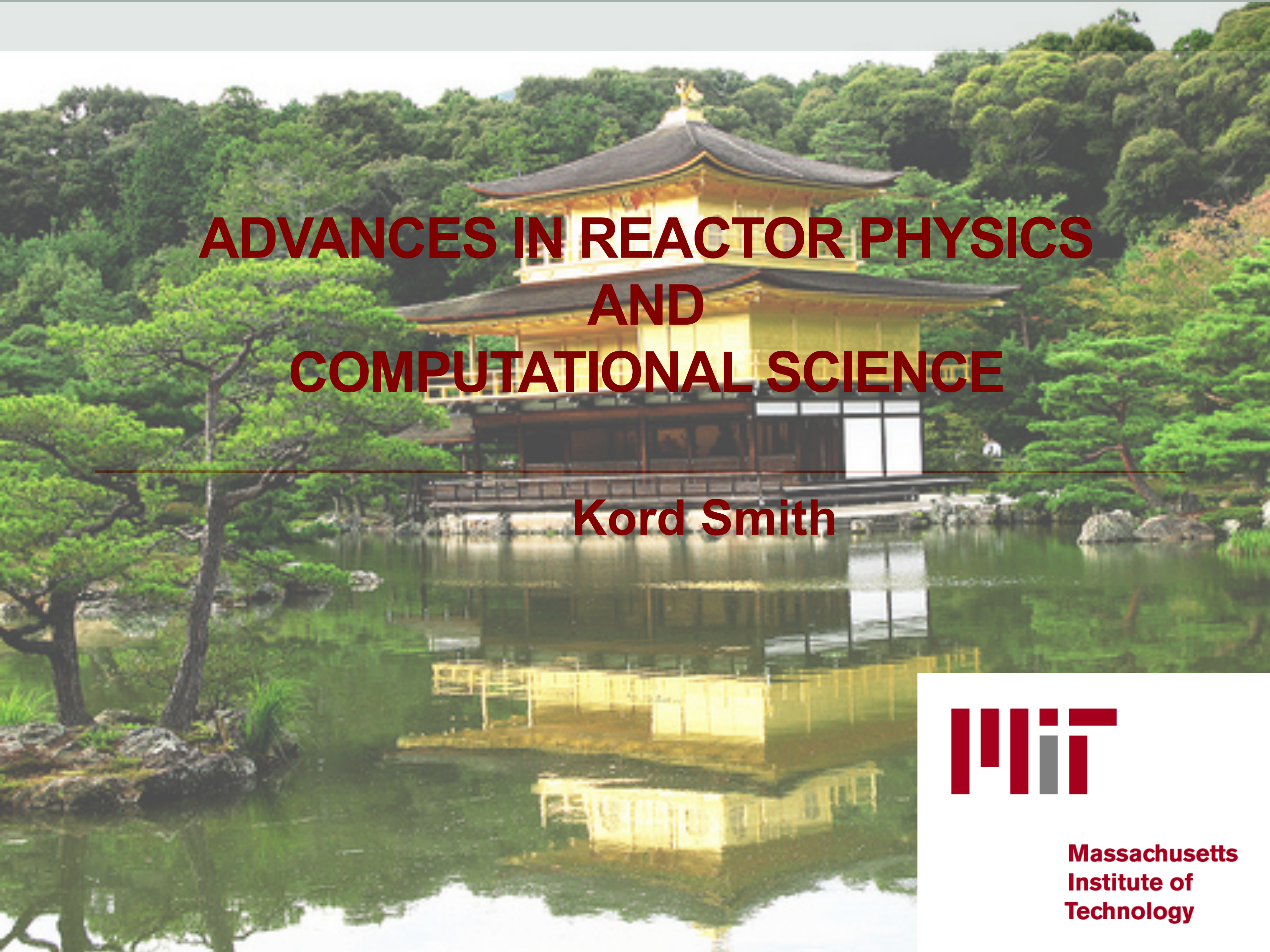
ADVANCES IN REACTOR PHYSICS AND COMPUTATIONAL SCIENCE

Kord Smith



Massachusetts Institute of Technology

Goals of This Presentation

- **To briefly outline some of the:**
  - **Trends in advanced reactor analysis methods**
  - **Challenges faced by new analysis methods**
  - **Implications of modern computing platforms**

LWR analysis will be used as the framework for this introduction, and I apologize to those whose work is not mentioned due to the time constraints.

Reactor Physics Goals

- **To obtain a precise solutions to the Boltzmann neutron transport equation(s) for any reactor design and operational condition**

  (steady-state, depletion state, or transient condition)

- **To accommodate arbitrary-fine spatial variations in material properties provided by other physics fields**

  (temperature, density, nuclide inventory, geometric distortions, etc.)

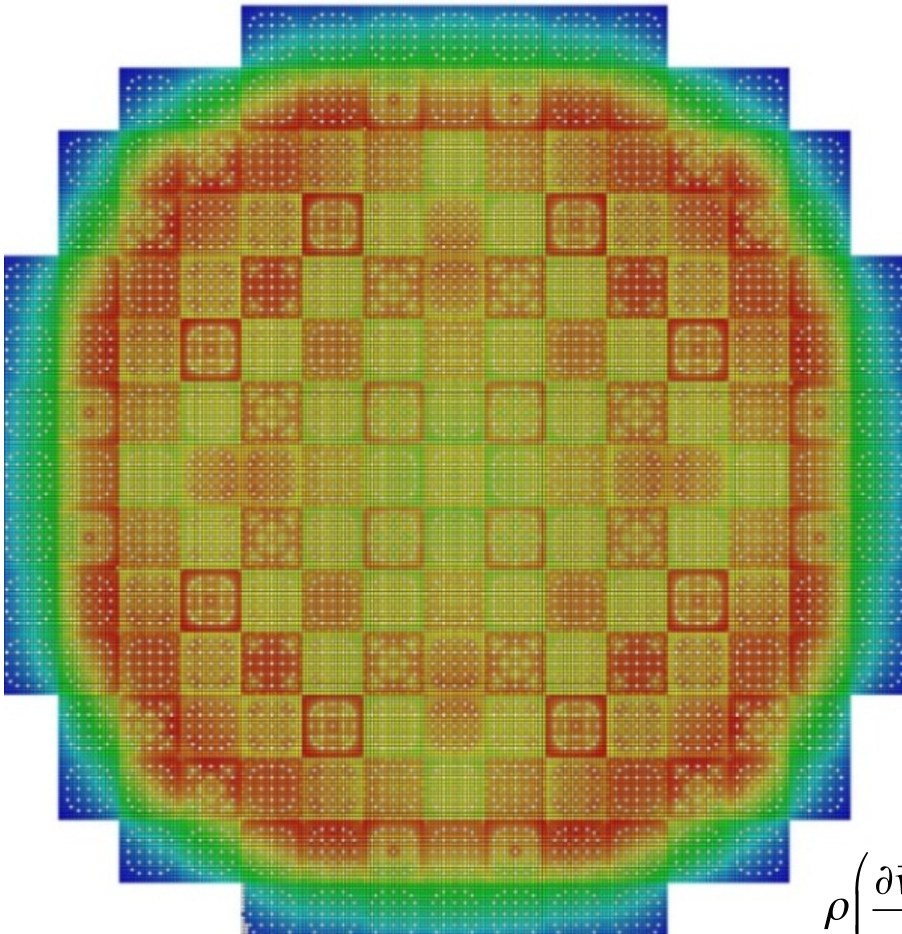
- **To account for known and unknown sources of uncertainty on predicted core physics parameters**

  (nuclear cross sections, construction deviations, corrosion/crud deposition, irradiation growth, etc.)

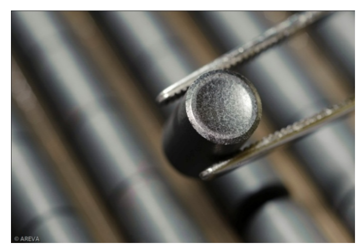
Boltzmann Transport coupled to Fuel Conduction/Depletion/Fluid Flow

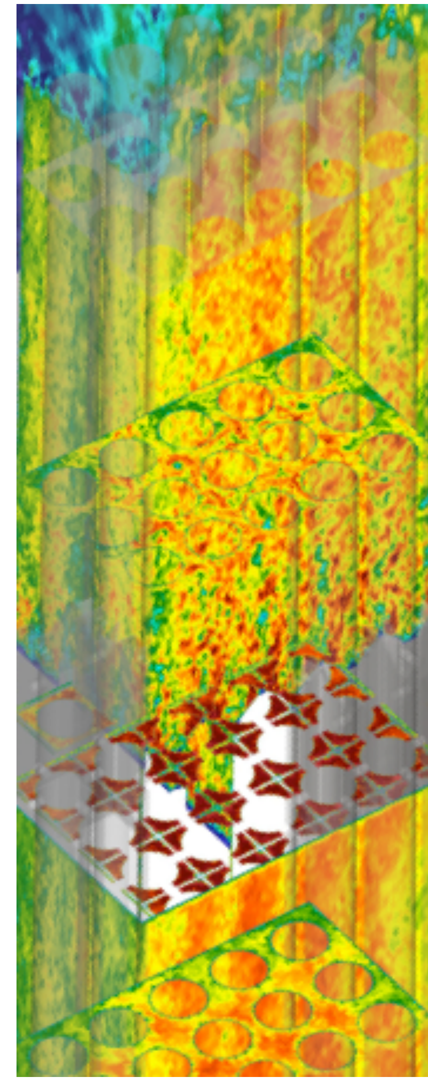
$$\frac{1}{v(E)}\frac{\partial}{\partial t}\psi(\vec{r},E,\vec{\Omega},t)+\vec{\Omega}\cdot\nabla\psi(\vec{r},E,\vec{\Omega},t)+\Sigma_t(\vec{r},E,t)\psi(\vec{r},E,\vec{\Omega},t)$$

$$=\int dE'\int d\vec{\Omega}'\left[\left(\frac{\chi(E)}{k_{eff}}\nu\Sigma_f(\vec{r},E',t)+\Sigma_s(\vec{r},\vec{\Omega}\rightarrow\vec{\Omega},E'\rightarrow E,t)\right)\psi(\vec{r},E',\vec{\Omega},t)\right]$$



$$\rho c_p(T)\frac{\partial T(\vec{r},t)}{\partial t}=$$
$$\nabla\cdot k(T)\nabla T(\vec{r},t)+\dot{q}(\vec{r},t)$$

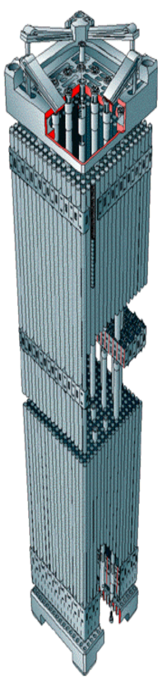


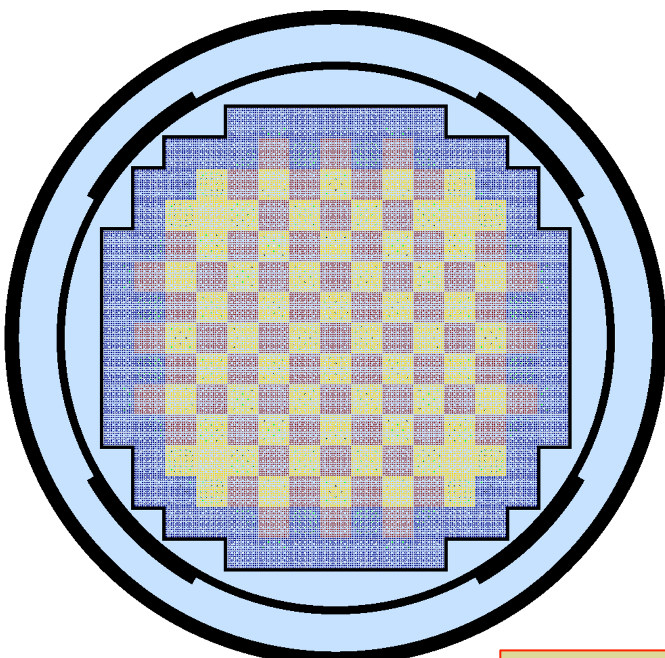


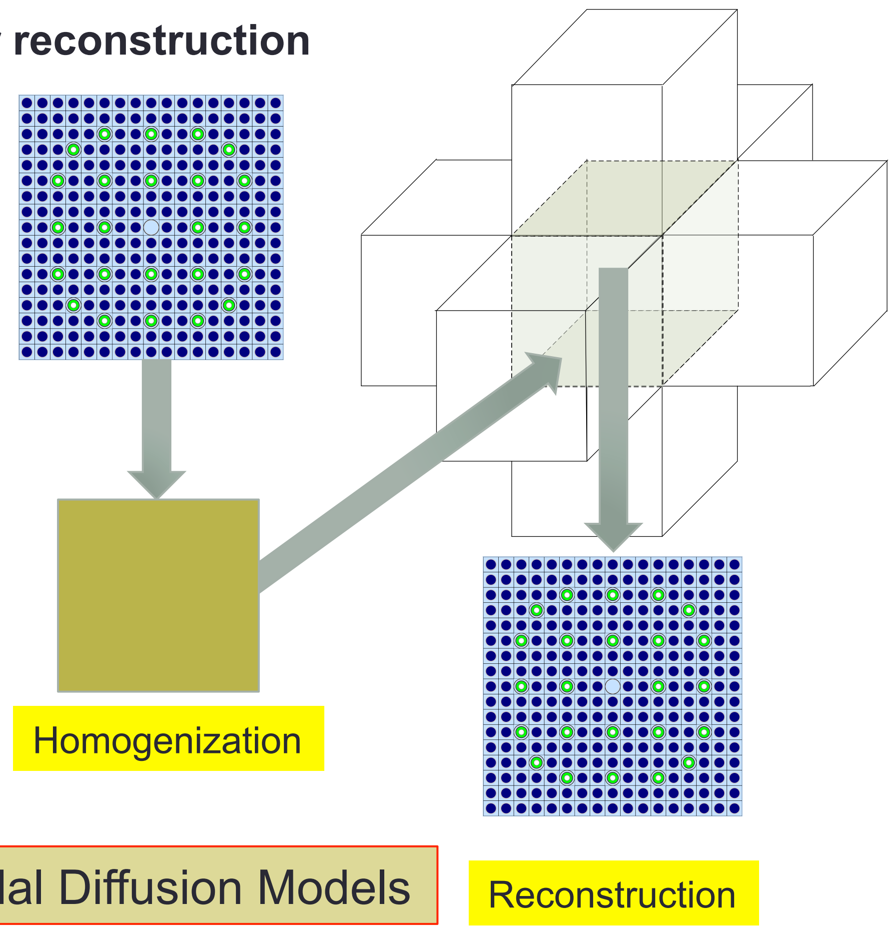
$$\rho\left(\frac{\partial\vec{v}(\vec{r},t)}{\partial t}+\vec{v}(\vec{r},t)\cdot\nabla\vec{v}(\vec{r},t)\right)=-\nabla p(\vec{r},t)+\mu\nabla^2\vec{v}(\vec{r},t)+\vec{f}(\vec{r},t)$$

Traditional Nodal Models: Eliminating The Weak Links

1) Lattice resonance approximations (isotope interference, spatial self-shielding)
2) Assembly homogenization approximations (typically single-assembly geometry)
3) Equivalent homogenized baffle/reflector data
4) One characteristic thermal-hydraulic channel per assembly
5) Simplified fuel depletion/spectrum interactions
6) Factorization approximations in pin power reconstruction
7) Few-group homogenized diffusion theory







Current Nodal Diffusion Models

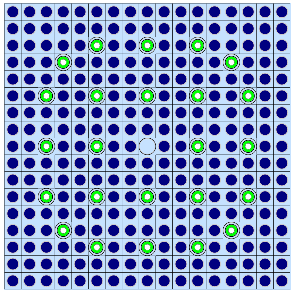
Using Monte Carlo to Replace Deterministic Lattice Calculations

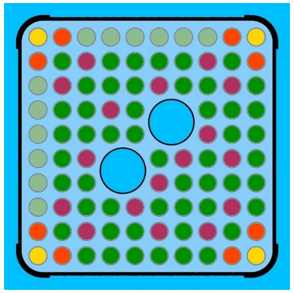
Serpent

a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code

Huge Advantages:

- Eliminates many lattice resonance approximations
- Integrated and accurate nuclide depletion module
- On-the-fly cross section temperature treatment
- Direct treatment of resonance up-scattering effects



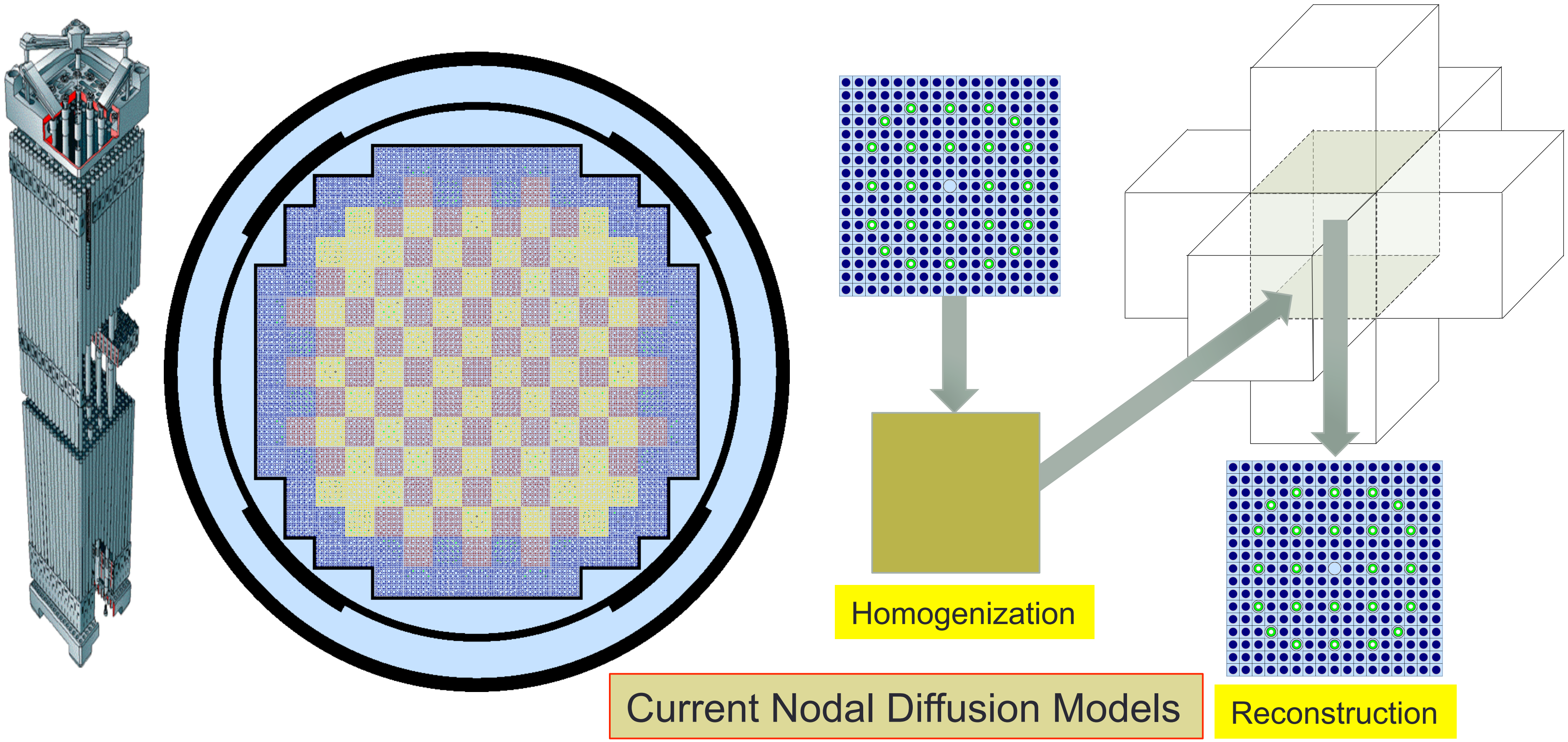


Remaining Challenges:

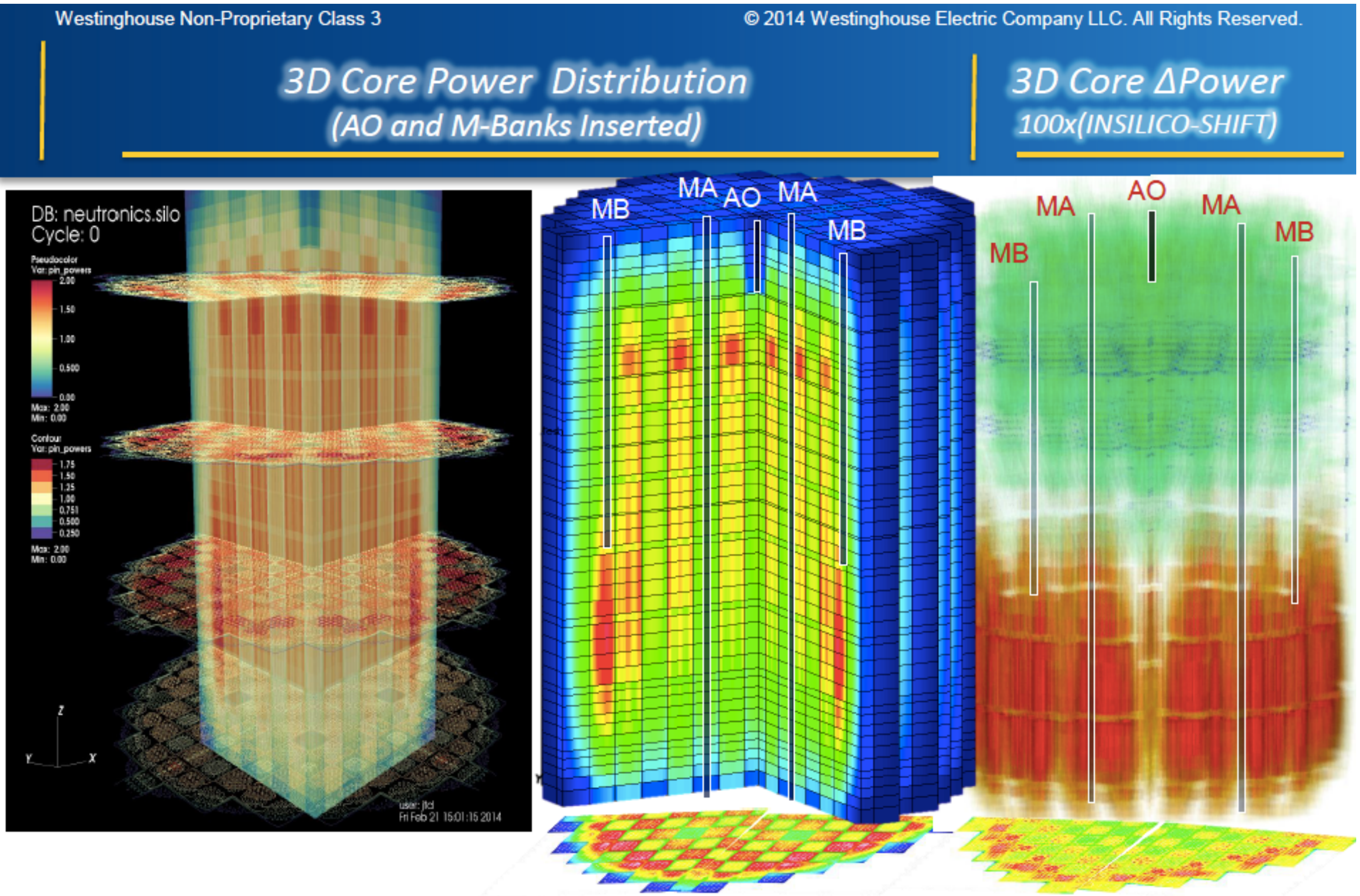
- Avoiding multi-assembly geometries
  - Calculations must remain user-friendly
  - Accurate definition of multi-group homogenized diffusion coefficients, transport cross section, or P_N scattering moments
  - Incorporation of many subtle features of “traditional” homogenization
- Direct tallying of few-group data without using many-group tallies
  - Traditional B_1 spectrum calculation and subsequent diffusion coefficient or transport cross section collapse to few groups
- Reducing execution times and/or resources requirements

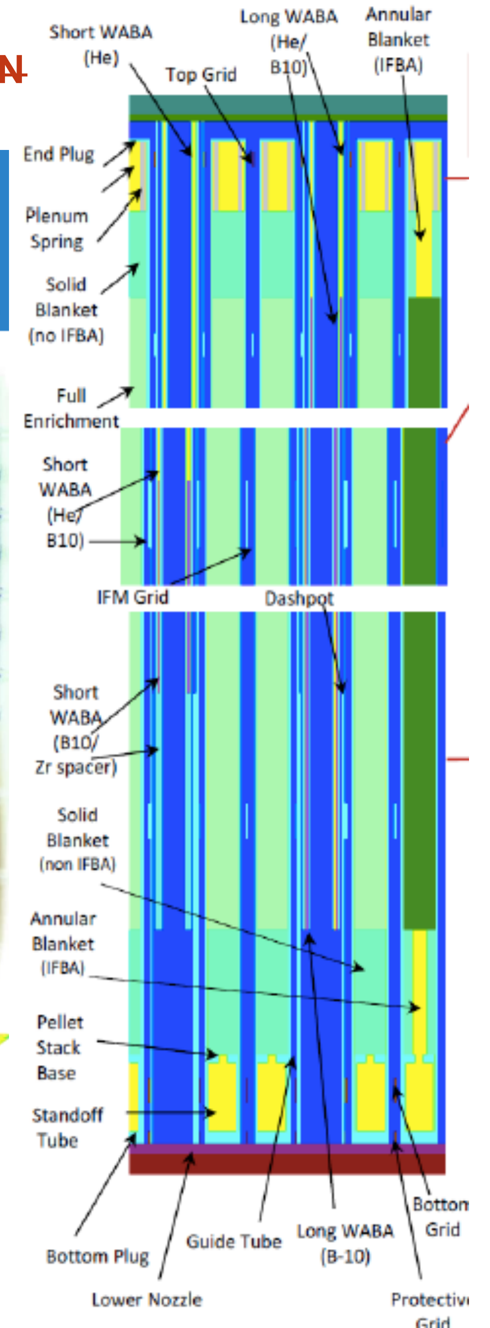
Trend to Move From Current Models → Higher-Fidelity Tools

1) **No up-front lattice calculations (1000s vs. burnup, history, temperature, rods, etc.)**
2) **No homogenization of fuel assemblies or fuel pins**
3) **No baffle/reflector calculations for generation of equivalent reflector data**
4) **Fuel pin and channel level hydraulic feedback**
5) **Pellet-level isotopic depletion and Doppler feedback**



AP1000 INSILICO Tests of Homogenized Pin-cell SP_N



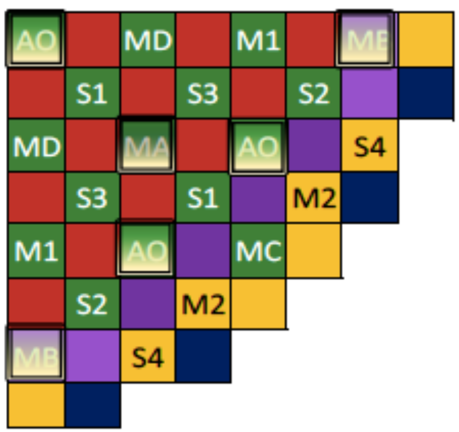


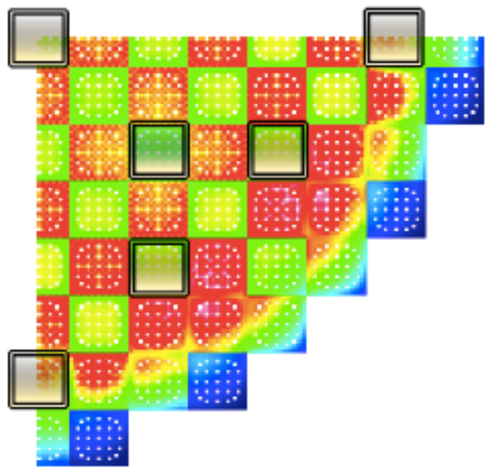
Westinghouse

CASL
A DOE Energy Innovation Hub

AP1000 INSILICO Testing of 3D Homogenized Pin-cell SP_N

	K_{eff}	AO (%)	ΔK_{eff} (pcm)	Δ AO (%)	RMS/Max ΔP Axial "Node" (%)	RMS/Max ΔP Asm (%)	RMS/Max ΔP Pin (%)	RMS/Max ΔP Cell (%)	ΔP Hot Spot (%)
SHIFT	1.00141	-0.8	Ref	Ref	Ref	Ref	Ref	Ref	Ref
KENO	1.00090	-0.7	-50	-0.1	0.1/0.2	0.4/1.0	0.4/1.1	0.5/3.0	1.0
INSILICO	1.00078	-1.7	-63	-0.9	1.0/2.9	0.4/0.7	0.5/3.0	1.2/5.8	1.9



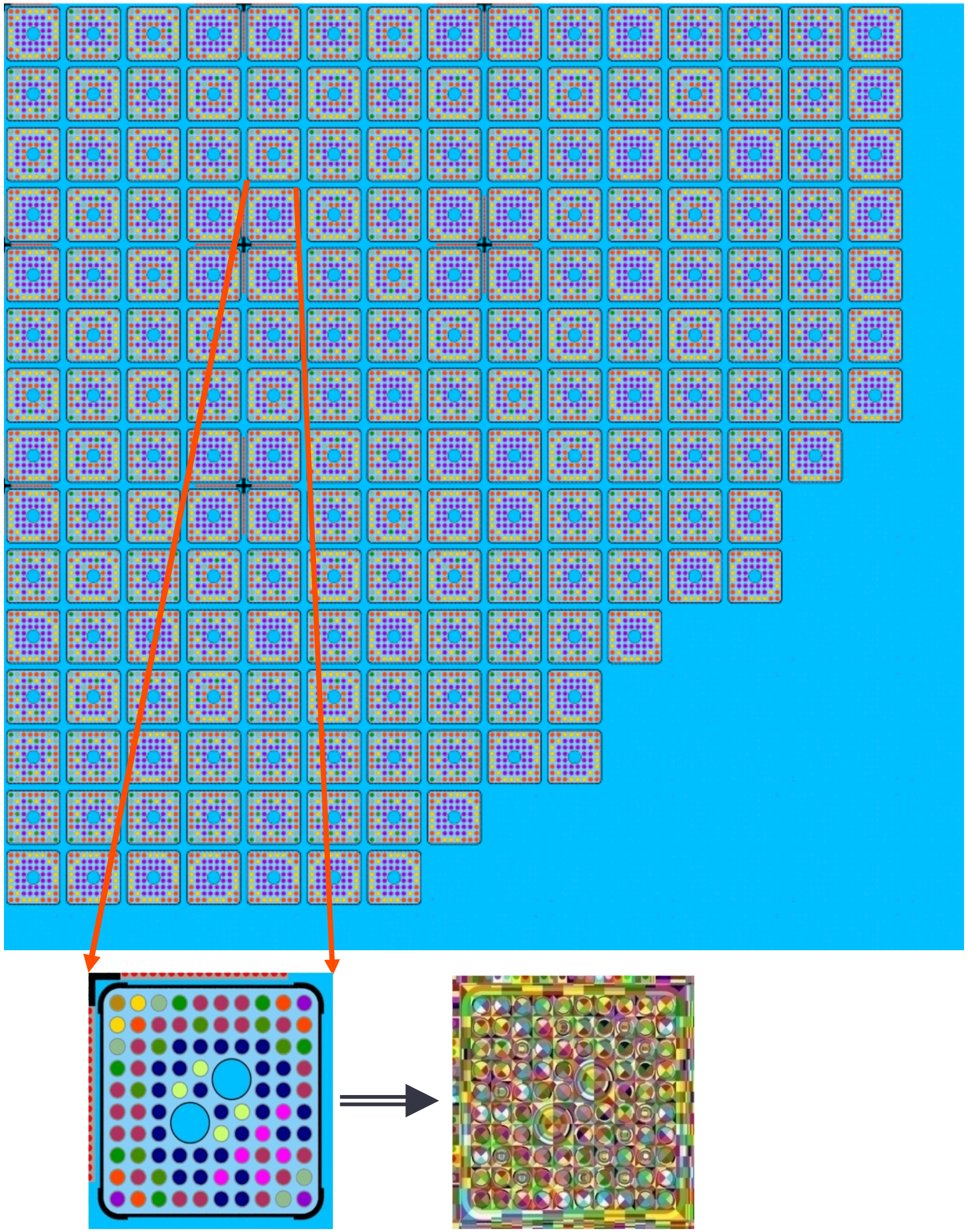


MA (Gray) Fully Inserted
MB (Gray) ~ 60% Inserted
AO (Black) ~ 15% Inserted
Boron at ~1250 ppm
HZP Temperatures

The AP100 results are far more accurate than most expect or can explain.

Homogenized SP_N has had limited over many years with mixed success.
But many choose not to agonize over applicability of pin-cell homogenization

Fully-Resolved Deterministic 2D Transport Calculations



2D MOC in use for >10 years

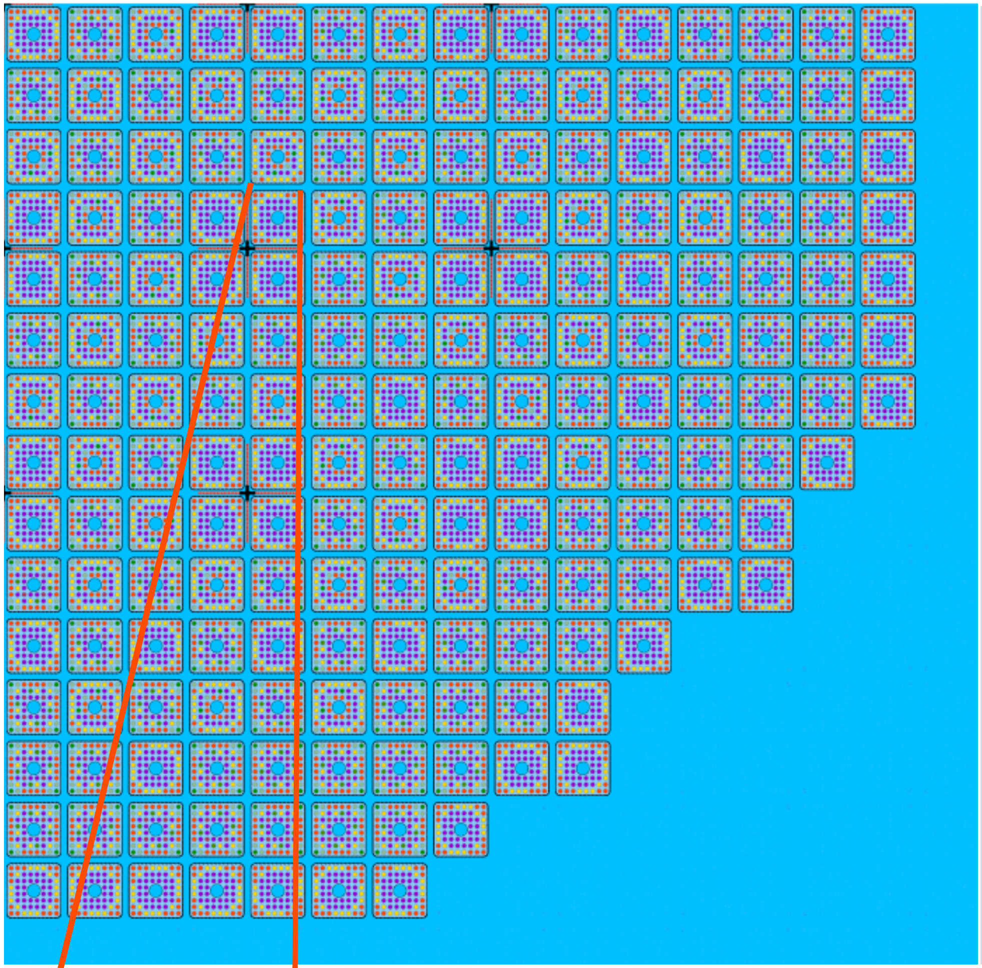
Advantages:

- No up front lattice calculations
- Very fine radial mesh solutions
- No homogenization approximations
- Depletion on sub-pin basis
- Local T-H data can be treated
- Radial mesh is geometrically constrained by physical geometry
- Few core-hours execution per state-point have been achieved

Disadvantages:

- Deterministic resonance models
- 2D applications are very limited

Full-Core Fully-Resolved 3D Deterministic Transport Calculations



3D MOC seems very natural

Challenges:

- Axial axial source mesh and fine ray spacing: **x1000**
- More polar angles needed in 3D: **x5**
- Domain decomposition for memory

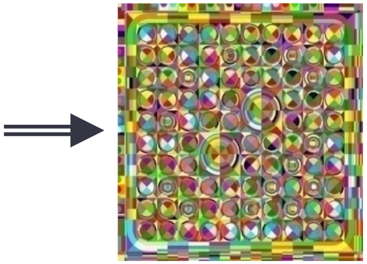
3-D Discrete S_N (LD, FEM, EP)

Advantages:

- High-order spatial approximations may be advantageous axially

Disadvantages:

- Meshing for air gaps, IFBA regions require far more mesh than MOC



Bottom line: No deterministic LWR transport solution (converged in space, and angle) with credible energy resolution has been published.
Problem size is currently overwhelming

MC21 (KAPL/BETTIS) Full-Core Monte Carlo Calculations

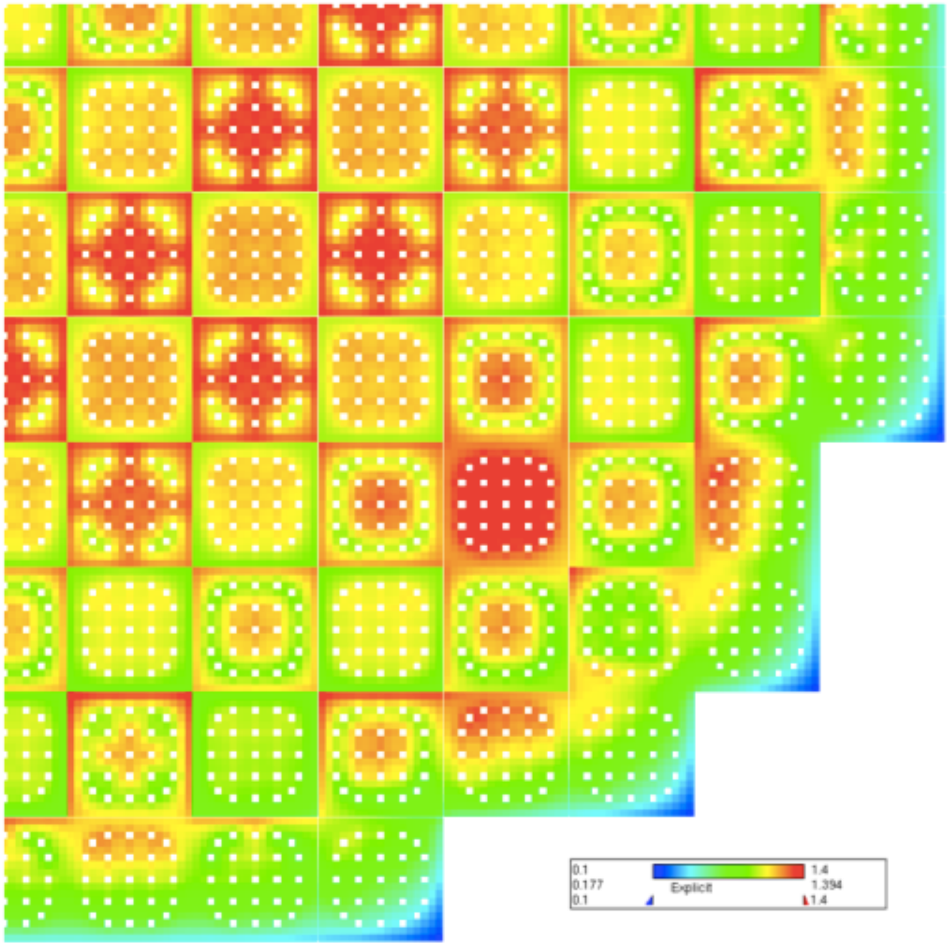


Figure 17. MC21 pin wise relative power density at day 92.

3D MC is attractive:

Advantages:

- **Direct resonance treatment**
- **No meshing to resolve flux gradients**
- **Fine spatial mesh coupling for thermal-hydraulic and depletion physics**

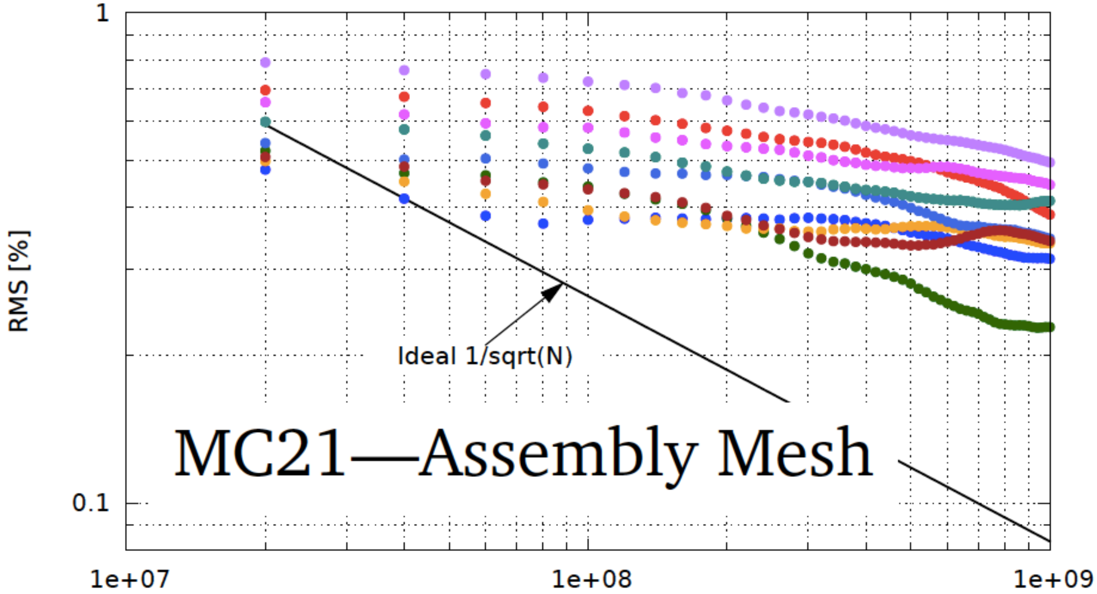
Challenges:

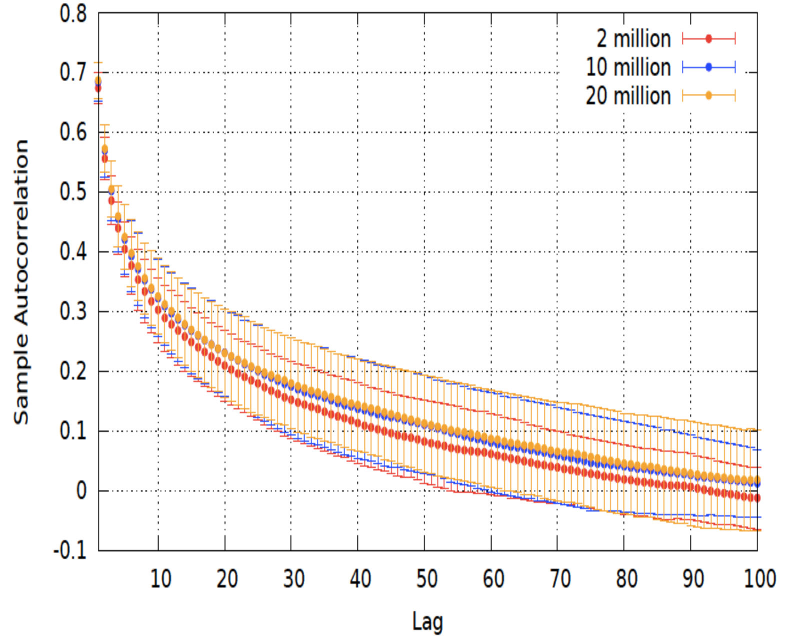
- **Cross section temperature modeling**
- **Converging source distributions in high dominance ratio LWRs**
- **Obtaining reliable estimates of local uncertainties**
- **TB size tallies for depletion**

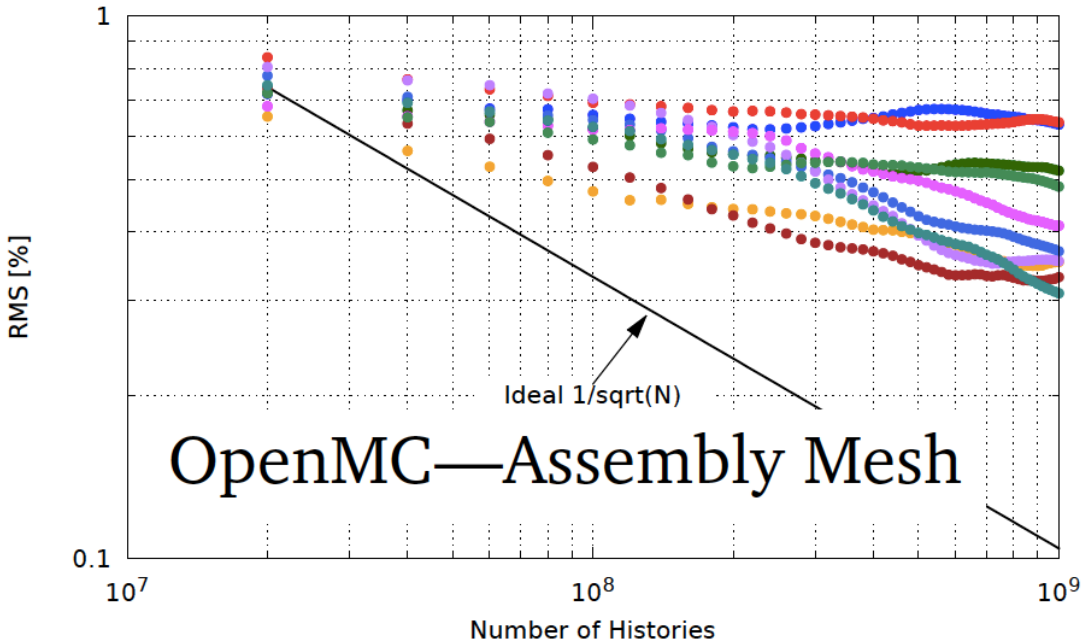
- **~50,000 of core-hours per step**

Bottom line: Monte Carlo has, at least temporarily, surpassed deterministic methods for fully-resolved reactor depletion with thermal feedback

Monte Carlo Fission Source Correlations Effects







Bottom line:

- **MC spatial results do not converge as as 1/sqrt(N)**
- **Traditional tally uncertainty estimates are unrealistic**
- **Independent realizations are needed to be confident**
- **Massive # of neutrons are required per batch**

Be Mindful of the Difference Between Scalability and Efficiency

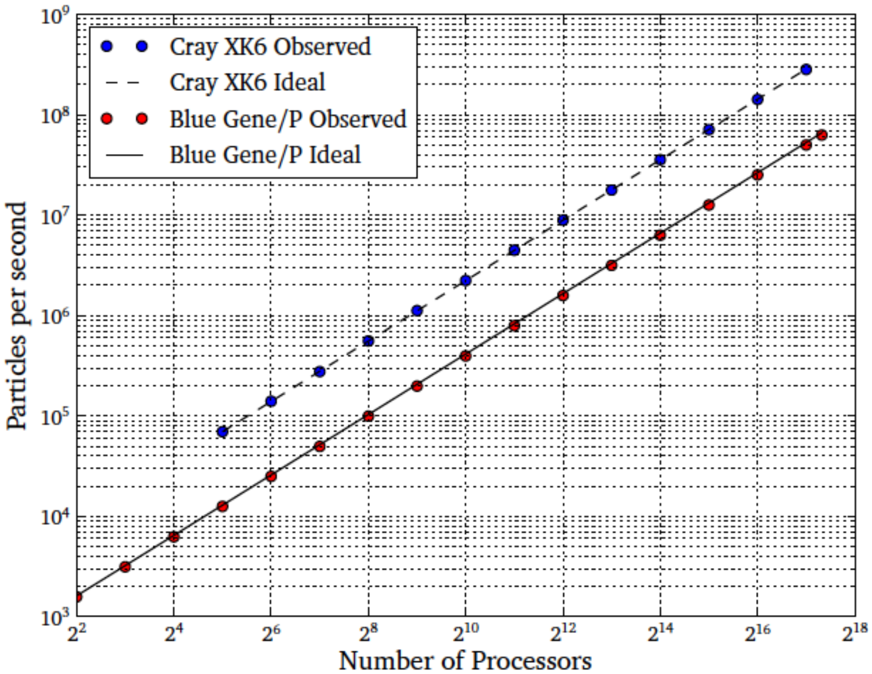
- Currently Monte Carlo cross section linear interpolation consists of the following sequence:

  Zero the material macroscopic cross section

  Loop over 400 Isotopes

  Loop over 3 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

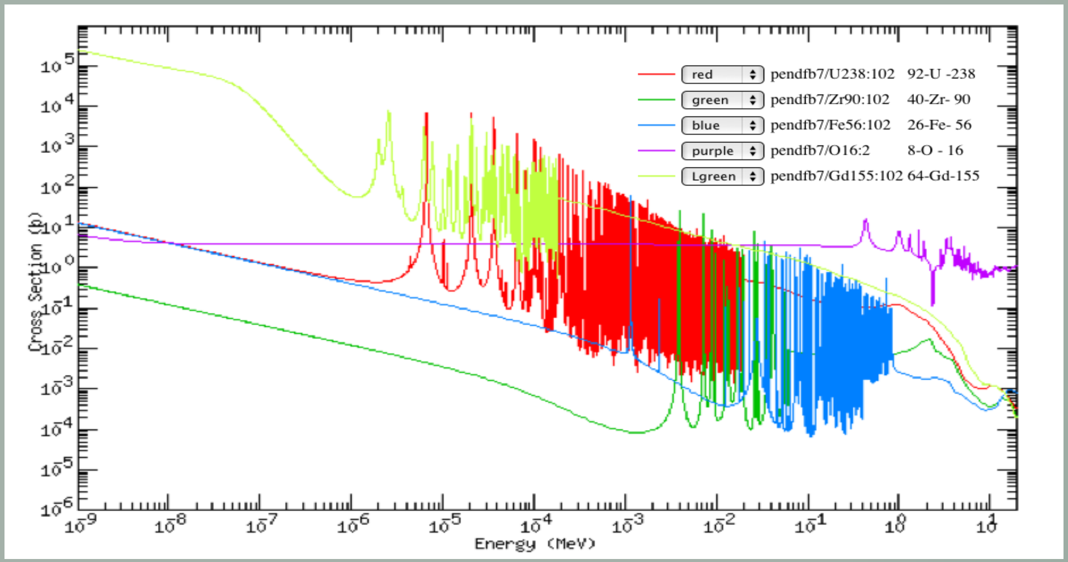


Bytes/FLOP are miserably large for Monte Carlo

Scalability ≠ Efficiency

HPC Flops Are "Free": If Data Movement from Cache/Memory Is Avoided

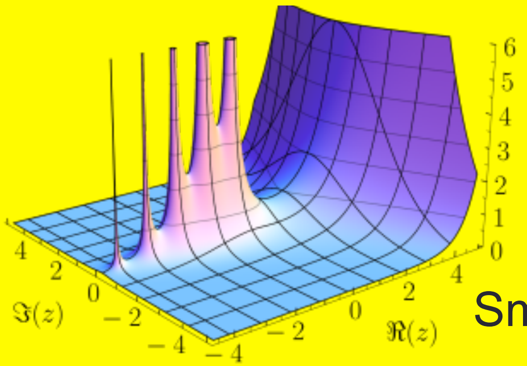
Simple point-wise data tables for temperature interpolations



$$\sigma_x(E,T) = \frac{1}{4}\left[\begin{matrix}\sigma_x(E_n,T_l) + \sigma_x(E_{n+1},T_l) \\ \sigma_x(E_m,T_{l+1}) + \sigma_x(E_{m+1},T_{l+1})\end{matrix}\right]$$

Every data access is a cache miss

Store resonance parameters and reconstruct cross sections



$$\sigma_x(E,T) = \frac{1}{E}\sum_{l,J}\sum_{\lambda=1}^{N}\sum_{i=1}^{2(l+1)} \Re\left[\frac{e^{-2i\phi_l} R_x \sqrt{\pi}\, W(z_0) - \frac{iR_t}{\sqrt{\pi}} C\left(\frac{z}{\sqrt{\xi}}, \frac{u}{\sqrt{\xi}}\right)}{2\sqrt{\xi}}\right]$$

Small data stays in cache, movement from bulk memory avoided

More Needs To Be Done To Make Monte Carlo Practical

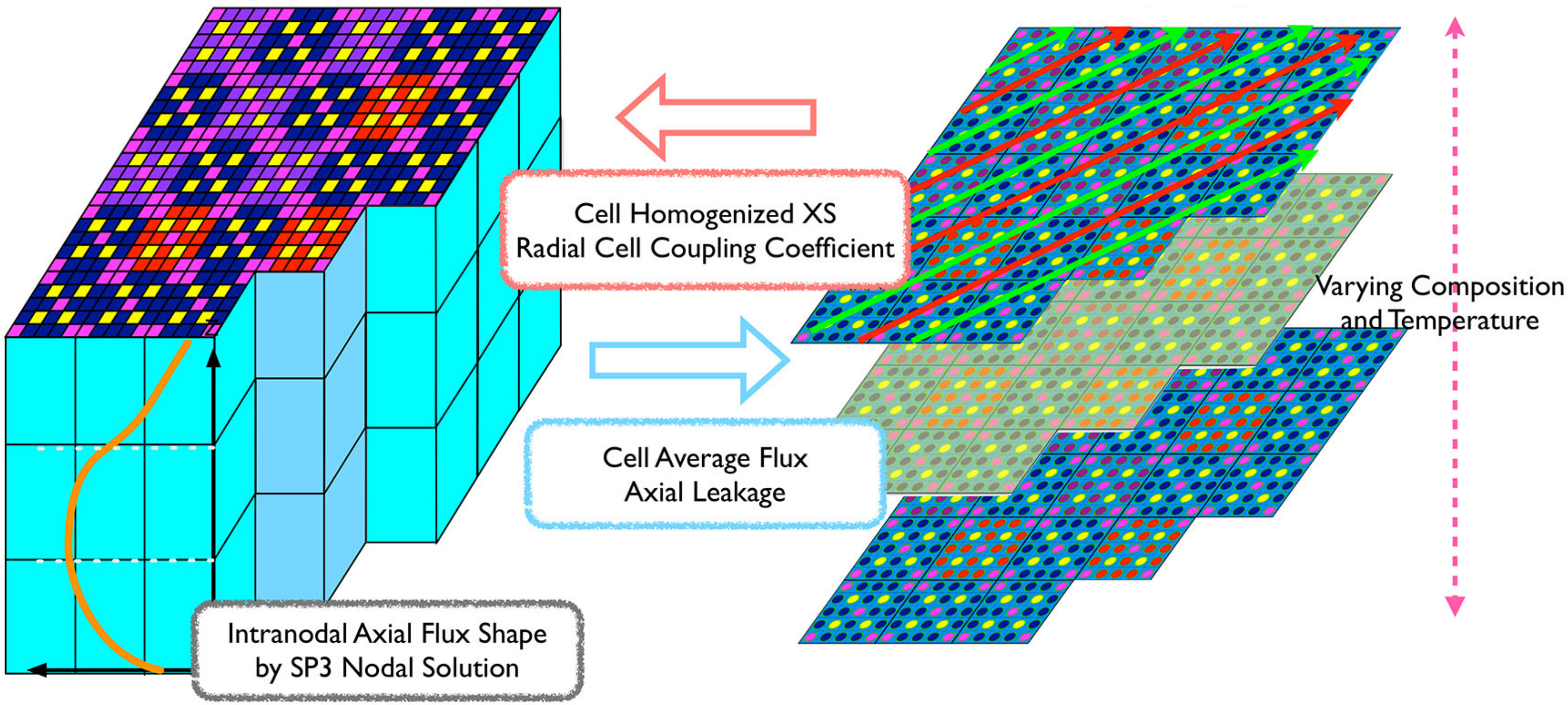
- **Inactive cycle convergence estimators more reliable than Shannon Entropy**
- **Variance estimators that treat batch correlation**
- **Improved methods for accelerating convergence of active cycles**
- **Efficient Doppler Broadening of full energy-range cross sections**
- **Domain decomposition (or functional equivalent) for massive tallies (nuclide depletion of sub-pellet spatial regions)**
- **Improved data structures to replace ACE-type formats, eliminate redundant data, and accommodate new functional data types**

Execution time remain a primary obstacle for broad-scale MC reactor applications

2D/1D Methods (n-TRACER, MPACT, DeCART, etc.)

3-D CMFD Calculation with Axial SP3 Kernel
to Resolve Global Balance and Generate 3-D Power Distribution♪

Planar MOC Calculations
to Generate Plane-wise Pin-cell Homogenized XS



3D CMFD Solver
incorporating with Axial SP3 Nodal Method

Planar MOC Solver

- In-stream sub-group resonance models
- Non-uniform pellet temperature profiles
- Sub-channel thermal fluid/heat conduction
- Predictor/Corrector nuclide depletion

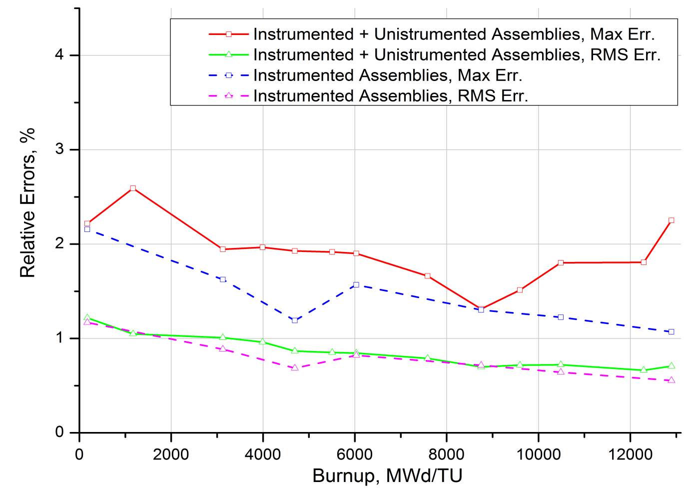
SNU Reactor Physics Laboratory
Advancing Innovation in Fission and Fusion Neutronics

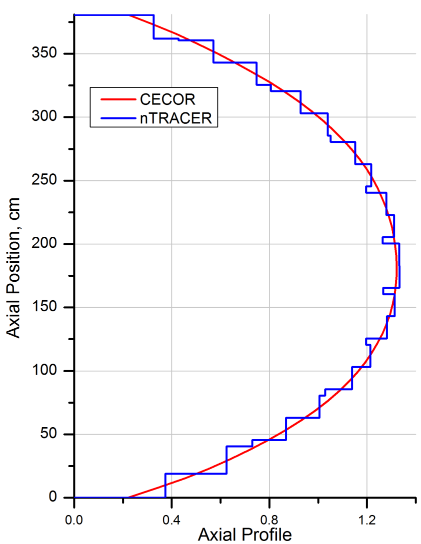
Prof. Han Gyu Joo (Seoul National) n-Tracer Comparisons with Plant Data

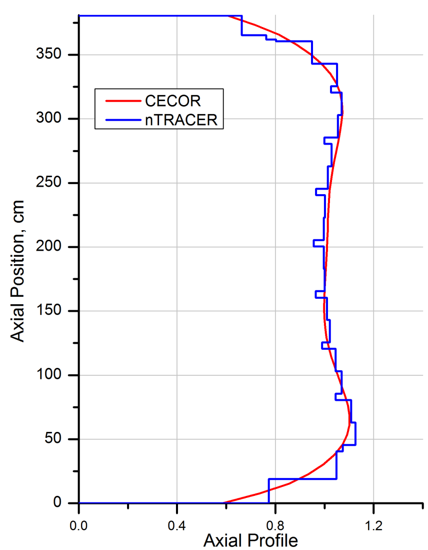
0.738 0.733 *0.005* *0.73*	**0.928** 0.933 *-0.006* *-0.60*	**1.088** 1.104 *-0.015* *-1.41*	**0.794** 0.803 *-0.010* *-1.20*	**1.143** 1.132 *0.011* *0.95*	**1.061** 1.059 *0.002* *0.14*	**1.271** 1.266 *0.005* *0.36*	**1.076** 1.077 *-0.001* *-0.10*
0.928 0.933 *-0.006* *-0.60*	**1.124** 1.116 *0.008* *0.67*	**0.784** 0.799 *-0.015* *-1.96*	**1.195** 1.181 *0.014* *1.16*	**0.817** 0.827 *-0.010* *-1.24*	**1.212** 1.232 *-0.020* *-1.68*	**1.229** 1.231 *-0.003* *-0.22*	**0.912** 0.918 *-0.006* *-0.69*
1.088 1.104 *-0.015* *-1.41*	**0.784** 0.799 *-0.015* *-1.96*	**1.087** 1.083 *0.004* *0.33*	**0.770** 0.778 *-0.008* *-1.00*	**1.142** 1.140 *0.002* *0.20*	**0.862** 0.881 *-0.019* ***-2.22***	**1.187** 1.187 *0.000* *0.01*	**0.608** 0.612 *-0.004* *-0.69*
0.794 0.803 *-0.010* *-1.20*	**1.195** 1.181 *0.014* *1.16*	**0.770** 0.778 *-0.008* *-1.00*	**1.106** 1.101 *0.005* *0.47*	**0.827** 0.835 *-0.009* *-1.05*	**1.301** 1.288 *0.014* *1.04*	**1.090** 1.069 *0.022* *1.99*	
1.143 1.132 *0.011* *0.95*	**0.817** 0.827 *-0.010* *-1.24*	**1.142** 1.140 *0.002* *0.20*	**0.827** 0.835 *-0.009* *-1.05*	**1.198** 1.183 *0.015* *1.22*	**1.170** 1.145 *0.025* *2.16*	**0.621** 0.620 *0.001* *0.22*	
1.061 1.059 *0.002* *0.14*	**1.212** 1.232 *-0.020* *-1.68*	**0.862** 0.881 *-0.019* ***-2.21***	**1.301** 1.288 *0.014* *1.05*	**1.170** 1.145 *0.025* *2.16*	**0.740** 0.726 *0.014* *1.94*		
1.271 1.266 *0.005* *0.36*	**1.229** 1.231 *-0.003* *-0.21*	**1.187** 1.187 *0.000* *0.01*	**1.090** 1.069 *0.022* *2.00*	**0.621** 0.620 *0.001* *0.22*			
1.076 1.077 *-0.001* *-0.09*	**0.912** 0.918 *-0.006* *-0.69*	**0.608** 0.612 *-0.004* *-0.68*					

Max Err, % 2.22
RMS Err. % 1.22

x.xxx	nTRACER
x.xxx	CECOR
x.xxx	*Abs. Err*
x.xx	*Rel. Err %*







2D/3D Methods

Advantages:

- **Preserves MOC radial fidelity**
- **Captures 3D pin-wise t-h effects**
- **In-stream resonance modeling**
- **Sufficient accuracy for LWRs**
- **Execution in ~500 core-hr/step**

Disadvantages:

- **Do not rigorously converge to 3D transport solutions**

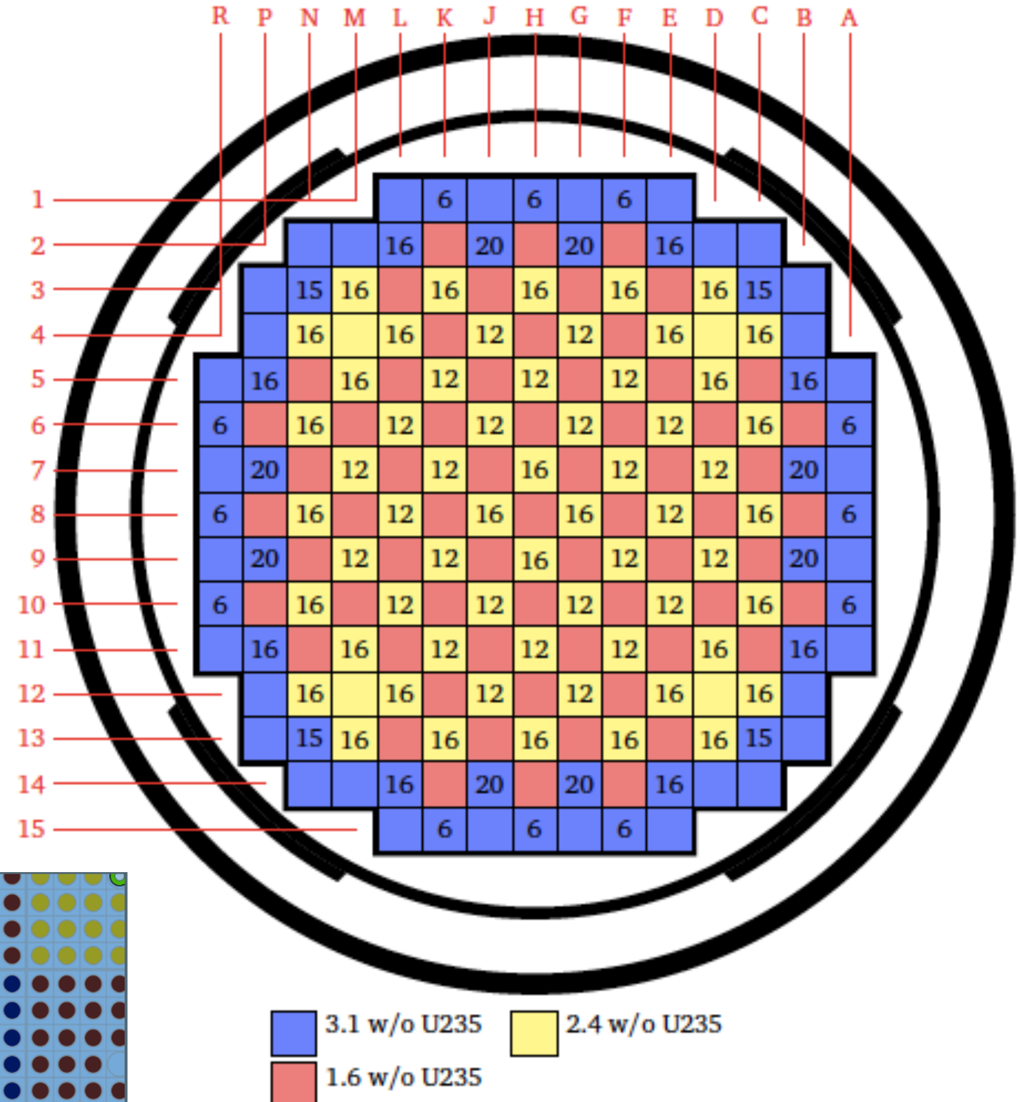
Remember It Is 2014 - not 1970. Manufactured Solutions and Numerical Benchmarks Are Useful, But No Longer Sufficient

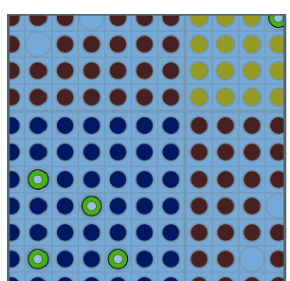
MIT

Benchmark for
Evaluation
And
Validation of
Reactor
Simulations

RELEASE rev. 1.0.1

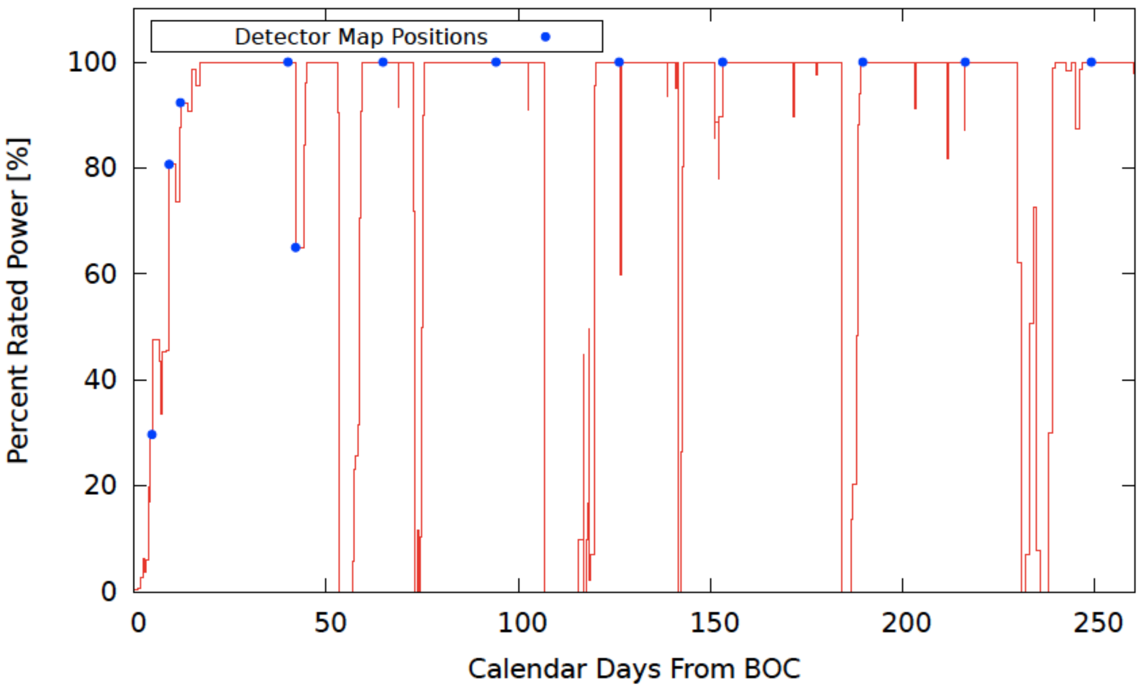
MIT Computational Reactor Physics Group

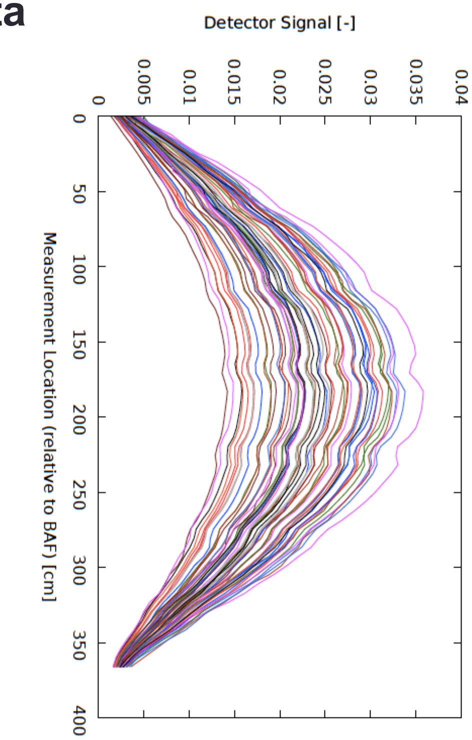




BEAVRS: Two-Cycle Operational LWR Benchmark

- **Cycle-1 Hot Zero Power (HZP) can be simulated without feedback**
- **Hot Full Power (HFP) requires neutronic/fluid coupling & cross section feedback**
- **Cycle simulation required detailed nuclide depletion and equilibrium Xenon**
- **Cycle-2 requires core fuel assembly shuffling of deletion data**





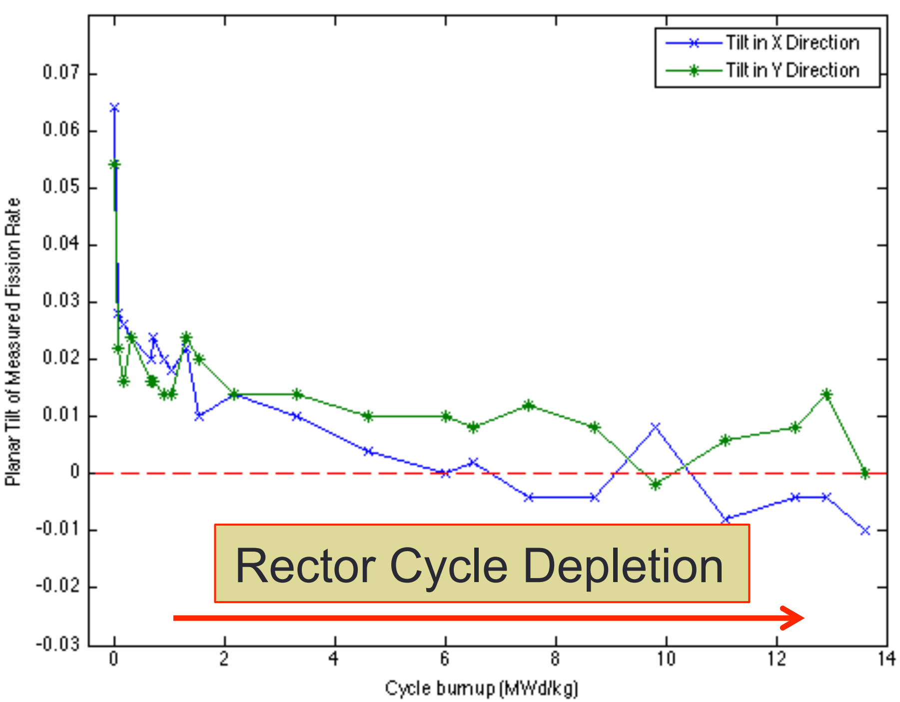
- **Comparison with measured data provides useful V&V/UQ testing of methods/codes**
- **Benchmark provides a challenge for both deterministic or Monte Carlo neutron transport – coupled to fuels behavior, nuclide depletion, and core/vessel fluid flow.**

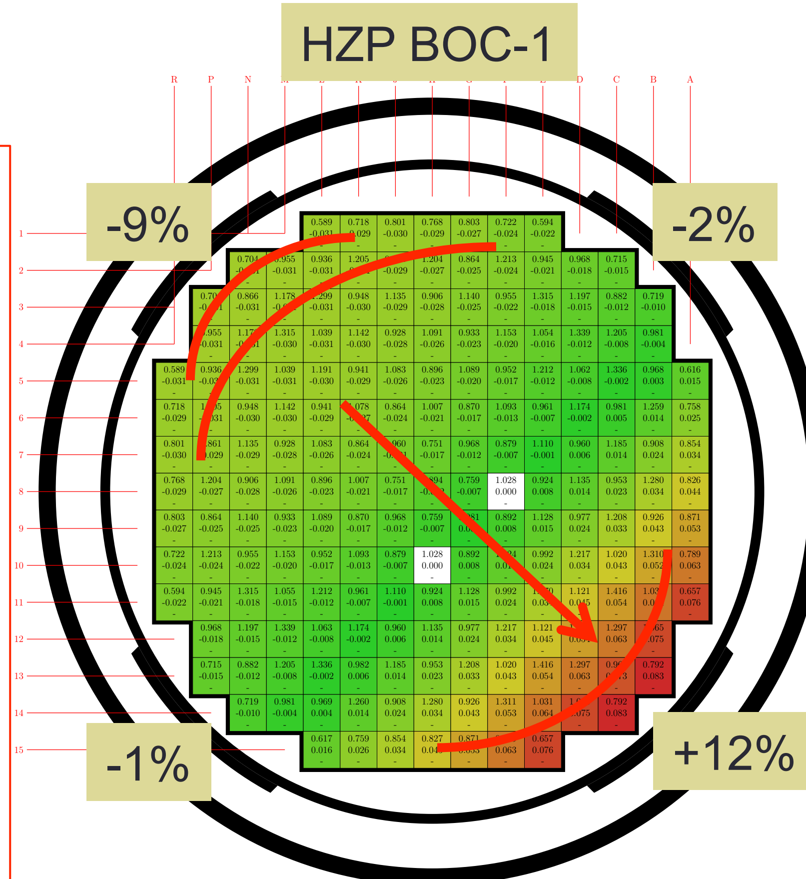
VV/UQ and the Real World

BEAVRS in-core fission rate distributions display a nearly pure x-y linear tilt:

- **Tilt is +/- 6.0% in both x and y directions at HZP BOC1**
- **Tilt becomes +/- 2.5% at HFP conditions**
- **Tilt rapidly depletes to +/- 1.0%**

Directional Tilts vs. Cycle Burnup





Spatial uncertainties are driven by geometrical, not cross section uncertainty

What Is Needed For Neutronics UQ

- **Methods for quantification of not only random geometrical uncertainties, but also systematic manufacturing/construction geometrical deviations - that are directly observable.**

- **Methods for quantification of geometrical distortions from CRUD deposition and irradiation-induced fuel skeleton growth**

- **Depletion reactivity uncertainties from cross sections that account for the fact that Evaluated Nuclear Data has been previously "adjusted" by evaluators to produce LWR cold critical eigenvalues of nearly unity. (e.g., >500 pcm uncertainties are not realistic)**

Bottom Line: We need UQ that gracefully handles multi-physics effects and produces realistic (not wildly conservative) uncertainty estimates.

Multi-physics Applications are Driving Current Developments

- **While full spatial resolution reactor neutronics has yet to be fully realized, numerous high-accuracy methods have been fully developed and deployed.**
- **Achieving coupled multi-physics simulations with <u>balanced computational effort</u> between the physics modules is key to continued progress.**
- **Multi-physics tool/toolkits (e.g., SALOME, MOOSE, VERA, etc.) being developed/deployed show promise for efficient multi-physics implementation with minimal engineering burden. Such developments will require substantial time and funding to achieve full maturity.**
- **We must assure that new models/tools are more accurate that existing tools, and are practical in the end-user's work environment.**



Remember What Nuclear Plant Owner/Operators Desire From Reactor Physics

- **To have sufficiently accurate knowledge of reactor behavior to enable safe and economic operation of every nuclear plant**

  (over the plants anticipated and/or extended lifetime)

- **To be confident that reactor physics personnel can successfully respond to many yet unknown operational plant challenges**

  (plant problems, changes in economics, licensing, plant availability)