Deterministic Transport MFEM-Miniapp: Advancing Fidelity of Fusion Energy Simulations

MFEM Community Workshop – Virtual Meeting

CASC
Center for Applied Scientific Computing

Milan Holec & GSN-Team

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Abstract

We introduce a new multi-dimensional discretization in MFEM enabling efficient high-order phase-space simulations of various types of Boltzmann transport. In terms of a generalized form of the standard discrete ordinate SN method for the phase-space, we carefully design discrete analogs obeying important continuous properties such as conservation of energy, preservation of positivity, preservation of the diffusion limit of transport, preservation of symmetry leading to rays-effect mitigation, and other laws of physics. Finally, we show how to apply this new phase-space MFEM feature to increase the fidelity of modeling of fusion energy experiments.

GSN TEAM

PI Milan Holec

Co-PI Terry Haut

Summer interns

Alex Mote

Veselin Dobrev

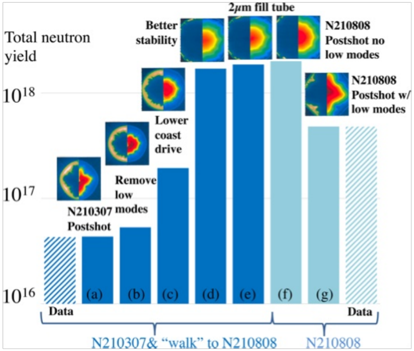
Yohann Dudouit

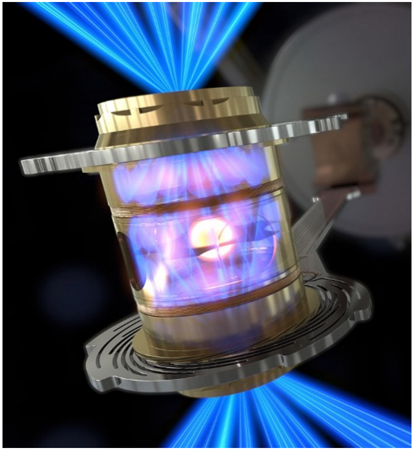
Colby Fronk

- Applied math & Physics & HPC & Reduced Order modeling (GNN)
- Pushing the limits of **DETERMINISTIC TRANSPORT**

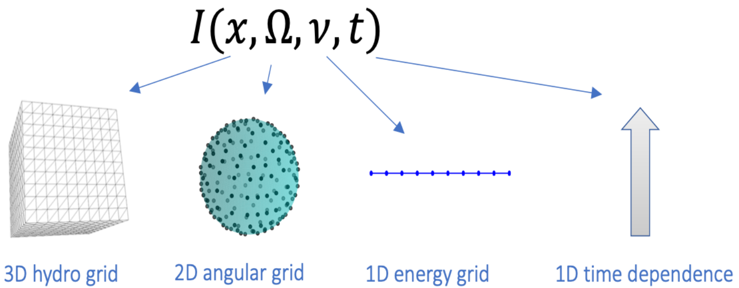
Breakthrough in Fusion Energy

- National **Ignition** Facility at LLNL.
- Dec 5^{th} 2022 **Fusion Ignition** Energy yield 3.15 MJ, $\mathbf{Q > 1.5}$.
- Jul 30^{th} 2023 **Fusion** Record Energy yield 3.88 MJ, $\mathbf{Q > 1.9}$.
- Every ICF experiment repeat $\mathbf{Q > 1}$.
- Only **5%** of the combustible burned.
- How to improve? Simulations fidelity?

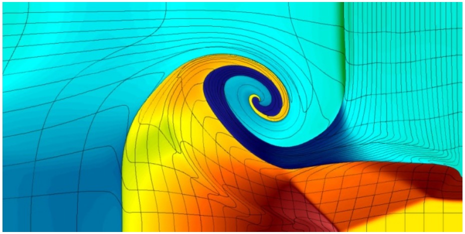




High-order multi-dimensional DG

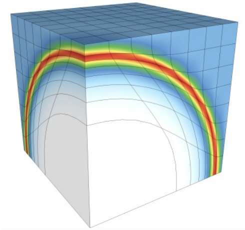


- Lagrangian curved mesh[1]
- High-order accuracy space+angles+energy
- Matrix-free (Yohann)
- **Novel GSN method** $\sim 1000\times$ **less dofs**

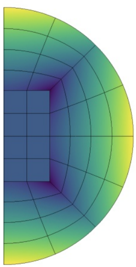


[1] Haut, High-Order Finite Elements for TRT on Curved Meshes, LDRD-ER, 18-ERD-002.

SPACE



Cartesian 3D

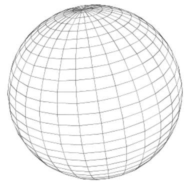


Axisymmetric 2D

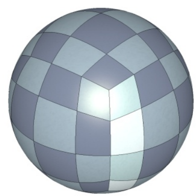
slab/sphere 1D

×

ANGLE



Product quadrature



P_N exact quadrature

1D polar

×

ENERGY

Phase-space
6D mesh
3D×2D×1D

N-dimensional MFEM!

Multi-Dimensional High-Order DG in MFEM

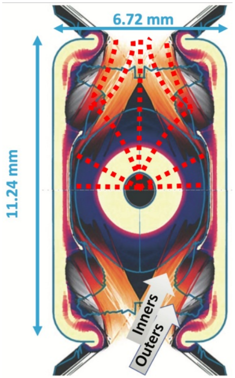
Krook's-type multidimensional transport

$$\partial_t \psi + \sum_{i=1}^{N} \partial_{x_i}(a_i \psi) = \sigma(B - \psi),$$

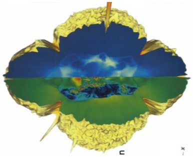
- **N-dimensional** product mesh
- **N-dimensional** user defined advection field
- MFEM: solvers, time integrators, visualization
- Generic programming abstraction, performance
- Matrix-free, GPU-portable
- **Example: polar-SN in 6D on 50 lines!**

```
////////////////////////////////////////////////
// Deterministic Transport Mesh
Mesh space_mesh("cart3D.mesh");
Mesh angle_mesh("sphere-product.mesh");
Mesh energy_mesh("energy1D.mesh");
auto mesh = MakeDTMesh(space_mesh, angle_mesh, energy_mesh);

////////////////////////////////////////////////
// Deterministic Transport Finite Element Space
FiniteElementOrders< o_rho, o_theta, o_phi > space_os;
FiniteElementOrders< o_polar, o_azim > angle_os;
FiniteElementOrders< o_energy > energy_os;
// Finite element
auto finite_element = MakeDTLegendreFiniteElement(space_os, angle_os, energy_os);
// Finite element space
auto fe_space = MakeDTFiniteElementSpace(mesh, finite_element);

////////////////////////////////////////////////
// Deterministic Transport Integration Rule
IntegrationRuleNumPoints< o_rho + 2, o_theta + 2, o_phi + 2 > quad_space;
IntegrationRuleNumPoints< o_polar + 2, o_azim + 2 > quad_angle;
IntegrationRuleNumPoints< o_energy + 2 > quad_energy;
// High-dimension integration rule
auto int_rules = MakeDTIntegrationRule(quad_space, quad_angle, quad_energy);

////////////////////////////////////////////////
// Deterministic Transport Operator and RHS
auto adv_lb = [=]( auto & X, Real (& a)[6] )
{
   coords(X, rho, theta, phi, mu, omega, eps);
   a[0] = rho * rho * sin(theta) * mu;
   a[1] = rho * sin(theta) * sqrt(1.0 - mu * mu) * cos(omega);
   a[2] = rho * sqrt(1.0 - mu * mu) * sin(omega);
   a[3] = rho * sin(theta) * (1.0 - mu * mu);
   a[4] = - rho * sqrt(1.0 - mu * mu) * sin(omega) * cos(theta);
   a[5] = 0.0;
};
// Operator
auto operator = MakeMassAdvectionOperator(fe_space, int_rules, adv_lb, sigma_lb);
// Evaluate the right hand sides
FiniteElementVector rhs(fe_space);
rhs = MakeLinearForm(fe_space, legendre_int_rules, sigmaB_lb);

////////////////////////////////////////////////
// Solve 6D problem
GMRESSolver solver;
solver.SetOperator(operator);
FiniteElementVector sol(fe_space);
solver.Mult(rhs, sol);
```

Why is the kinetics such a challenge in fusion?



Capsule at peak compression
30x shrank in radius



Kritcher *et al.*,PRE 98,053206,2018.
HYDRA simulation.

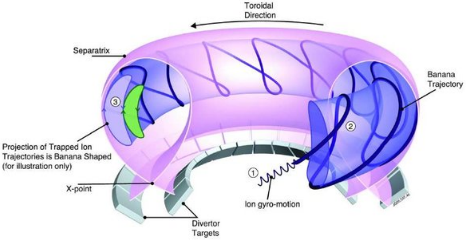
Rotating angular coordinates

$$\begin{bmatrix} q^x \\ q^y \\ q^z \end{bmatrix} := \begin{bmatrix} r\cos(\phi) \\ r\sin(\phi) \\ z \end{bmatrix}$$

$$\begin{bmatrix} p^x \\ p^y \\ p^z \end{bmatrix} := \mathbf{R} \begin{bmatrix} \epsilon\cos(\omega)\sqrt{1-\mu^2} \\ \epsilon\sin(\omega)\sqrt{1-\mu^2} \\ \epsilon\mu \end{bmatrix}$$

General phase-space coordinates transformation **J**

Transport along B-field lines in tokamaks



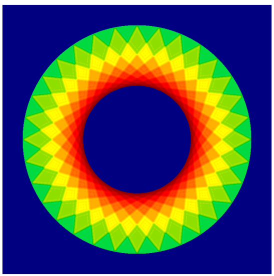
General transfer operator

Transformed **Conservative** transfer operator

$$\vec{\Omega}\cdot\vec{\nabla}\psi = \tilde{\Omega}^T\cdot\tilde{\mathbf{J}}^{-T}\cdot\tilde{\nabla}\tilde{\psi} = \frac{1}{|\tilde{\mathbf{J}}|}\tilde{\nabla}^T\cdot(|\tilde{\mathbf{J}}|\tilde{\mathbf{J}}^{-1}\cdot\tilde{\Omega}\tilde{\psi})$$

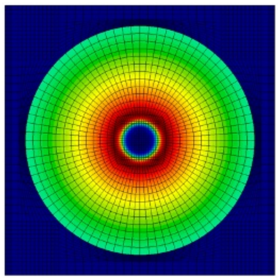
Comparing standard SN vs. GSN in MFEM

32 directions

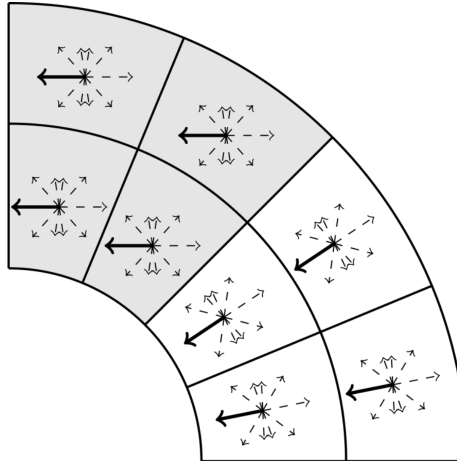


"Eulerian" angular mesh

4 directions



"Lagrangian" angular mesh

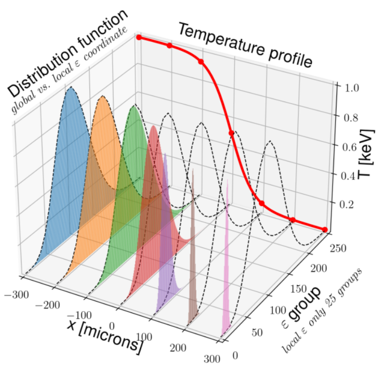


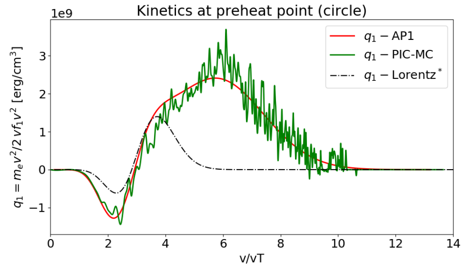
Standard-SN (gray) vs. Polar-SN (white)

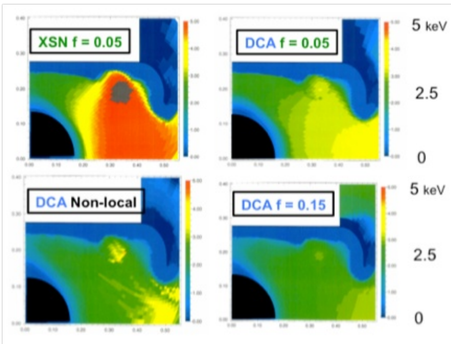
Spatially varying rotation $\mathbf{R}(\vec{x})$ pointing to the origin corresponds to polar-SN.

"Lagrangian-like" transformation of energy

Full potential of GSN: local energy $\varepsilon_{loc}(\vec{x}) = \frac{\varepsilon_{glob}}{k_B T(\vec{x})} \Rightarrow \vec{\Omega} \cdot \vec{\nabla} \varepsilon_{loc} \partial_{\varepsilon_{loc}} \psi = \varepsilon_{loc} \frac{\vec{\nabla} T}{T} \partial_{\varepsilon_{loc}} \psi$





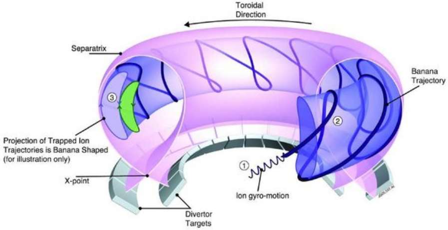


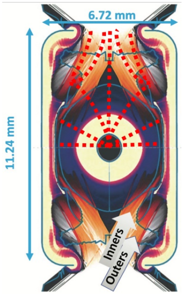
Quoting Mordy Rosen: "Given the inherent non-local nature of long mean-free-path large-velocity heat-flow-carrying electrons, there is a clear need to replace the **fundamentally flawed approach** of a local description of heat flow and the flux-limiter crutch upon which it stands."

Rosen, HEDP, 2011. Holec, PoP, 2018. Holec, arXiv, 2018.

Flux-GSN: Radition drive, charged particles transport

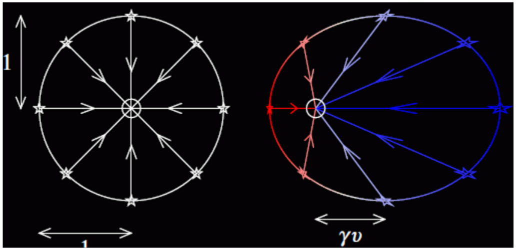
$$\begin{bmatrix} q^{\tilde{j}}_{,\hat{i}} & 0 \\ p^{\tilde{\beta}}_{,\hat{\gamma}} \left((Rf)^{\hat{\gamma}}_{,\tau^{\tilde{m}}} \tau^{\tilde{m}}_{,\tilde{k}} + (Rf)^{\hat{\gamma}}_{,p^*} p^*_{,\tilde{k}} \right) q^{\tilde{k}}_{,\hat{i}} & p^{\tilde{\beta}}_{,\hat{\alpha}} \end{bmatrix} \begin{bmatrix} p^{\hat{i}} \\ a^{\hat{\alpha}}_L \end{bmatrix}$$





Fluid-GSN: Relativistic radiation transport

$$\frac{1}{c} D_t \psi + \mu \partial_z \psi - \underbrace{\frac{1}{c} \left(\mu \partial_z v \mu \varepsilon \partial_\varepsilon \psi + \mu \partial_z v (1 - \mu^2) \partial_\mu \psi - 3\mu \partial_z v \mu \psi \right)}_{O(v/c) \text{ correction by } \partial_\varepsilon \psi,\ \partial_\mu \psi,\ \partial_z v}$$

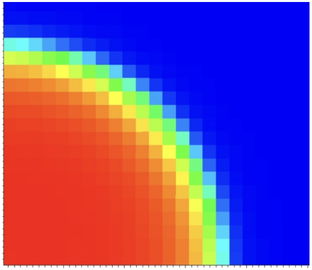


Buchler, JQSRT, 1983. Gentile, ICTT, 2019. Holec, CSE, 2019. Holec, PoP, 2018. Holec, arXiv, 2018.

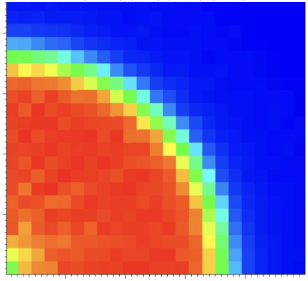
Non-negotiable physics: how to get it right?

Energy conservation

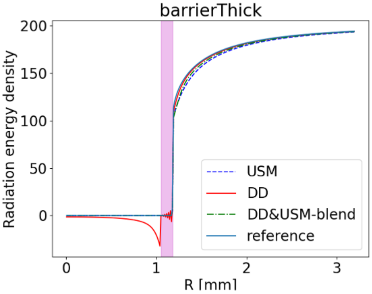
Conservative



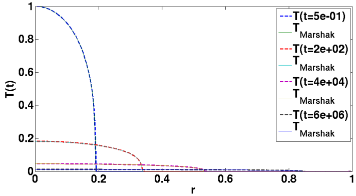
Non-conservative



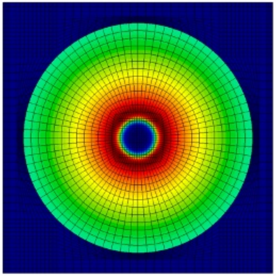
Positivity preservation



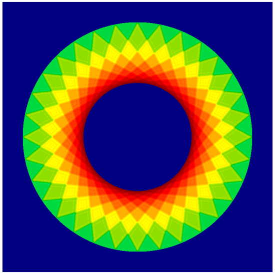
Diffusion limit



Symmetry preservation



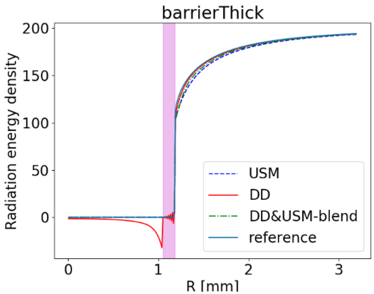
Rays-effect



MFEM-Miniapp example: 5D gray-transport in perfect hohlraum

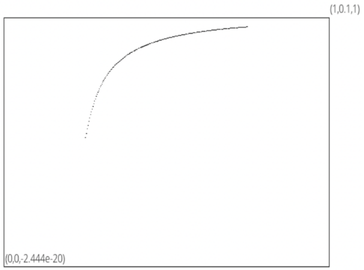
Polar-SN (**R**-to-origin) with spatial ρ, θ, ϕ and angular μ, ω coordinates

$$\overline{a} = \rho^2 \sin(\theta) \left[\mu, \frac{\sqrt{1-\mu^2}\cos(\omega)}{\rho}, \frac{\sqrt{1-\mu^2}\sin(\omega)}{\rho\sin(\theta)}, \frac{1-\mu^2}{\rho}, -\sqrt{1-\mu^2}\sin(\omega)\frac{\cot(\theta)}{\rho} \right]$$



1D $\left(\mu\partial_\rho\psi + \frac{1-\mu^2}{\rho}\partial_\mu\psi\right)$

Perfect hohlraum



5D MFEM-Miniapp

Conclusions & Future Work

New features in MFEM:

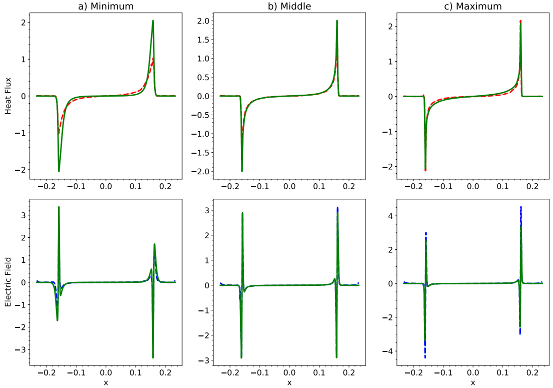
- **N-dimensional** product mesh & anisotropic DG
- MFEM: mesh, solvers, time integrators, visualization
- Generic programming abstraction, performance
- Matrix-free, GPU-portable

More is comming!

- **N-dimensional** advection-diffusion
- Integro-differential equations
- **N-dimensional** adaptive-mesh-refinement

Machine Learning - Graph-Neural-Networks

$10^6\times$ faster than phase-space FEM simulations



Credit: Colby Fronk and Alex Mote

Anyone can relate to this?

MFEM wolrd-wide community ... pick your language :)

Thank you for your attention. Any questions?

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