Neutronics Code Development at Argonne National Laboratory

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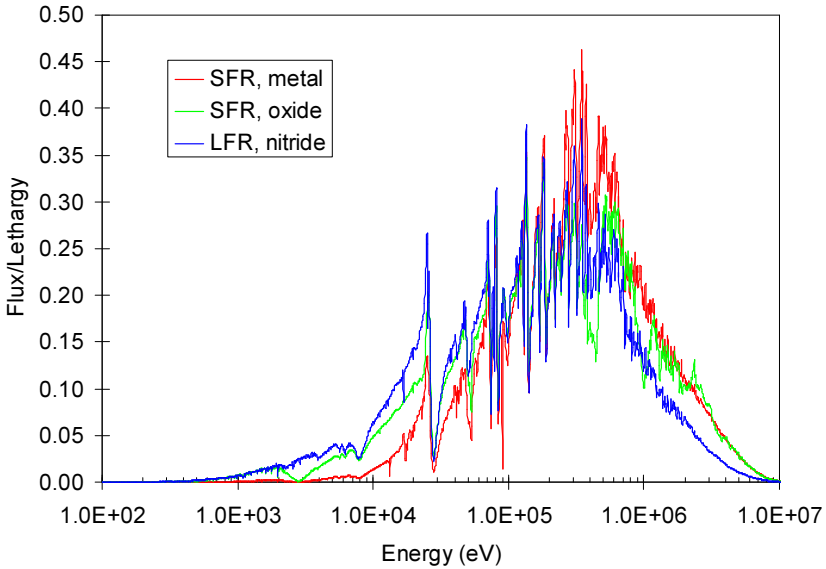
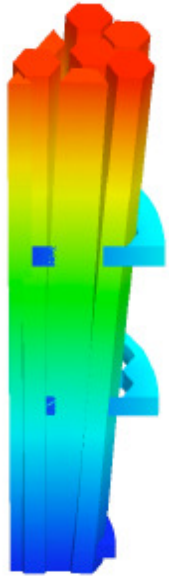
Fast Reactor Modeling and Simulation Challenges

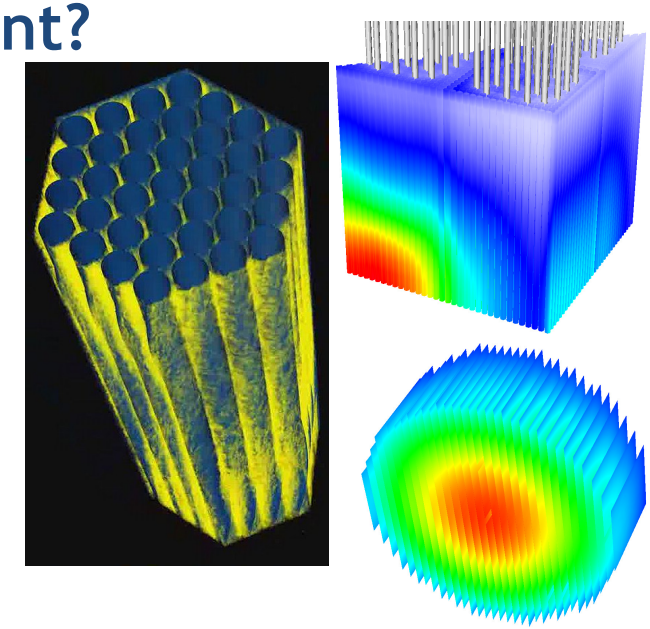
- Detailed energy modeling
  - Lack of a 1/E spectrum as a basis for resonance absorption calculation
  - Inelastic, (n,2n), anisotropic scattering are of great importance
- Long neutron mean free paths
  - Neutron leakage is enhanced, 25% at moderate sizes
  - Local reactivity effects impact entire core



- High leakage and heterogeneous core configurations challenge design methods
  - Transport effects are magnified
  - Spectral and directional transitions at the core and reflector interface are hard to model
  - Core reactivity is sensitive to minor geometric changes
    - Integration with thermal-hydraulics and structural mechanics analyses to account for reactivity feedbacks due to geometry deformation accurately



High Fidelity Modeling, What is the point?

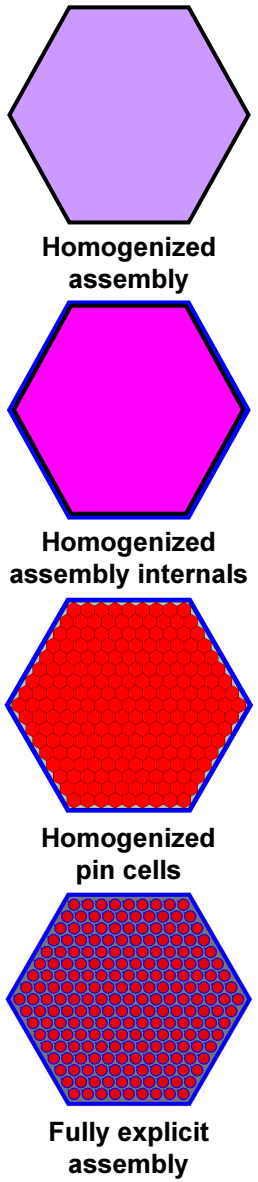


- The existing approach: Homogenized assembly
  - Vast reduction of space-angle-energy dofs
  - Focused on producing the global gradient
  - Reconstruct: local and global solution must be merged
- Explicit geometry core calculations?
  - $>10^{10}$ degrees of freedom requires some parallelism
  - Few large problems have been attempted
- Can we improve the existing calculation accuracy?
  - Not really concerned about depletion in short term
    - Errors in cross section data? Multi-group processing?
  - Material loading uncertainties
    - Are we solving a contrived problem; i.e. predicting the weather?
    - Not the case for ZPR and other similar benchmarks. Production reactors?
- Safety analysis was identified as one area of weakness that can be improved
  - Radial thermal expansion is generally treated poorly in neutronics
  - Above core mixing (thermal induced stress) is poor in CFD
  - Modeling of seismic event impacts on core and plant?

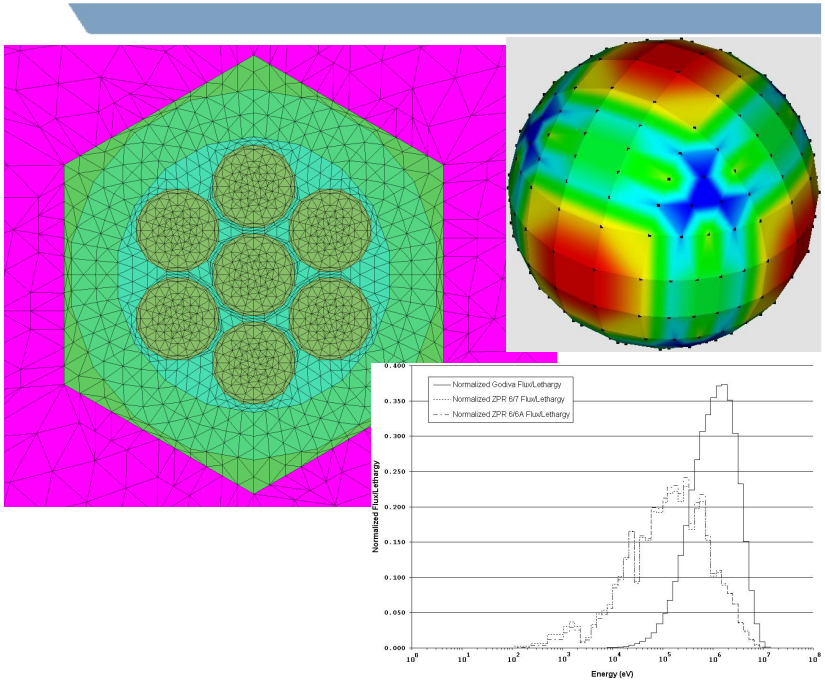
➢ Considerable development lead time before significant results can be achieved

Status of UNIC Code Development

- "Allow the existing reactor analysis work to transition smoothly from assembly level homogenization to less crude homogenization and eventually to fully heterogeneous descriptions"
  - Diffusion theory structured geometry solver (NODAL)
    - Reproduce nodal diffusion capability in existing tools
    - Can be extended to 1st order S_N or VARIANT
  - Even-parity transport equation with spherical harmonics (PN2ND)
    - Immediate use on problems with significant homogenization
  - Method of Characteristics (MOCFE)
    - Long term deployment and use on problems without homogenization
  - Even-parity transport equation with discrete ordinate (SN2ND)
    - Modeling transition region between PN2ND and MOCFE solvers
    - Still has the second-order limitations (voids?)
    - We still prefer to homogenize similar regions
- MC^2-3 module for in-line multi-group cross section generation
  - Hyperfine (~400,000) group transport capability for homogeneous mixture and 1-D slab and cylindrical geometries. Started 2-D work.



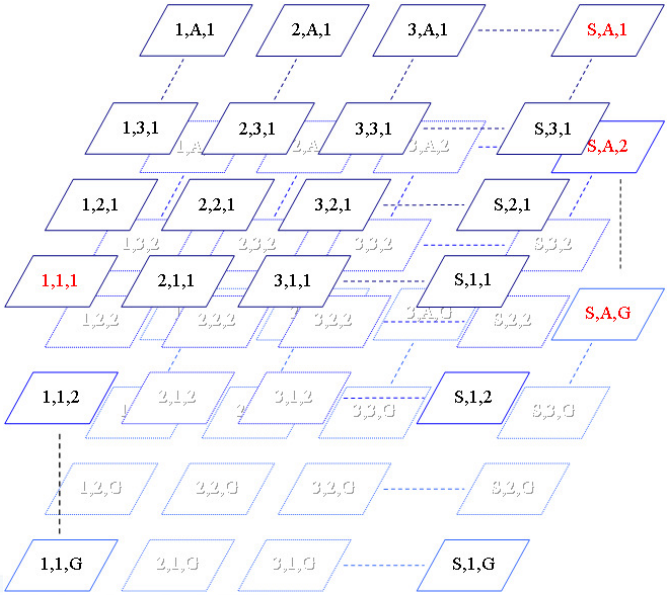
Parallelism in UNIC



- Novel?
  - Parallel transport studied for well over a decade
    - LANL, Sandia, French, Japanese,…
  - Production tools?
    - Unstructured mesh capabilities?
    - Parallel capabilities?
- Lessons learned at ANL
  - Parallelization in space-angle-energy is necessary
  - There are small, medium, and large parallel machines
    - Spatial domain decomposition is not best for all
    - Angle decomposition for S_N is generally good up to a limit
    - We have not studied energy decomposition at this point
  - Focused parallelization of L is not necessarily best idea

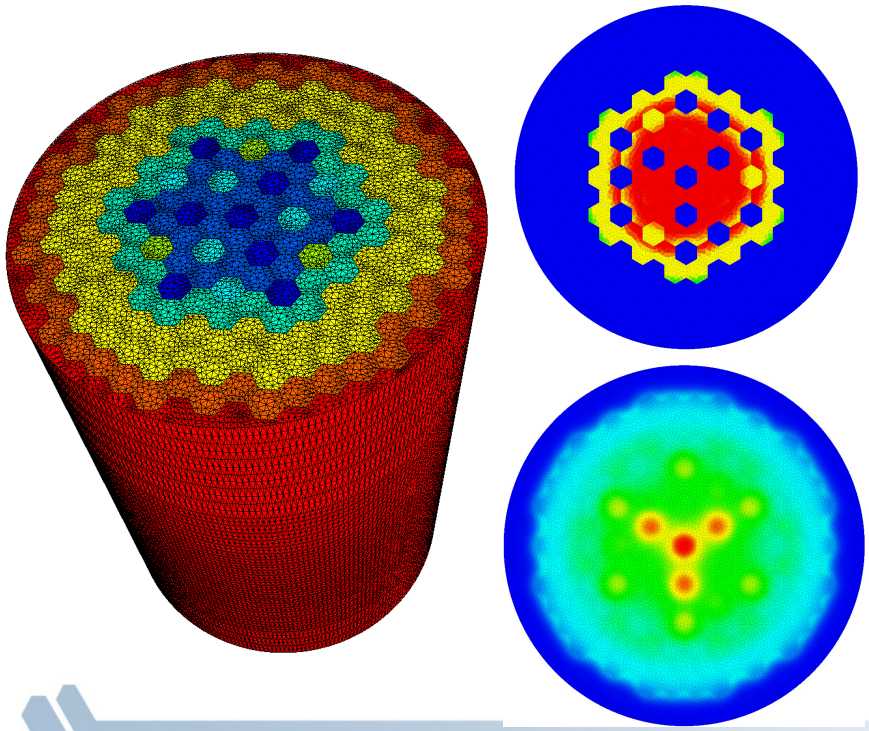
$$\left\{\begin{bmatrix} A_1 & 0 & 0 \\ \vdots & \ddots & 0 \\ W_{1\to G} & \cdots & A_G \end{bmatrix} + \begin{bmatrix} W_{1\to 1} & \cdots & W_{G\to 1} \\ 0 & \ddots & \vdots \\ 0 & 0 & W_{G\to G} \end{bmatrix}\right\}\begin{bmatrix} \Psi_1 \\ \vdots \\ \Psi_G \end{bmatrix} = \begin{bmatrix} S_1 \\ \vdots \\ S_G \end{bmatrix}$$

- Capabilities
  - PN2ND: 500-3,000 processors (2007)
  - SN2ND: 1,000-300,000+ processors
  - MOCFE and NODAL: unknown



Existing Approach (Assembly Homogenization)

- Typical approach used in fast reactor physics today
  - VARIANT residual error is due to P_N order and source approximation
    - Used 4th order source, 8th order flux, and 3rd order leakage
  - PN2ND residual error is due to P_N order and spatial mesh refinement
    - Used 109,740 hexahedral elements with 461,219 vertices
  - SN2ND residual error is due to spatial mesh refinement
    - Used Carlson even-moment (level symmetric) cubature



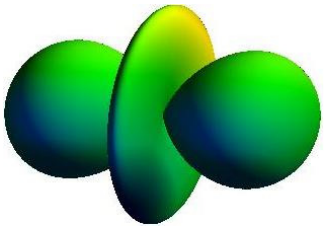
ABTR 33 group (120 periodic)

Eigenvalue error (pcm)

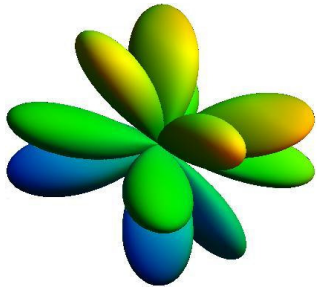
Angular Resolution	VARIANT	PN2ND	SN2ND
1	-1588	-1594	-192
2	-237	-249	-1
3	-91	-109	-69
4	-47	-70	-47
5		-55	-51

Assembly Level Homogenization (cont...)

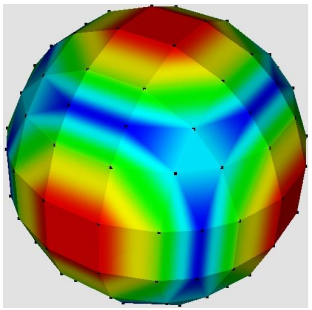
- VARIANT can easily out perform PN2ND and SN2ND
  - Uses hybrid finite element (nodal) combined with spherical harmonics
    - Spatial approximation includes discontinuities in even- and odd-parity flux
    - Defines much fewer degrees of freedom in assembly homogenized problems
  - Not currently ideal for all problems
    - 1/6 hexagonal ABTR with 230G, P_5-S_5 requires 14 hours of cpu time ($5 \cdot 10^8$ dofs)
    - ZPR drawer homogenized problems have convergence problems
    - Cannot treat void or pure scattering regions



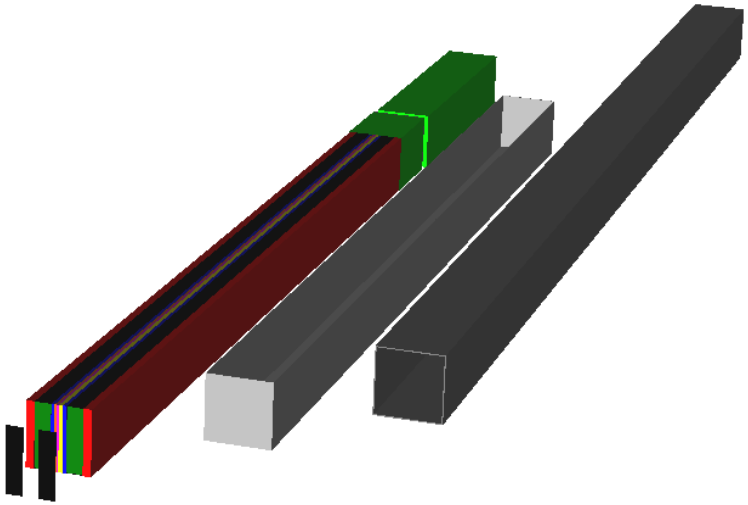
- PN2ND uses UFE combined with spherical harmonics
  - Even-parity unstructured mesh treatment assumes continuous even-parity flux
    - Requires careful boundary layer meshing (key weakness of method)
    - Increased memory storage relative to VARIANT and bandwidth limited flop rate
  - Uses a parallel CG operation on the WG space-angle system
    - Preconditioner is just diagonal angular sub-system
    - Use SSOR in parallel CG solver from PETSc on each angular sub-system



- SN2ND uses UFE combined with discrete ordinates
  - Mesh related problems are identical to PN2ND
  - Uses a scattering source iteration on WG space-angle system (CG on L^{-1})
    - Uses diagonal angular sub-system preconditioner
    - Uses SSOR via parallel CG solver in PETSc
    - Started development of multi-level h multi-grid preconditioner



ZPR6 Assembly 6A



Single ZPR6 Drawer

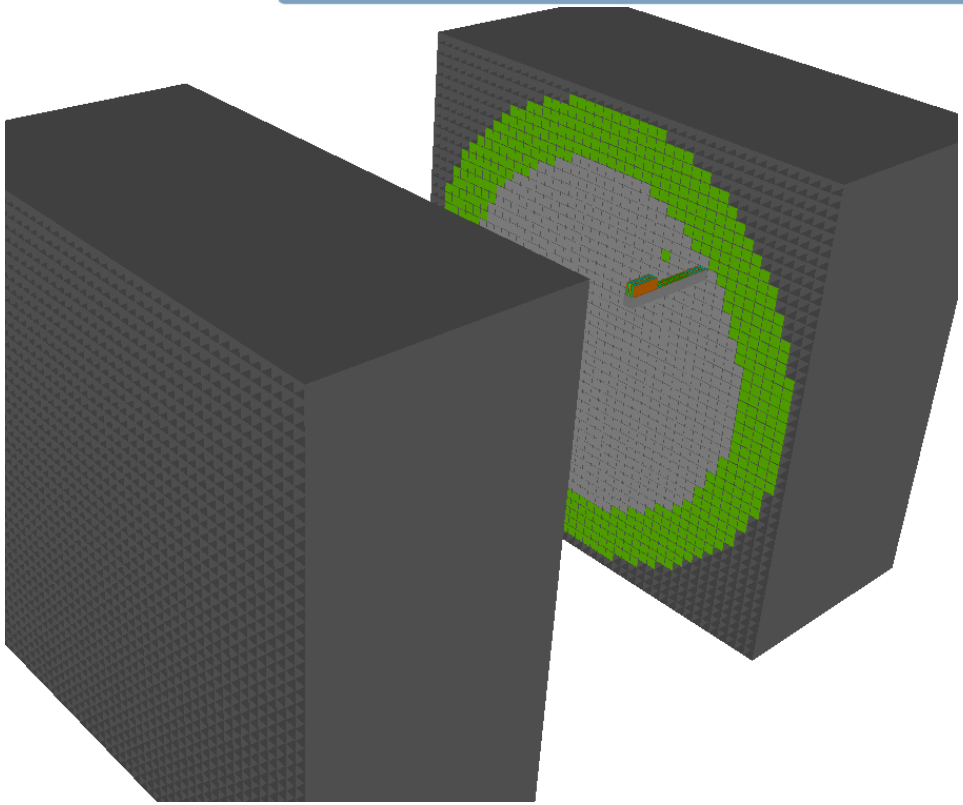
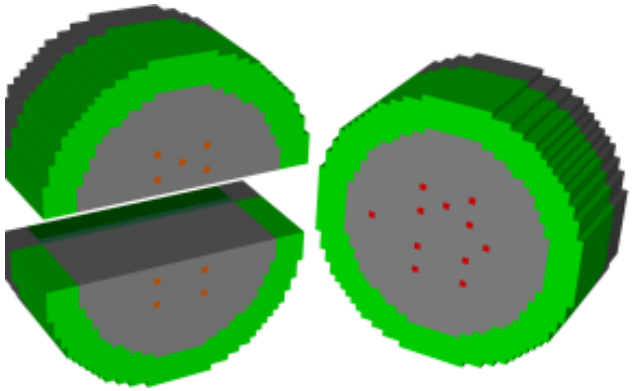


Plate by Plate ZPR6 Geometry

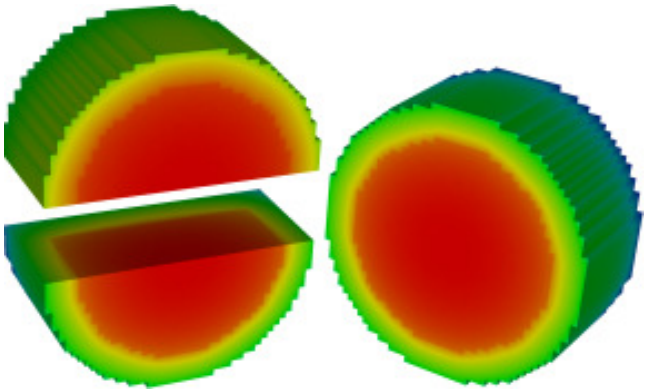
- Over a period of 30 years, more than a hundred ZPR critical assemblies were constructed at Argonne National Laboratory: ZPR-3, ZPR-6, ZPR-9 and ZPPR.
- The geometrical information for selected loadings is now widely available (ICSBEP)
- Materials are very well known compared with existing production reactors.
- In addition to experimental validation we can compare with CE MCNP/VIM solutions
- No concerns for multi-physics coupling

Standard Homogenized Approach

- Used 1-D “equivalent” lattice cell calculation to generate cross sections in MC^2-3
  - Homogeneous solution only gives the global gradient
  - Done to capture foil reaction rates and compare other reactor physics parameters
  - Need to combine global gradient with lattice cell calculation to extract solution
- Reference solution is experiment (i.e. critical)
  - SN2ND: 0.99966 VIM: CE 0.99981±0.00025
  - Ignoring plate heterogeneity
    - SN2ND: 0.99344 VIM CE: 0.99400±0.00020
- We have obtained similar results on ZPR 6/7 and ZPPR-15
- We are focused on using 2-D MOC for future cross section generation



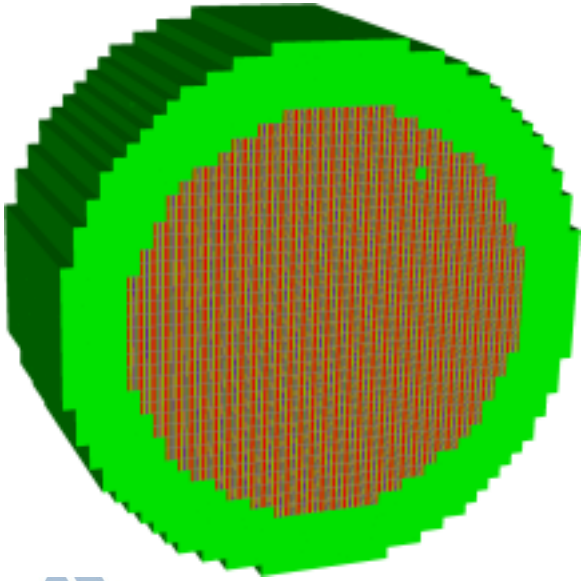
Geometry

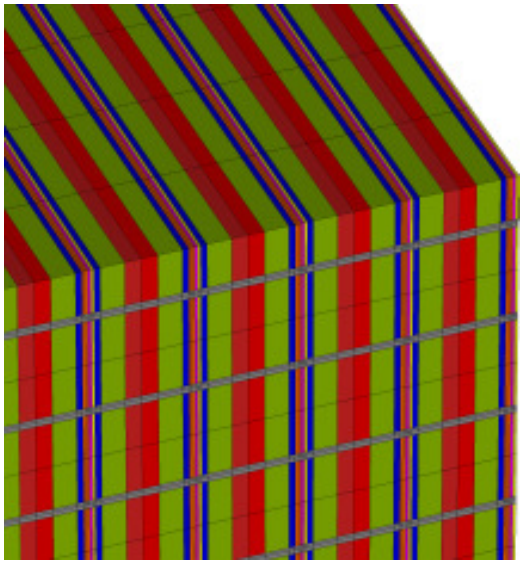


Power on a Log Scale

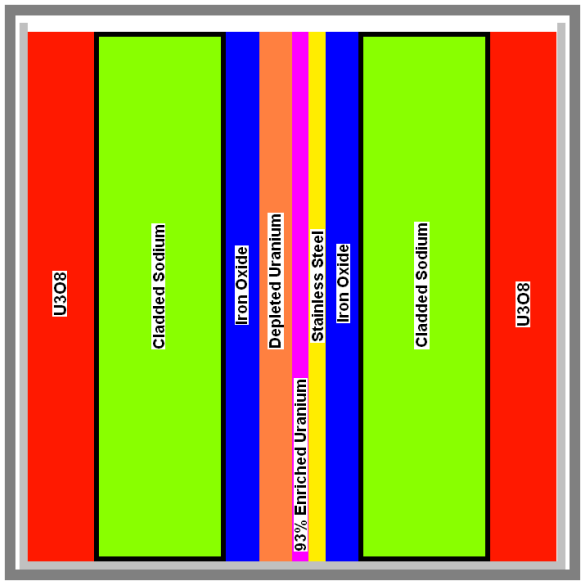
Plate-by-Plate ZPR6 Assembly 6A

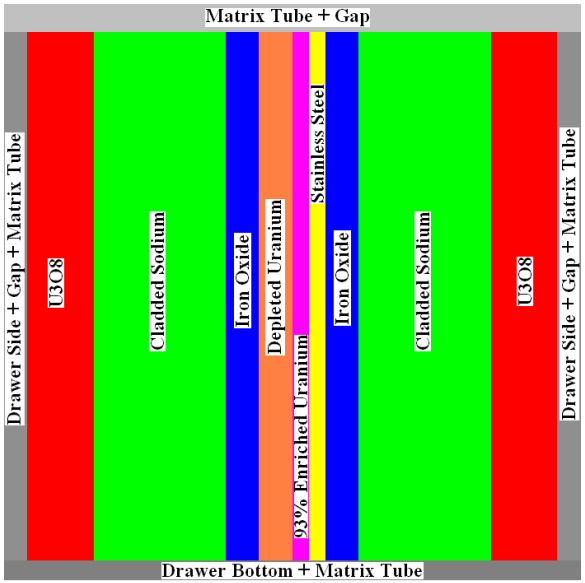
- SN2ND cannot handle explicit voids
  - Not really an issue for this problem
  - Development: $2 \cdot 10^6 \rightarrow +50 \cdot 10^6$ vertex mesh
  - 33 group calculation requires ~40 minutes on full parallel machine (~700 billion dof)
- Cross sections generated with 1-D lattice cell
  - The implementation of these cross sections in the explicit geometry model is not consistent.
  - The cross section data representation is inaccurate





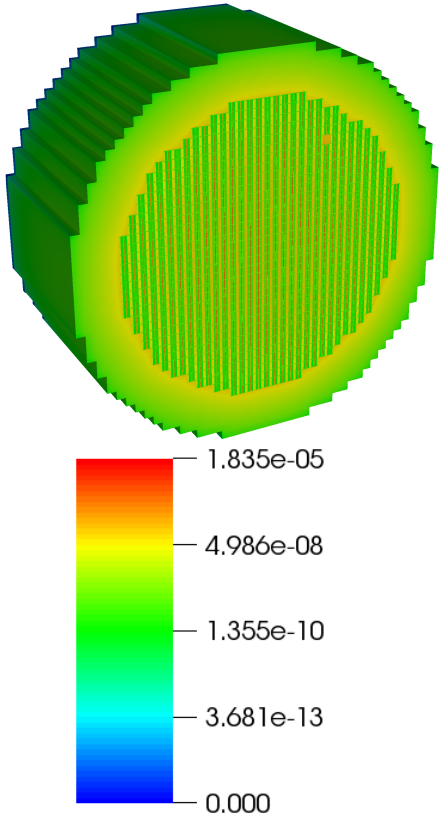
Exact Geometry

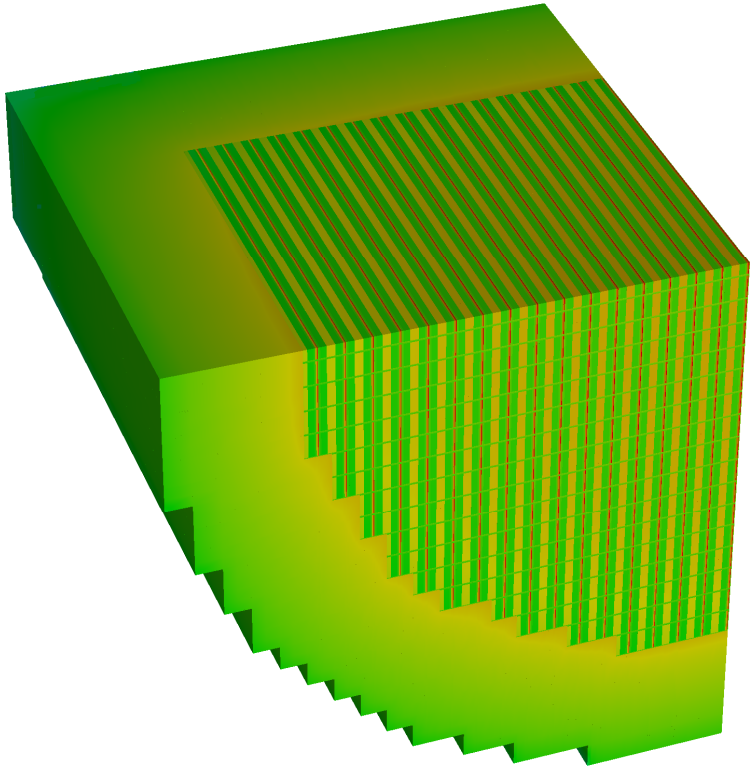


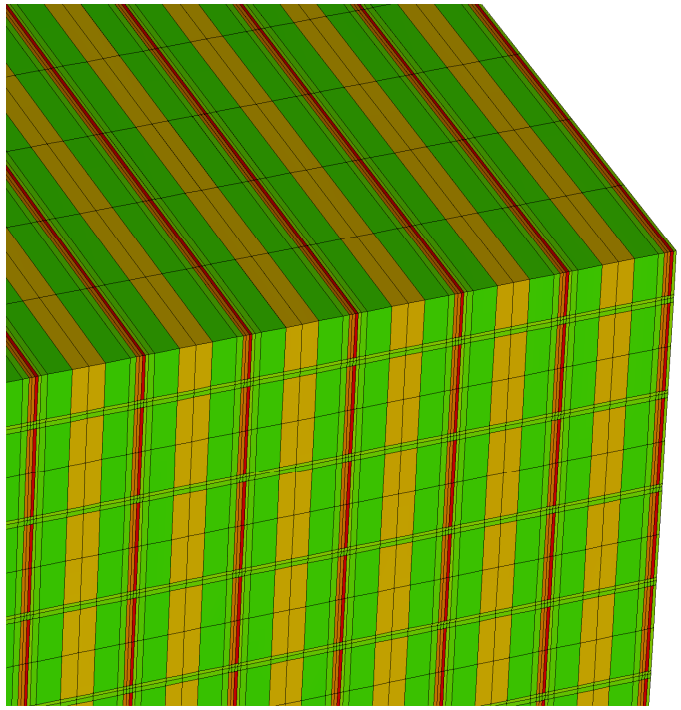


SN2ND Geometry

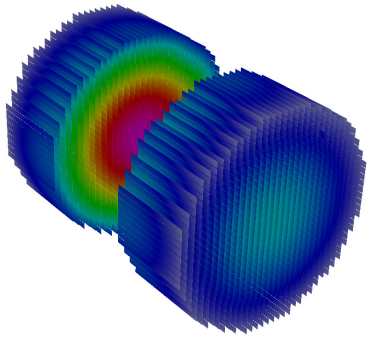
Plate by Plate ZPR-6 Assembly 6A, cont…





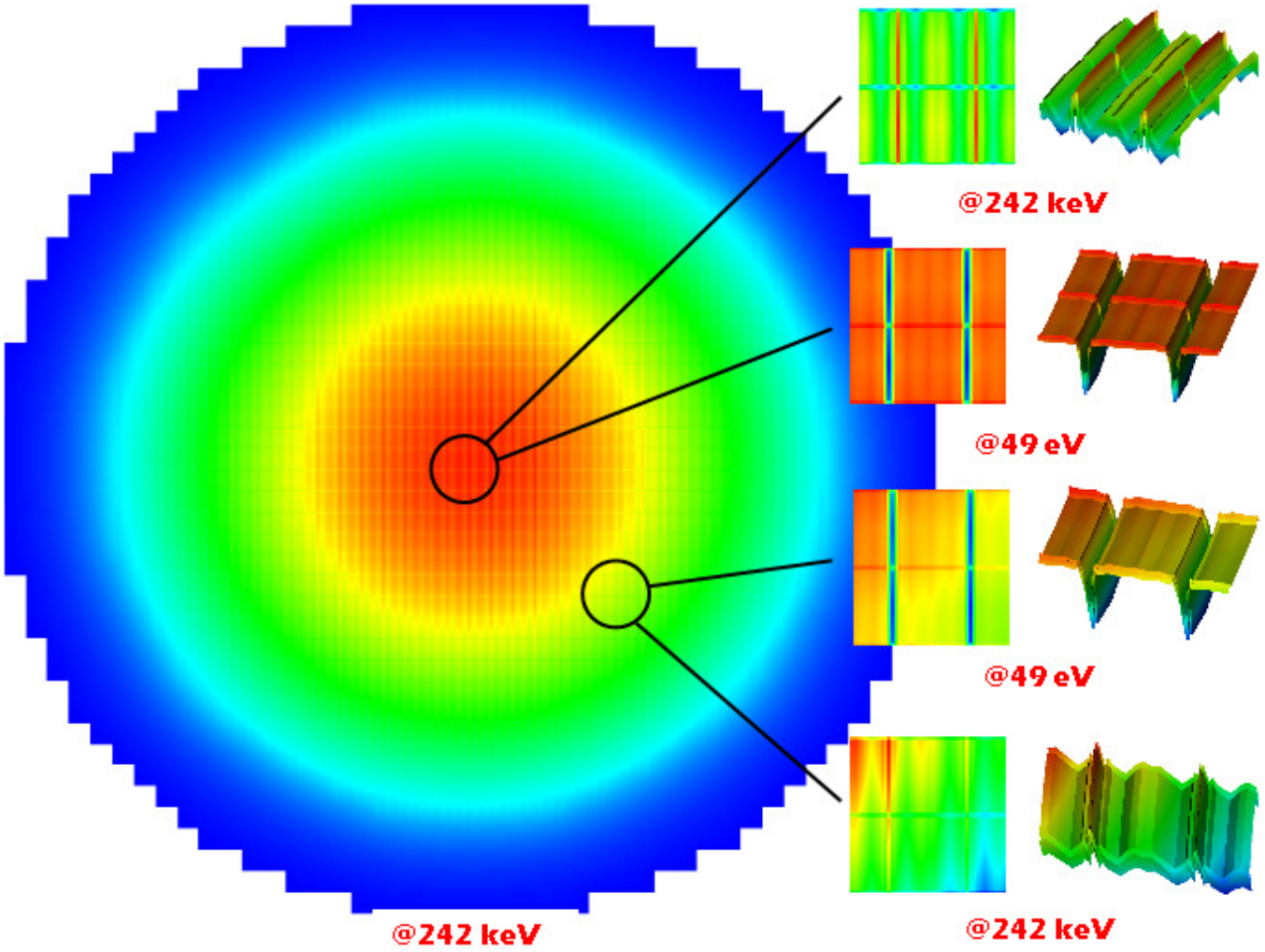


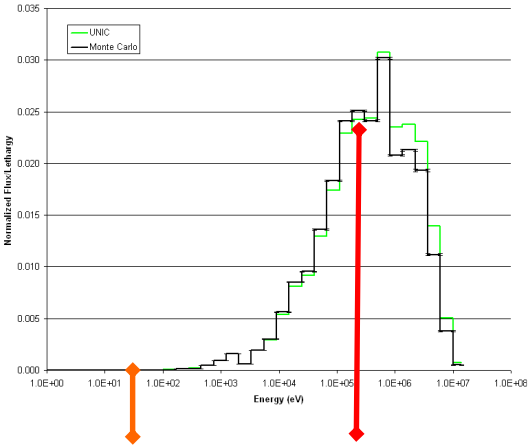
- Maximum of 116 group with P_5 scattering (9, 33, 70, 116)
- Maximum 50,000,000 vertex mesh (cubic hexahedrons)
- Maximum S_{28}, (LT or DLT)



Just EU plates

Flux Solution for ZPR6 Assembly 6A Experiments





49 eV **242 keV**

- Local gradients on drawers exhibit global gradient
- Resolved spatial gradients should result in better foil reaction rates

SN2ND Parallel Performance

- Strong spatial scaling of 94% on BlueGene/P-ANL

Total Cores	Vertices/ Process	Total Time (seconds)	Parallel Efficiency
8,192	7,324	2,402	100%
16,384	3,662	1,312	92%
24,576	2,441	873	92%
32,768	1,831	637	94%

Mainly measurement of PETSc

Strong scaling in angle is <75%

Diffusion equation needs further partitioning

- Weak angle scaling of 75% on XT5. 76% on BlueGene/P 294,912 cores JSC

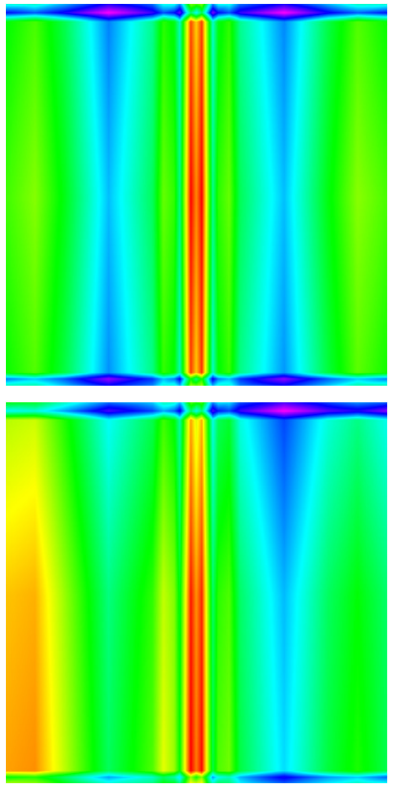
Total Cores	4π Angles	Total Time (seconds)	Weak Scaling
16,512	32	1891	100%
37,152	72	1901	99%
66,048	128	1829	103%
103,200	200	2050	92%
148,608	288	2298	82%
222,912	432	2517	75%

Weak scaling in space means mesh refinement for us

This can be good and bad. Refinement of bad aspect ratio elements produced >95%

Lessons Learned from ZPR

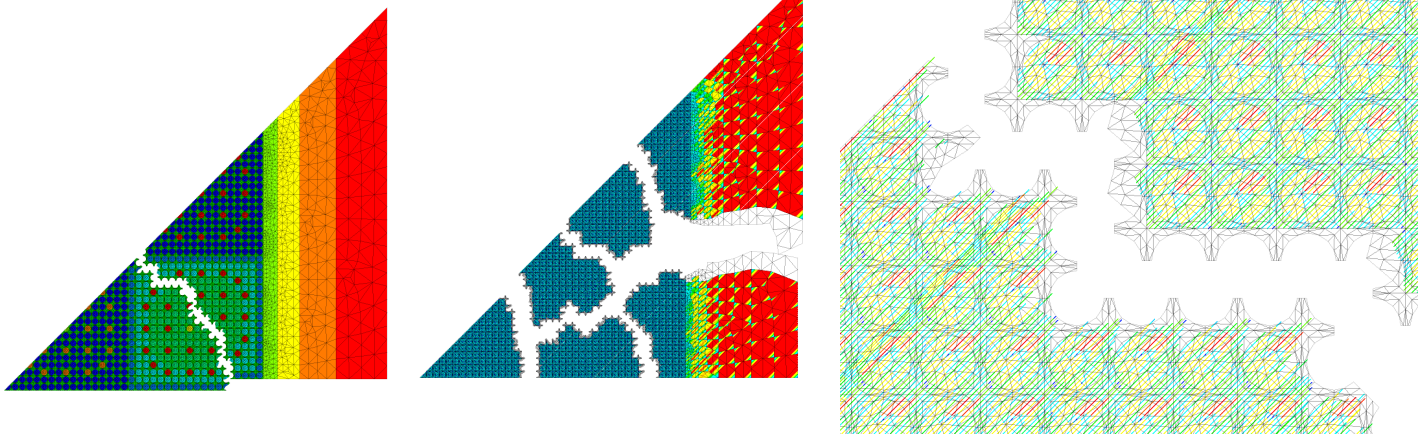
- Cross sections are not sufficiently accurate
  - 1-D model is appropriate and proves to be accurate for drawer average cross sections
  - Equivalence theory used to generate self-shielded ultrafine group cross sections is approximate
    - A hyperfine group (i.e., pointwise) calculation can help
  - Plate-by-plate cross sections may reduce the error, but the fundamental issue is that the global gradient is not seen in the cell lattice problem (either 1-D slab or 2-D MOC)
- New approach: Improve accuracy of legacy methodology
  - Incorporate global and local gradients via a 2-D MOC solution
    - Generate drawer homogenized cross sections
  - Use SN2ND or improved VARIANT to solve global homogenized problem
- With new capability we will research using plate-dependent cross sections in the radial plane

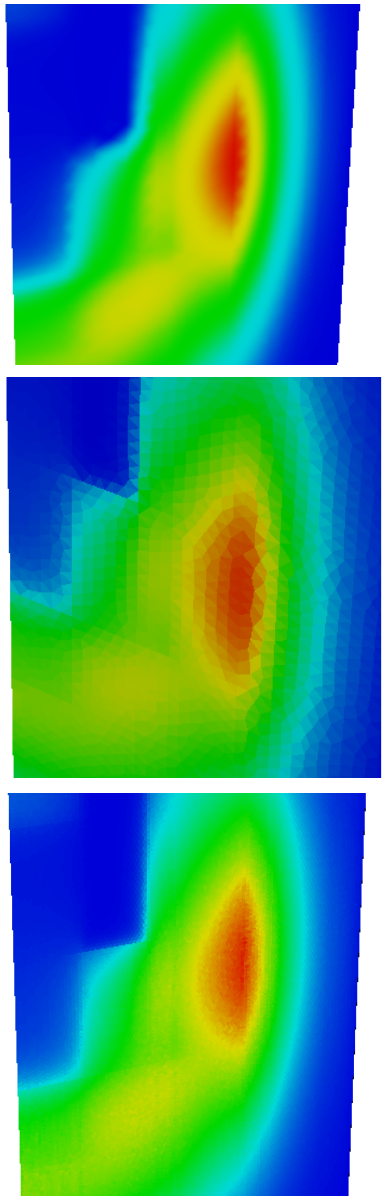


Flux at 243 keV
on Log Scale
Top is ~lattice calc.
Bottom is real world

The Future for Fast Reactor Cross Sections?

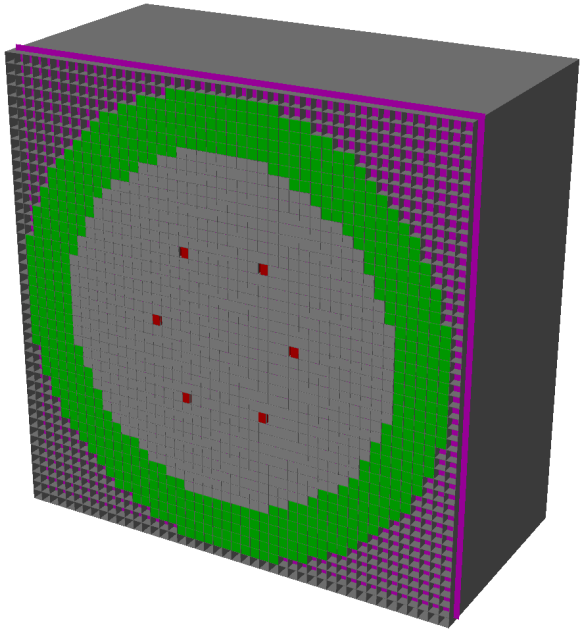
- In 2007 we researched a 3-D MOC for fine level solution
  - 10,000 to 1 element comparison with SN2ND
  - Parallel algorithm is relatively immature; ours was not scaling
- In 2009 we rebuilt 2D and 3D MOCFE solver
  - Easier to modify/maintain/develop
  - Faster ray tracing, exact domain surface discretization
  - Assumed a Krylov subspace method for spatial decomposition
    - More appropriate path for large scale parallelism
    - Assumes trajectory splitting and communication of trajectory flux
    - Needs research into good preconditioner (synthetic diffusion?)

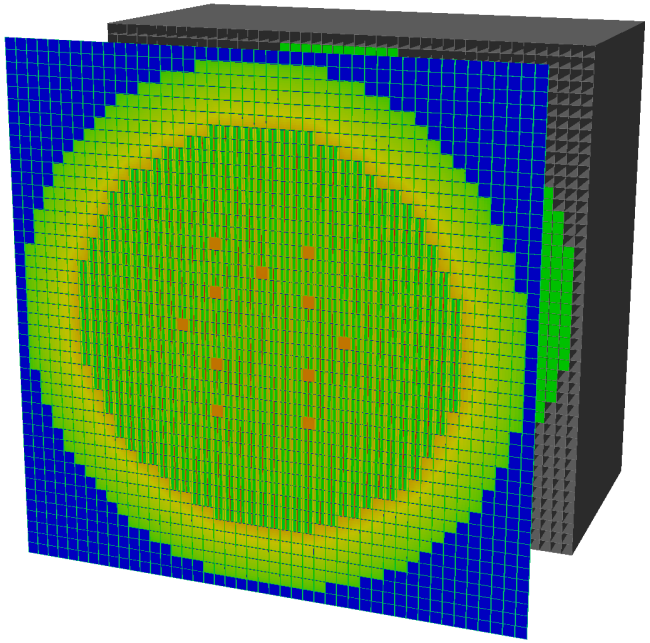


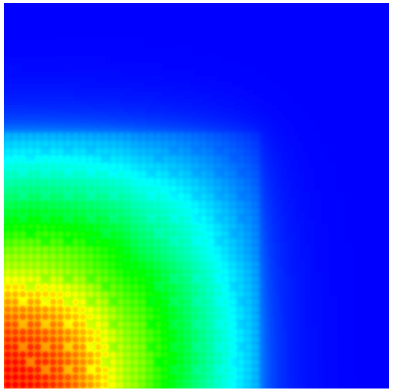


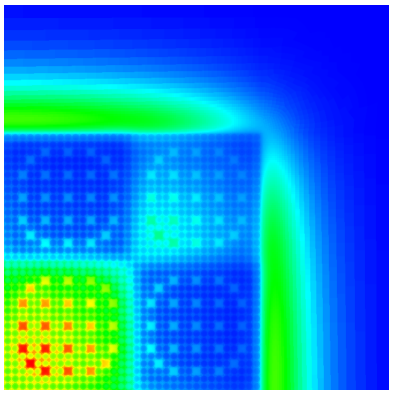
MOCFE continued

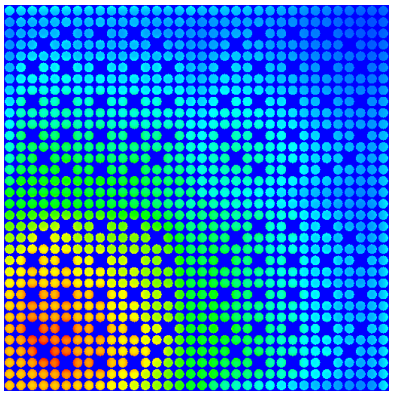
- New version is >10 times faster than old version
- Validated “accuracy” on C5G7, CANDU, ABTR geometries
- Working on PWR, BWR, VHTR, and ZPR geometries
- Haven’t tested out any parallel options
- Haven’t tested out the Krylov solver options
- Have no clue how well it compares to other MOC solvers











Future Work and Key Issues

- SN2ND
  - Implement multi-level h-multigrid preconditioner scheme
  - Implement error estimator for intelligent mesh refinement and accuracy assessment
  - Investigate parallel decomposition of energy with Krylov subspace methodology
  - ➢ Even with ~300,000 cores, direct whole core transport calculations are not practical yet
- Cross Section Generation
  - Optimize MC^2-3 code for speed and investigate parallel execution of work
  - Fully validate 1-D, 2-D, and 3-D MOCFE for parallel execution of space-angle-energy
  - Investigate option to use localized hyperfine-group spectrum calculation with fine-group whole core transport calculation
- "Intermediate" fidelity methods to perform routine design calculations (<<1000 processors)
  - 2D MOC calculation for cross section generation
    - New homogenization and group collapsing schemes
  - PN2ND or SN2ND calculation with homogenized pin-cell
  - Improved NODAL based code with assembly homogenization
    - Is there a potential for 2D/1D coupled schemes like DeCART?