HIGH PERFORMANCE COMPUTING CHALLENGES ENCOUNTERED IN HIGH-RESOLUTION REACTOR CORE SIMULATION

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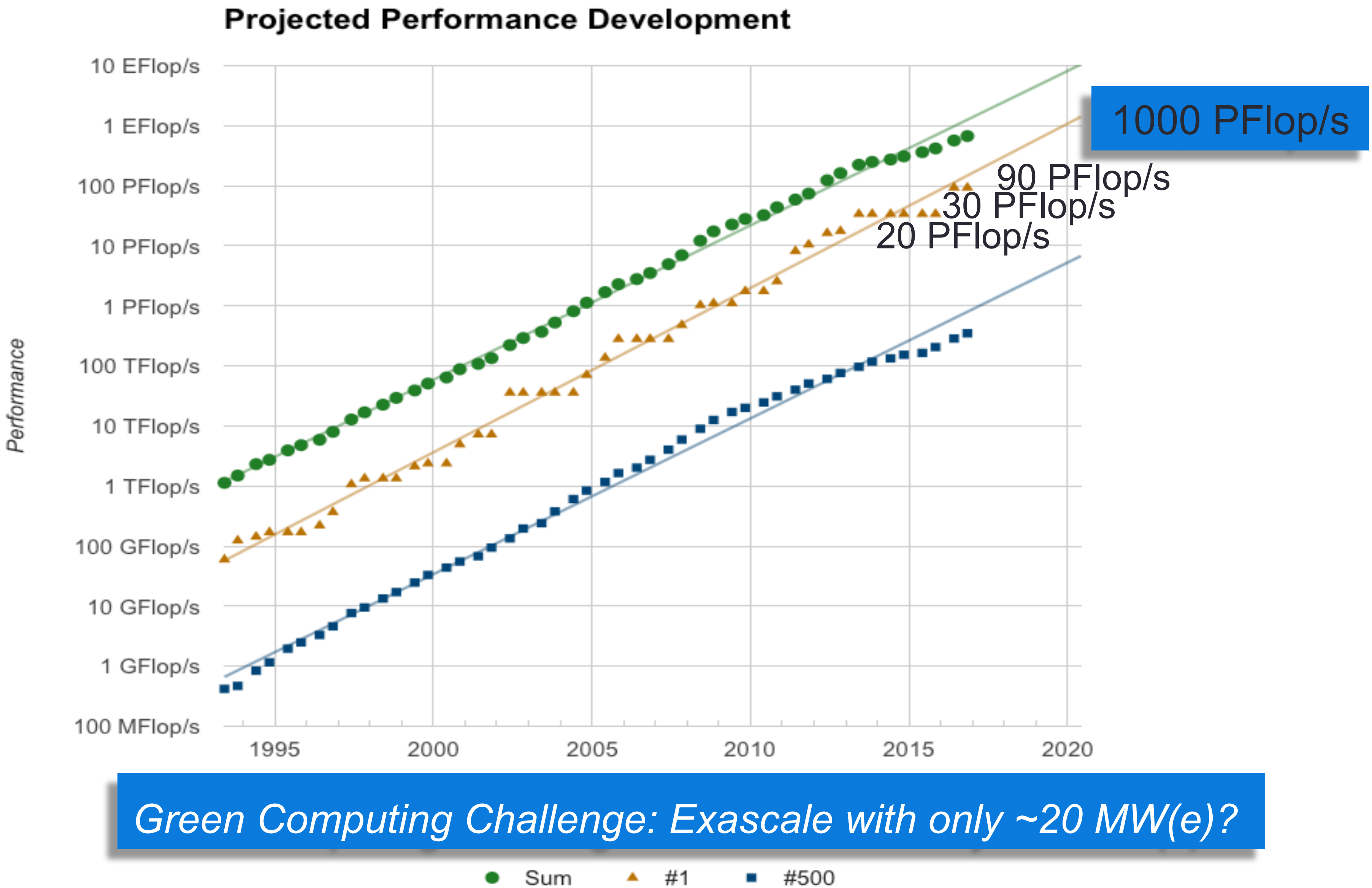
Presentation Outline

- *Some HPC machine and programming perspectives*
- *Nuclear reactor multi-physics HPC challenges*
    - *Stochastic (Monte Carlo) neutron transport*
    - *Deterministic neutron transport*
    - *Hybrid transport methods*
- *Lessons from historical reactor methods development*
- *Summary*

HPC Leadership Class Machines - lots of cores

Titan	Tianhe-2	TaihuLight
Cray XK7 2.2 GHz AMD Opteron	Intel 2.2 GHz Ivy Bridge	Sunway 1.45 GHz Sunway
~300,000 cores	~3,000,000 cores	~11,000,000 cores
19,000 NVIDIA K20x GPUs	900,000 Intel Xeon Phis	-
8 MW(e) 19 PFlop/s	18 MW(e) 34 PFlop/s	15 MW(e) 93 PFlop/s

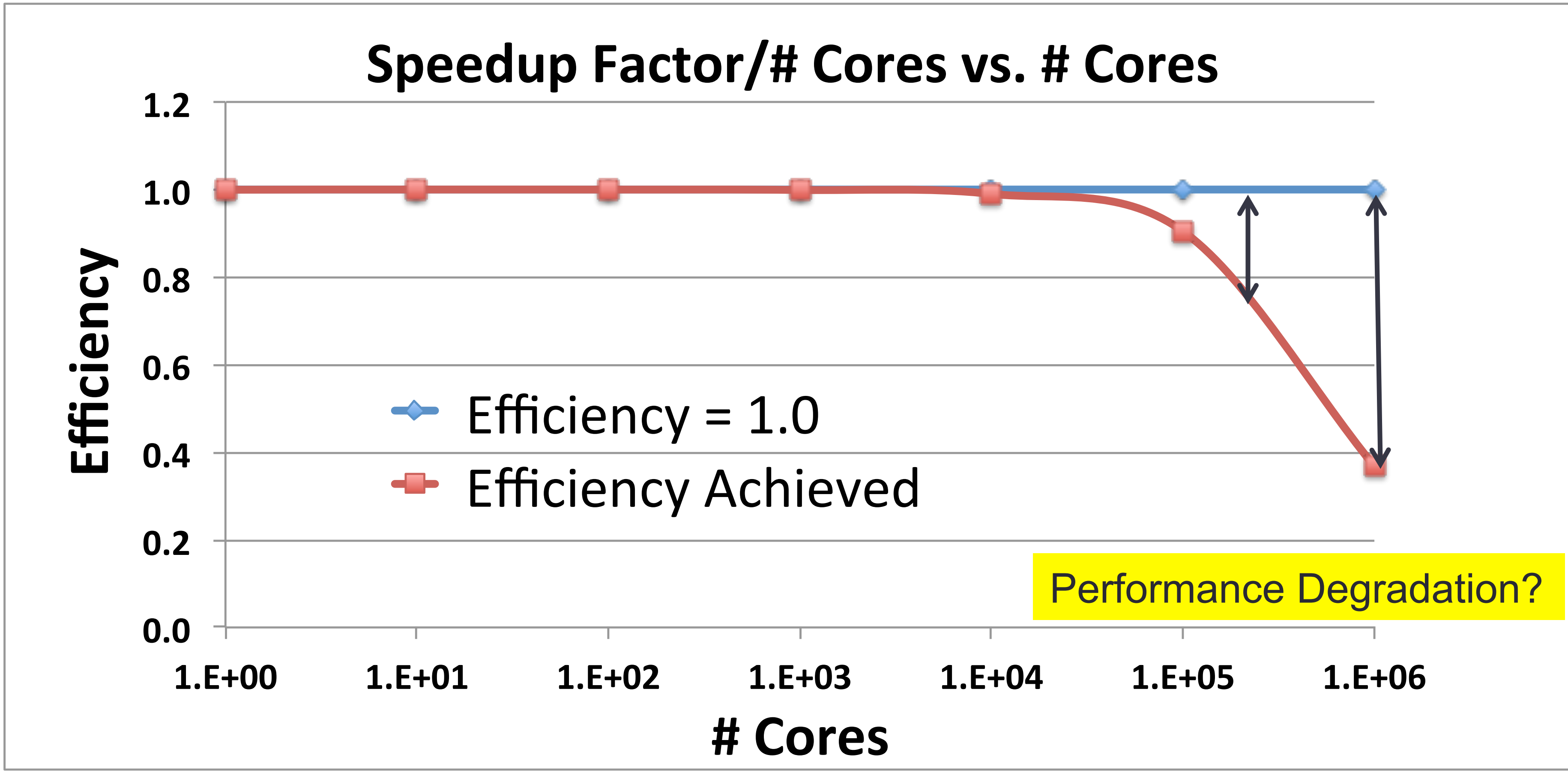
TOP 500: The Exascale Machine Trajectory



Green Computing Challenge: Exascale with only ~20 MW(e)?

Are Real Problems Looking For HPC Machines, or is HPC Looking For Real Problems?

Code Scalability vs. Cores

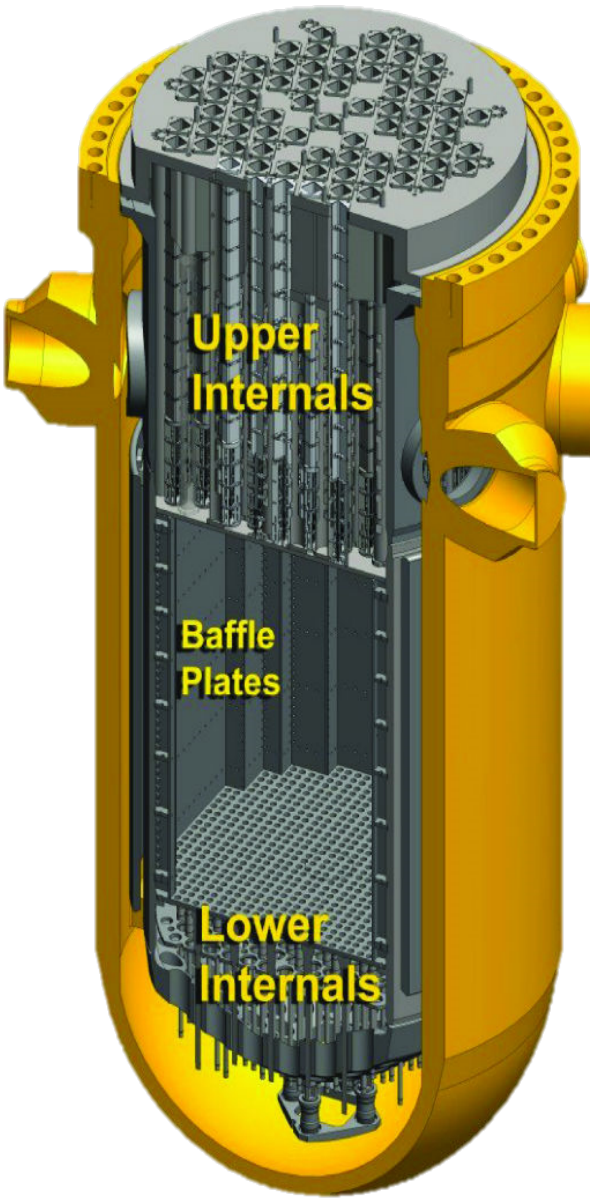


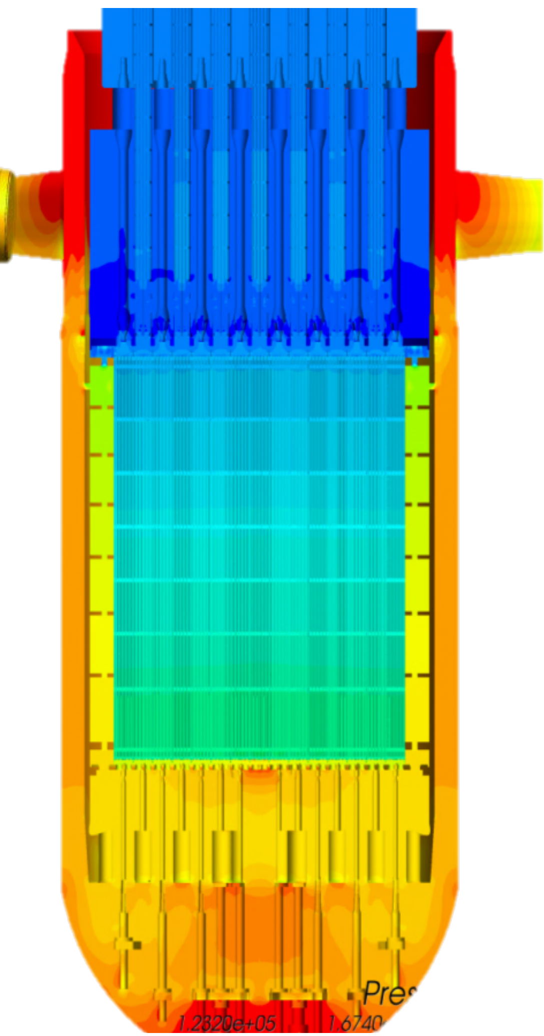
Will code scalability decrease when using 100s of millions or billions of cores?

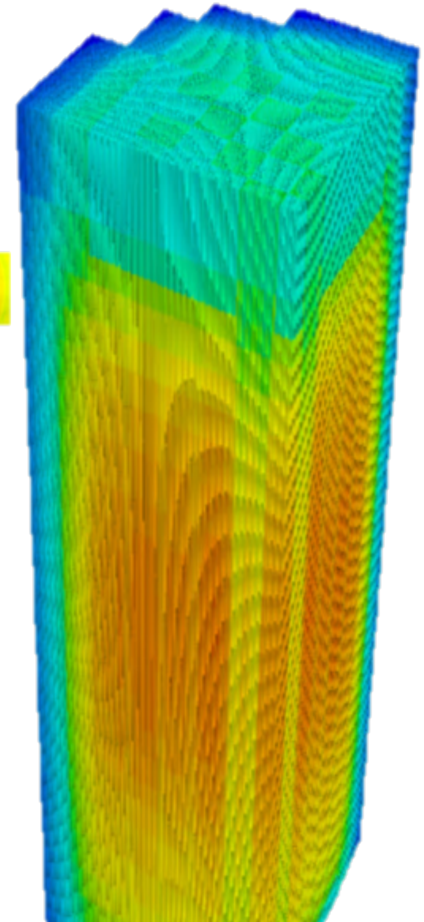
Programming Questions to Ask

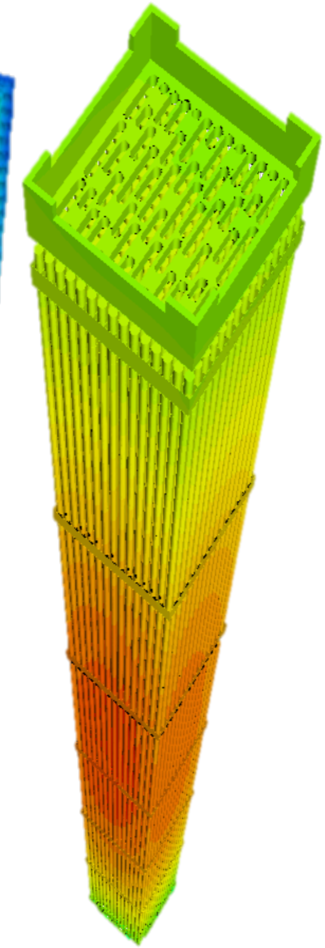
- *Do you really need to use so much memory?*
- *Are you using all cache hierarchies as efficiently as possible?*
- *Do you need double precision for all variables?*
- *Have you lost control of memory locality by over using objects?*
- *Are you using dynamically memory allocation at too low of level?*
- *Should you re-compute rather than store some of your data?*
- *Are Krylov methods (e.g., many back vectors) really the most efficient?*
- *Is code maintenance ultimately more important than code efficiency?*
- *Is it time to start from scratch with new algorithms and codes?*

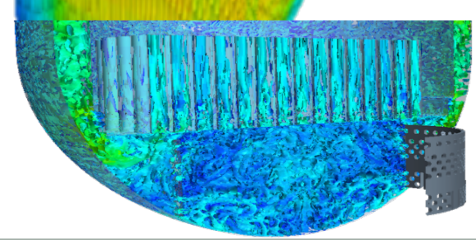
One of DOE’s Exascale Projects: ORNL/ANL/MIT



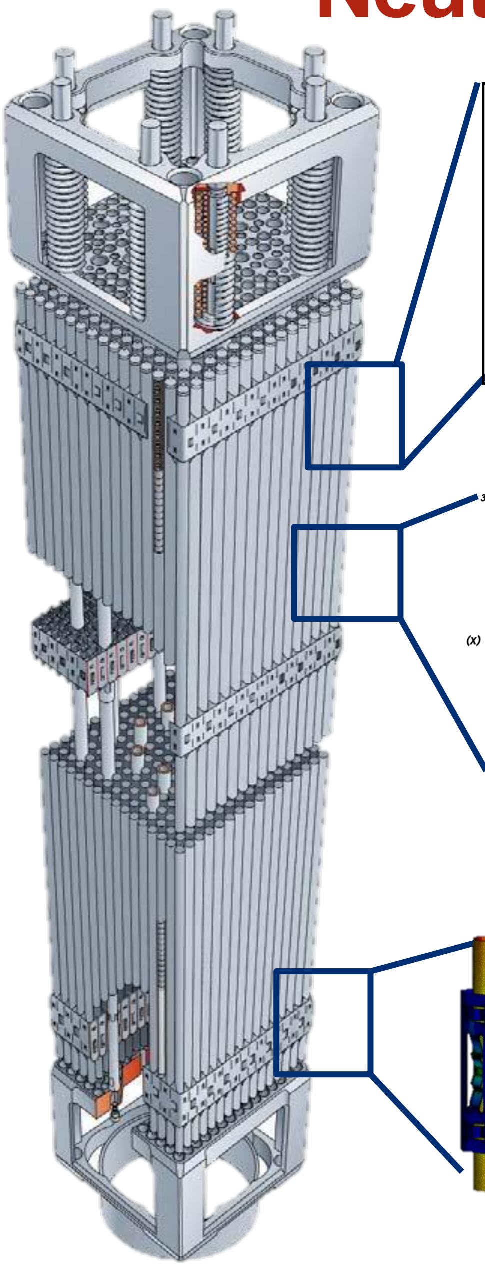


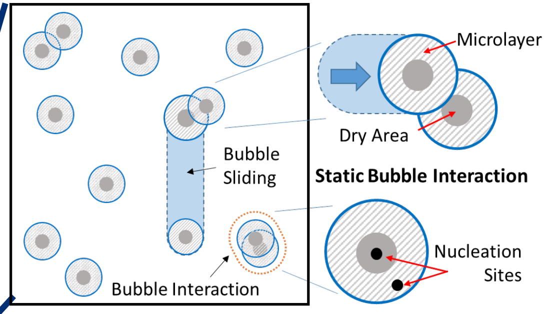




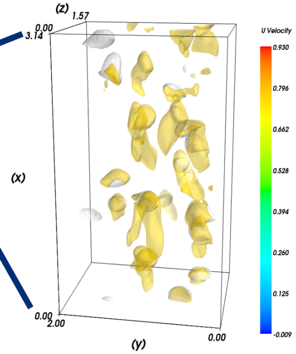


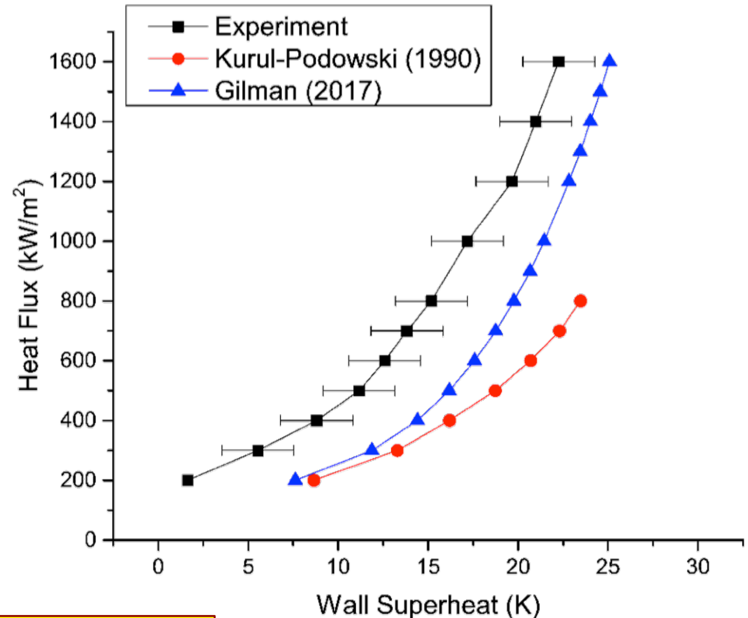
Neutronics / 2-Phase Flow / CHF



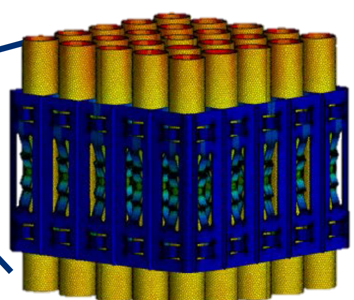


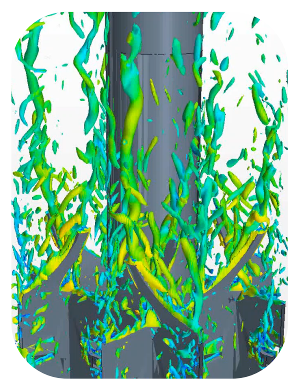
2-Phase

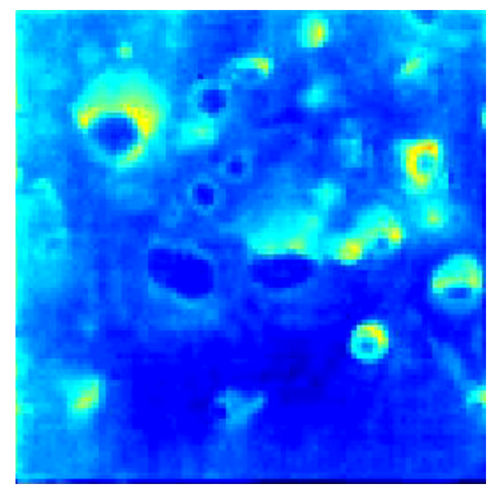




Predict CHF?

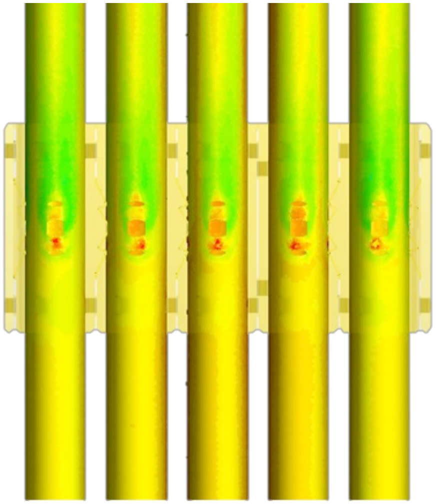




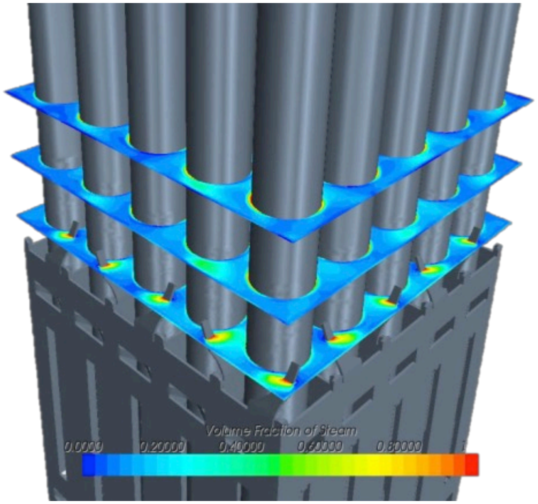


Baglietto, Bucci, et.al, MIT

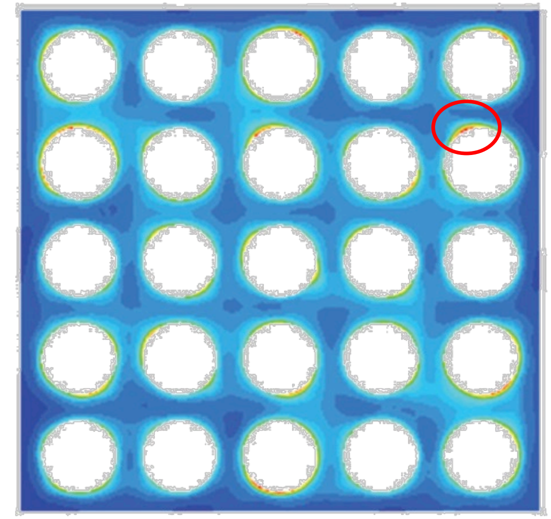
Coupled Physics Modeling: Balance Required



boiling heat transfer



void fraction



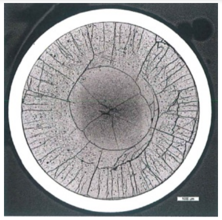
DNB

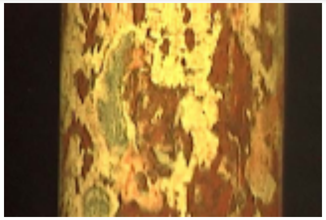
Higher accuracy neutronics requires using local fluid properties / fuel temperatures

- *Production nodal methods with pin reconstruction are limited in local accuracy*

Higher accuracy fluids requires more localized neutronics and fuel heat fluxes

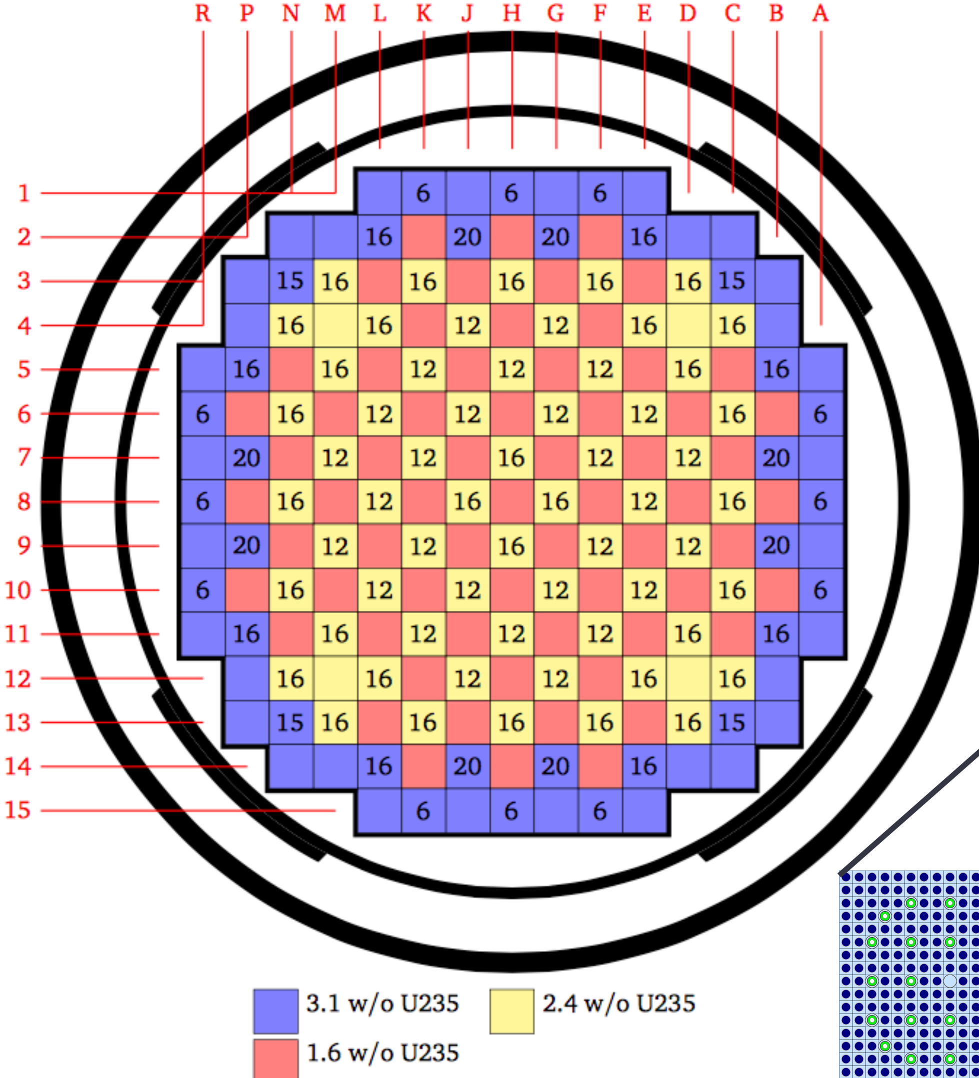
CHF and DNBR require improvements in neutronics, fluids, and fuels modeling

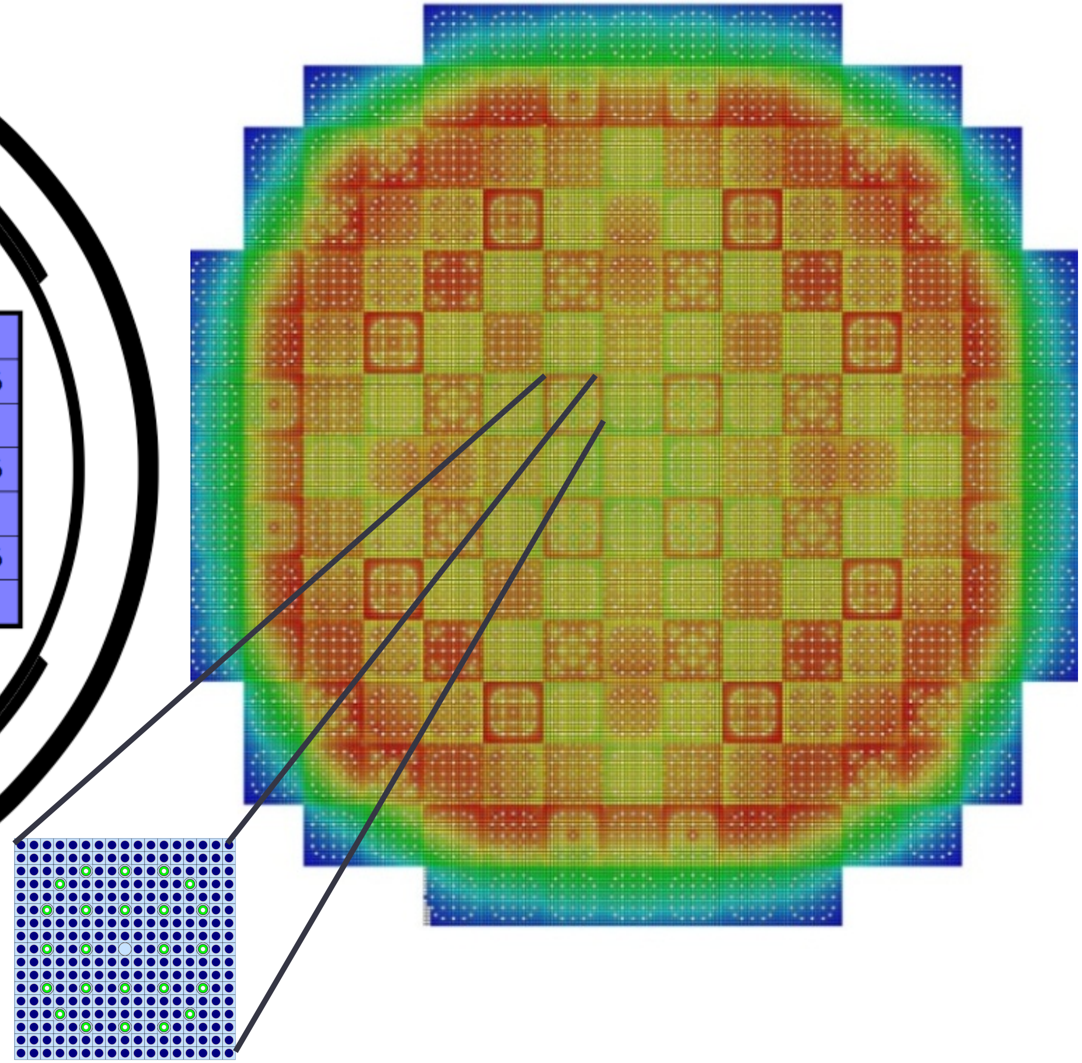




Some effects (e.g. pellet cracking and crud growth) are incredibly hard to model precisely!

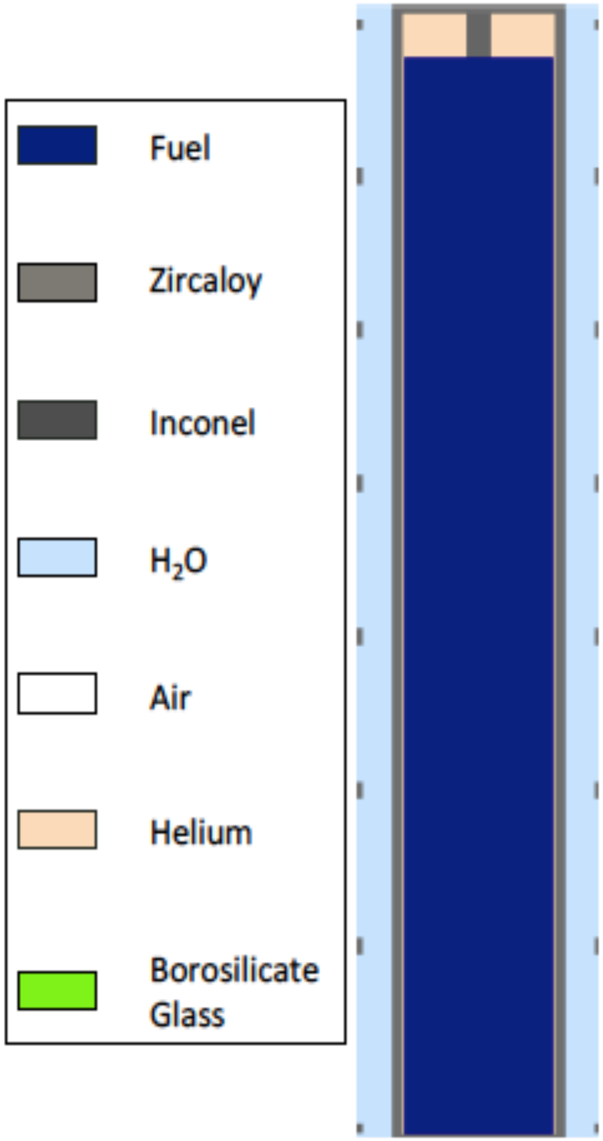
Core Neutronics: Full 3-D Neutron Transport





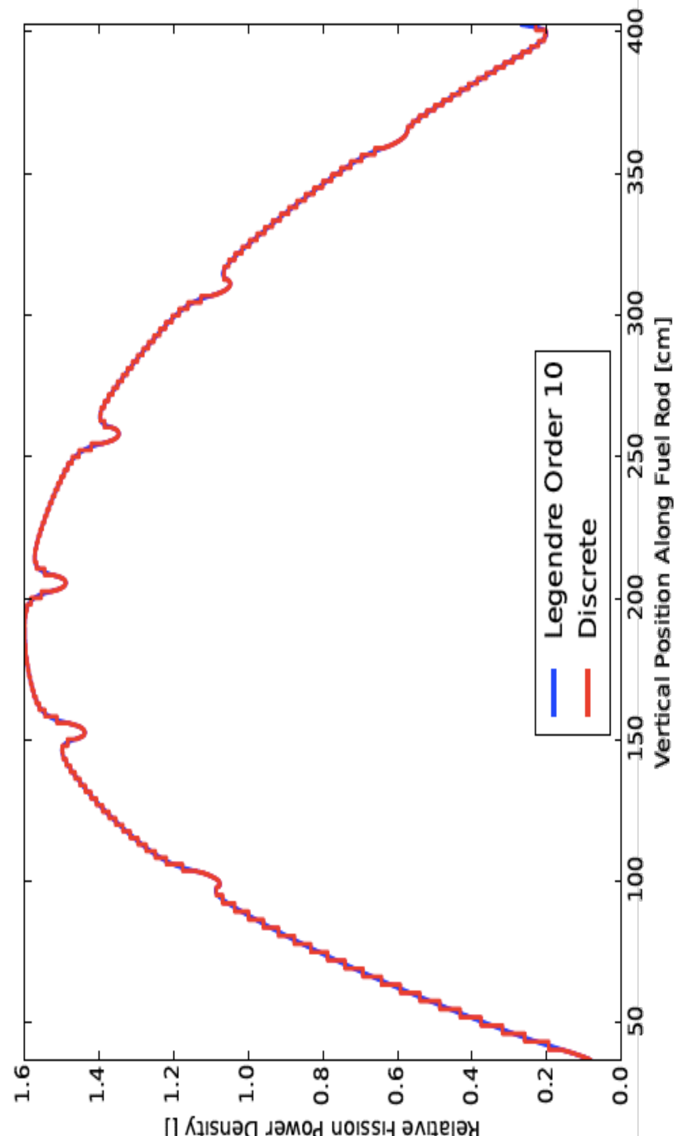
Lattice detail now used for full 3-D transport without homogenization or 2-D/1-D models

Neutronic Challenges from Thermal Feedback

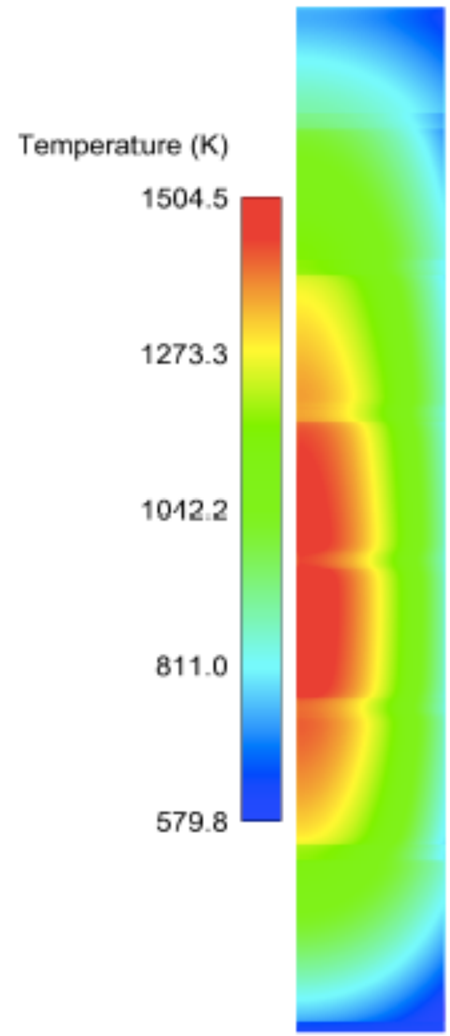


(a) Fundamental geometry

Fuel Pin Heat Sources



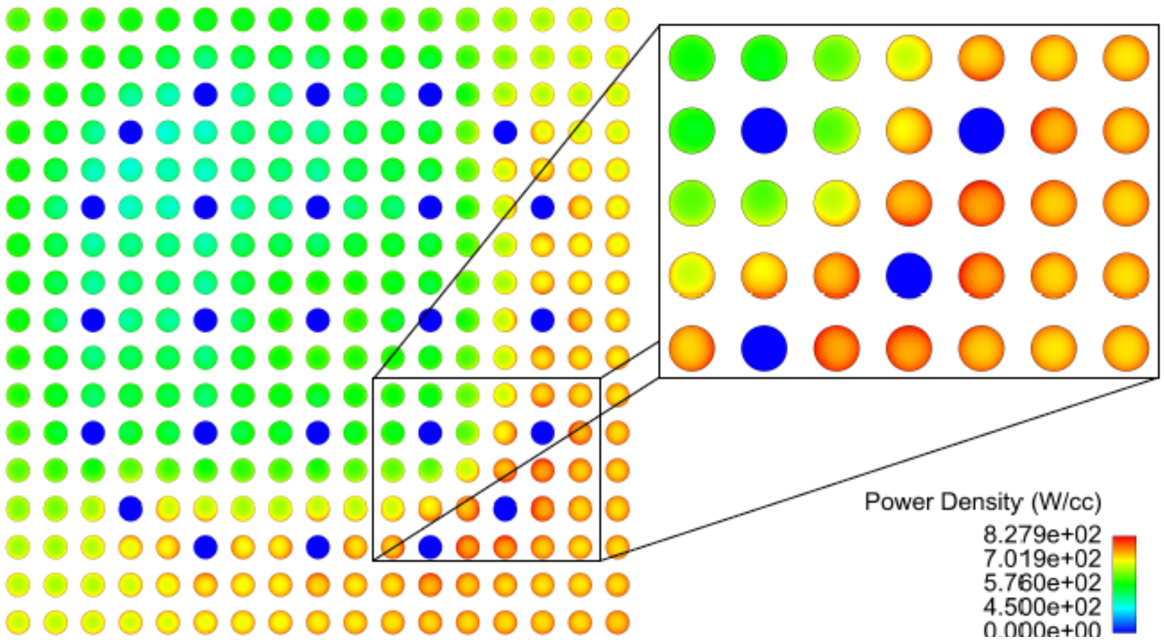
Fuel Pin Temperatures



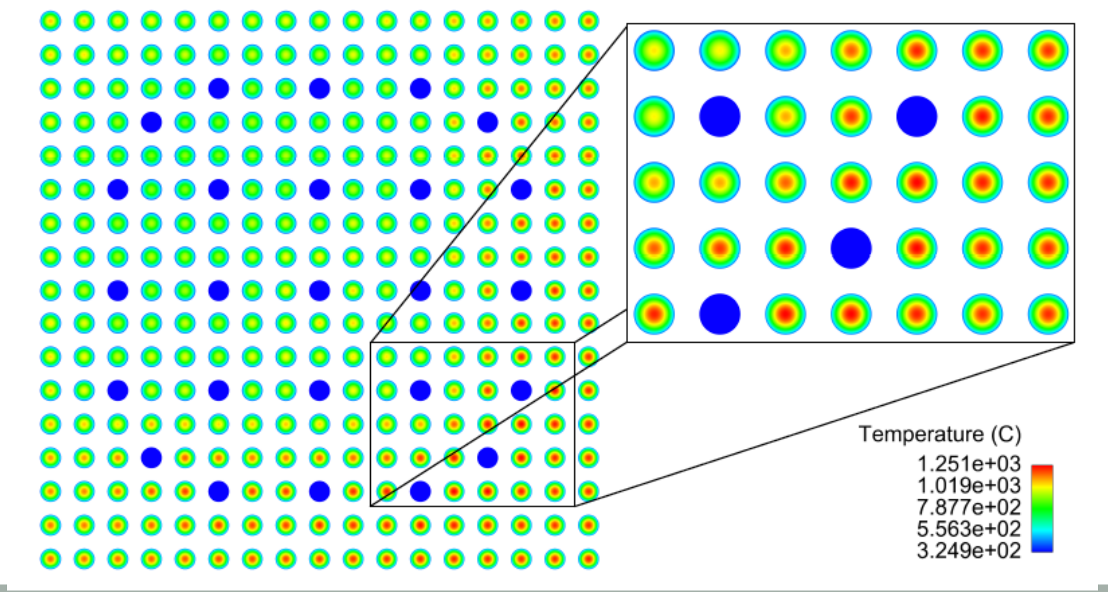
(b) Temperature (L_{10}:Z_{10}^0)

Matt Ellis, MIT

Radial Fission Rates (*q'''*) and Fuel Temperatures

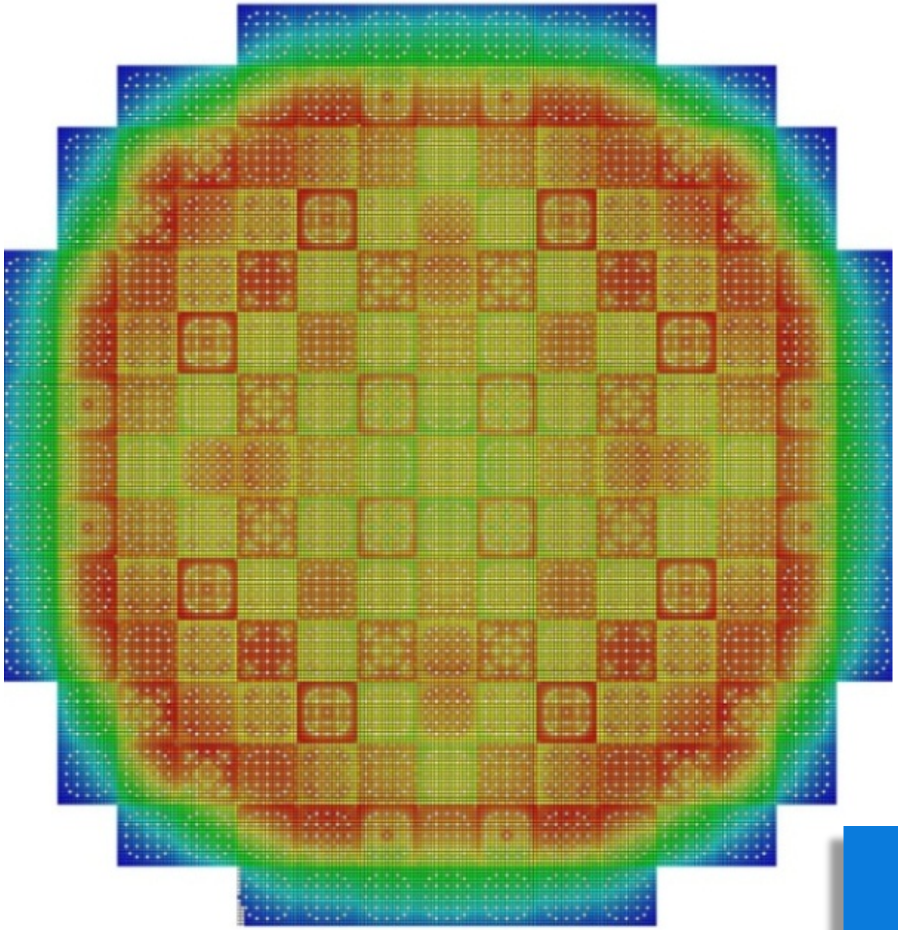


High-resolution requires full local detail



Matt Ellis, MIT

Fuel Depletion: Nuclide Storage Requirements

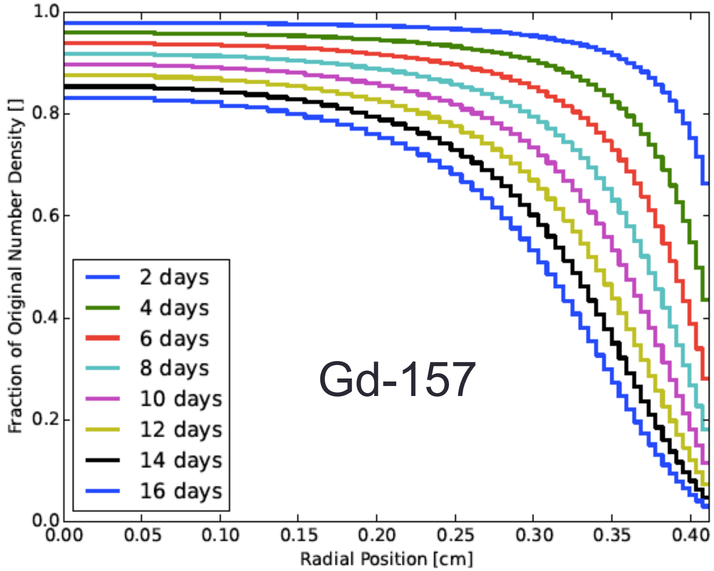


- 193 Fuel assemblies
- 264 Pins/assembly
- 200 Axial pellets/pin
- 10 Radial regions/pellet
- 400 Nuclides/region
- 5 Reactions/nuclide
- 8 Bytes/reaction

= ~1.6 T-Bytes of data

Massive on-node storage
or
Spatial domain decomposition?

Discretize or Functionalize?



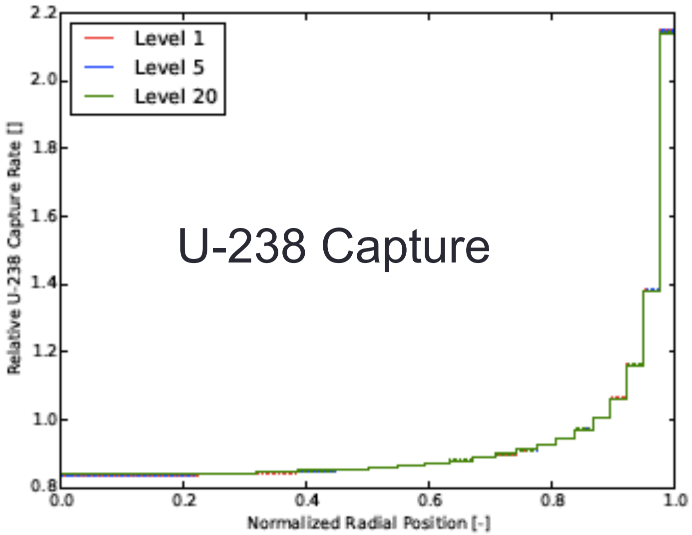


Figure 3.18.. U-238 absorption rate in the eighth axial zone in twenty equal volume ring tallies for the first, fifth, and twentieth axial slices in the eigenvalue calculation.

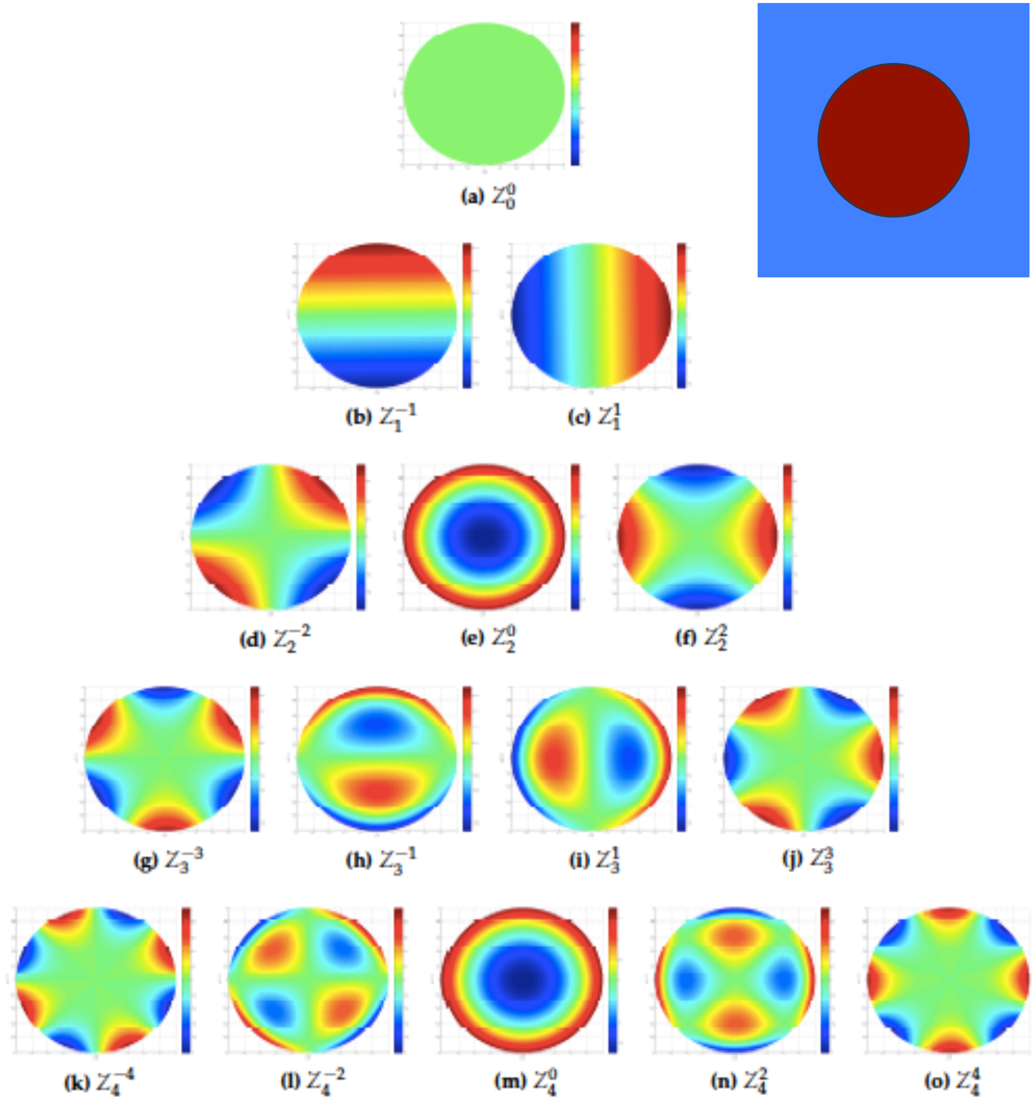


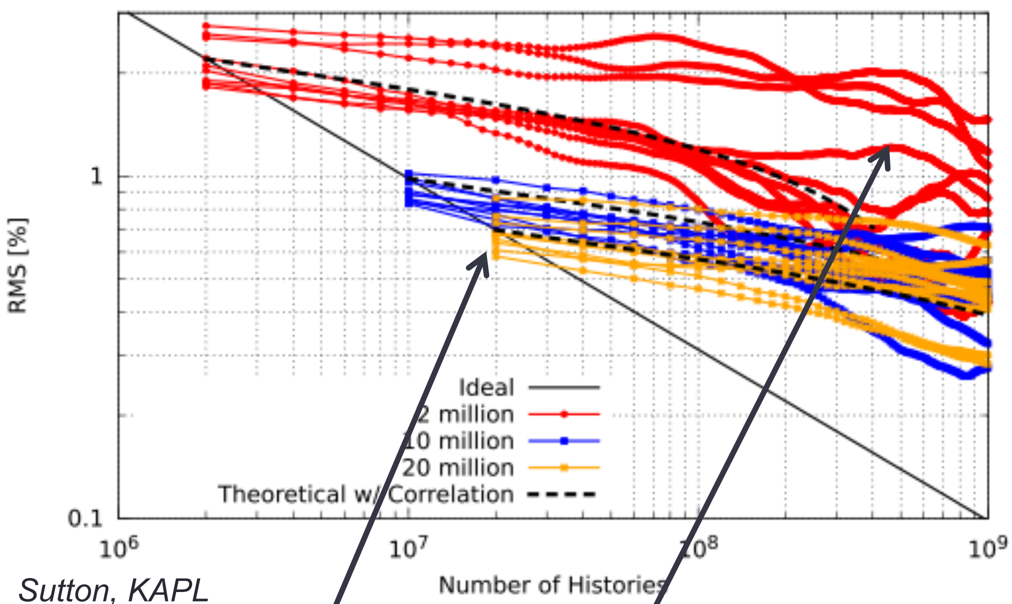
Figure 2.2.. Zernike polynomial orders zero through four

Challenges for Monte Carlo Eigenvalue Problems

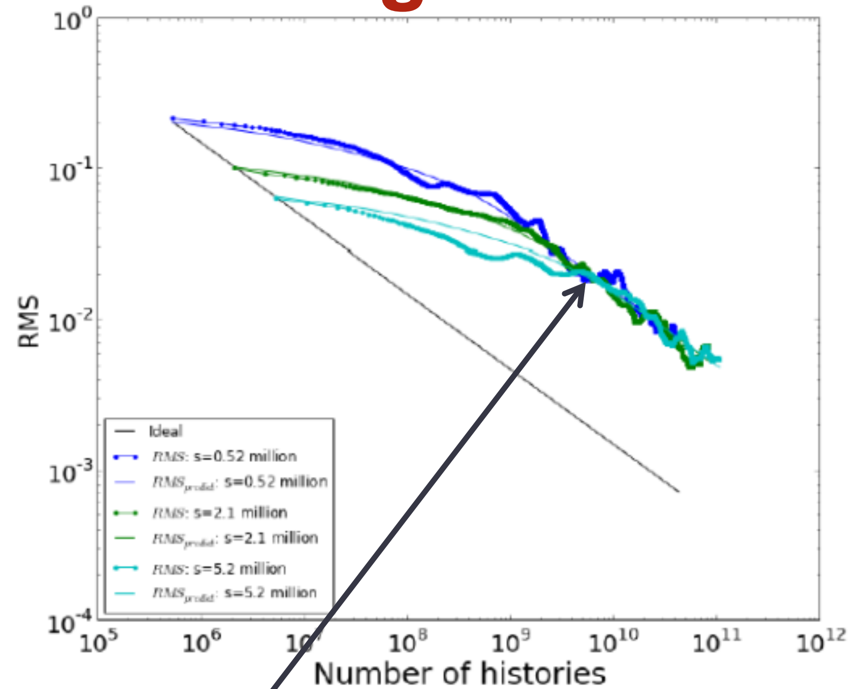
- *Accelerate "convergence" of sources (inactive batches)*
- *Achieve 1% statistical uncertainties of on local spatial tallies*
- *Track efficiently with > 1 TB depletion tallies*
- *Treat coupled physics from fuel and coolant fields*
  - *Treat temperature-dependent cross sections*
  - *Converge efficiently in multi-physics environment*
- *Modeling of distorted geometries*
- *Extensions to time-dependent problems*

For reactors, k-eff is a byproduct of convergence - not the statistical objective!

Monte Carlo's Correlated Fission Sources Lead to Poor Convergence/Misleading Statistics



Sutton, KAPL
Forget, et.al., MIT

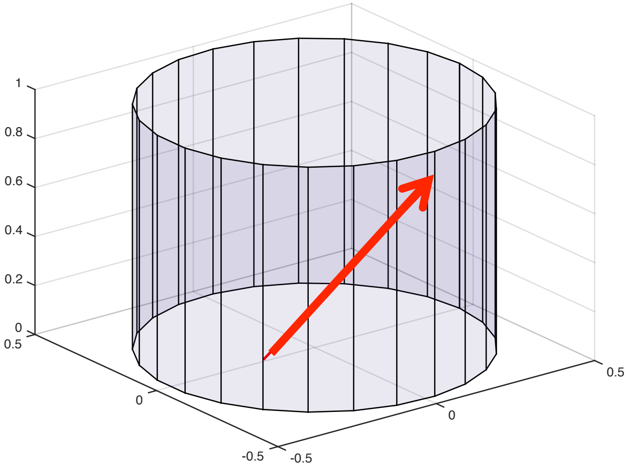


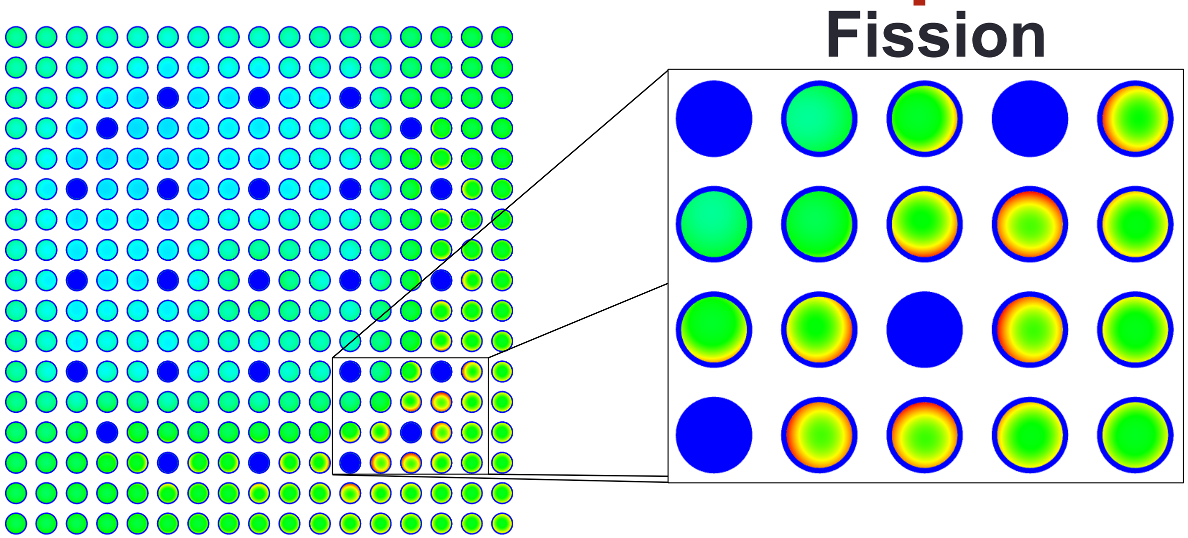
- *More histories per batch reduce the initial uncertainties*
- *Many batches are required before 1/N variance is achieved*
- *Use independent simulations to determine credible statistics?*
- *Under-sampling is a problem for tallies in small spatial regions*

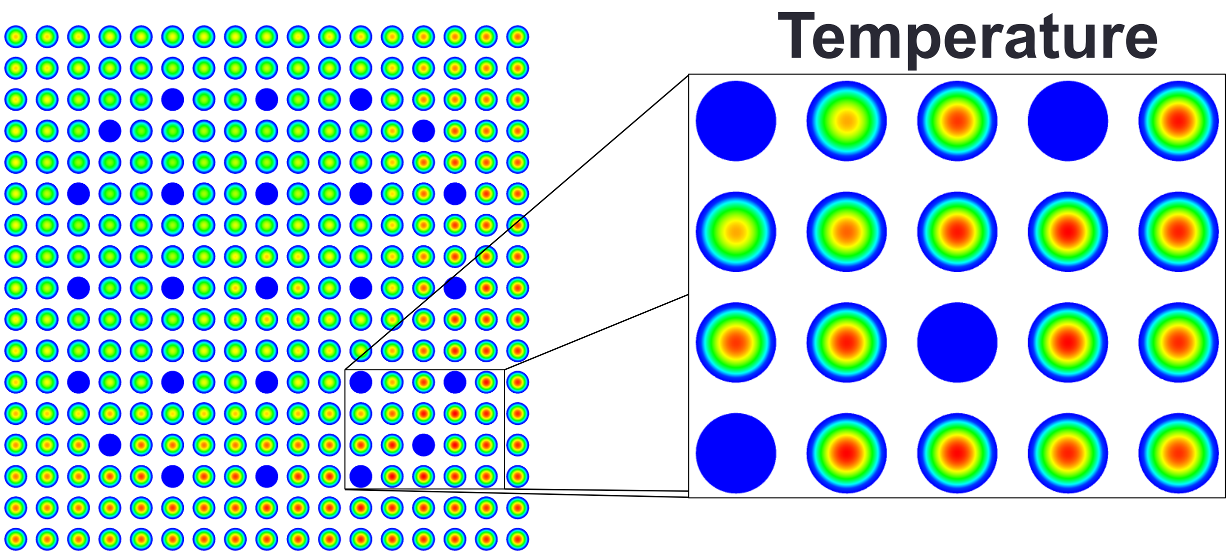
Continuous Material Tracking (e.g., FETs) for Monte Carlo and Deterministic Transport?

$$\hat{\tau} = -ln(1 - G\xi)$$

$$\hat{\tau} = \int_0^s \Sigma(x')dx'$$







Griesheimer and Martin, U of M
Matt Ellis, MIT

Remember the Difference Between Scalability and Computational Efficiency

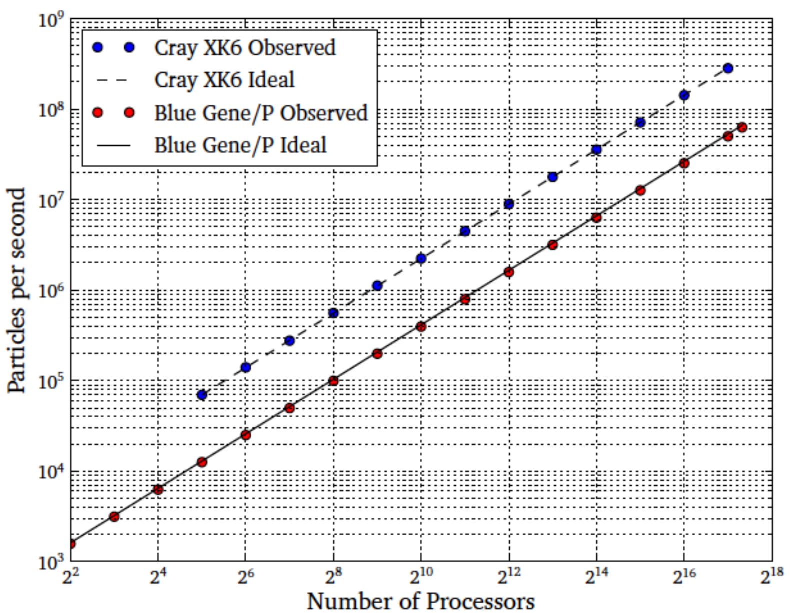
- Currently Monte Carlo cross section linear interpolation consists of the following sequence:

  Zero the material macroscopic cross section

  Loop over 400 Isotopes

    Loop over reaction types

    1. Load the energy vector needed for a binary search
    2. A small number of FLOPS and ifs (e.g. ~10) for a binary search for data index
    3. Load cross section data
    4. A few FLOPS for actual data interpolation
    5. A few FLOPS to add microscopic to macroscopic cross section



Scalability ≠ Efficiency

Bytes/FLOP are miserably large for Monte Carlo

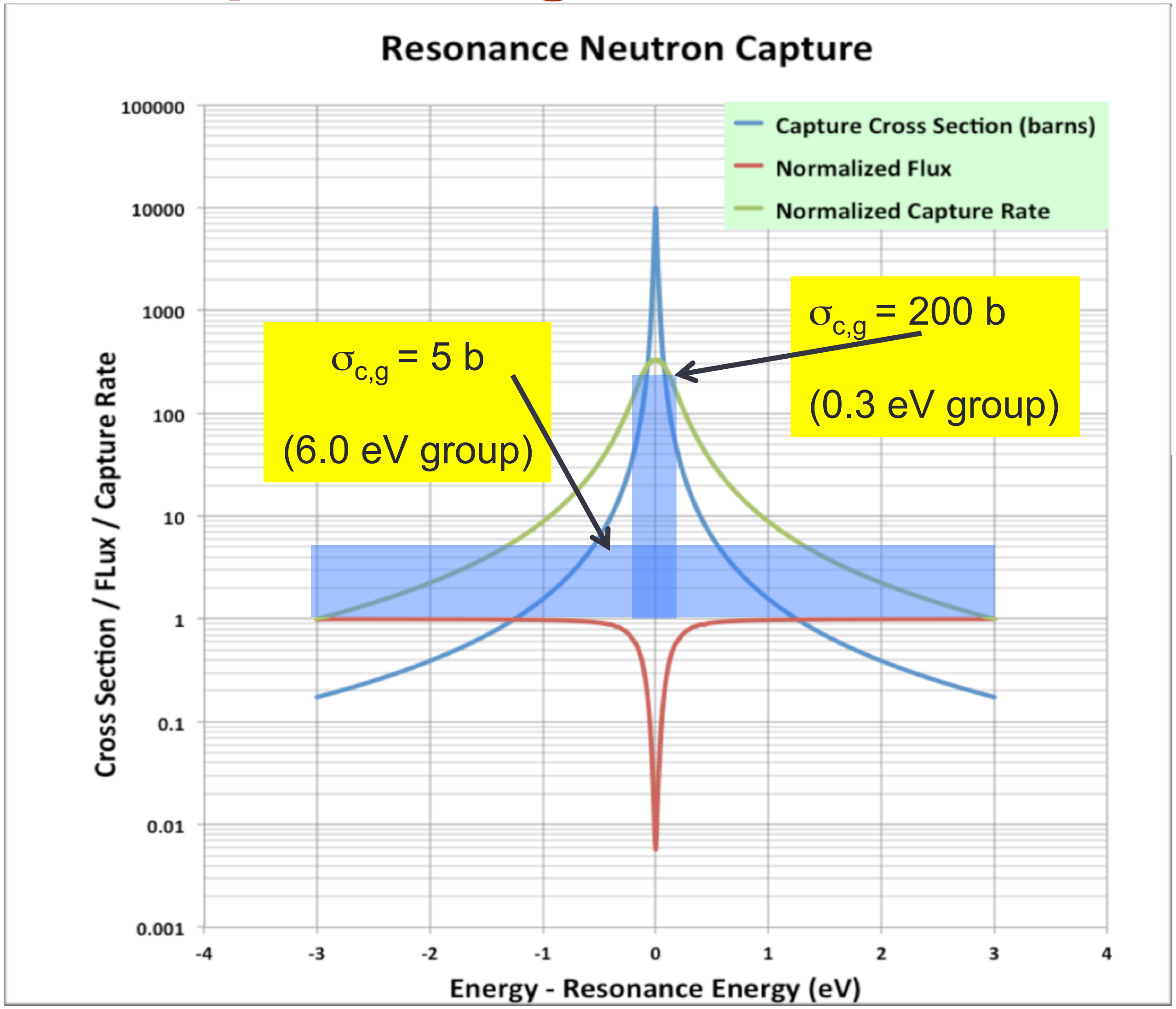
Romano and Forget, MIT

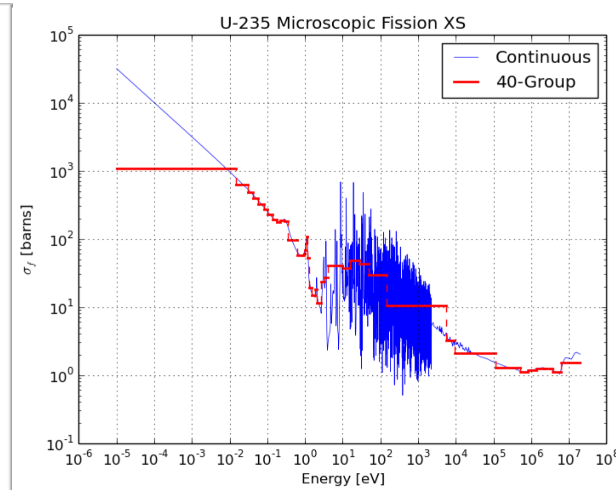
Challenges for Deterministic Transport

- *Modeling feedback effects on multi-group cross sections*
- *Intra-pellet discretization for nuclide depletion and temperature tracking*
- *Modeling of distorted geometries*
- *Accurate temporal integration schemes*

- *Selection of appropriate group structure for libraries of cross sections*
- *Generation of accurate multi-group cross sections*
- *Generation of appropriate equivalence parameters*
- *Approximation of anisotropic scattering or P_0 transport cross sections*
- *Converge in angles (1000's are needed)*
- *Converge in spatial source regions*

200 pcm Jungle: Multi-group Resonance Cross Sections





$$\sigma_{c,g} \equiv \frac{\int_{E_{g-1}}^{E_g} \sigma_c(E)\,\phi(E)\,dE}{\int_{E_{g-1}}^{E_g} \phi(E)\,dE}$$

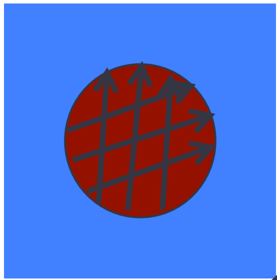
$$\phi_g^{N.R.} = \frac{\left(\sigma_{pot,f}+\sigma_e\right)}{\sigma_{c,g}+\left(\sigma_{pot,f}+\sigma_e\right)}$$

$$\phi_g^{N.R.} \cong \frac{75b}{\sigma_{c,g}+75b}$$

As group width increases, resonance absorption has smaller impact on multi-group flux

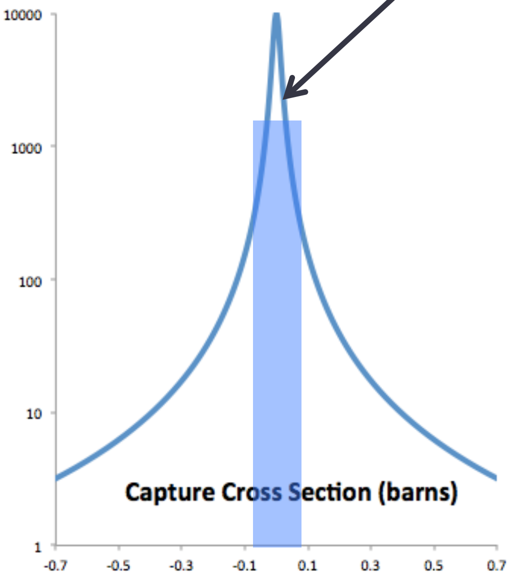
Equivalence for Multi-Group Cross Sections

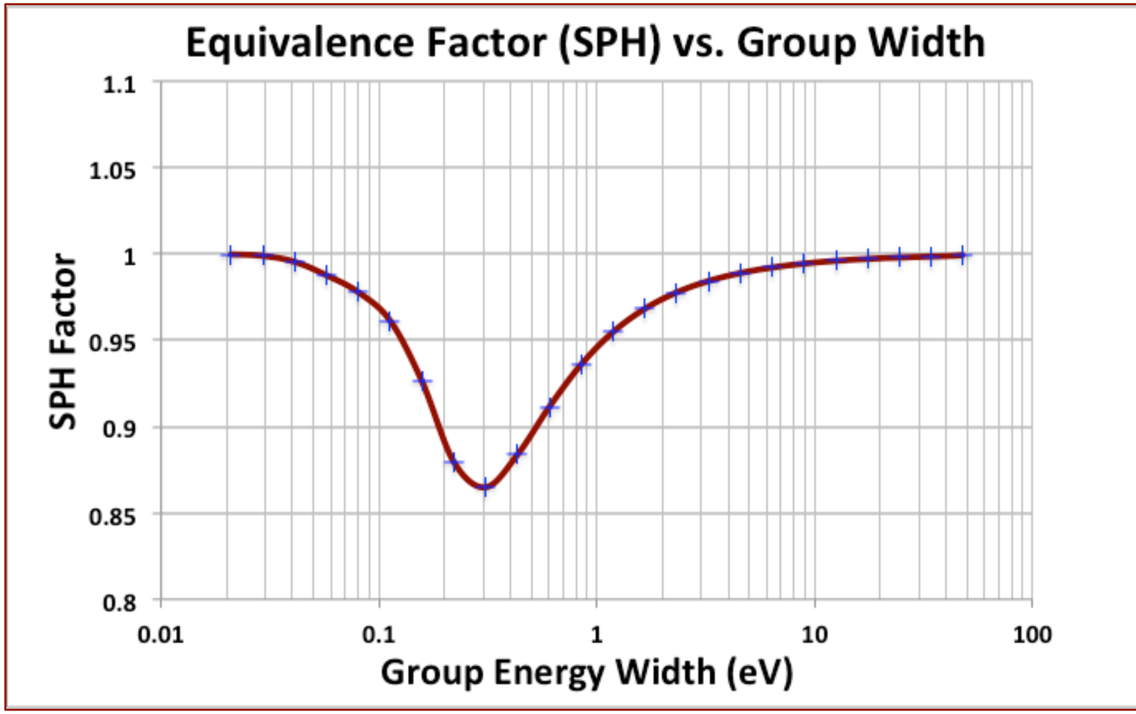
$$\int_{E_{g-1}}^{E_g} \Sigma(E)\,\phi^{MC}(E)\,dE = \Sigma_g \phi_g^{MC} \neq \Sigma_g \overline{\phi}_g^{Multi-group}$$



$$\int_{E_{g-1}}^{E_g} e^{-\Sigma(E)\tau/\mu}\,dE \neq e^{-\Sigma_g\tau/\mu}\int_{E_{g-1}}^{E_g} dE$$

$$\int_{E_{g-1}}^{E_g} e^{-\Sigma(E)\tau/\mu}\,dE \equiv e^{-SPH\,\Sigma_g\tau/\mu}\int_{E_{g-1}}^{E_g} dE$$

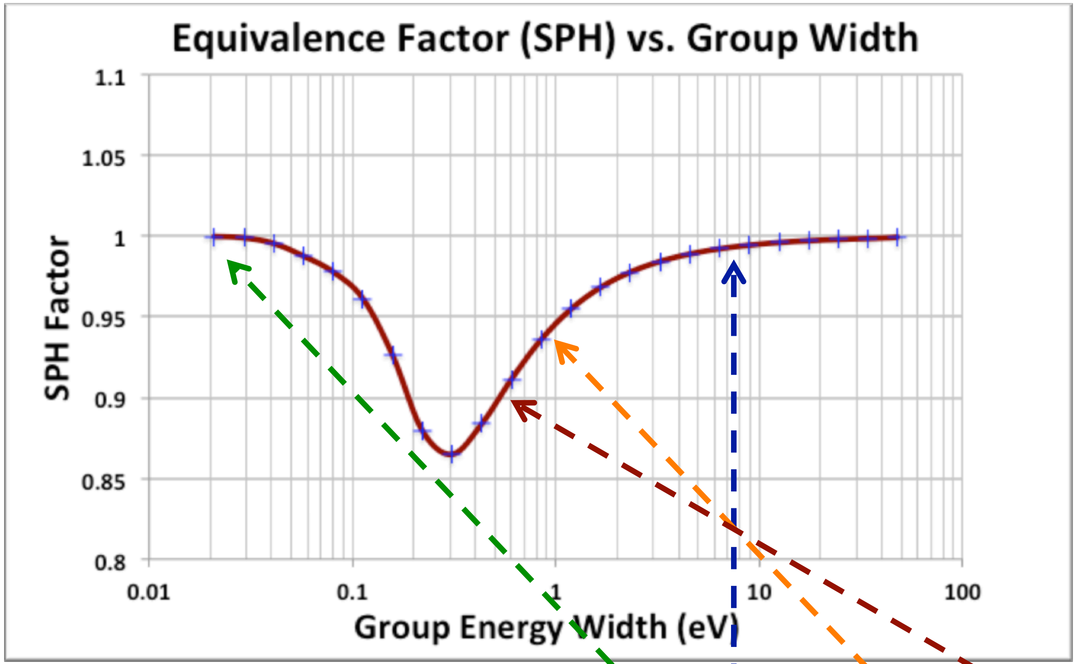


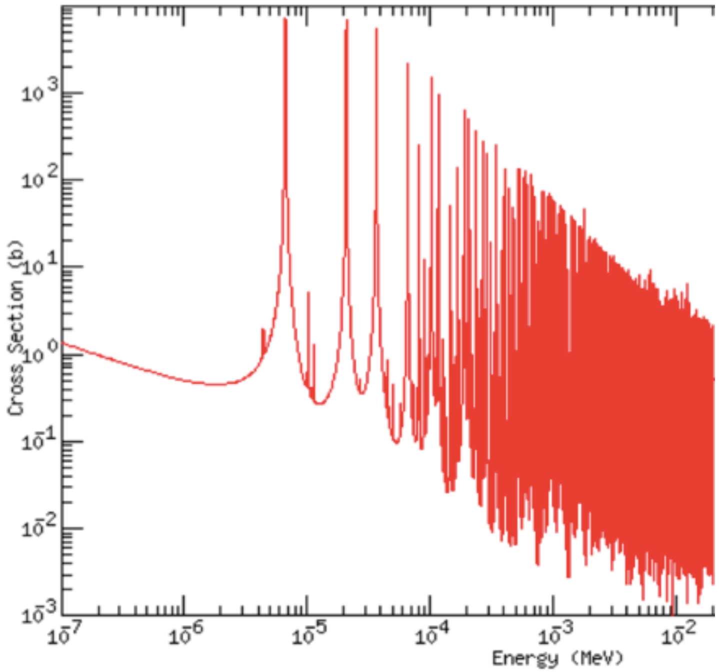


$$\hat{\Sigma}_g \equiv SPH \cdot \Sigma_g$$

$$\Sigma_g \phi_g^{MC} = \hat{\Sigma}_g \overline{\phi}_g^{Multi-group}$$

Selecting Multi-Group Energy Boundaries



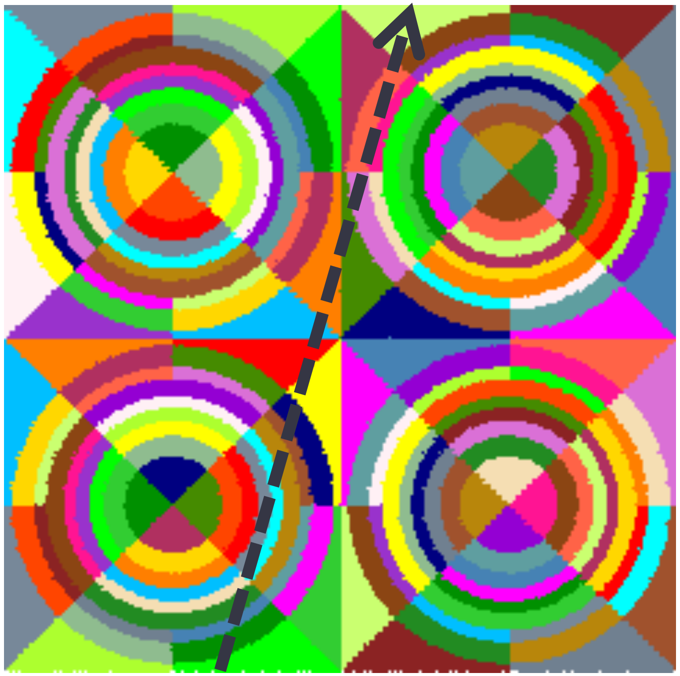


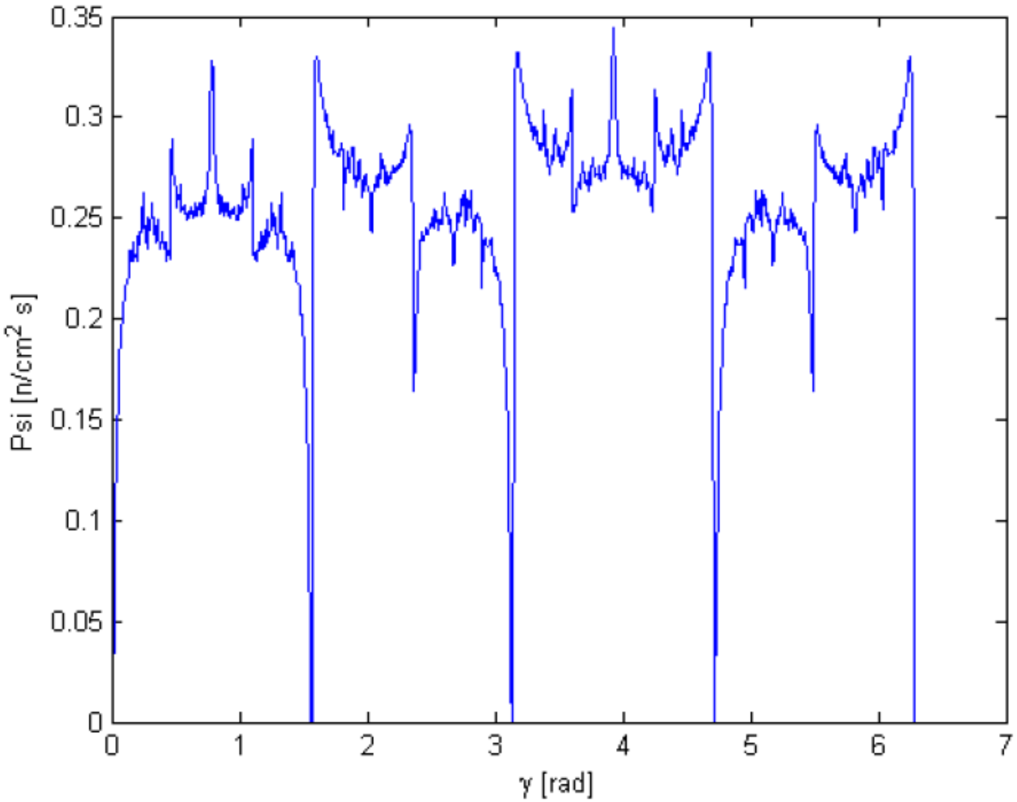
U-238 Resonance	Energy Group Widths (eV) Near Resonance Peak Energy			
Energy (eV)	WIMS-69	SHEM-361	XMAS-172	CASL-51
36.68	10.30	~0.05	3.50	18.30
20.87	11.70	~0.01	3.15	16.60
6.67	5.90	~0.01	0.8 - 1.4	0.3 - 0.8

1000's of energy groups are needed to blindly overcome group boundary sensitivities

Intermediate group widths produce results that are sensitive to "equivalence factors"

Angular Convergence of Deterministic Transport





- *Pin-to-pin self shielding leads to discontinuous angular fluxes*
- *High-order quadrature is ineffective for azimuthal angular expansions*
- *Convergence is usually linear in the number of angles*

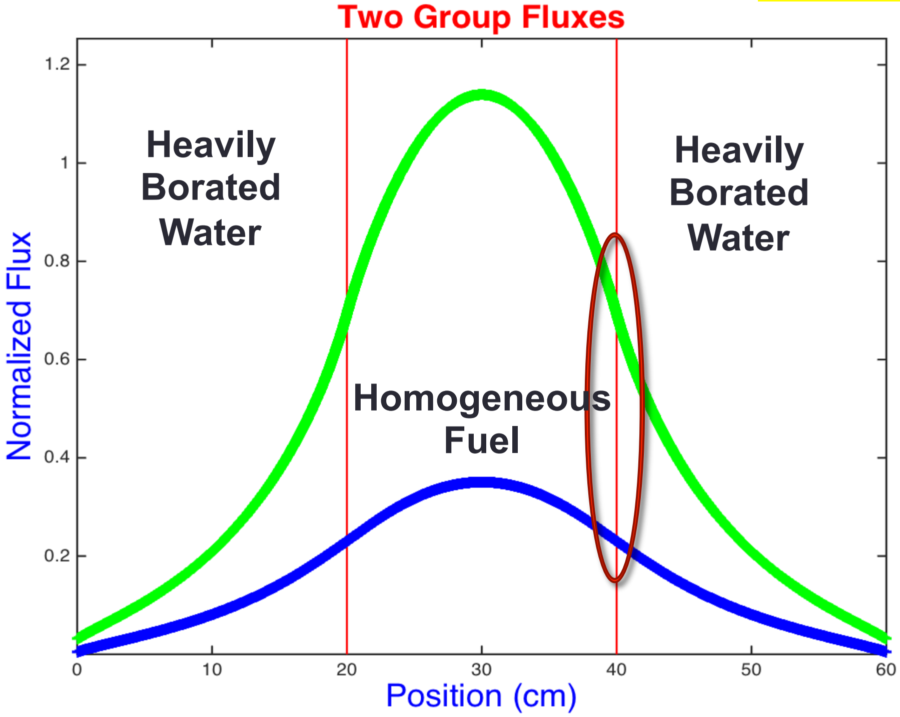
Spatial Convergence for Deterministic Transport Models (e.g. 1-D Diamond-Difference)

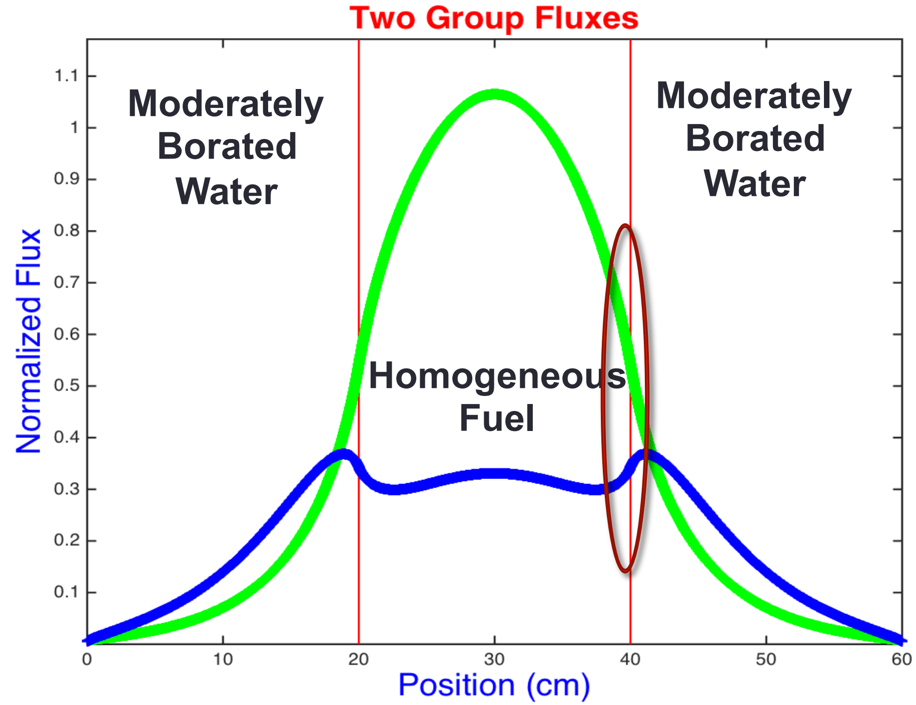
$$\int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \mu_n \frac{\partial \psi_n(x)}{\partial x} + \Sigma_{t,i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \psi_n(x) = \frac{1}{2}\left[\Sigma_{s,i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \phi(x) + \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, S(x)\right]$$

$$\mu_n\left[\psi_{i+1/2,n} - \psi_{i-1/2,n}\right] + \Delta_i \Sigma_{t,i} \bar{\psi}_{i,n} = \frac{\Delta_i}{2}\left[\Sigma_{s,i}\bar{\phi}_i + \bar{S}_i\right] \equiv \bar{Q}_i$$

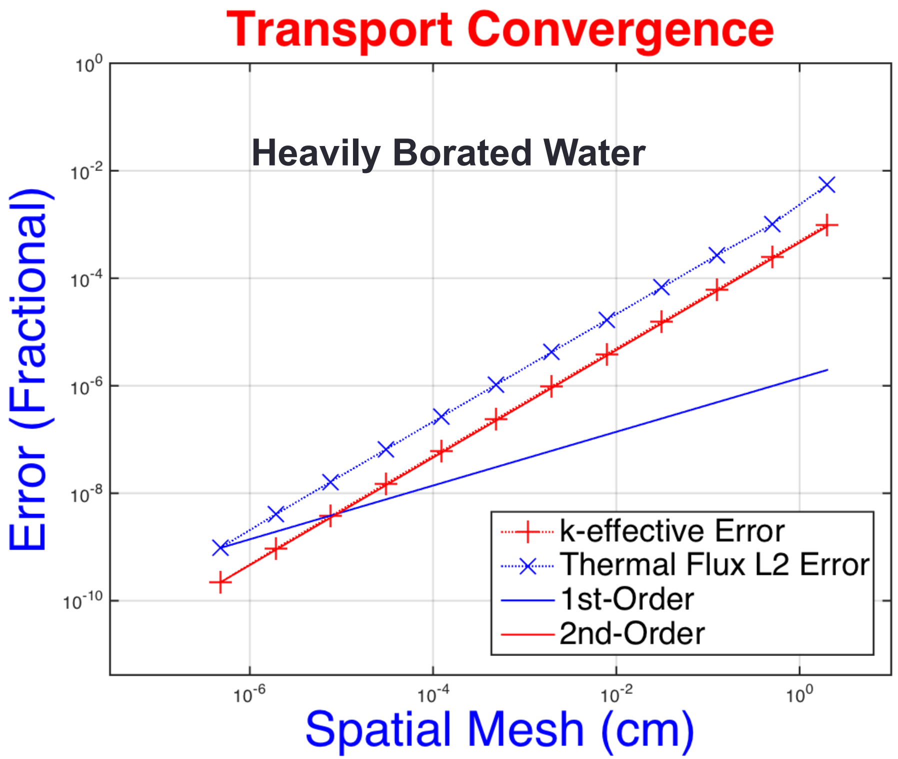
$$\bar{\psi}_{i,n} \cong \frac{1}{2}\left[\psi_{i+1/2,n} + \psi_{i-1/2,n}\right]$$

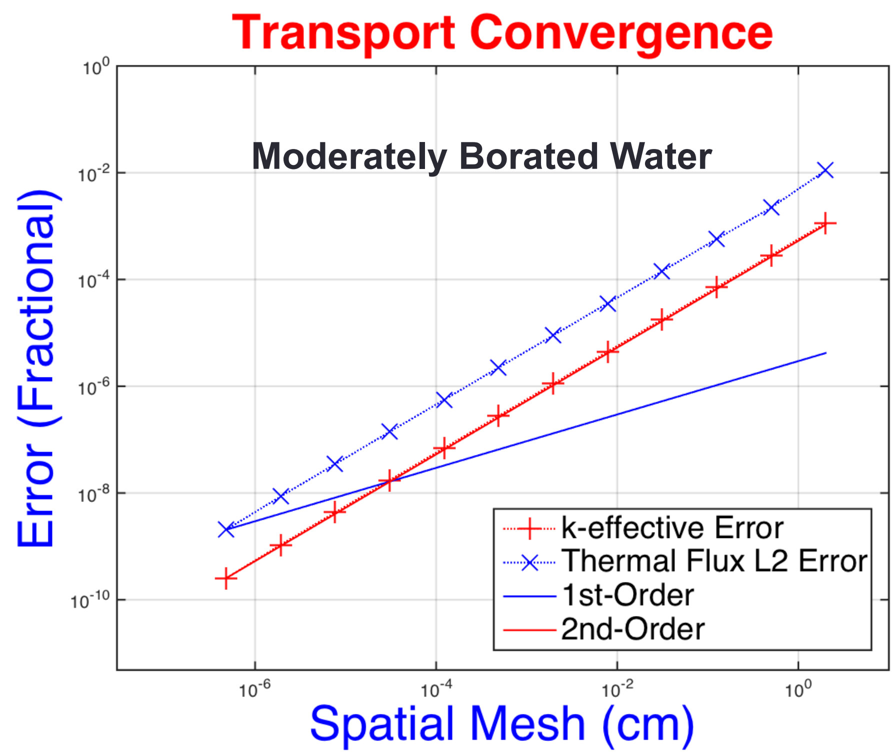
$$\Rightarrow \psi_{i+1/2,n} = \left[\frac{\psi_{i-1/2,n}\left(2|\mu_n| - \Delta_i \Sigma_{t,i}\right) + 2\Delta_i \bar{Q}_i}{2|\mu_n| + \Delta_i \Sigma_{t,i}}\right]$$





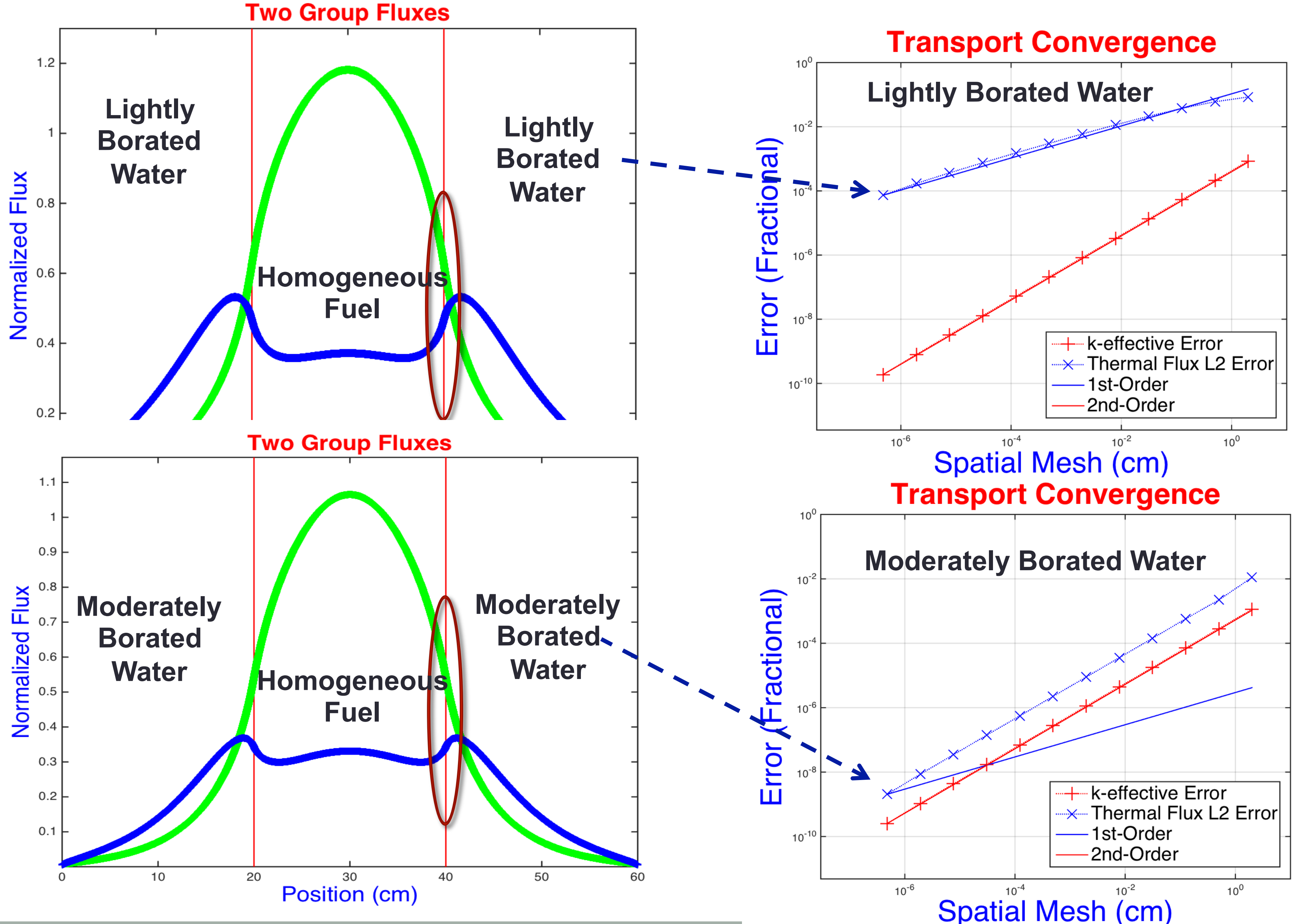
Spatial Convergence is 2nd Order – Duh?



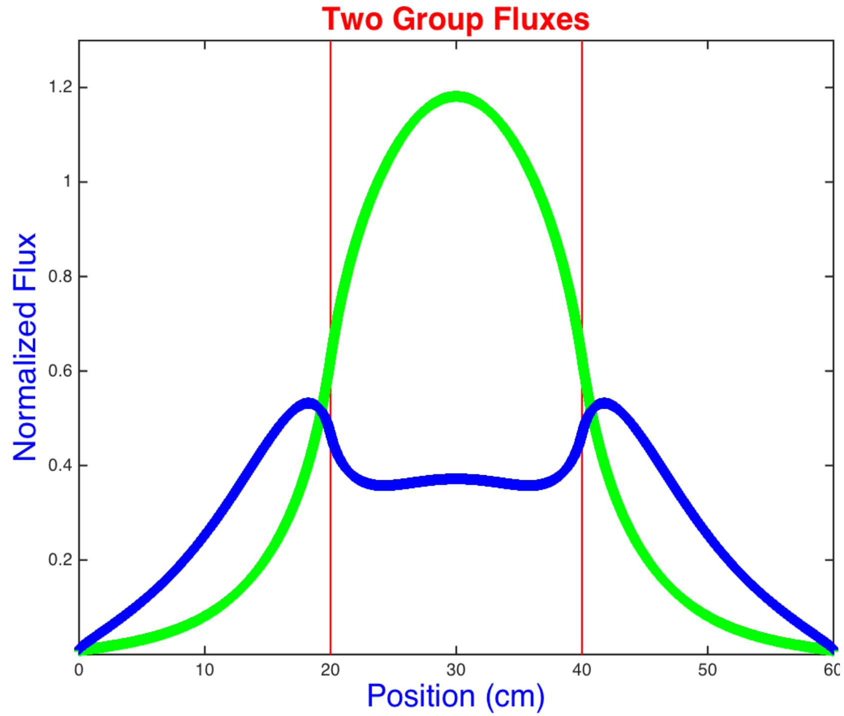


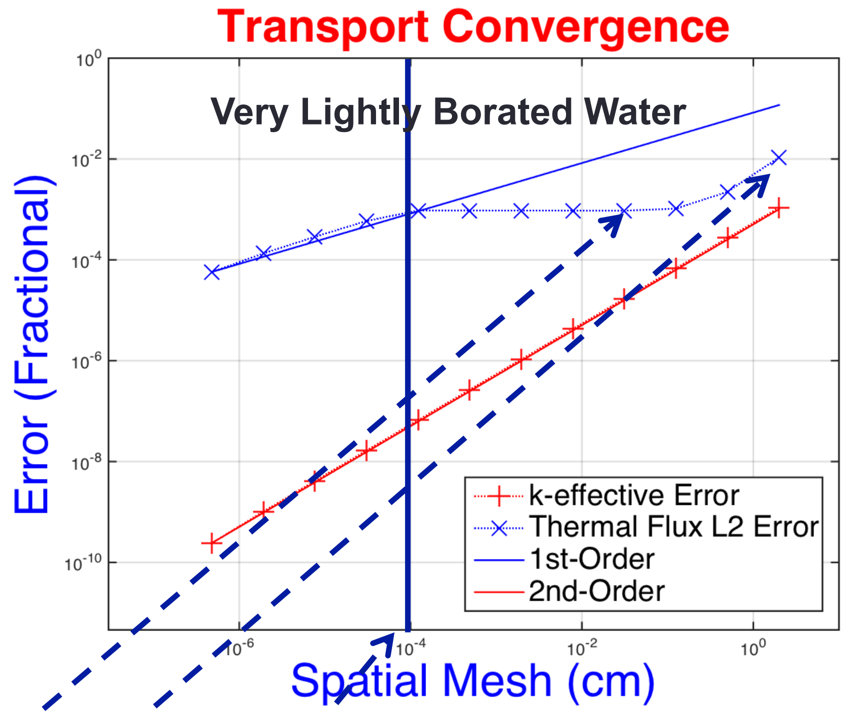
Second-order convergence: Larsen and Miller's published results of 1979

But – Does Convergence Depends on Boron?



What Drives Transition of Order of Convergence?



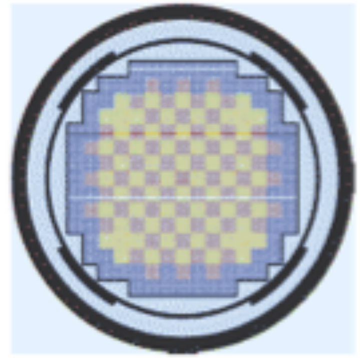


- *What are the implications of order-of-convergence depending on reflector boron?*
- *Can you reliably predict the shape of mesh dependence of convergence?*
- *Can you predict the leading order term of convergence?*
- *How confident are you in your favorite transport method's order of convergence?*

Since simple 1-D problem requires 10^{-4} cm mesh to achieve asymptotic convergence, will we able to demonstrate convergence of real 3D core models on HPC machines?

Hybrid Methods to Avoid the 200 pcm Jungle?

OpenCG

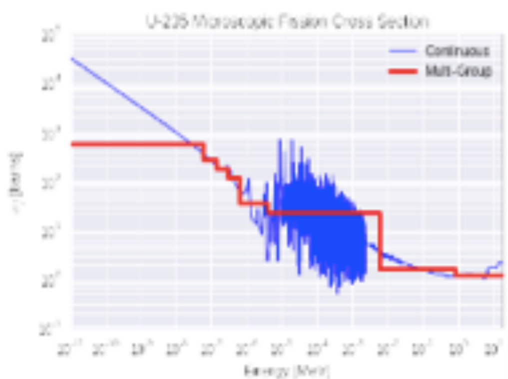


- Model reactor geometry
- Transfer data across meshes

Loosely converge a
3D Monte Carlo core model

Fully-converge a
3-D deterministic core model

OpenMC

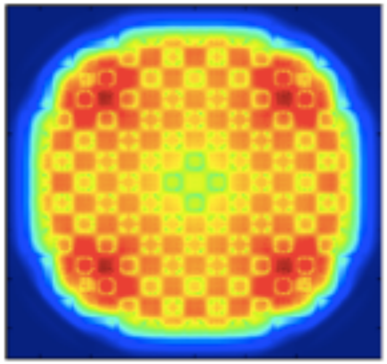


- Generate MGXS library
- Compute reference solution

python

Monte-Carlo cross sections
for deterministic models

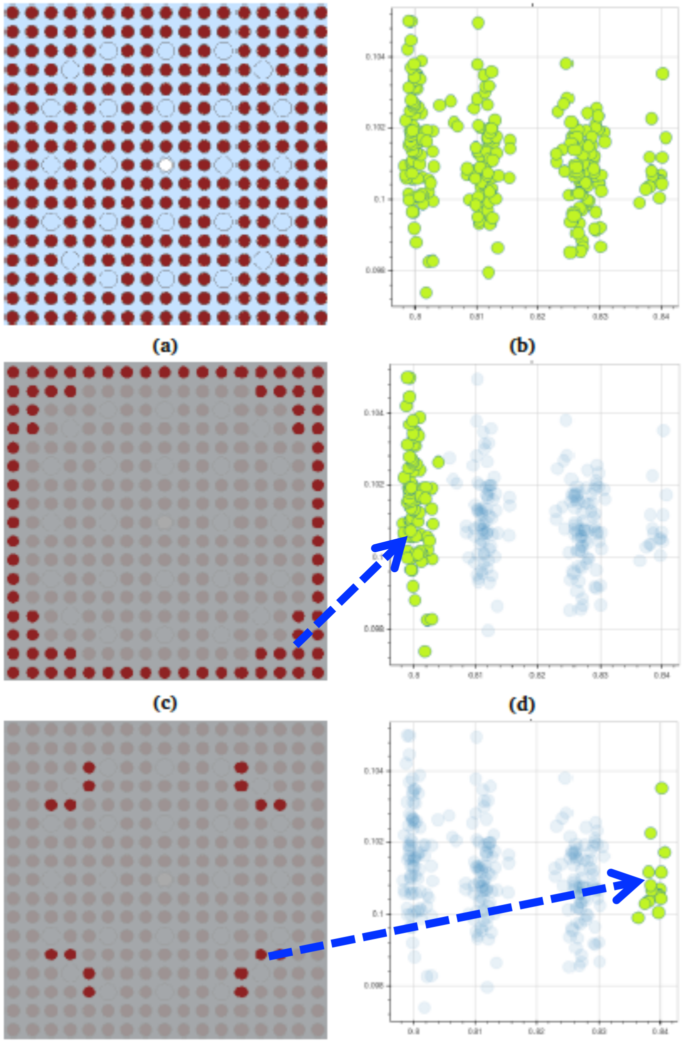
OpenMOC



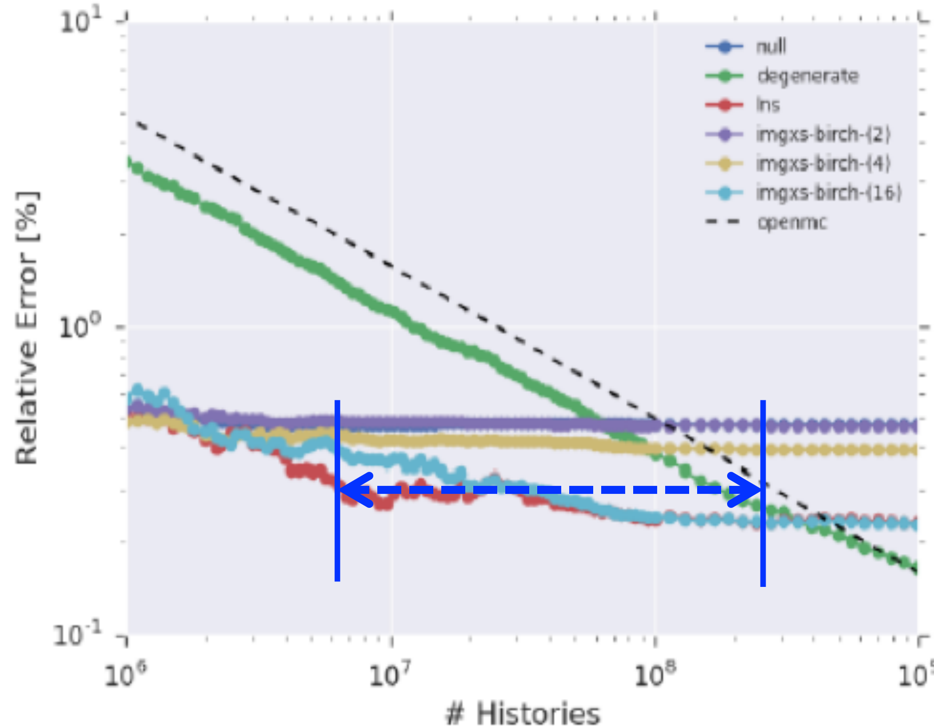
- Deterministic multi-group transport simulation

Will Boyd, MIT

Hybrid Method with Monte Carlo Cross Sections



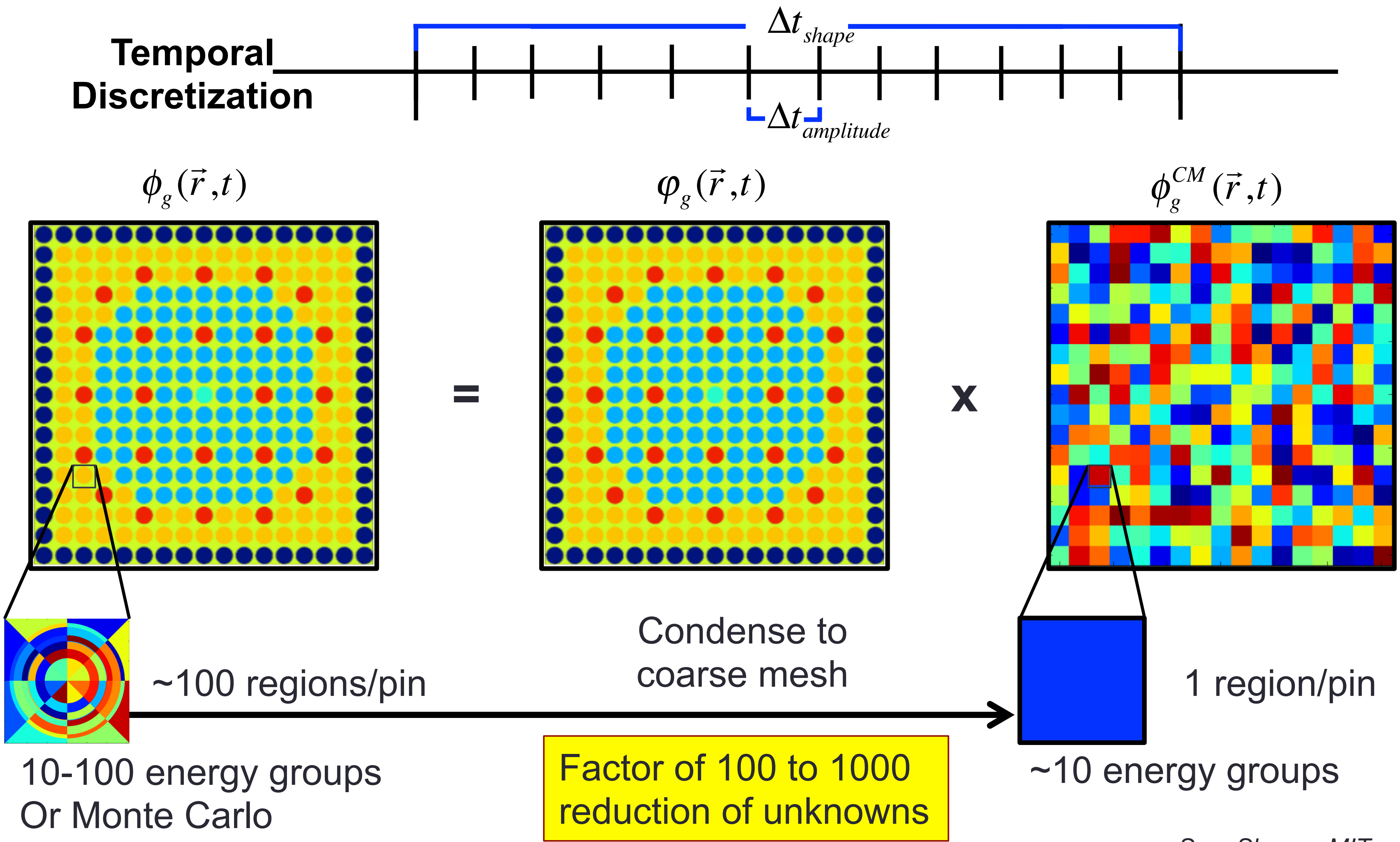
Use machine learning to determine "optimum" clusters of multi-group cross sections



Will Boyd, MIT

Achieve desired accuracy faster than direct Monte Carlo by using clustered cross sections in a 3-D a deterministic core transport model?

Time-Dependent Monte Carlo or Deterministic Transport Using Yamamoto's Multi-grid Amplitude Function (MAF)?



Sam Shaner, MIT

Often Humbling Lessons in Core Neutronics

- *The most scalable methods can be hiding large underlying inefficiencies (e.g., Monte Carlo cache misses)*
- *Small problem success can lead to unwarranted optimism regarding scalability (e.g., C5G7 transport problem vs. large dominance ratio LWRs)*
- *Premature optimization of single-physics methods makes researchers reluctant to move on to challenges arising in multi-physics modeling (e.g., neutron transport sweeps without acceleration or thermal feedback)*
- *Practical problems arising from nuclide depletion should be addressed as early as possible (e.g., massive data handling issues)*
- *High-fidelity multi-physics methods may start out less accurate than current low-fidelity methods (e.g., Doppler feedback in LWRs)*
- *Transient methods may not be direct extensions of steady-state methods (e.g., time-dependent Monte Carlo)*

Engineers Value Short Turnaround Times

Waiting…..

Waiting…..

Waiting…..

Waiting….

Waiting……….

- *“Hero runs” are rare: design, analysis, and testing require fast turnaround times*
- *Real engineering projects require simultaneous execution of many jobs*
- *Mid-range HPC machines often provide “best” turnaround today*
- *Most HPC machine queues need to dramatically improve many-user performance*

Other Challenges for HPC in Nuclear Engineering

- *Fast-access mass storage devices for saving "checkpoint" or "restart" files*
- *Long-term (and cheap) storage devices for saving/accessing reactor history data*
- *Compliers that are more robust and less error prone*
- *QA procedures for production "middleware"*
- *Extended software and hardware life-cycles*

Costs for Using HPC Machines

$300 Million/5 year lifetime = 60 $M/yr
15 Mw(e) x 24 hr/d x 365 d/yr x 100 $/Mw-hr = 13 $M/yr

73 $M/yr x 3 /(365 x 24 hours/yr x 10^7 cores) = 0.0025 $/core-hr

One 10^6 core-hour job x 0.0025 $/core-hr = $2,5000/job

What 10^6 core-hr simulation is worth $2,500 to your boss?
Make sure you have a paying "customer" !

Thank you!

Have a great time at M&C 2017

Questions?