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

MFEM Community Workshop – Virtual Meeting

October 26, 2023
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\textsuperscript{th} 2022 **Fusion Ignition** Energy yield 3.15 MJ, \( Q > 1.5 \).
- Jul 30\textsuperscript{th} 2023 **Fusion** Record Energy yield 3.88 MJ, \( Q > 1.9 \).
- Every ICF experiment repeat \( Q > 1 \).
- Only 5\% of the combustible burned.
- How to improve? Simulations fidelity?

![Diagram showing neutron yield and experiment outcomes]
High-order multi-dimensional DG

\[ I(x, \Omega, \nu, t) \]

- Lagrangian curved mesh\(^1\)
- High-order accuracy space+angles+energy
- Matrix-free (Yohann)
- **Novel GSN method \( \sim 1000 \times \text{less dofs} \)**

\(^1\) 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 $\times$ 2D $\times$ 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!
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

\[
\begin{bmatrix}
q_x^x \\
q_y^y \\
q_z^z
\end{bmatrix}
:=
\begin{bmatrix}
r \cos(\phi) \\
r \sin(\phi) \\
z
\end{bmatrix}
\]

\[
\begin{bmatrix}
p_x^x \\
p_y^y \\
p_z^z
\end{bmatrix}
:=
R
\begin{bmatrix}
\epsilon \cos(\omega) \sqrt{1 - \mu^2} \\
\epsilon \sin(\omega) \sqrt{1 - \mu^2} \\
\epsilon \mu
\end{bmatrix}
\]

General phase-space coordinates transformation \( J \)

Transport along B-field lines in tokamaks
General transfer operator

Transformed **Conservative** transfer operator

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

Comparing standard SN vs. GSN in MFEM

32 directions

4 directions

"Eulerian" angular mesh

"Lagrangian" angular mesh

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

Spatially varying rotation \( \mathbf{R}(\mathbf{x}) \) pointing to the origin corresponds to polar-SN.
"Lagrangian-like" transformation of energy

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

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."

Flux-GSN: Radition drive, charged particles transport

\[
\begin{bmatrix}
q_{\alpha j}^j \\
p_{\alpha j}^j (\langle Rf \rangle_{\gamma \alpha} + (Rf)_{\gamma, \alpha}^{\gamma}) q_{\alpha j}^j \\
0
\end{bmatrix}
\begin{bmatrix}
\partial_{t, \alpha} \\
\partial_{x, \alpha} \psi - \partial_{y, \alpha} \psi - \partial_{z, \alpha} \psi
\end{bmatrix}
\]

Fluid-GSN: Relativistic radiation transport

\[
\frac{1}{c} D_t \psi + \mu \partial_z \psi - \frac{1}{c} \left( \mu \partial_z \nu \mu \varepsilon \partial_\varepsilon \psi + \mu \partial_z \nu (1 - \mu^2) \partial_\mu \psi - 3 \mu \partial_z \nu \mu \psi \right)
\]

O(\nu/c) correction by \( \partial_\varepsilon \psi, \partial_\mu \psi, \partial_z \nu \)

Non-negotiable physics: how to get it right?

Energy conservation
Conservative

Positivity preservation

Symmetry preservation
Rays-effect

Diffusion limit

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

Polar-SN (R-to-origin) with spatial $\rho, \theta, \phi$ and angular $\mu, \omega$ coordinates

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

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 coming!
- **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?

Do you know how frustrating it is to have to translate everything in my head before I say it?

Do you even know how smart I am in Spanish?

MFEM worldwide community ... pick your language :)

Lawrence Livermore National Laboratory
LLNL-PRES-856356
CASC
NNSA
Thank you for your attention. Any questions?

Disclaimer: This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees make any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.