Unstructured Finite Element Neutron Transport using MFEM

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Outline

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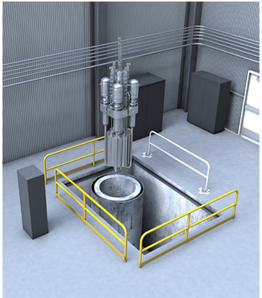
Microreactors

- Relatively small electrical output ($<$10 MW).
- Geometrically compact.
- Varied designs.
  - Thermal, epithermal, and fast neutron spectra.
  - Unique cooling designs (e.g., heat pipes).
  - Space applications.

MARVEL Microreactor

- Development led by Idaho National Laboratory (INL) for construction on-site.
- 18 kW to 25 kW electric output.
- Cylinder with 50 cm height and 120 cm diameter.
- UZrH HALEU fuel.
- Thermal spectrum.
- Liquid NaK eutectic coolant.



Why MFEM?

- Exascale Computing Project (ECP).
- GPU support.
- Library support (e.g., HYPRE, PETSc, SLEPc, AmgX, etc.).
- Rapid prototyping.
  - Essential for research computer programs.
  - Dozens of solver methods implemented.

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Neutron Transport Equation

- Steady-state Boltzmann equation.
- 6 independent variables:
  - 3 space.
  - 2 direction (angle).
  - 1 energy.
- Eigenvalue problem for eigenvalue λ and eigenfunction $\psi(\mathbf{r}, \hat{\Omega}, E)$.
- Coefficients are "cross sections." Interaction probabilities.

$$\hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}, E) + \Sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, \hat{\Omega}, E) = \frac{\chi(\mathbf{r}, E)}{\lambda} \int_0^\infty \nu\Sigma_f(\mathbf{r}, E') \int_{4\pi} \psi(\mathbf{r}, \hat{\Omega}', E')\, d\hat{\Omega}' + \int_0^\infty \int_{4\pi} \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}, E' \to E)\psi(\mathbf{r}, \hat{\Omega}', E')\, d\hat{\Omega}'\, dE'$$

Neutron Transport Equation – Multigroup Discretization

- Multigroup approximation in energy (e.g., 24 groups).
- Multigroup constants conserve reaction rates.

$$\hat{\Omega} \cdot \nabla \psi_g(\mathbf{r}, \hat{\Omega}) + \Sigma_{t,g}(\mathbf{r}) \psi_g(\mathbf{r}, \hat{\Omega}) =$$

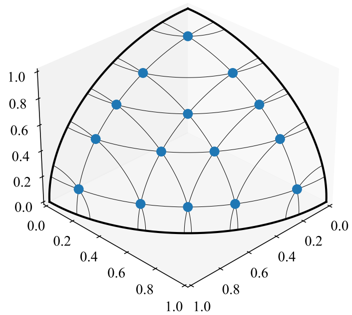
$$\frac{\chi_g(\mathbf{r})}{\lambda} \sum_{g'=1}^{N_G} \nu\Sigma_{f,g'}(\mathbf{r}) \int_{4\pi} \psi_{g'}(\mathbf{r}, \hat{\Omega}')\, d\hat{\Omega}' + \sum_{g'=1}^{N_G} \int_{4\pi} \Sigma_{s,g'\to g}(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\mathbf{r}, \hat{\Omega}')\, d\hat{\Omega}'$$

$$\psi_g(\mathbf{r}, \hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} \psi(\mathbf{r}, \hat{\Omega}, E)\, dE$$

Neutron Transport Equation – Discrete Ordinates Discretization

- Discrete ordinates (S_N) approximation in angle.
- Full derivation projects Σ_s onto spherical harmonics.

$$N_A = \begin{cases} N(N+2) & \text{3D} \\ \frac{N(N+2)}{2} & \text{2D} \end{cases}$$



Level-symmetric S_{10} quadrature.

$$\hat{\Omega}_n \cdot \nabla\psi_{g,n}(\mathbf{r}) + \Sigma_{t,g}(\mathbf{r})\psi_{g,n}(\mathbf{r}) =$$

$$\frac{\chi_g(\mathbf{r})}{\lambda} \sum_{g'=1}^{N_G} \nu\Sigma_{f,g'}(\mathbf{r}) \sum_{n'=1}^{N_A} w_n \psi_{g',n'}(\mathbf{r}) + \sum_{g'=1}^{N_G} \sum_{n'=1}^{N_A} S_{g'\to g, n'\to n}(\mathbf{r})\psi_{g',n'}(\mathbf{r})$$

Vector Dimension

- Number of unknowns per spatial grid point.
- Unique to neutron transport due to underlying phase space.
- High-dimensional continuous phase space leads to high-dimensional discrete phase space.
- Example:
  - 24 group, S_{10} in 2D.
  - $N_G = 24$, $N_A = 60$. VDIM = 1440.
- Most DOF are due to energy & angle (not space).
- Linear finite elements. Spectral FEM likely not useful.

SAAF Equations for FEM

- Self-Adjoint Angular Flux (SAAF).
- Convert hyperbolic to elliptic.
- Second-order system of PDEs can be solved with continuous FEM.
- No sweep.

$$\int_{\mathcal{D}} \frac{1}{\Sigma_{t,g}(\mathbf{r})} \hat{\Omega}_n \cdot \nabla v(\mathbf{r}) \hat{\Omega}_n \cdot \nabla \psi_{g,n}(\mathbf{r})\, d\mathbf{r} + \int_{\mathcal{D}} v(\mathbf{r}) \Sigma_{t,g}(\mathbf{r}) \psi_{g,n}(\mathbf{r})\, d\mathbf{r} +$$

$$\frac{1}{2}\left(\oint_{\Gamma} v(\mathbf{r}) \psi_{g,n}(\mathbf{r}) \hat{\Omega}_n \cdot \hat{\mathbf{n}}\, d\Gamma + \oint_{\Gamma} v(\mathbf{r}) \psi_{g,n}(\mathbf{r}) \left| \hat{\Omega}_n \cdot \hat{\mathbf{n}} \right| d\Gamma \right) =$$

$$\frac{1}{\lambda}\left(\int_{\mathcal{D}} \chi_g(\mathbf{r}) \sum_{g'=1}^{N_G} \nu\Sigma_{f,g'}(\mathbf{r}) \sum_{n'=1}^{N_A} w_{n'} \psi_{g',n'}(\mathbf{r})\, d\mathbf{r} + \int_{\mathcal{D}} \frac{\hat{\Omega}_n \cdot \nabla v(\mathbf{r})}{\Sigma_{t,g}(\mathbf{r})} \chi_g(\mathbf{r}) \sum_{g'=1}^{N_G} \nu\Sigma_{f,g'}(\mathbf{r}) \sum_{n'=1}^{N_A} w_{n'} \psi_{g',n'}(\mathbf{r})\, d\mathbf{r} \right)$$

$$\int_{\mathcal{D}} v(\mathbf{r}) \sum_{g'=1}^{N_G} \sum_{n'=1}^{N_A} S_{g'\to g, n'\to n}(\mathbf{r}) \psi_{g',n'}(\mathbf{r})\, d\mathbf{r} + \int_{\mathcal{D}} \frac{\hat{\Omega}_n \cdot \nabla v(\mathbf{r})}{\Sigma_{t,g}(\mathbf{r})} \sum_{g'=1}^{N_G} \sum_{n'=1}^{N_A} S_{g'\to g, n'\to n}(\mathbf{r}) \psi_{g',n'}(\mathbf{r})\, d\mathbf{r} -$$

$$\frac{1}{2}\left(\oint_{\Gamma} v(\mathbf{r}) \psi^{\text{inc}}_{g,n}(\mathbf{r}) \hat{\Omega}_n \cdot \hat{\mathbf{n}}\, d\Gamma - \oint_{\Gamma} v(\mathbf{r}) \psi^{\text{inc}}_{g,n}(\mathbf{r}) \left| \hat{\Omega}_n \cdot \hat{\mathbf{n}} \right| d\Gamma \right)$$

Solver Methodologies

Generalized Eigensolver.

- All-at-once.
- PETSc + SLEPc.
- Generalized Davidson.
- Approx. 100 GMRES iteration preconditioning.
- NVIDIA AmgX library.
- HYPRE+GPU in development.

Challenge:

Memory limited.

Source Iteration.

- One group at-a-time (all angle).
- Gauss-Seidel in energy.
- "Lagged" source term.
- Scattering iterations with Diffusion Synthetic Acceleration (DSA).
- HyprePCG + HypreBoomerAMG.
- Approx. 10 000 PCG solves.

Challenges:

Parallelism.
Runtime.

Source Iteration Algorithm

```
while Power Iterations not converged do
    Update fission & upscattering source.
    for g = 1 ... N_G do
        Update downscattering source.
        while Scattering Iterations not converged do
            Update selfscattering source.
            Assemble neutron source in b_g vector.
            Solve A_g ψ_g = b_g.
            Update scattering iterations convergence criteria.

    Update λ.
    Update power iterations convergence criteria.
```

~15 scattering iteration.

N_G (~20) energy iteration.

~40 power iteration.

Methods Comparison

Source Iterations

- N_G block diagonal, SPD matrices.
- Slow convergence (approx. 10 000 solves).
- Diffusion Synthetic Acceleration (DSA).

"Multigroup"

Jacobi in Energy

- Maintain SPD structure.
- Slow convergence in energy.

Combined Energy

- Asymmetric, requires GMRES.
- Improved convergence in energy.

Generalized Eigensolver

- Enormous memory requirement.
- Highly efficient algorithms (e.g., Generalized Davidson).
- Massively parallelizable.

Increasing Memory →

← Increasing "Matrix-free"

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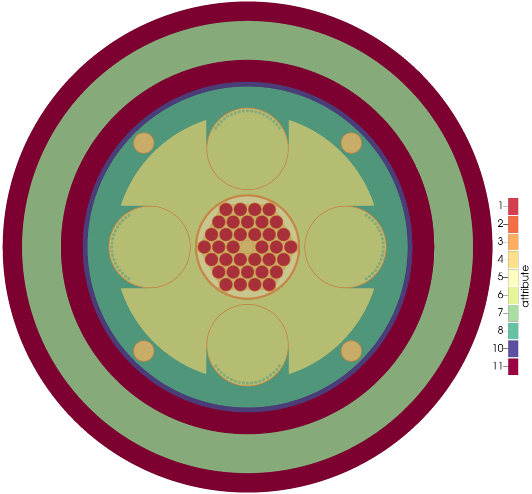
MARVEL Reactor Model

- Series of two-dimensional meshes generated with Gmsh.
- 24 and 238 group cross sections generated with data from SCALE.
- All results use 24 group structure.
- Large gaseous region (approx. 12 % by volume).
- Gas density artificially increased 100 ×.

Refinement	h_{inner} [cm]	h_{outer} [cm]	Elements	Vertices
R0	0.5	1.0	45 204	22 791
R1	0.25	0.5	439 168	220 333
R2	0.125	0.25	6 322 912	3 164 449
R3	0.0625	0.125	96 378 000	48 200 969

MARVEL Reactor Geometry



MARVEL Reactor Results

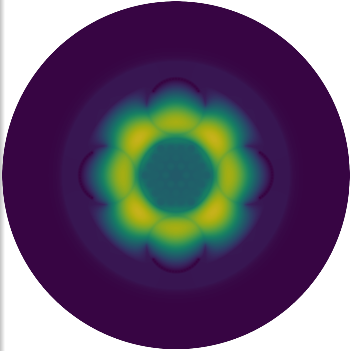
- Source iteration solver necessary.
- Most refined results require 256 Summit nodes (10 752 MPI ranks) and 6 h.
- More spatially refined results desirable.
- Observed convergence rate $O(h^{1.340})$.

Refinement	S_2	S_4	S_6	S_8	S_{10}
R0	1.325 219	1.326 908	1.326 742	1.326 872	1.327 017
R1	1.335 505	1.336 675	1.336 745	1.336 790	1.336 872
R2	1.339 502	1.340 601	1.340 697		
Ref.†	1.342 042	1.343 240	1.343 278		

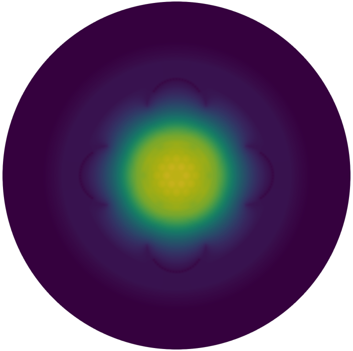
† Richardson extrapolation.

Refinement	S_2	S_4	S_6	S_8	S_{10}
R0	2.19 M	6.56 M	13.13 M	21.88 M	32.82 M
R1	21.15 M	63.46 M	126.91 M	211.52 M	317.28 M
R2	303.79 M	911.36 M	1.82 B	*	

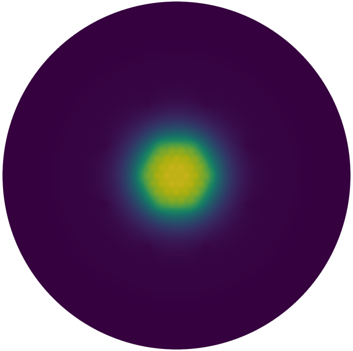
MARVEL Reactor Results



Thermal scalar flux.
$E < 0.625\,\text{eV}$



Epithermal scalar flux.
$0.625\,\text{eV} < E < 6\,\text{keV}$



Fast scalar flux.
$E > 6\,\text{keV}$

Mesh Refinement Effects

Two entirely separate effects:

1. Better describe curved geometry.
2. Decrease characteristic mesh size.

- 1.64 % fuel volume error for R0 mesh.
- Brief investigation of "mesh correction" methods.
  - Equidistant vertices.
  - Volume preserving meshes.
  - Cross section correction.
- Eigenvalue change due to refinement is mostly attributable to improved mass conservation.

Refinement	Corrected	Uncorrected	Difference [pcm]
R0	1.334 091	1.326 872	721.88
R1	1.338 354	1.336 790	156.41

MARVEL 2D S_8 Results.

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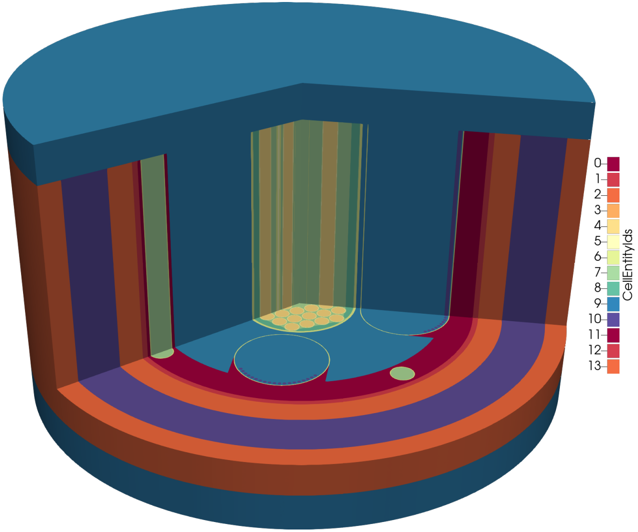
MARVEL 3D Model



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Next Steps

- Improved GPU utilization.
  - HYPRE+GPU.
  - “Partial”/tensor assembly of linear forms on GPUs.
- “Large” meshes.
- Heat conduction multiphysics feedback.
- Demonstration of three-dimensional results.

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Thank You!

Thank you all for your attention this afternoon!

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