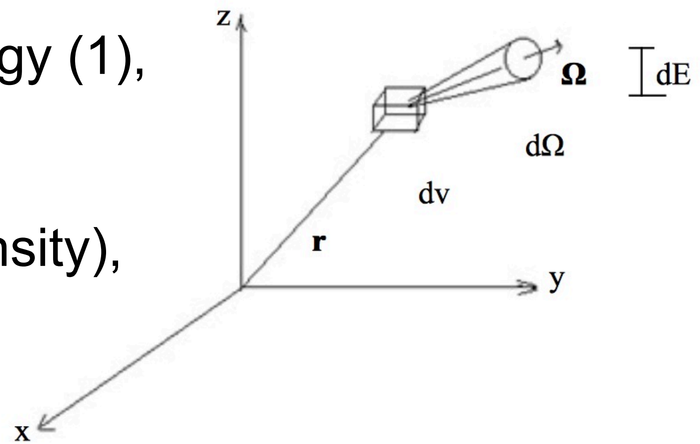
# Rattlesnake: A MOOSE/LibMesh based Multiscale Neutronics Application

Sebastian Schunert, Yaqi Wang, Mark DeHart

Idaho National Laboratory

# The Radiation Transport Equation (RTE)

- Describes transport of uncharged particles (neutrons, photons) in a host medium
- Phase space 7-dimensional! Space (3), energy (1), direction of motion (3), time (1)
- Solve for angular flux ψ (speed * neutron density), typically # DoFs high




$$\frac{1}{v}\frac{\partial\psi}{\partial t}+\hat{\Omega}\cdot\nabla\psi+\sigma_t(\vec{r},t)\psi(\vec{r},E,\hat{\Omega},t)=\int_0^\infty\int_{4\pi}\sigma_s(\vec{r},t,E',\hat{\Omega}'\rightarrow E,\hat{\Omega})\psi(\vec{r},E',\hat{\Omega}',t)\,d\hat{\Omega}'\,dE'$$

- Linear integro-differential equation, first order, hyperbolic
- Nonlinearity comes from coupling: cross sections depend on temperatures, density changes etc.

# Alternative Forms of the RTE

1. Diffusion approximation:
   1. Approximation of transport equation => linearly anisotropic
   2. Diffusion type equation for each energy group
2. SAAF equations:
   1. 2nd order form of the transport equation
   2. Elliptical set of equation (as opposed to hyperbolic)
3. Operator Notation:

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \boxed{L}\psi = \boxed{S}\psi + \boxed{F}\psi$$

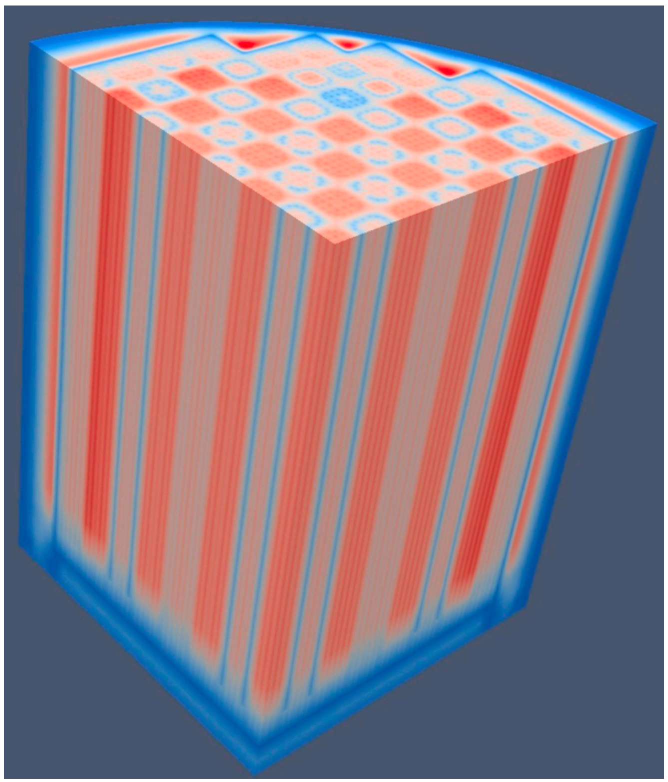
Streaming & Collision
Lower triangular

Scattering

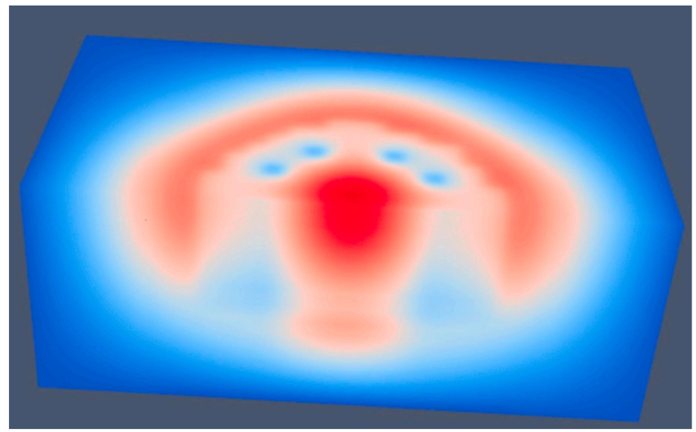
Fission

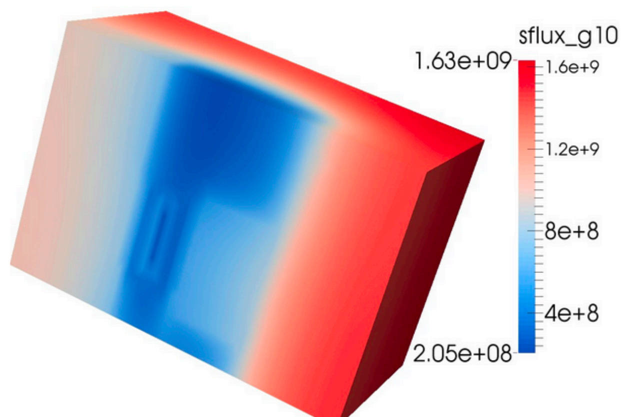
# Rattlesnake Applications

*PWR: BEAVRs benchmark RMS: 4% (OPENMC: 5.4%)*

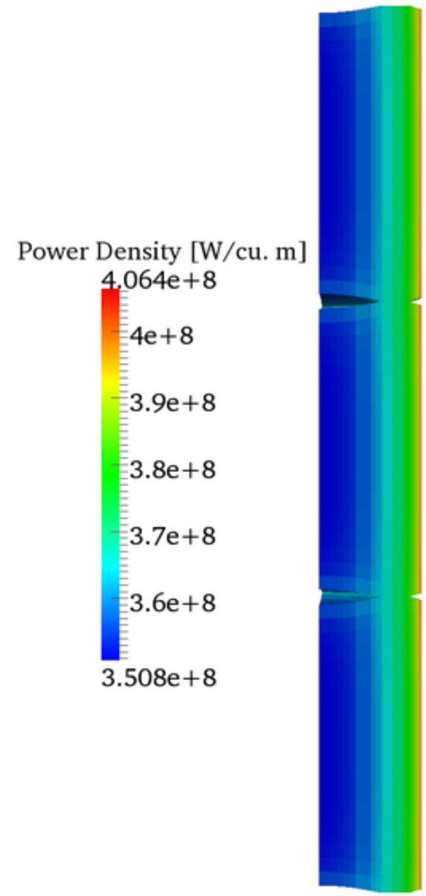


*TREAT transient analysis & experiment modeling*



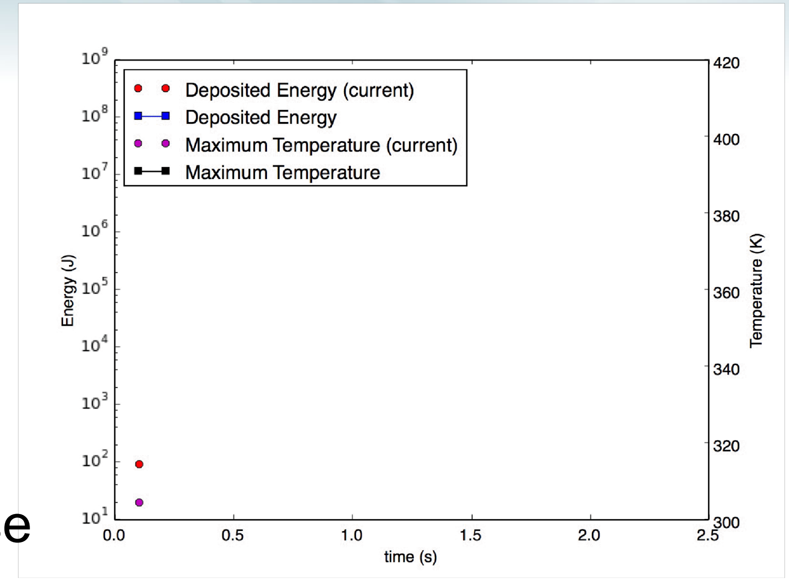


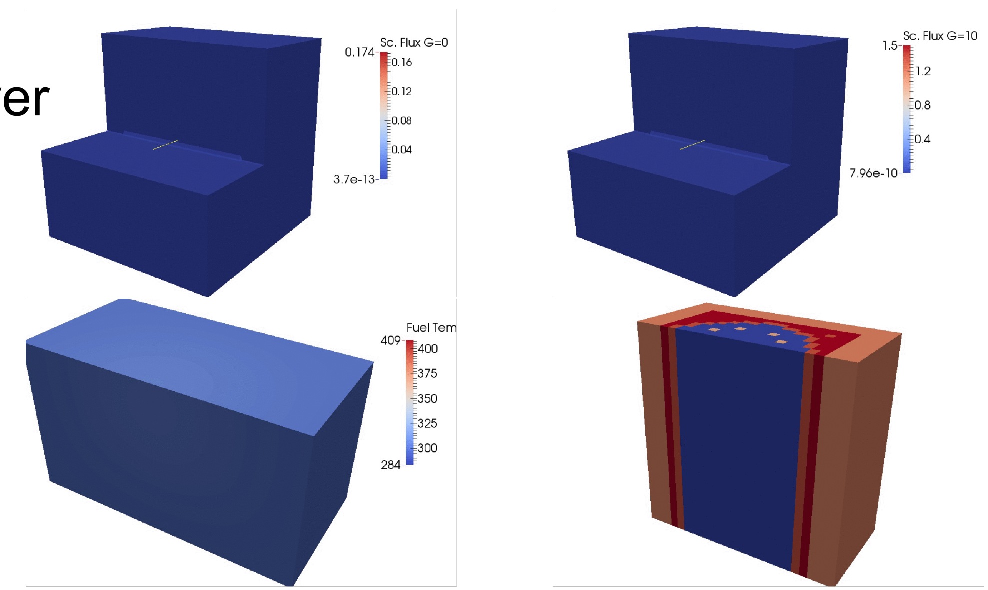

*Drive Fuel Performance*



# Transient-15

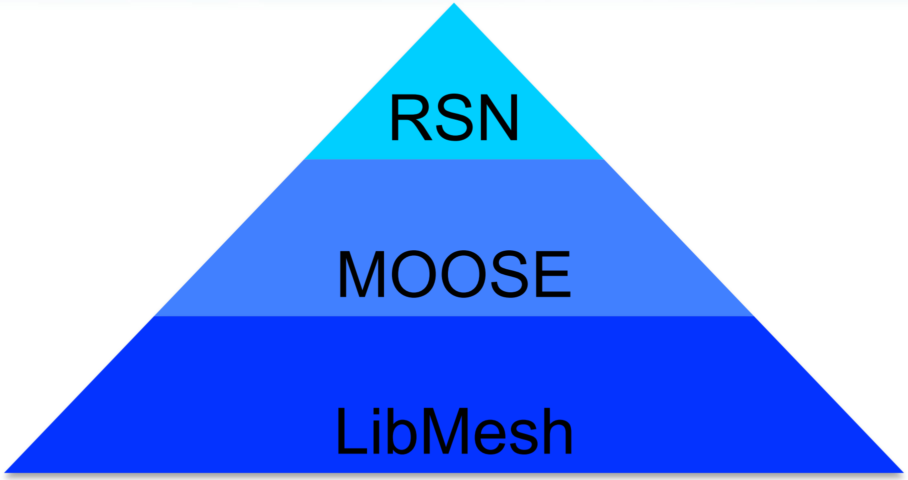
- TREAT: transient reactor for fuel testing
- Graphite with tiny fuel particles
- Experiment contains tested fuel
- Insert reactivity => power increase (10-20 GW)
- Thermal shift kill reactor power



# Why is Rattlesnake different?

*Oscillating Godiva Experiment*




| Rattlesnake | Standard transport code |
|---|---|
| Built on LibMesh | Custom spatial discretization |
| Natural coupling with MOOSE apps | Customized via (fragile) interface |
| Full Newton, Picard, loose coupling | Loose coupling or Picard |
| Material properties evaluated at Qps | Constant element properties |
| 2nd order mixed mesh fully supported | 1st order mesh, one or few element types |
| Inherits timestepping, AMR etc. | Usually focused on transport only |
| Framework performance penalty | Streamlined |

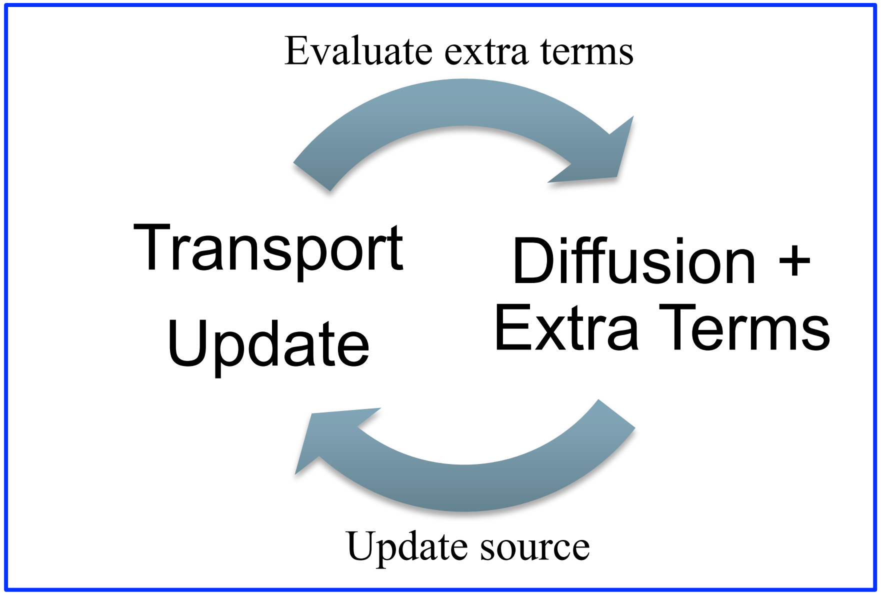
# *Flexible Nonlinear Diffusion Acceleration (NDA)*

- Transport Update

$$Q = S\psi^{p,n+1} + F\psi^{p,n+1}$$

$$\psi^{p+1,n+1} = L^{-1}Q$$

- $L^{-1}$ computed via
  - transport sweep (1st order)
  - BoomerAMG V-cycles (SAAF)
- Flexible 1st order NDA method
  - Transport: DGFEM discretization
  - Diffusion: interior penalty DGFEM (advantage: linear/ quadratic expansion)
- Allows transport & diffusion shape functions & mesh to be different

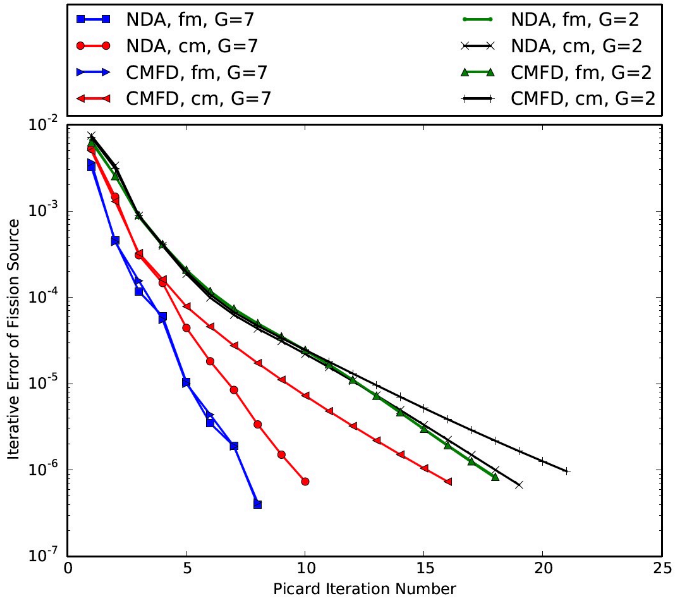


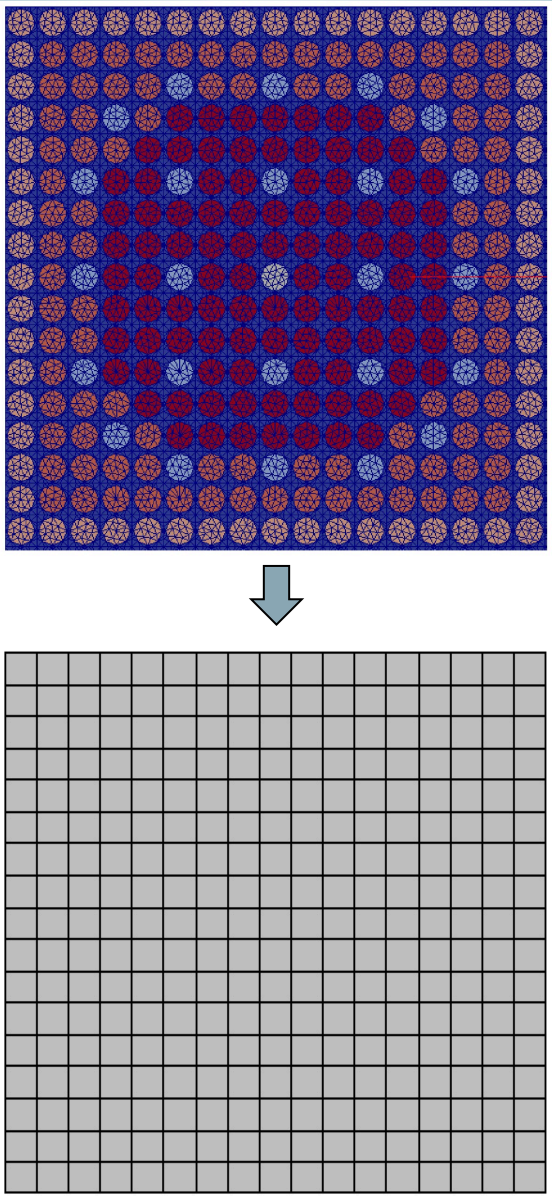

*Picard iteration scheme*

# Flexible NDA – 2 (Example)

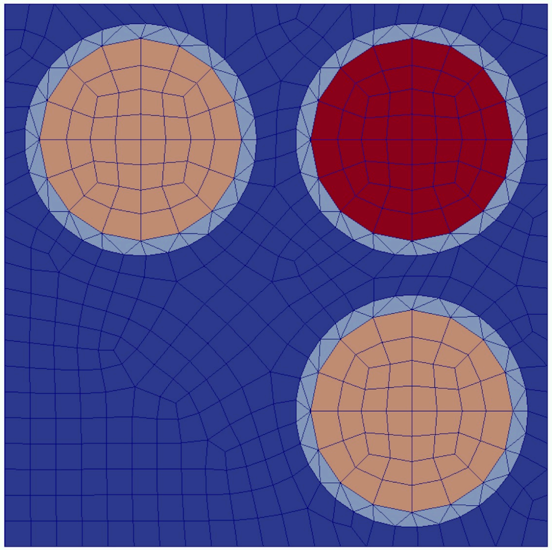
- Flexibility from FEM Projection & Prolongation
- C5G7 with pin-cell homogenized diffusion
- Results: Flexible NDA better than standard for pin-cell homogenized diffusion

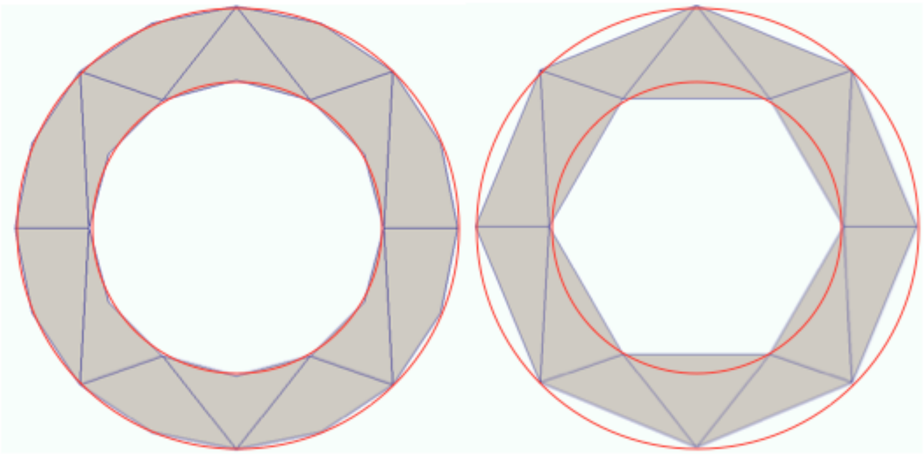
| | NDA | CMFD |
|---|---|---|
| Fine | 8 | 8 |
| Coarse | 10 | 16 |



# Second Order Sweeps - 1



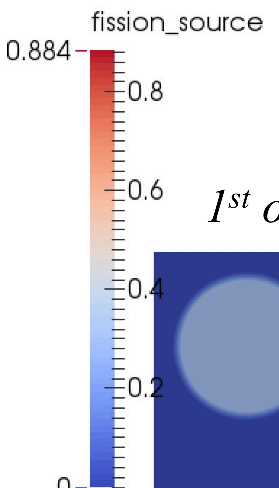



- $2^{nd}$ order mesh: edges are not straight lines but $2^{nd}$ order curves
- Highly beneficial for typical light water reactor geometries (pin/cladding)
- Ideas:
  - GMRES solution on $2^{nd}$ mesh; precondition with sweep on $1^{st}$ mesh
  - Use NDA [diffusion & transport source], sweep on $1^{st}$ mesh
  - Both approaches are novel (to our knowledge)

# Second Order Sweeps - 2

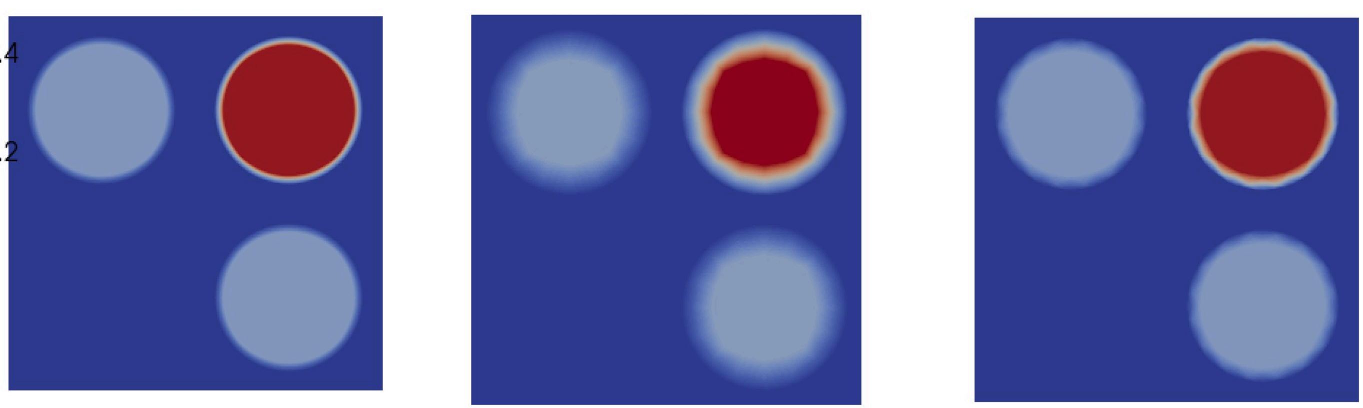
- Results using 1st order mesh, 2nd order mesh, 2nd mesh / sweep 1st mesh
- Multiplication factor $k_{eff} = \dfrac{\text{Neutron Production}}{\text{Neutron Losses}}$

| keff | Direct (sweep prec.) | NDA | Reference |
|---|---|---|---|
| 1st order | 0.710411 | 0.710411 | 0.733041 |
| 2nd order | 0.733685 | 0.733683 | - |
| 2nd order/ 1st sweep | 0.733685 | 0.733683 | - |

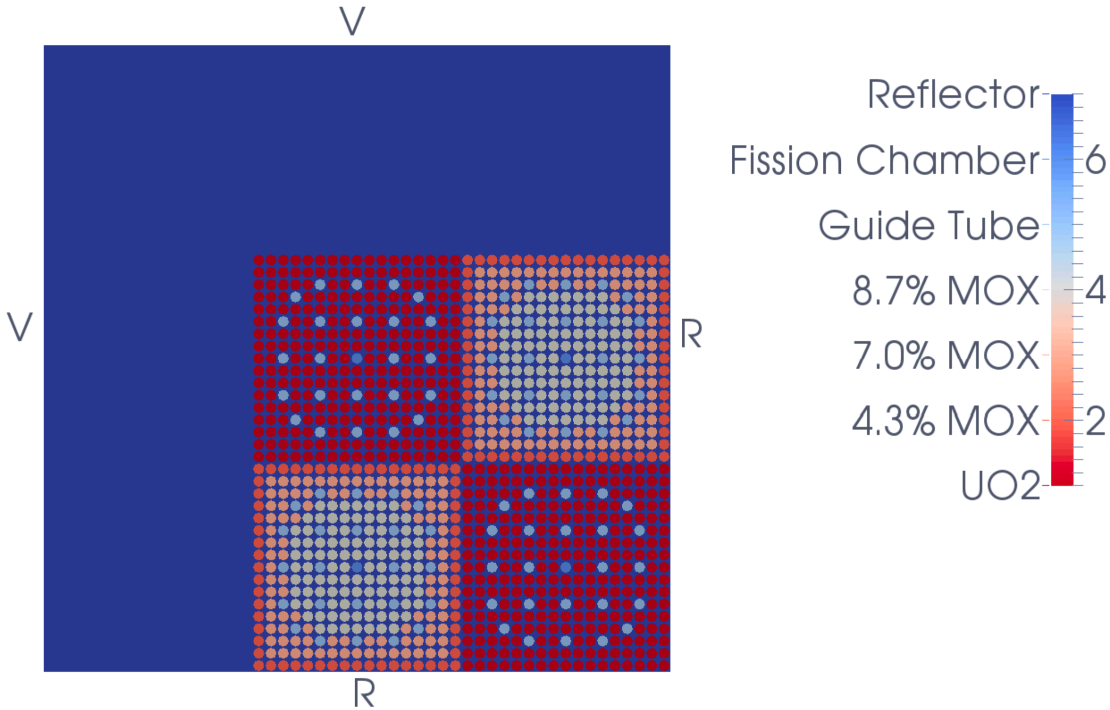


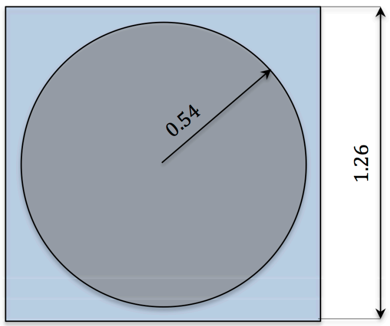

## Fission Source Distribution

*1st order reference*    *1st order*    *2nd order*



# C5G7 Solutions with SAAF-$S_N$

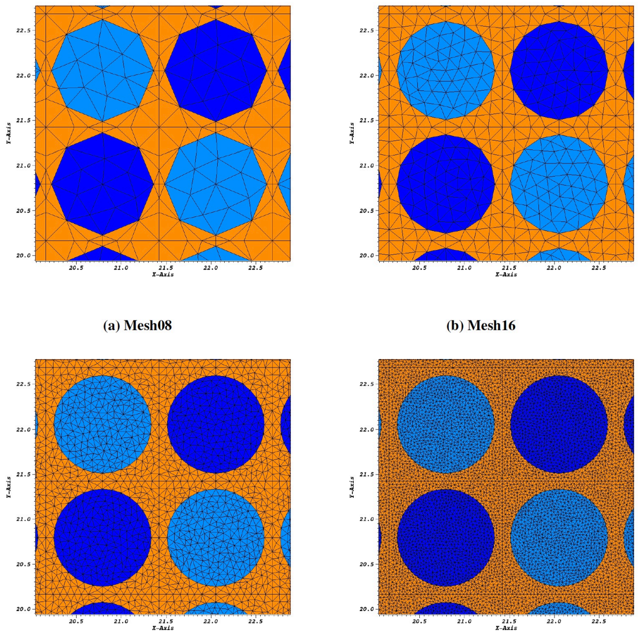



- C5G7 is a 2D neutronics benchmark, 2x2 assemblies minicore
- Rattlesnake SAAF-SN solution with up to 4.5 x $10^{10}$ DoFs (45 billion)
- Largest all-in-one PETSc system?

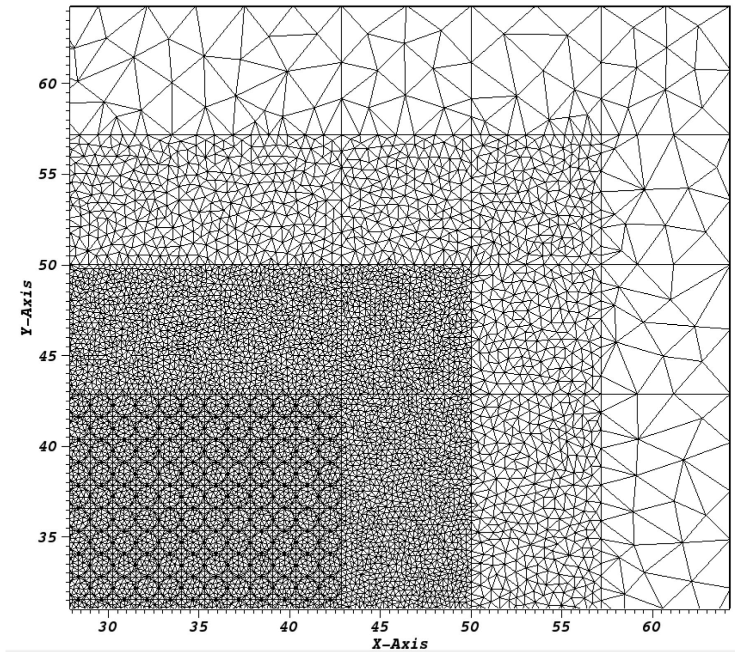
# C5G7 Solutions with SAAF-$S_N$ - Discretization

| Mesh | #elem |
|---|---|
| 8 | 87,108 |
| 16 | 265,577 |
| 32 | 1,033,668 |
| 64 | 4,216,587 |



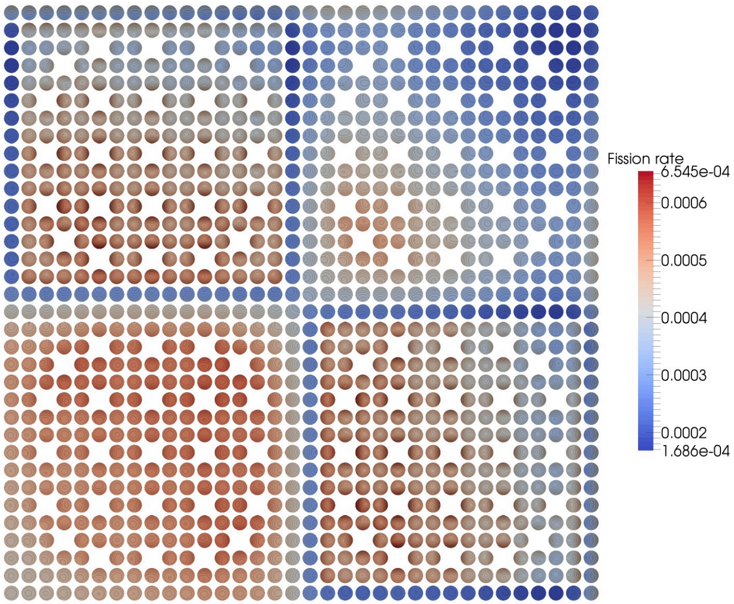
(a) Mesh08

(b) Mesh16




- Angular Discretization (# direction): NA=8-64, Np=2-5, (1280 directions)
- SAAF a coupled system of elliptical equations
- K-eigenvalue calculations (forced steady-state) solved via NDA ($L^{-1}$ via multiple V-cycles & BoomerAMG)

# C5G7 Solutions with SAAF-$S_N$ - Results




*Fission rate, Second order elements, Mesh 32, $N_A$ = 64, $N_p$=4*

| Notable Results | |
|---|---|
| Error $k_{eff}$ (%) | <$10^{-3}$ % |
| Avg. Pin Power (%) | 0.004 |
| RMS Pin Power (%) | < 0.001 |
| Mean Rel. Pin power (%) | 0.005 |
| # Picard NDA iterations | ~7 |
| Runtime (45 billion DoFs) (2376 CPUs) | 5.6 h |

- Reference: MCNP5 Monte Carlo calculation
- Nailed the eigenvalue to < 1pcm
- Nailed power distribution to < 0.001 %
- Efficient execution using < 10h & < 10 (NDA) Picard iterations

## Conclusions

- Rattlesnake is a LibMesh/MOOSE based radiation transport solver
- Designed for multiphysics applications & unique coupling capabilities
- Strong focus on transient capabilities
- Unique examples in this talk
  - Effective & flexible NDA method & application to C5G7
  - Second order sweep capabilities (novel approach)
  - Largest (?) PETSc system ever solver in SAAF-$S_N$ C5G7 solution
- Unique challenges: solve highly specialized, huge systems in a general framework!