P} = \int_{\mathbb{S}^2} (\cdot)\, d\vec{\Omega}.$$

Discretize Over Angle with Quadrature

$$\partial_t \psi_k + \vec{\Omega}_k \cdot \nabla_{\vec{x}} \psi_k + \sigma_{\mathrm{t}} \psi_k = \frac{\sigma_{\mathrm{s}}}{4\pi} \sum_{\ell=1}^{K} \omega_\ell \psi_\ell + q_k,$$

$$(k = 1, \ldots, K)$$

Vector Notation

$$\partial_t \boldsymbol{\psi} = -\left(\boldsymbol{\mathcal{L}} - \boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{P}}\right)\boldsymbol{\psi} + \boldsymbol{q},$$

$$\boldsymbol{\psi} = \left[\psi_1, \ldots, \psi_K\right]^T \qquad \boldsymbol{q} = \left[q_1, \ldots, q_K\right]^T$$

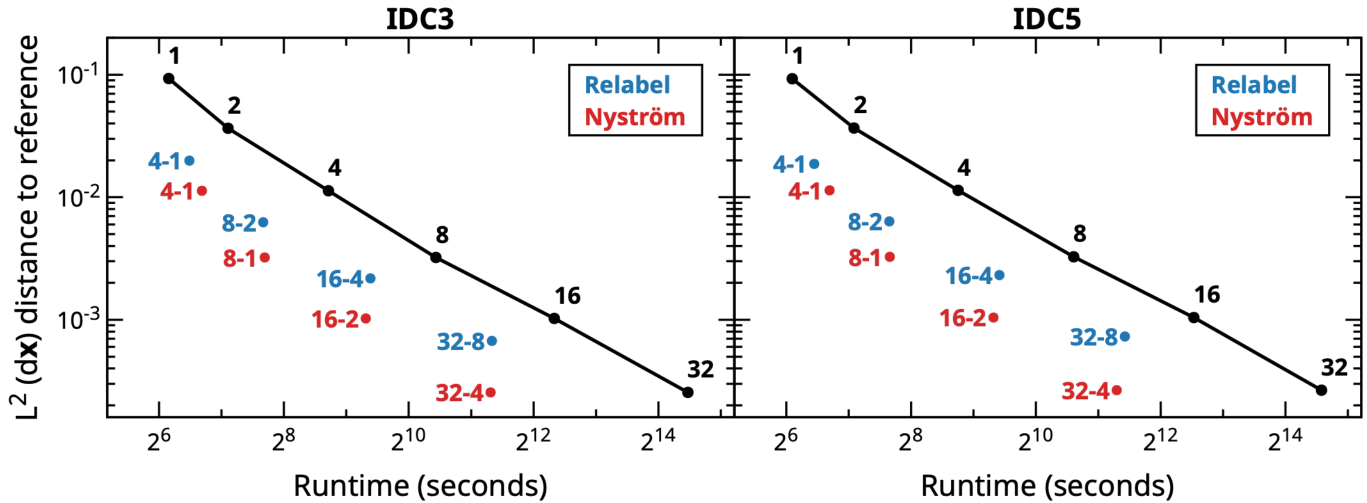
$$\boldsymbol{\mathcal{L}} = \mathrm{Diag}\left(\mathcal{L}_1, \ldots, \mathcal{L}_K\right) \qquad \mathcal{L}_k = \vec{\Omega}_k \cdot \nabla_{\vec{x}} + \sigma_{\mathrm{t}}$$

$$\boldsymbol{\mathcal{S}} = \left[\frac{\sigma_{\mathrm{s}}}{4\pi}, \ldots, \frac{\sigma_{\mathrm{s}}}{4\pi}\right]^T \qquad \boldsymbol{\mathcal{P}} = \left[\omega_1, \ldots, \omega_K\right]$$

Big Idea

- Develop a splitting into a cheap solve (transport) and an expensive solve (collisional update)
- Create cheap surrogate model for expensive solve
- Create a conservative mapping between the cheap solve and the surrogate (where the magic is)
- Use defect correction to remove the errors of the splitting, mapping and surrogate.

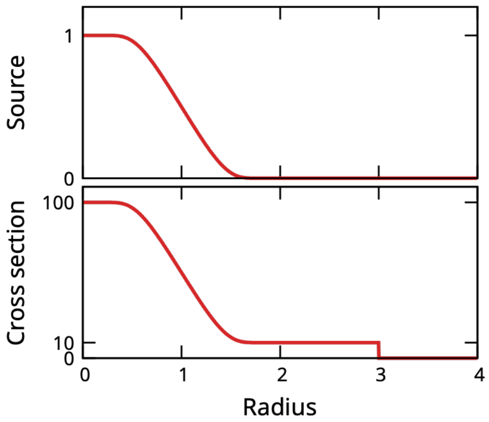
Start with the END of the Story

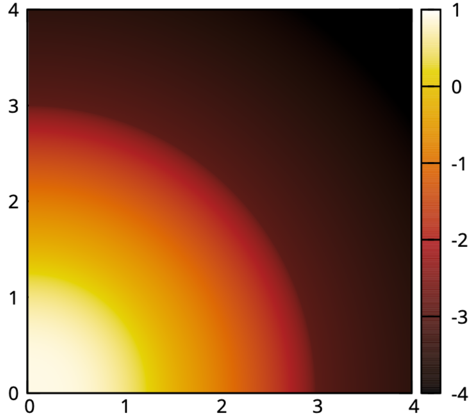


- Two orders of magnitude faster than a conventional Discrete Ordnance (DO) method with equivalent computational accuracy.
- 3 to 5 times faster than the best hybrid methods based on DO.

Only splitting of this type that can:

Capture the transition from collisional to free streaming regimes without loss of accuracy.





How it Works

- Start with First Collision Source Technique [1]

$$
\begin{aligned}
\partial_t \psi_{\mathrm{u}} + \vec{\Omega} \cdot \nabla_{\vec{x}} \psi_{\mathrm{u}} + \sigma_{\mathrm{t}} \psi_{\mathrm{u}} &= q, \\
\partial_t \psi_{\mathrm{c}} + \vec{\Omega} \cdot \nabla_{\vec{x}} \psi_{\mathrm{c}} + \sigma_{\mathrm{t}} \psi_{\mathrm{c}} &= \frac{\sigma_{\mathrm{s}}}{4\pi} \left[\langle \psi_{\mathrm{u}} \rangle + \langle \psi_{\mathrm{c}} \rangle \right]
\end{aligned}
$$

- **In collisionless regimes**: Need high number of angles; Can use fast sweeping.
- **In collisional regimes**: Need low number of angles; replace implicit high angular update with cheaper implicit low angular resolution update

[1] R. E. Alcouffe, "A first collision source method for coupling Monte Carlo and discrete ordinates for localized source problems," in *Monte-Carlo Methods and Applications in Neutronics, Photonics and Statistical Physics* (R. Alcouffe, R. Dautray, A. Forster, G. Ledanois, and B. Mercier, eds.), vol. 240 of *Lecture Notes in Physics*, pp. 352–366, Springer, Berlin, Heidelberg, 1985.

In Operator Notation

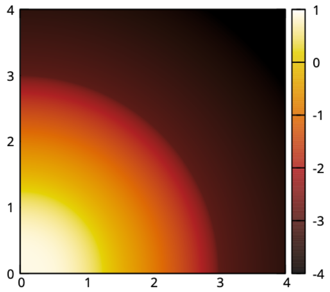
Let $\{\vec{\Omega}_{\mathrm{u},k}, \omega_{\mathrm{u},k}\}_{k=1}^{K_\mathrm{u}} \subset \mathbb{S}^2 \times \mathbb{R}$ $\quad \{\vec{\Omega}_{\mathrm{c},k}, \omega_{\mathrm{c},k}\}_{k=1}^{K_\mathrm{c}} \subset \mathbb{S}^2 \times \mathbb{R}$

$$\partial_t \boldsymbol{\psi}_\mathrm{u} = -\boldsymbol{\mathcal{L}}_\mathrm{u} \boldsymbol{\psi}_\mathrm{u} + \boldsymbol{q},$$
$$\partial_t \boldsymbol{\psi}_\mathrm{c} = -(\boldsymbol{\mathcal{L}}_\mathrm{c} - \boldsymbol{\mathcal{S}}_\mathrm{c} \boldsymbol{\mathcal{P}}_\mathrm{c}) \boldsymbol{\psi}_\mathrm{c} + \boldsymbol{\mathcal{S}}_\mathrm{c} \boldsymbol{\mathcal{P}}_\mathrm{u} \boldsymbol{\psi}_\mathrm{u},$$

Maps $\boldsymbol{\mathcal{P}}_\mathrm{u} \boldsymbol{\psi}_\mathrm{u}^n$ into K_c angles
$K_c << K_u$

$$\boldsymbol{\psi}_\mathrm{u} = [\psi_{\mathrm{u},1}, \ldots, \psi_{\mathrm{u},K_\mathrm{u}}]^T$$
$$\boldsymbol{\psi}_\mathrm{c} = [\psi_{\mathrm{c},1}, \ldots, \psi_{\mathrm{c},K_\mathrm{c}}]^T$$
$$\boldsymbol{q} = [q_1, \ldots, q_{K_\mathrm{u}}]^T$$

Obvious difficulty
for problems such as



Using Backwards Euler

$$\left(\boldsymbol{\mathcal{L}}_\mathrm{u} + \frac{1}{\Delta t}\right) \boldsymbol{\psi}_\mathrm{u}^n = \frac{1}{\Delta t} \boldsymbol{\psi}_*^{n-1} + \boldsymbol{q}^n \quad \left(\boldsymbol{\mathcal{L}}_\mathrm{c} + \frac{1}{\Delta t} - \boldsymbol{\mathcal{S}}_\mathrm{c} \boldsymbol{\mathcal{P}}_\mathrm{c}\right) \boldsymbol{\psi}_\mathrm{c}^n = \boldsymbol{\mathcal{S}}_\mathrm{c} \boldsymbol{\mathcal{P}}_\mathrm{u} \boldsymbol{\psi}_\mathrm{u}^n$$

Remapping from collided to un-collided

- In [2], Cory Hauck introduced the idea of Remapping with First Collision Source Technique.

- At the end of a time step:

$$\boldsymbol{\psi}_*^n = \boldsymbol{\psi}_{\mathrm{u}}^n + \boldsymbol{\mathcal{R}}\boldsymbol{\psi}_{\mathrm{c}}^n$$

where $\mathcal{R}$ must be a conservative map

[2] C. D. Hauck and R. G. McClarren, “A collision-based hybrid method for time dependent, linear, kinetic transport equations,” *Multiscale Modeling and Simulation*, vol. 11, no. 4, pp. 1197–1227, 2013.

Defect Correction (SDC, IDC and space time)

- In reference [3], we developed defect correction to raise the order in time through successive corrections for [2] and proved the method was Asymptotic Preserving and high order.
- Using residual to write down an equation for the error.
- It will take form of original PDE.
- Solve error equation and raise the order by $O(\Delta t^p)$ where P is the order of method used to solve error equation.

[3] M. M. Crockatt, A. J. Christlieb, C. K. Garrett, and C. D. Hauck, "An arbitrary-order, fully implicit, hybrid kinetic solver for linear radiative transport using integral deferred correction," *Journal of Computational Physics*, vol. 346, pp. 212–241, Oct. 2017.

Simplest form of Defect Correction

$$y' = f(t, y), \quad y(t_0) = y^0$$

Apply Backwards Euler:

$$u^{n,[0]} = u^{n-1,[0]} + \Delta t f\left(t_0 + c_n \Delta t, u^{n,[0]}\right)$$

Define residual and error as:

$$r = \hat{u}' - f(t, \hat{u})$$

$$e' = y' - \hat{u}'$$

$$\left(e + \int_0^t r(\tau) d\tau\right)' = f(e + \hat{u}) - f(\hat{u})$$

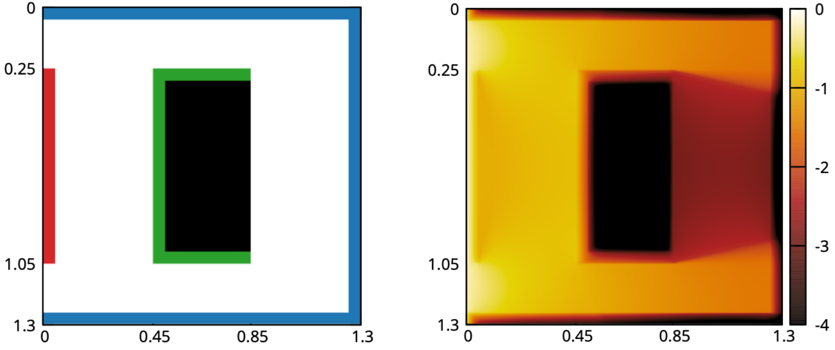
Lifts order by Δt with each correction

Apply Backwards Euler to get update $u^{n,[p+1]}$ given $u^{n,[p]}$

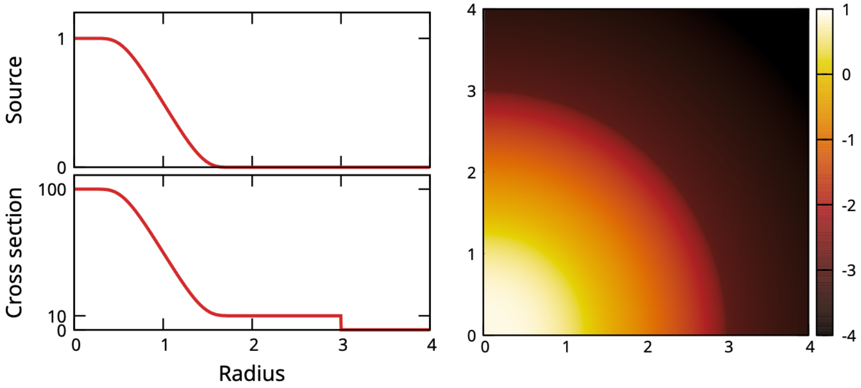
$$\left(e^n + \hat{u}^{n,[p]}\right) - \left(e^{n-1} + \hat{u}^{n-1,[p]}\right) - \int_{t_{n-1}}^{t_n} f(\tau, \hat{u}) d\tau = \Delta t(f(e^n + \hat{u}^{n,[p]}) - f(\hat{u}^{n-1,[p]}))$$

Results

Worked Great!



Did not work Great!



Michael realized that First Collision Source Technique is close to the two grid methods for Integral Equations out of the 1970's.

To not suffer order reduction, key is $\mathcal{R}$

Consider an Integral equation of the form

$$\lambda x(s) - \int_D K(s,t)x(t)dt = y(s), \quad s \in D$$

Appling quadrature

$$\lambda \bar{x}(s) - \sum_j^N w_j(s)\bar{x}(t_j) = y(s)$$

Compute the solution at the quadrature points

$$\lambda \bar{x}(t_i) - \sum_j^N w_j(t_i)\bar{x}(t_j) = y(t_i)$$

Nyström Interpolation [4]

$$\bar{x}(s) = \frac{y(s)}{\lambda} + \frac{1}{\lambda}\sum_j^N w_j(s)\bar{x}(t_j)$$

Under assumptions on K, which our problem satisfy, This is a high order, Positivity Preserving, Conservative Map

This allows us to go from course to fine angular representation.

$$\psi_*^n = \psi_u^n + \mathcal{R}\psi_c^n$$

[4] K. E. Atkinson, *The Numerical Solution of Integral Equations of the Second Kind*, vol. 4 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge, United Kingdom: Cambridge University Press, 1997.

Prediction

for $n = 1, \ldots, N$ **do**

Solve for $\boldsymbol{\psi}_{\mathrm{u}}^{n,[0]}$:

$$\left(\boldsymbol{\mathcal{L}}_{\mathrm{u}} + \frac{1}{h_n \Delta t}\right) \boldsymbol{\psi}_{\mathrm{u}}^{n,[0]} = \frac{1}{h_n \Delta t} \boldsymbol{\psi}_{*}^{n-1,[0]} + \boldsymbol{q}^{n}$$

128 angles sweep

Solve for $\boldsymbol{\psi}_{\mathrm{c}}^{n,[0]}$:

$$\left(\boldsymbol{\mathcal{L}}_{\mathrm{c}} + \frac{1}{h_n \Delta t} - \boldsymbol{\mathcal{S}}_{\mathrm{c}} \boldsymbol{\mathcal{P}}_{\mathrm{c}}\right) \boldsymbol{\psi}_{\mathrm{c}}^{n,[0]} = \boldsymbol{\mathcal{S}}_{\mathrm{c}} \boldsymbol{\mathcal{P}}_{\mathrm{u}} \boldsymbol{\psi}_{\mathrm{u}}^{n,[0]}$$

4 angles BE solve

Solve for $\boldsymbol{\psi}_{*}^{n,[0]}$:

$$\left(\boldsymbol{\mathcal{L}}_{\mathrm{u}} + \frac{1}{h_n \Delta t}\right) \boldsymbol{\psi}_{*}^{n,[0]} = \boldsymbol{\mathcal{S}}_{\mathrm{u}} \left(\boldsymbol{\mathcal{P}}_{\mathrm{u}} \boldsymbol{\psi}_{\mathrm{u}}^{n,[0]} + \boldsymbol{\mathcal{P}}_{\mathrm{c}} \boldsymbol{\psi}_{\mathrm{c}}^{n,[0]}\right) + \frac{1}{h_n \Delta t} \boldsymbol{\psi}_{*}^{n-1,[0]} + \boldsymbol{q}^{n}$$

128 angles Reconstruction Sweep

Correction [p] -> $\boldsymbol{\psi}_*^{N,[P]}$

for $p = 1, \ldots, P$ **do**

for $n = 1, \ldots, N$ **do**

Solve for $\boldsymbol{e}_{\mathrm{u}}^{n,[p-1]}$:

$$\left(\widetilde{\boldsymbol{\mathcal{L}}}_{\mathrm{u}} + \frac{1}{h_n \Delta t}\right) \boldsymbol{e}_{\mathrm{u}}^{n,[p-1]} = \frac{1}{h_n \Delta t}\left(\boldsymbol{\psi}_*^{n-1,[p]} - \boldsymbol{\psi}_*^{n,[p-1]}\right) - \sum_{\ell=1}^{N} \frac{\gamma_{n,\ell}}{h_n}\left[(\boldsymbol{\mathcal{L}}_{\mathrm{u}} - \boldsymbol{\mathcal{S}}_{\mathrm{u}}\boldsymbol{\mathcal{P}}_{\mathrm{u}})\boldsymbol{\psi}_*^{\ell,[p-1]} - \boldsymbol{q}^{\ell}\right]$$

128 angles
sweep

Solve for $\boldsymbol{e}_{\mathrm{c}}^{n,[p]}$:

$$\left(\widetilde{\boldsymbol{\mathcal{L}}}_{\mathrm{c}} + \frac{1}{h_n \Delta t} - \boldsymbol{\mathcal{S}}_{\mathrm{c}}\boldsymbol{\mathcal{P}}_{\mathrm{c}}\right) \boldsymbol{e}_{\mathrm{c}}^{n,[p-1]} = \boldsymbol{\mathcal{S}}_{\mathrm{c}}\boldsymbol{\mathcal{P}}_{\mathrm{u}}\boldsymbol{e}_{\mathrm{u}}^{n,[p-1]}$$

4 angles
BE solve

Solve for $\boldsymbol{\psi}_*^{n,[p]}$:

$$\left(\boldsymbol{\mathcal{L}}_{\mathrm{u}} + \frac{1}{h_n \Delta t}\right) \boldsymbol{\psi}_*^{n,[p]} = \boldsymbol{\mathcal{S}}_{\mathrm{u}}\left(\boldsymbol{\mathcal{P}}_{\mathrm{u}}\boldsymbol{e}_{\mathrm{u}}^{n,[p-1]} + \boldsymbol{\mathcal{P}}_{\mathrm{c}}\boldsymbol{e}_{\mathrm{c}}^{n,[p-1]}\right) + \frac{1}{h_n \Delta t}\boldsymbol{\psi}_*^{n-1,[p]} + \boldsymbol{\mathcal{L}}_{\mathrm{u}}\boldsymbol{\psi}_*^{n,[p-1]} - \sum_{\ell=1}^{N} \frac{\gamma_{n,\ell}}{h_n}\left[(\boldsymbol{\mathcal{L}}_{\mathrm{u}} - \boldsymbol{\mathcal{S}}_{\mathrm{u}}\boldsymbol{\mathcal{P}}_{\mathrm{u}})\boldsymbol{\psi}_*^{\ell,[p-1]} - \boldsymbol{q}^{\ell}\right]$$

128 angles
Reconstruction
Sweep

end for

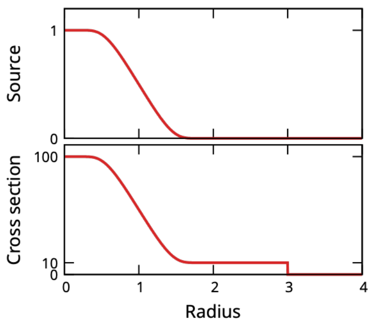
end for

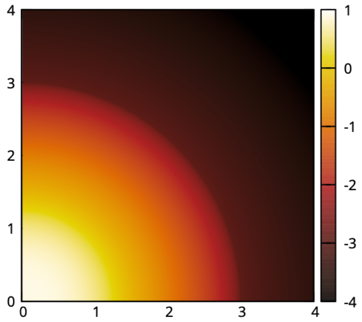
Results

Bench Marked 6 ways from Sunday (submitted)

Compared with unsplit

- BE DG
- ARK DG
- DIRK DG
- Space Time DG





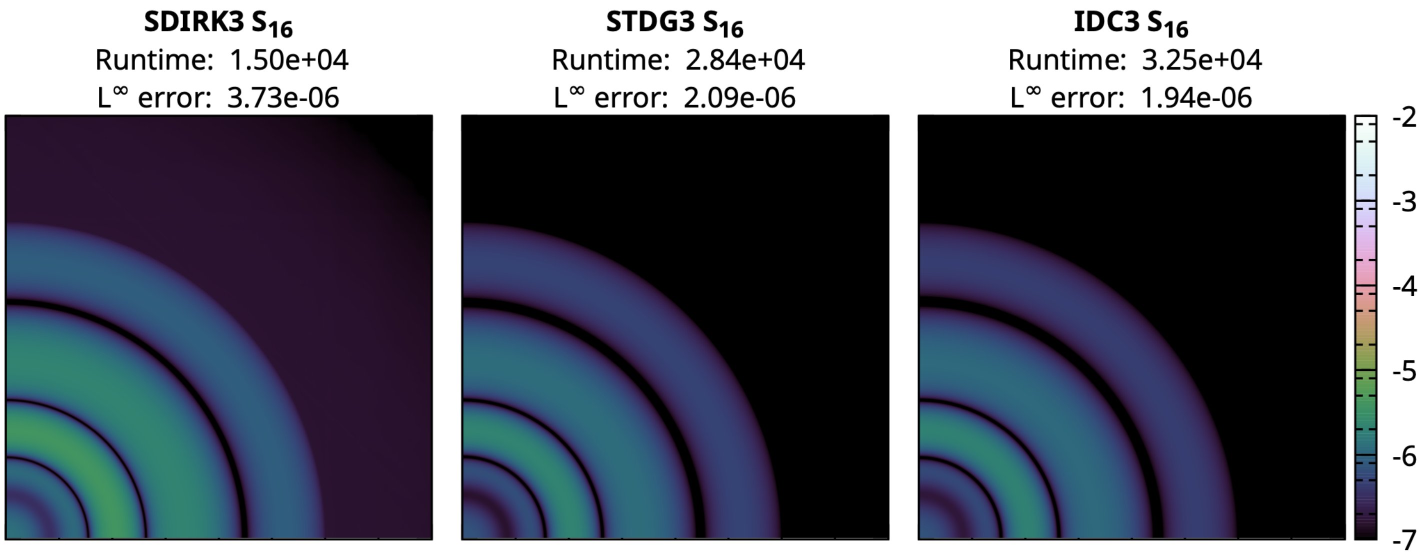
Compared with hybrid with **Nyström reconstruction**

- BE DG
- ARK DG
- DIRK DG
- Space Time DG

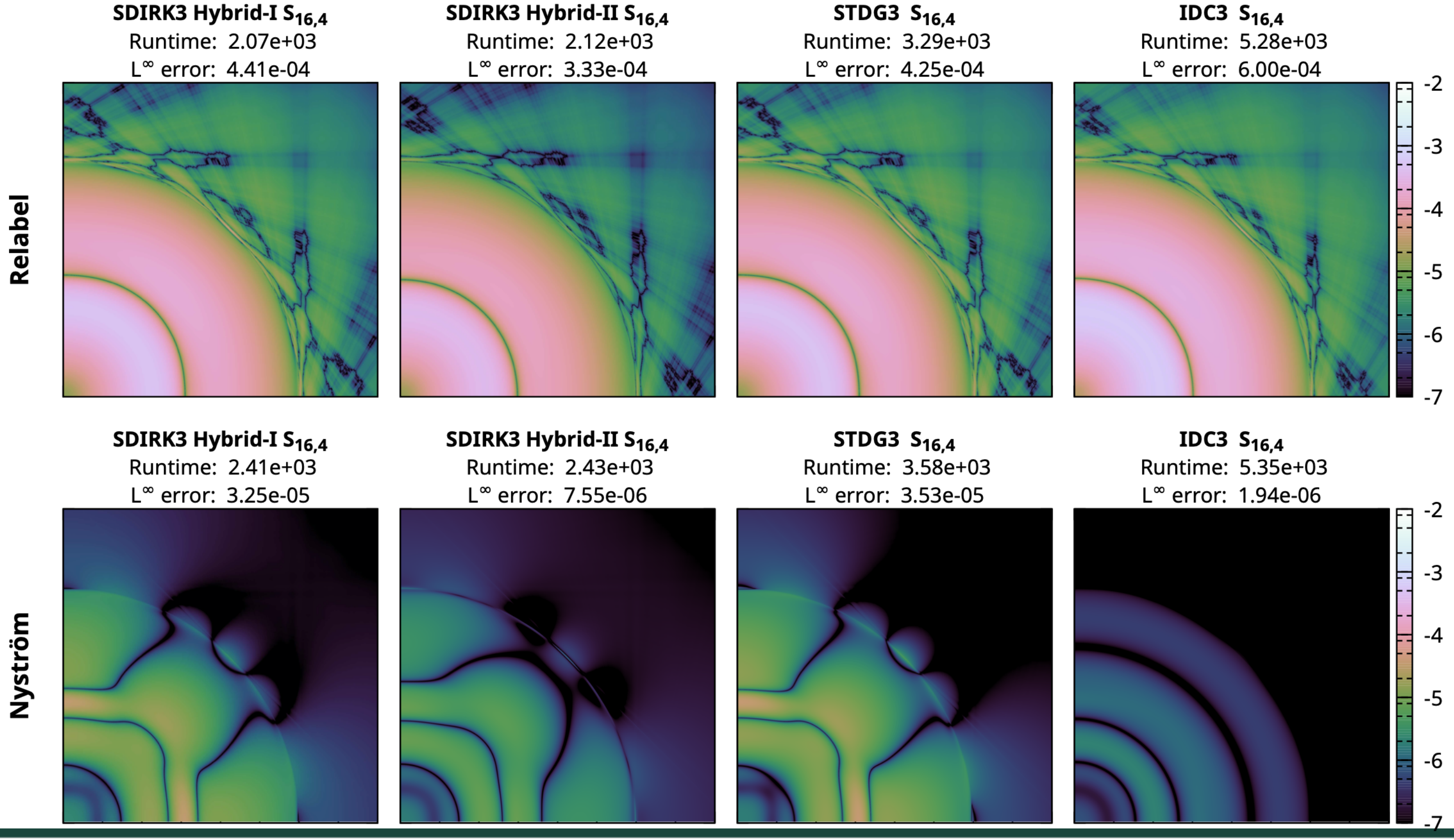
[5] MM Crockatt and AJ Christlieb, “Low-Storage Integral Deferred Correction Methods for Scientific Computing”, SIAM Journal on Scientific Computing, 2018

Low storage Defect Correction [5] 3 to 5 times faster than the BEST of these methods for the same accuracy and lower storage

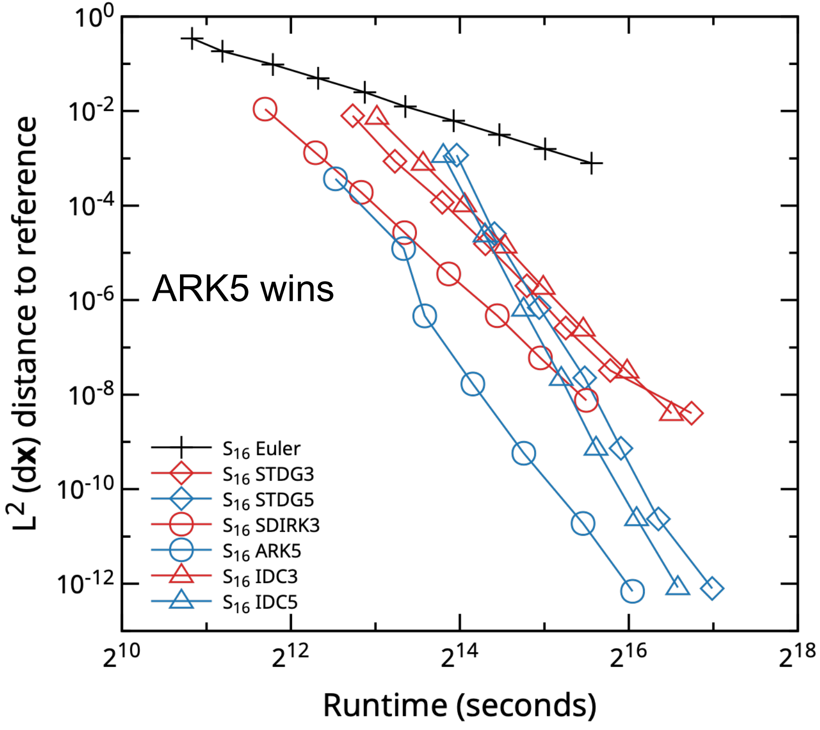
Error Plots Monolithic Methods

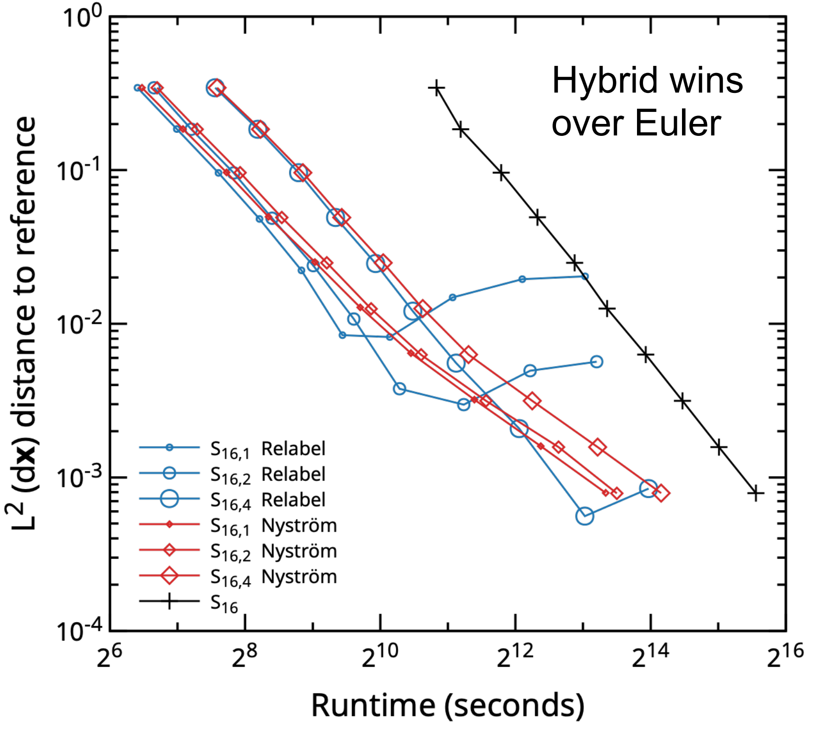


Error Plots Hybrid Methods



Run time vs L2 error-Monolithic and Hybrid Euler

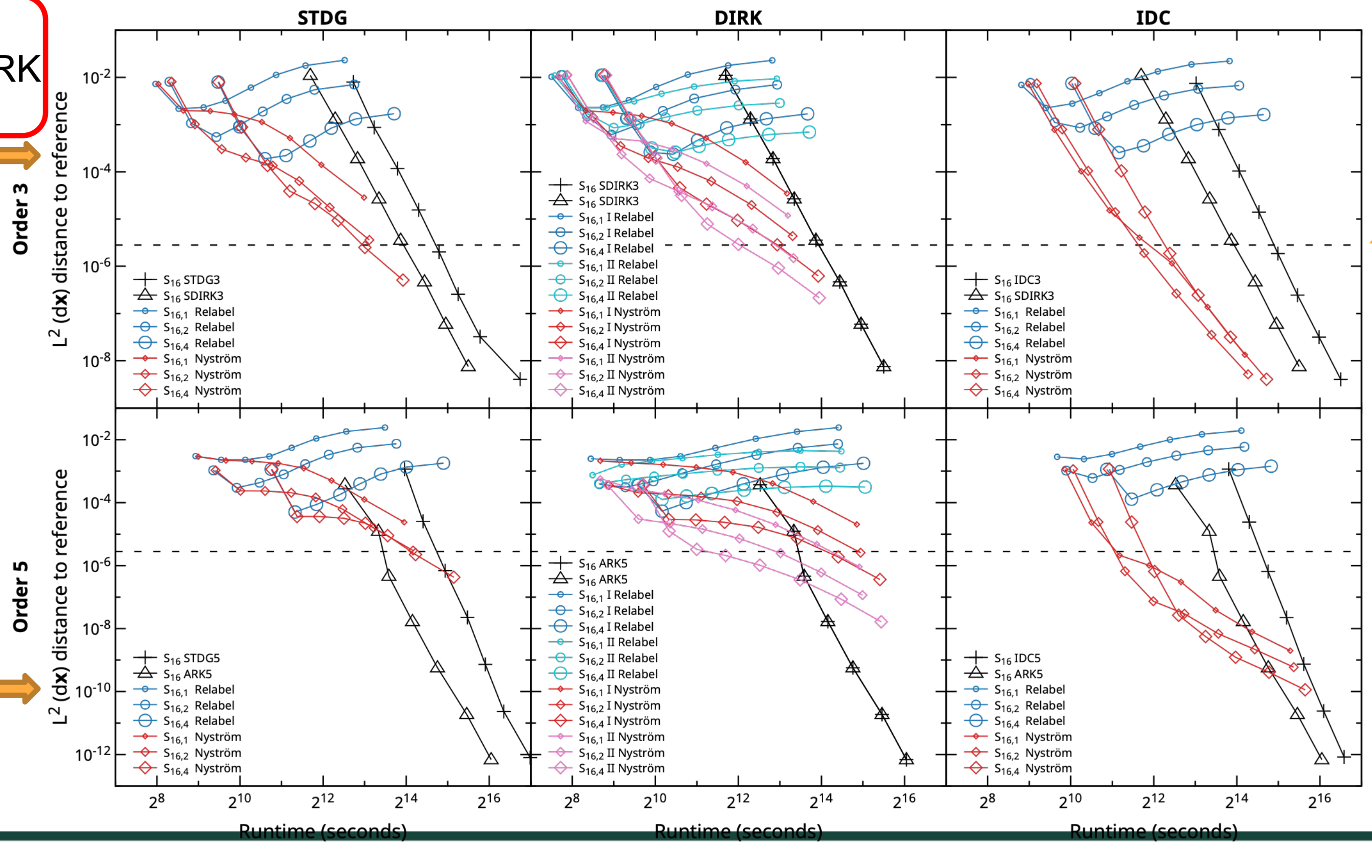




Run time vs L2 error optimal ARK (triangles)

Low storage Defect Correction << DIRK

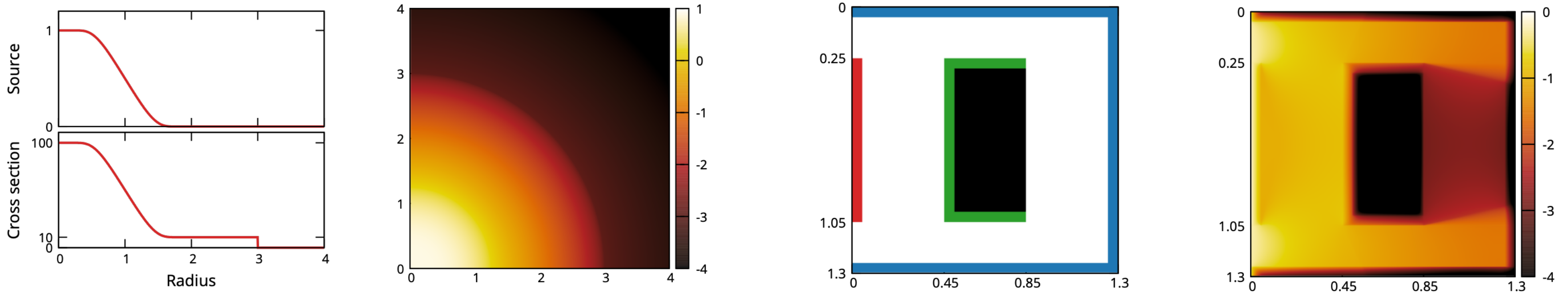
STDG and DIRK/ARK hybrid have order reduction even with Nystrom while IDC3 does not



Angular accuracy

Conclusions

- Physically accurate surrogate models have a key role to play in increased computational efficiency for Exa-scale computing.



New directions

- Luck Roberts
- Sean Couch
- Yingda Cheng
- Andrew Christlieb

NSF: A Data-driven Approach to Multiscale Methods for Scalable Transport in Neutron Star Mergers and Complex Plasmas, *recommended for funding*

***Goal: Push the idea of the* structure preserving surrogate models**

New directions we are pursuing:

- Cheap surrogate model for Collisional update
  - Can we replace the implicit update with "local" methods
    - ML based on constrained optimization

      Non-intrusive **reduced order modeling** of nonlinear problems using neural networks
      JS **Hesthaven**, S Ubbiali - Journal of Computational Physics, 2018
      Recurrent neural network closure of parametric POD-Galerkin **reduced-order models** based on the Mori-Zwanzig formalism
      Q Wang, N Ripamonti, JS **Hesthaven** - Journal of Computational Physics, 2020
    - Reduced order models

      Structure preserving **model reduction** of parametric **Hamiltonian** systems
      BM Afkham, JS **Hesthaven** - SIAM Journal on Scientific Computing, 2017
      Structure-preserving **model-reduction** of dissipative **hamiltonian** systems
      BM Afkham, JS **Hesthaven** - Journal of Scientific Computing, 2019
    - Reduced Basis Methods

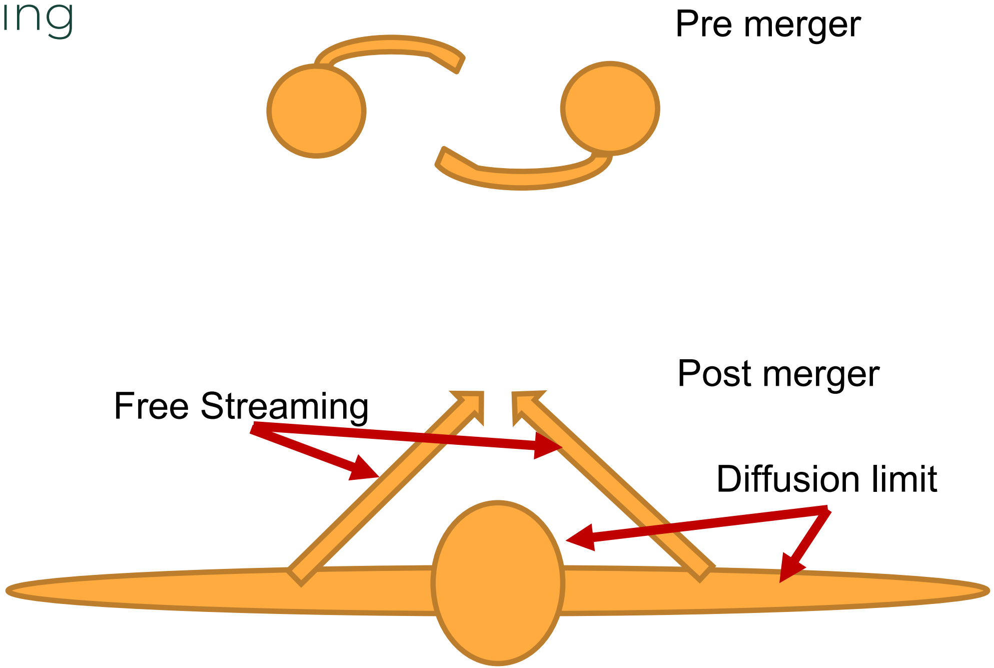
      Six-dimensional adaptive simulation of the **Vlasov** equations using a hierarchical **basis**
      E Deriaz, S Peirani - Multiscale Modeling & Simulation, 2018

Structure preserving surrogate

- Looking at data on N nearest nodes
  - Cheap surrogate model for Collisionless update
    - ML based on constrained optimization
    - Reduced order models
    - Reduced Basis Methods

Closure in M1 via structure preserving surrogate

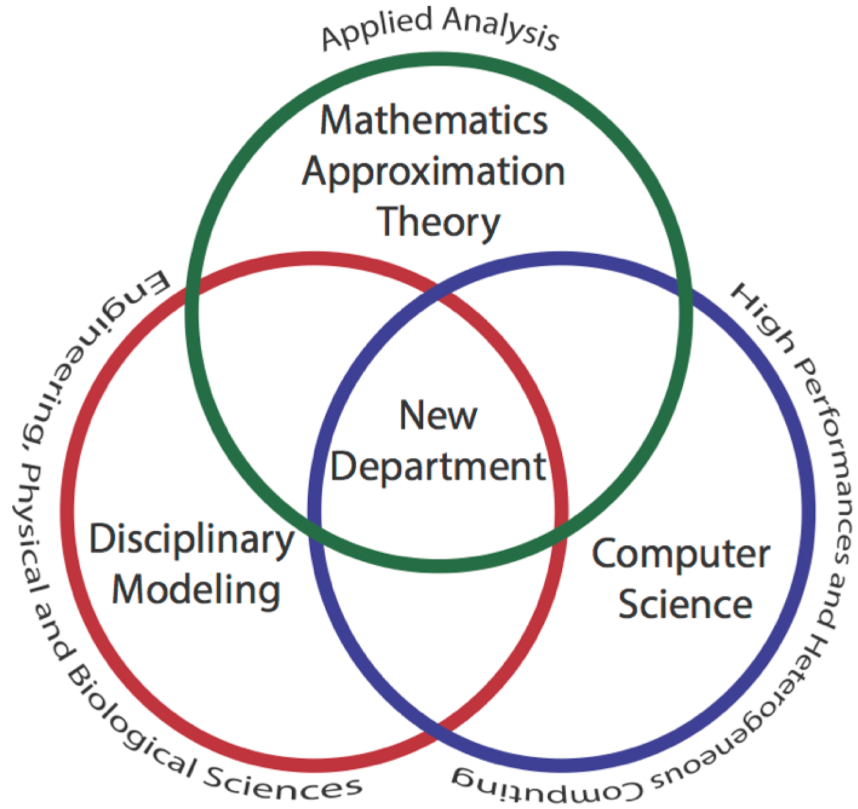
- Learn closure for M1 that can handle both diffusion and free streaming



What is CMSE?

- CMSE is the Department of Computational Mathematics, Science and Engineering.
- CMSE is Jointly administered department between the College of Natural Science and the College of Engineering at Michigan State University.

Computational Math, Science and Engineering



How does CMSE differ from Computer Science?

- Computer Science focuses on the science of computing
- **CMSE focuses on computing to do science**

Recruiting PhD students for 2021

- What will they study: (Starting Fall 2020 - 51 PhD students)
  - Data Science
  - Numerical Methods
  - Modeling
  - The interplay of all three and the application to STEM

CMSE videos

About CMSE:

1) https://www.youtube.com/watch?v=fNvUTyhwzFQ
2) https://www.youtube.com/watch?v=fjeXWg1qcwI

Faculty Highlights:

1) https://www.youtube.com/watch?v=azeGR4US07Y
2) https://www.youtube.com/watch?v=VdsKHhncXYw
3) https://www.youtube.com/watch?v=plOlK9CJWIc
4) https://www.youtube.com/watch?v=nkf-B3Aksak
5) https://www.youtube.com/watch?v=fZfkH8pkIPM
6) https://www.youtube.com/watch?v=McTHshJdrtM
7) https://www.youtube.com/watch?v=e4Op2hd5icY