MPACT Overview

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VERA Workshop

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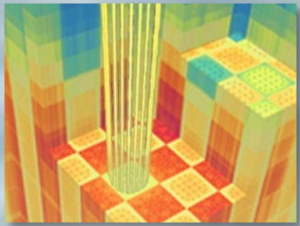
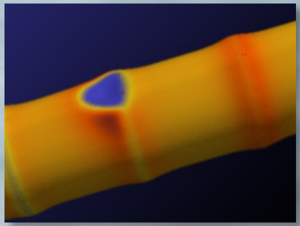
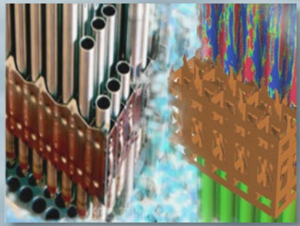




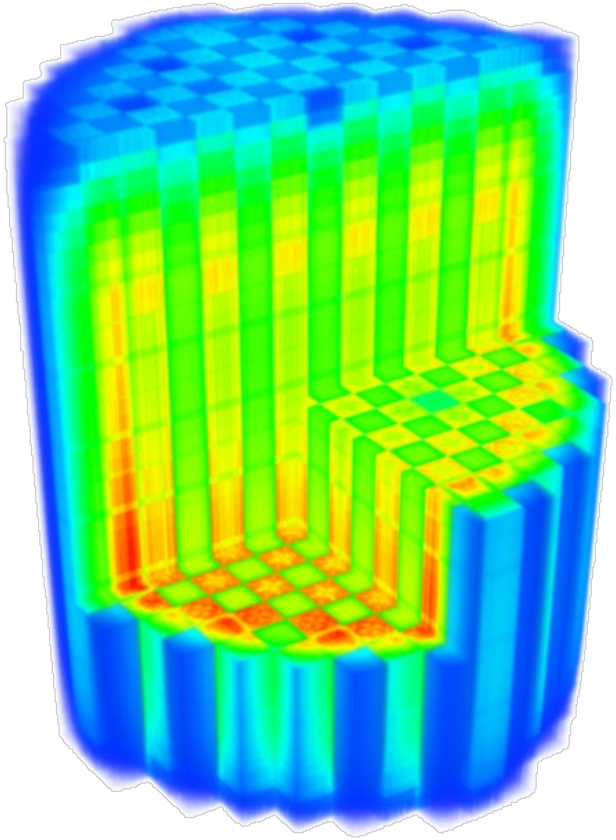


CASL The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

U.S. DEPARTMENT OF ENERGY

Outline

- Background
- 2D/1D Method
  - Radial and Axial Equations
  - Coarse Mesh Finite Difference
- Parallel Decomposition Approach
- XS Library Background
- Depletion/Shuffling
- Reflector Fidelity
- Transient Capability



AP1000 HFP Power Distribution

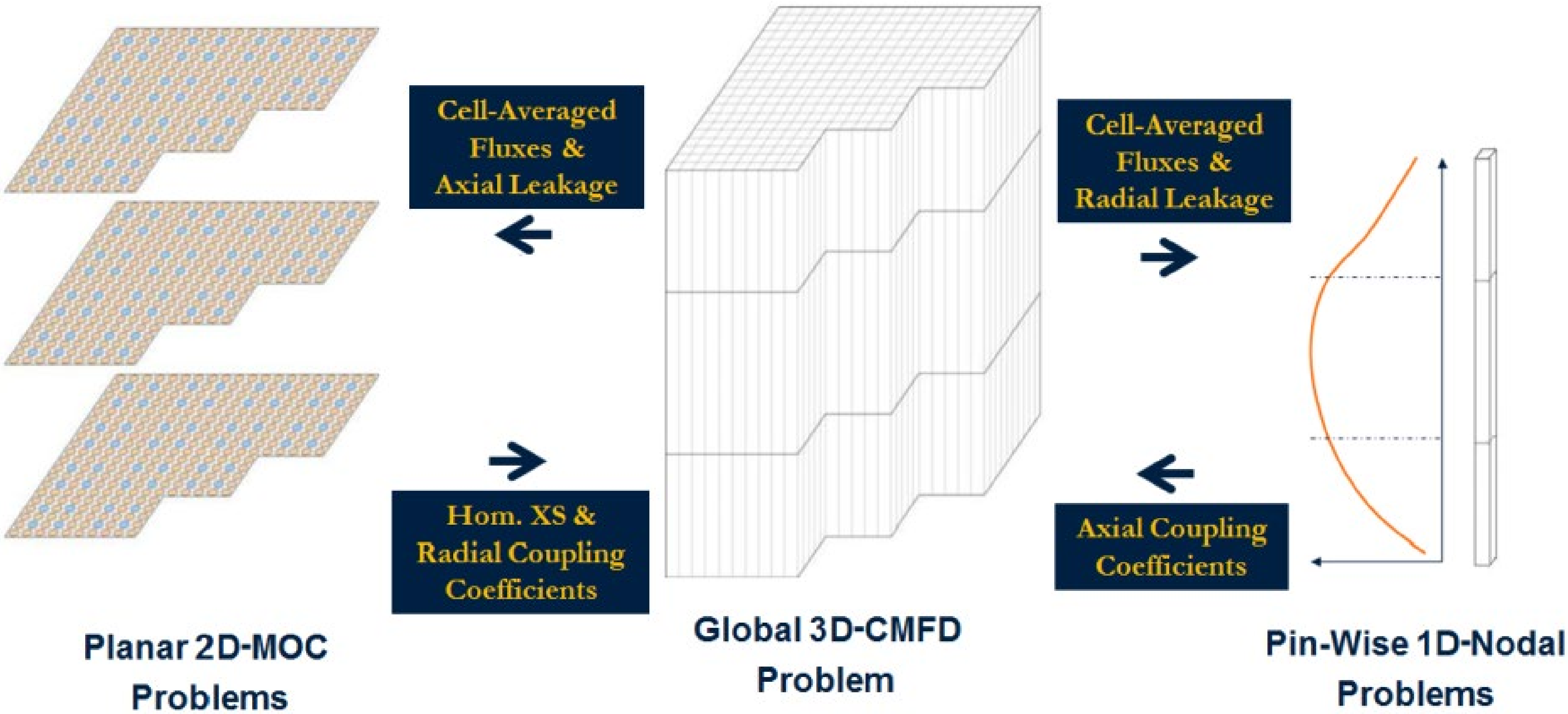
Background

- MPACT is a deterministic transport solver package that originally began development exclusively at the University of Michigan (~2011)
- Since 2014, development has been collaboratively driven by both ORNL and Michigan
- Goal to provide high-fidelity, pin-resolved flux and power distributions
- Several solvers are available, but the workhorse is the 2D/1D method
  - Decomposes 3D problems into an axial stack of radial planes
  - 2D-MOC used radially, and 1D-nodal methods used axially
  - Accelerated with 3D-coarse mesh finite difference (CMFD)

Comparison to Industry Neutronics Tools

Physics Model	Industry Practice	CASL (VERA-CS)
Neutron Transport	3-D diffusion (core) 2 energy groups (core) 2-D transport on single assy	3-D transport 51+ energy groups
Power Distribution	nodal average with pin-power reconstruction methods	explicit pin-by-pin
Xenon/Samarium	nodal average w/correction	pin-by-pin
Depletion	infinite-medium cross sections quadratic burnup correction history corrections spectral corrections reconstructed pin exposures	pin-by-pin with actual core conditions
Reflector Models	1-D cross section models	actual 3-D geometry
Target Platforms	workstation (single-core)	1,000 – 100,000 cores

2D/1D Illustration



Radial Equations

- Axially-Averaged Transport: $\varphi^{Z}_{g,l}(x,y) = \frac{1}{h_z}\int_{z_B}^{z_T} \varphi_{g,l}(x,y,z)dz$
  - μ_l denotes cosine of polar angle
  - α_l denotes azimuthal angle

$$\sqrt{1-\mu_l^2}\left(\cos(\alpha_l)\frac{\partial}{\partial x} + \sin(\alpha_l)\frac{\partial}{\partial y}\right)\varphi^{Z}_{g,l}(x,y) + \Sigma^{Z}_{t,g}(x,y)\varphi^{Z}_{g,l}(x,y) = \tilde{q}^{Z}_{g,l}(x,y)$$

$$\tilde{q}^{Z}_{g,l}(x,y) = \bar{q}^{Z}_{g,l}(x,y) + TL^{Z}_{g,l}(x,y)$$

Axial Transverse Leakage

$$TL^{Z}_{g,l}(x,y) = \frac{\mu_l}{h_z}\left(\varphi_{B,g,l}(x,y) - \varphi_{T,g,l}(x,y)\right)$$

Axial TL - Approximations

- Isotropic Approximation:

$$TL_{g,l}^{Z}(x,y) = \frac{J_{B,g}(x,y) - J_{T,g}(x,y)}{4\pi h_z}$$

- Flat Approximation:

$$TL_{g,l}^{Z}(x,y) = \frac{J_{B,g}^{XY} - J_{T,g}^{XY}}{4\pi h_z}$$

Method of Characteristics

- MOC is used to discretize the 2D transport equation and determine subpin level angular and scalar fluxes:

$$\mathbf{\Omega} \cdot \nabla\varphi(x,y) + \Sigma_t(x,y)\varphi(x,y) = Q(x,y)$$

- Casting this along a characteristic direction:
  - Can convert PDE into ODE
  - Assuming step characteristics: $\frac{\mathrm{d}\varphi}{ds} + \Sigma_t\varphi(s) = Q$
- The angular flux at any point s along this direction can be found:

$$\varphi(s) = \varphi_{in}e^{-\Sigma_t s} + \frac{Q}{\Sigma_t}\left(1 - e^{-\Sigma_t s}\right), \quad \varphi(0) = \varphi_{in}$$

Method of Characteristics

- Outgoing Angular Flux:

$$\varphi_{out,m} = \varphi(s = l_m) = \varphi_{in,m} e^{\Sigma_t l_m} + \frac{Q}{\Sigma_t}\left(1 - e^{-\Sigma_t l_m}\right), \quad l_m = t/\sin(\theta_m)$$

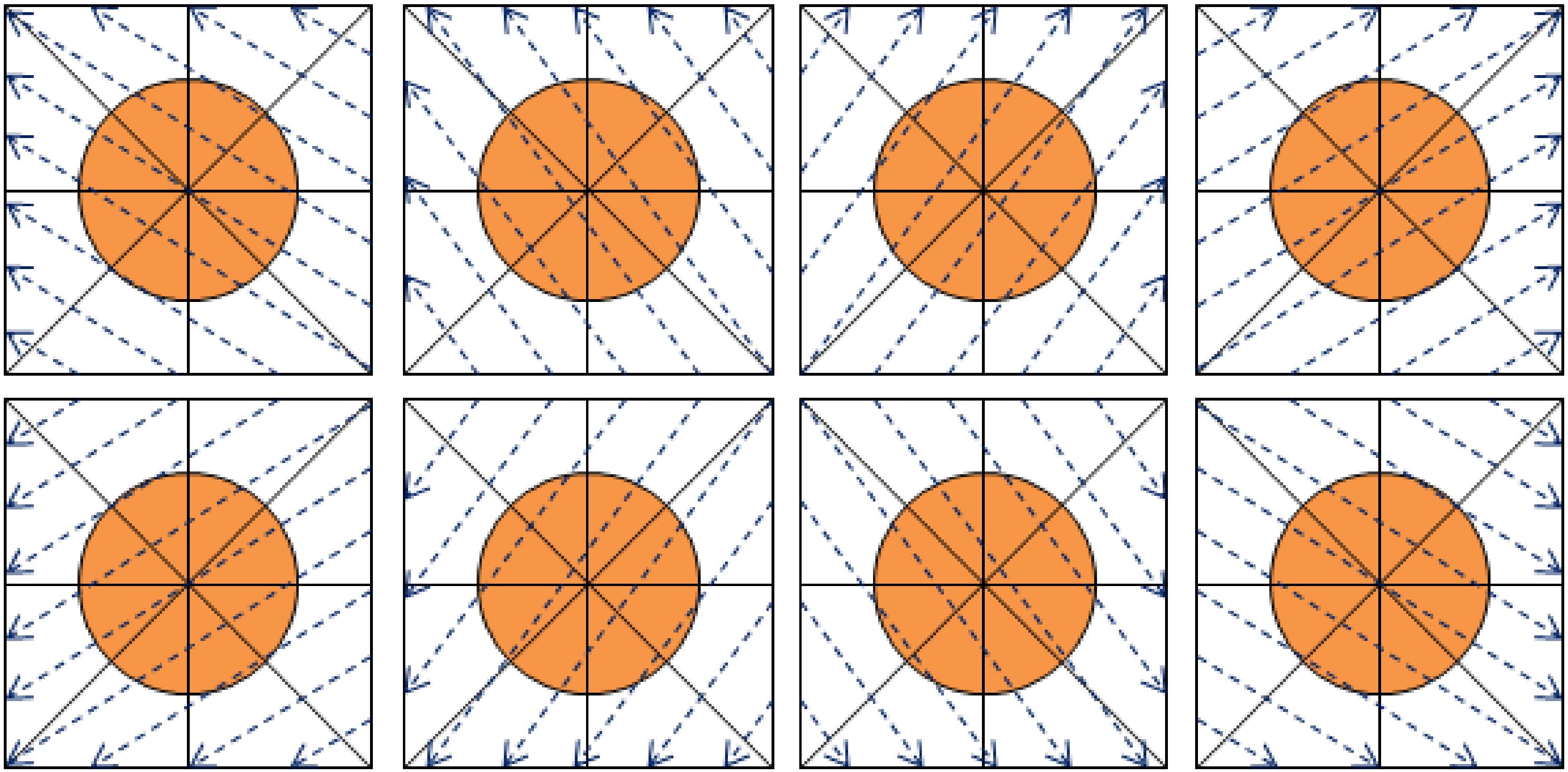
- Average Angular Flux along a segment:

$$\tilde{\varphi}_m = \frac{1}{l_m}\int_0^{l_m} \varphi(s)ds = \frac{Q}{\Sigma_t} + \frac{\varphi_{in,m} - \varphi_{out,m}}{\Sigma_t l_m}$$

- Scalar flux within a region:

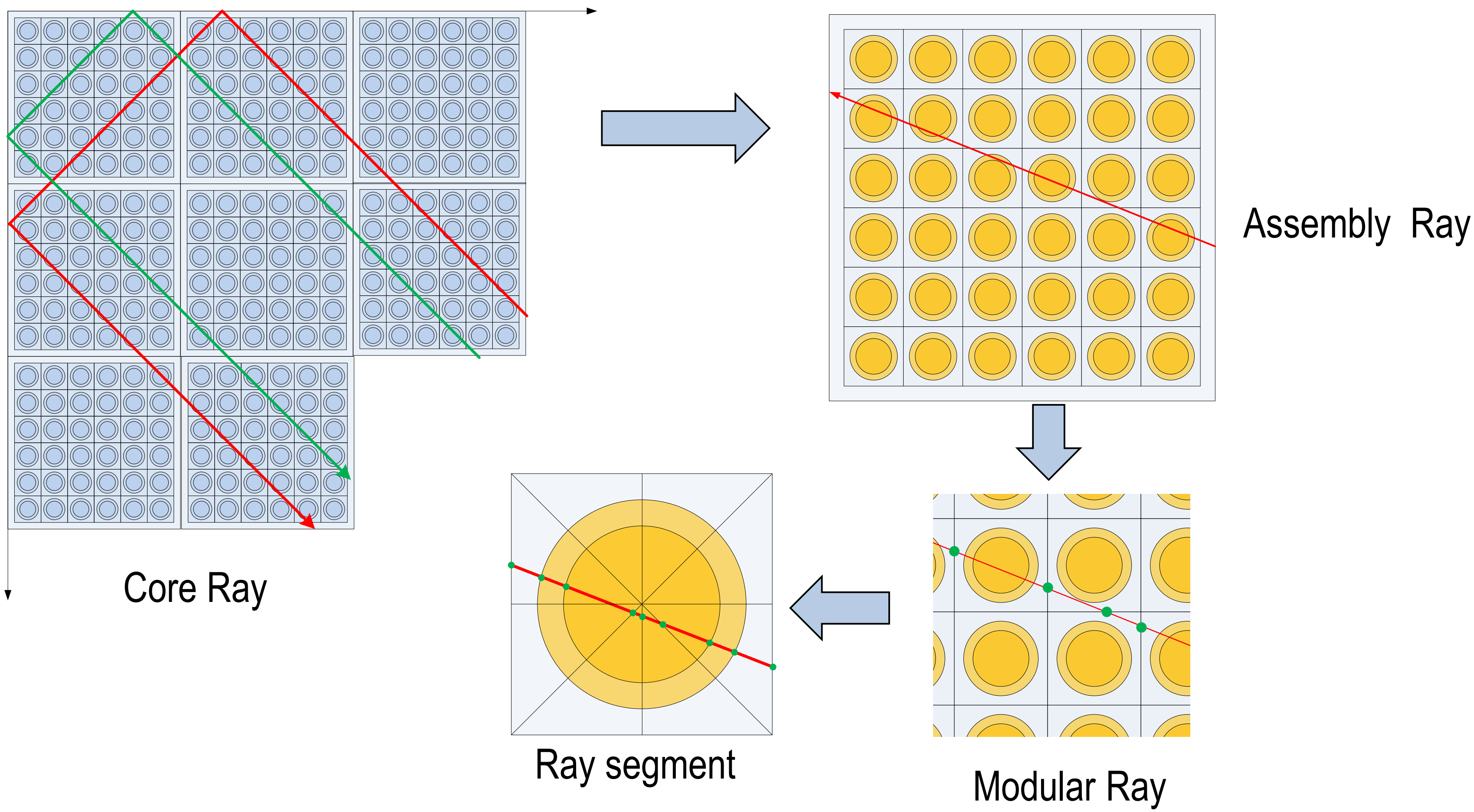
$$\bar{\varphi}_l = \frac{\sum_{r=1}^{N_{ray,l}} \delta_r l_r \tilde{\varphi}_{l,r}}{\sum_{r=1}^{N_{ray,l}} \delta_r l_{m,r}}, \qquad \bar{\phi} = \sum_{i=1}^{N_{ang}} w_i \bar{\varphi}_l$$

Method of Characteristics



- 16 regions, 8 azimuthal angles,

Modular Ray Tracing



Axial Equations

- Radially-Averaged Transport:

$$\varphi_{g,l}^{XY}(z) = \frac{1}{A_{xy}} \int_{y_L}^{y_R} \int_{x_L}^{x_R} \varphi_{g,l}(x,y,z)dxdy$$

$$\mu_l \frac{\partial}{\partial z} \varphi_{g,l}^{XY}(z) + \Sigma_{t,g}^{XY}(z)\varphi_{g,l}^{XY}(z) = \tilde{q}_{g,l}^{XY}(z)$$

$$\tilde{q}_{g,l}^{XY}(z) = \bar{q}_{g,l}^{XY}(z) + TL_{g,l}^{XY}(z)$$

Radial Transverse Leakage

- Total/transport cross section homogenized with scalar flux
- Diffusion approximation can be made for some solvers

Axial Equation

- In explicit form:
  - μ_l denotes cosine of polar angle
  - α_l denotes azimuthal angle

$$TL_{g,l}^{XY}(z) = -\frac{\sqrt{1-\mu_l^2}}{A_{xy}}\left(\begin{array}{c}\cos(\alpha_l)\int\limits_{y_L}^{y_R}\left(\varphi_{g,l}(x_R,y,z)-\varphi_{g,l}(x_L,y,z)\right)dy \\ +\sin(\alpha_l)\int\limits_{x_L}^{x_R}\left(\varphi_{g,l}(x,y_R,z)-\varphi_{g,l}(x,y_L,z)\right)dx\end{array}\right)$$

- Isotropic:

$$TL_{g,l}^{XY}(z) = \frac{1}{4\pi h_x}\left(J_{L,x,g}(z)-J_{R,x,g}(z)\right)+\frac{1}{4\pi h_y}\left(J_{L,y,g}(z)-J_{R,y,g}(z)\right)$$

- And Flat:

$$TL_{g,l}^{XY}(z) = \frac{1}{4\pi h_x}\left(J_{L,x,g}^{Z}-J_{R,x,g}^{Z}\right)+\frac{1}{4\pi h_y}\left(J_{L,y,g}^{Z}-J_{R,y,g}^{Z}\right)$$

Axial Transport Solver

- 1D P_N
  - Uses an N^{th} order polar expansion for the angular flux:

$$\varphi_g(z,\mu) = \sum_{m=0}^{N_{mom}} \frac{2m+1}{2} \varphi_{m,g}(z) P_m(\mu)$$

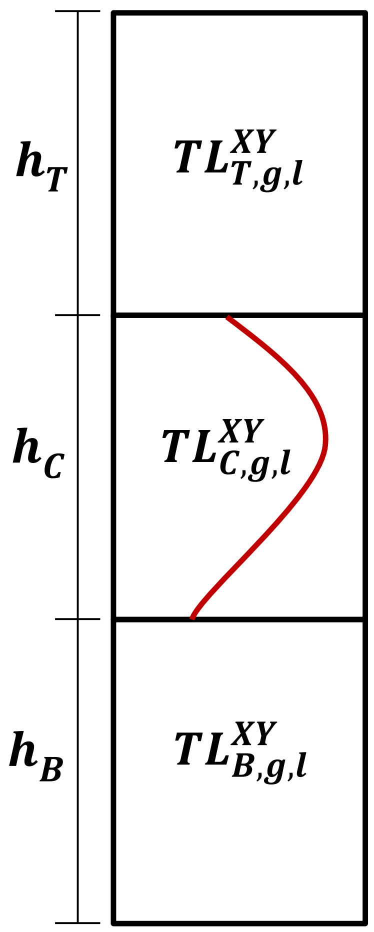
  - Wraps one-node NEM (4th order Legendre expansion) kernel for spatial representation
  - NEM-P_3:

$$-\frac{4D_{0,g}}{h^2}\frac{d^2}{d\xi}\Phi_{0,g}(\xi) + \Sigma_{r,g}\Phi_{0,g}(\xi) = Q_g(\xi) + 2\Sigma_{r,g}\Phi_{2,g}(\xi)$$

$$-\frac{4D_{2,g}}{h^2}\frac{d^2}{d\xi}\Phi_{2,g}(\xi) + \left(\Sigma_{t,g} + \frac{4}{5}\Sigma_{r,g}\right)\Phi_{2,g}(\xi) = -\frac{2}{5}\left(Q_g(\xi) - \Sigma_{r,g}\Phi_{0,g}(\xi)\right)$$

$$D_{0,g} = \frac{1}{3\Sigma_{tr,g}} \qquad D_{2,g} = \frac{9}{35\Sigma_{t,g}}$$

Radial TL Interpolation



- The currents used the generate the radial transverse leakages do not have axial dependence
- To compensate for this, a quadratic expansion for the leakage is formulated:

$$TL^{XY}_{g,l}(\xi) = \sum_{i=0}^{2} TL^{XY}_{g,l,i} P_i(\xi)$$

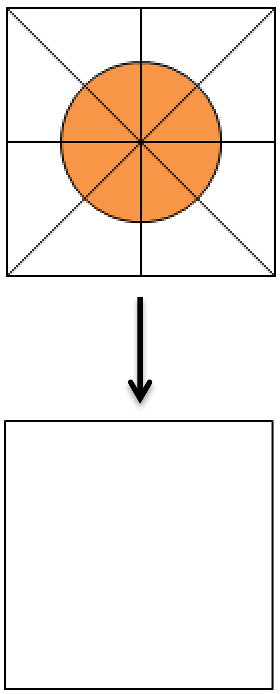
- Uses information from the upper and lower neighboring planes

Coarse Mesh Finite Difference

- CMFD is used as an accelerator to improve eigenvalue and scalar flux convergence in a wide range of transport solvers
- Pin-wise coarse cells
- Homogenization:

$$\bar{\Sigma}_{\mathrm{x,g,n}} = \frac{\sum_{i\in n}\Sigma_{x,g,i}V_i\phi_{g,i}}{\sum_{i\in n}V_i\phi_{g,i}}, \quad \bar{\phi}_{\mathrm{g,n}} = \frac{\sum_{i\in n}V_i\phi_{g,i}}{\sum_{i\in n}V_i}$$

- Projection: $\bar{\xi}_{\mathrm{g,i,n}} = \dfrac{\phi_{g,i}}{\bar{\phi}_{\mathrm{g,n}}}$



Coarse Mesh Finite Difference

- To perform a CMFD iteration, coupling coefficients are formulated:
  - Finite difference coupling coefficient:

$$\widetilde{D}_{g,n,i} = \frac{2D_{g,n}D_{g,n(i)}}{D_{g,n}h_{n(i),i} + D_{g,n(i)}h_{n,i}}$$

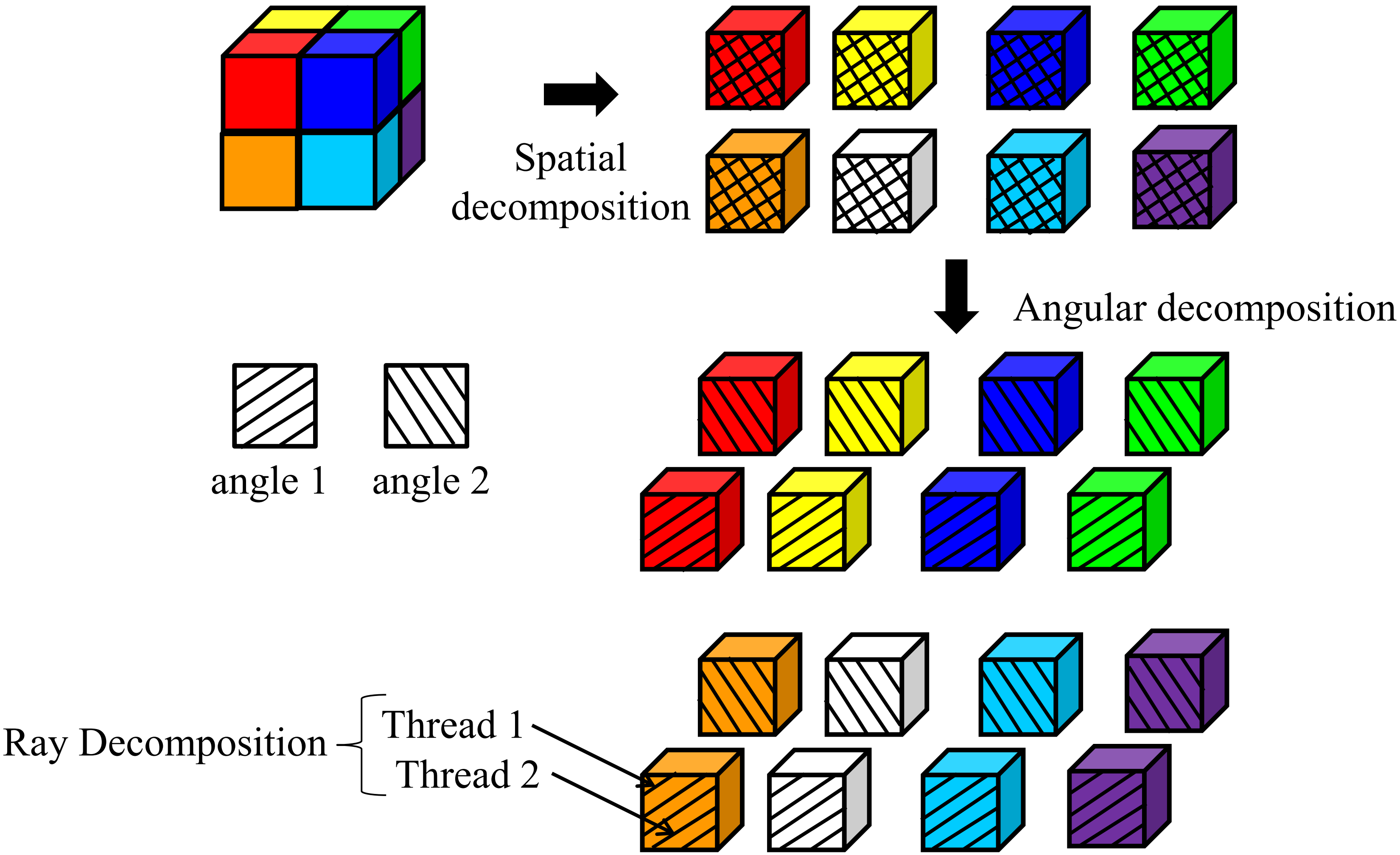
  - Current correction coupling coefficient

$$J_{s,g,n,i}^{transport} = -\widetilde{D}_{g,n,i}\left(\phi_{g,n} - \phi_{g,n(i)}\right) + \widehat{D}_{g,n,i}\left(\phi_{g,n} + \phi_{g,n(i)}\right)$$

$$\widehat{D}_{g,n,i} = \frac{J_{s,g,n,i}^{transport} + \widetilde{D}_{g,n,i}\left(\phi_{g,n} - \phi_{g,n(i)}\right)}{\phi_{g,n} + \phi_{g,n(i)}}$$

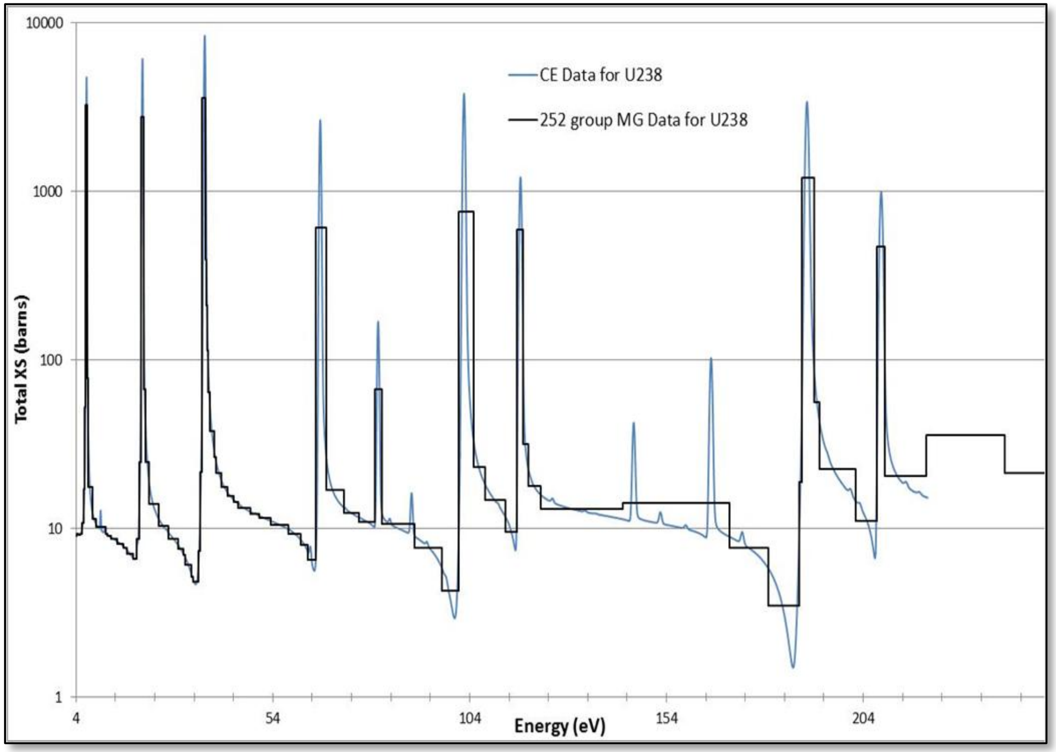
- Constructs and solves an nCell × nCell × nGroup matrix

Parallel Decomposition



XS Libraries and Scattering

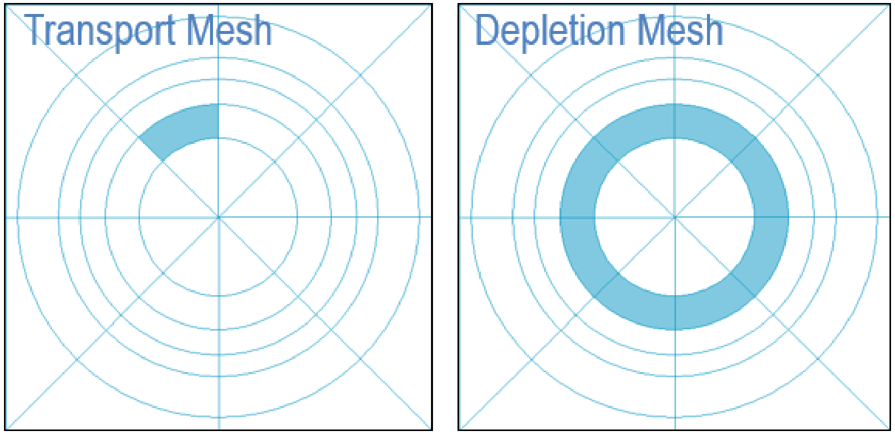
- ENDF-B/VII basic nuclear data library
  - Collapsed to a multi-group library (51/252 groups)
  - Library generated with SCALE codes



- Subgroup Resonance Self Shielding
- Default TCP_0 scattering (P_N available)

Depletion Methodology through ORIGEN

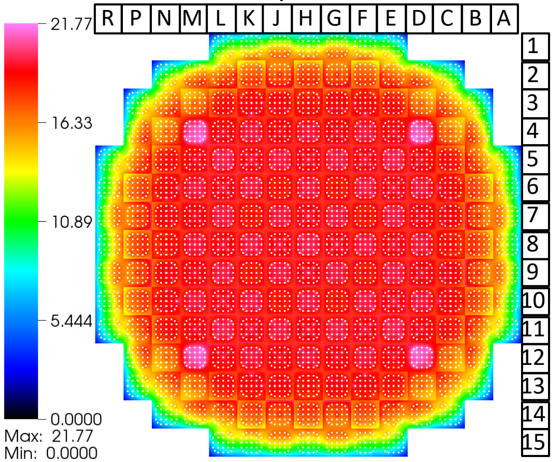
- Over 40 years of applications and validation bases within SCALE
- In-line depletion and decay of the fuel and burnable poisons
- Includes capability for activity, decay heat, radiation emission rates, and activation of structural materials
- Reduced isotope chain developed to improve run time and memory footprint
  - ~2200 → 263 isotopes



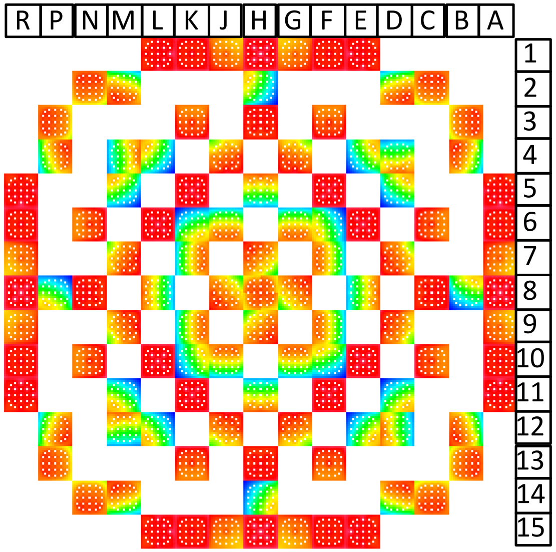
Fuel Shuffling Capability

- Depletion and fuel shuffle capability
  - Tracks isotopic transmutation in every region
  - Stores exact isotopics for entire core
  - Provides mechanism to shuffle full core correctly rotating isotopics
  - Decays all isotopes over outage
- Also manages shuffling and restart data for multiphysics calculations
  - CRUD restart information from MAMBA
  - Vessel fluence restart data from Shift
  - CTFFuel restart data

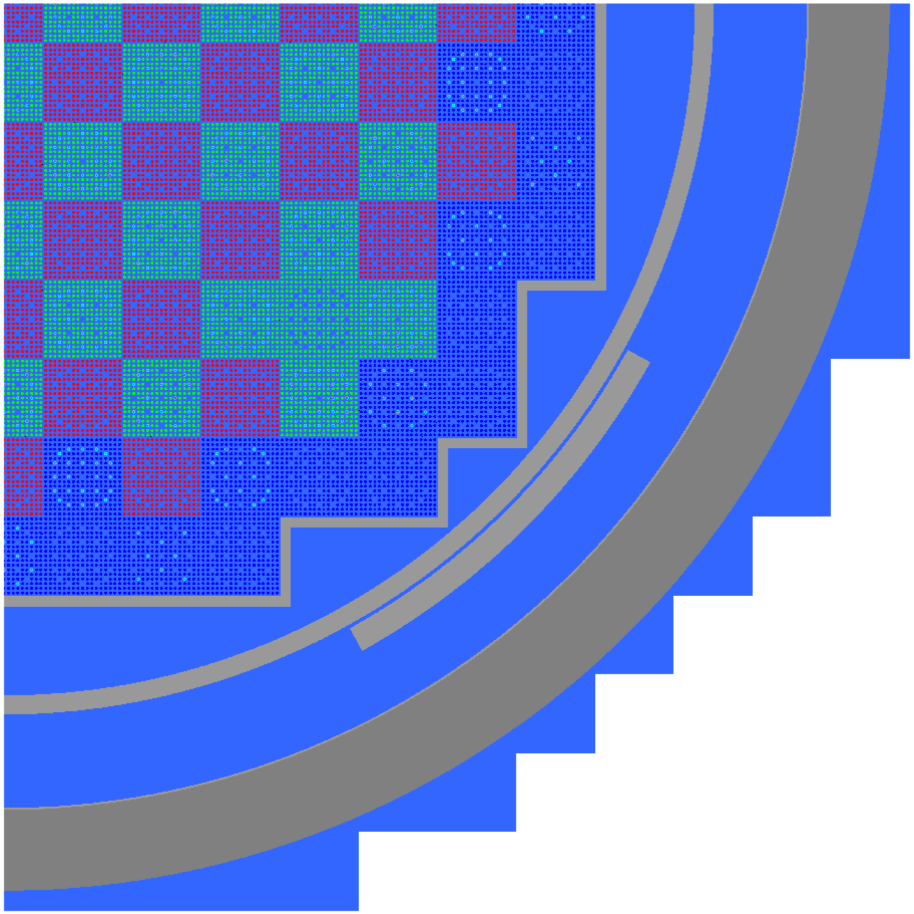
EOC 1 Pin-wise Exposure



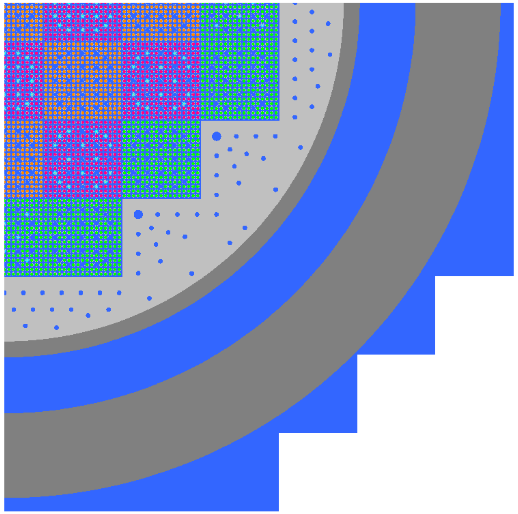
BOC 2 Pin-wise exposure



Reflector/Vessel Resolution



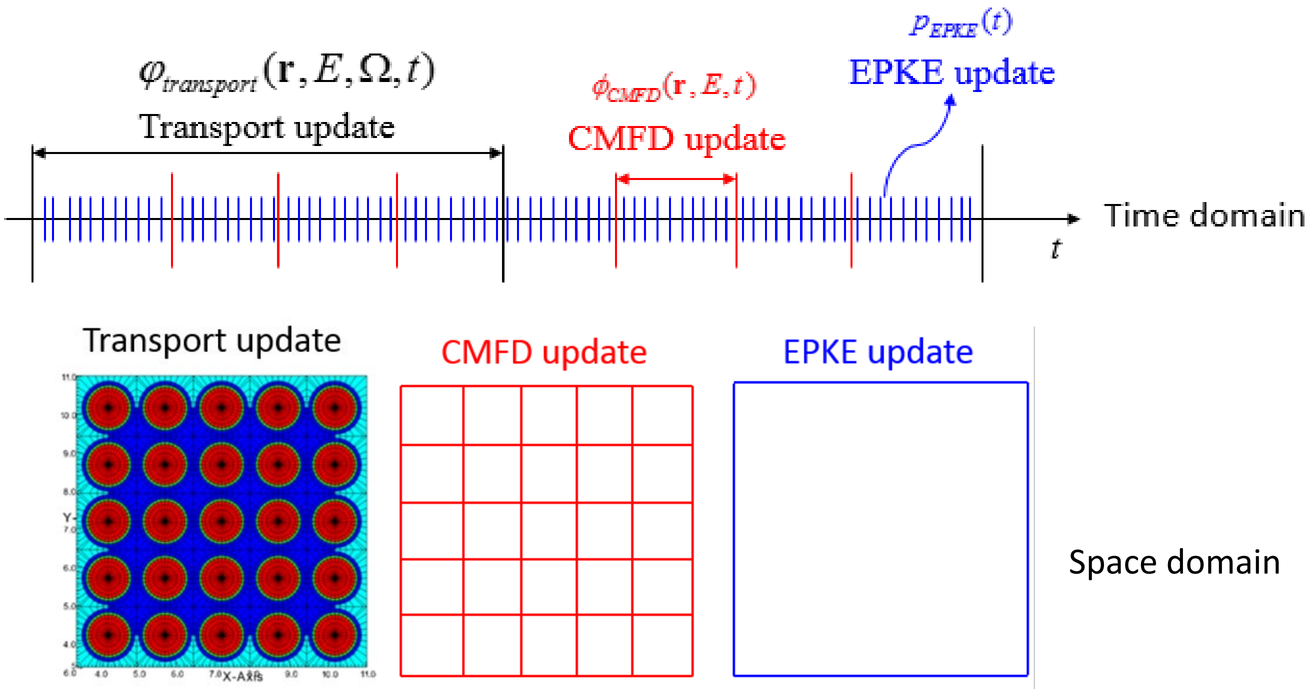
Watts Bar Unit 1 Slice



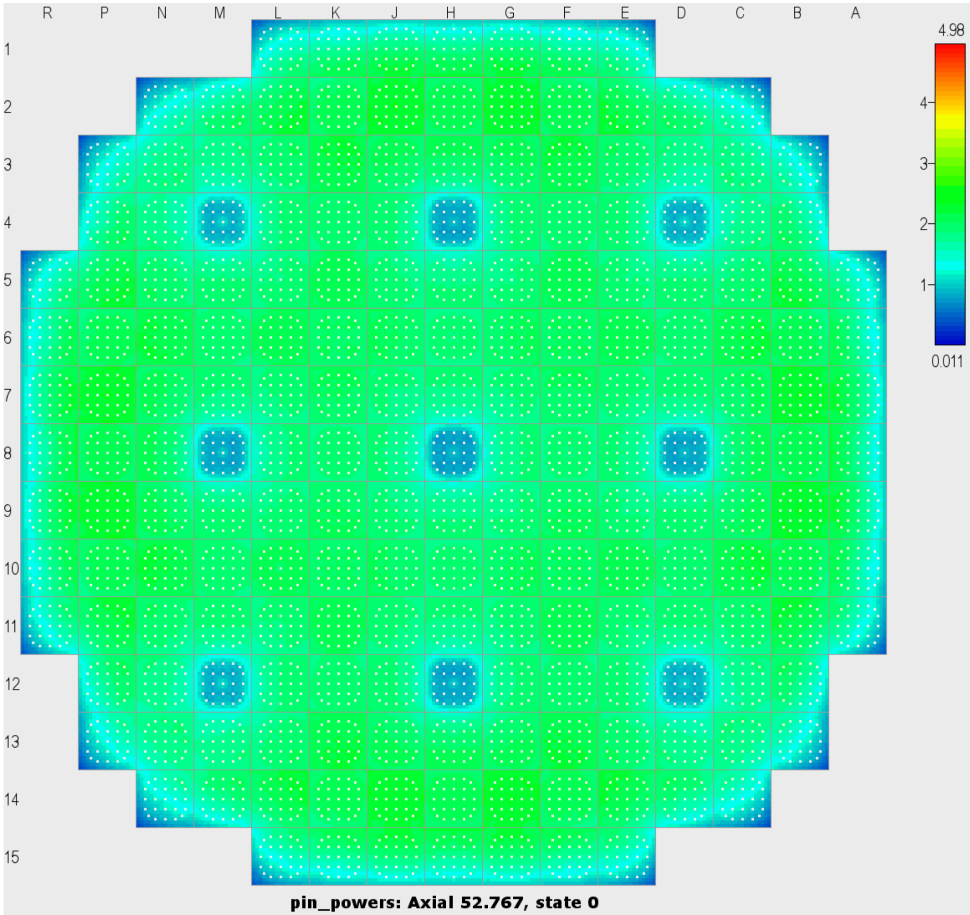
NuScale-like Slice

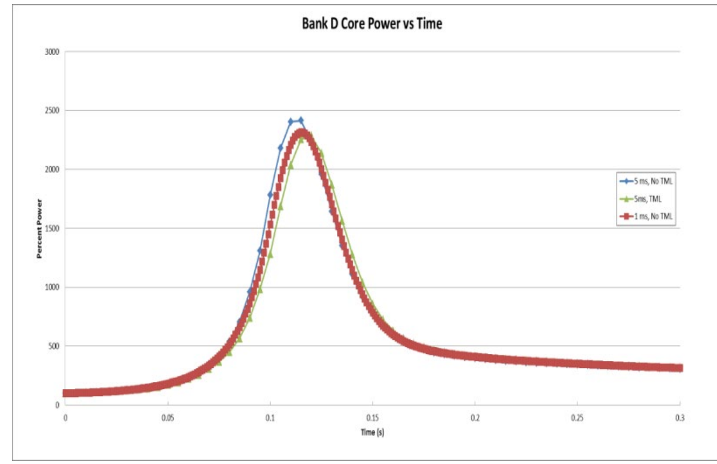
Transient Multi-level (TML) Method

- Pure transport transient calculation is computationally very expensive.
- Objective of the TML method is to use multi-level transient solvers to capture the physical phenomena in different time domains to maximize the numerical accuracy and computational efficiency.



Transient Application to Watts Bar





Time Step	TML Enabled	Runtime
1 ms	No	8.7 hours
5 ms	No	2.3 hours
5 ms	Yes	3.3 hours

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Summary

- Reviewed the 2D/1D equations
  - Approximations to Transport Equation
  - MOC, P_3, CMFD
  - Leakage Approximations
- Other key components
  - Depletion, Shuffling, Parallelization, XS Library
- Demonstrated transient capabilities
- Other MPACT capabilities are covered in later talks

Questions?