

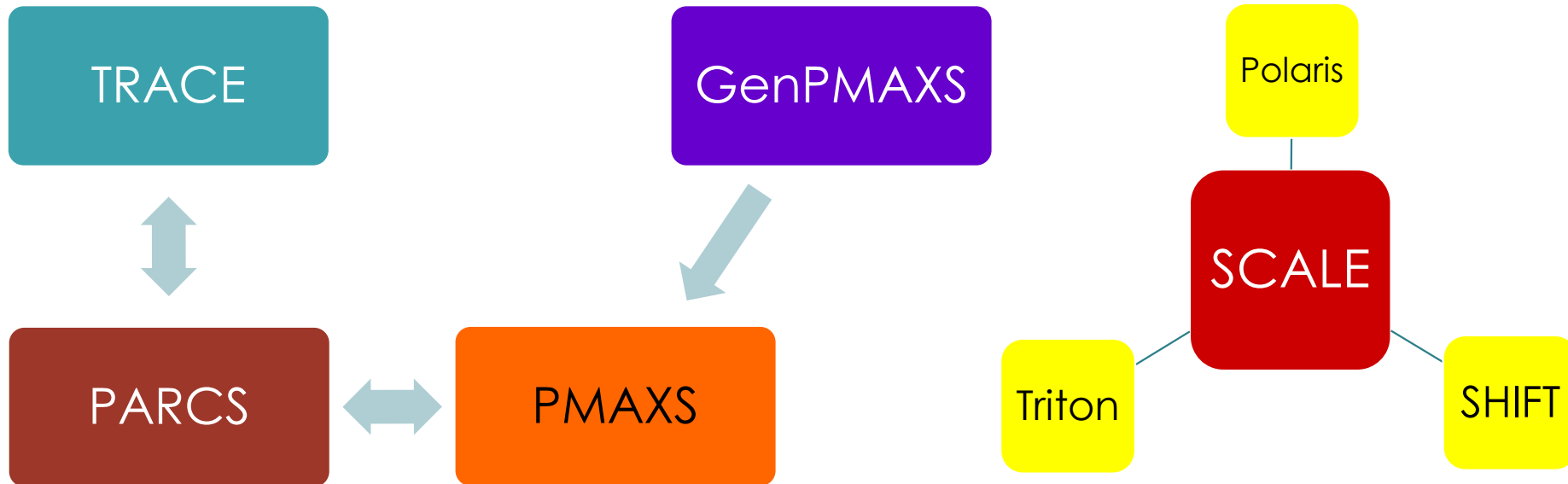
Overview of Polaris-GenPMAXS-PARCS calculation procedure

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Overview

- Diffusion & Two-Step Method
- Diffusion Methods in PARCS
 - Nodal Methods
 - CMFD
- Coupled Neutronics / Thermal-hydraulics
 - Cross Section Feedback
- Application & Assessments

U.S. NRC Coupled Code System



Coupled Neutron / Nuclide and Temperature/ Fluid Field Equations

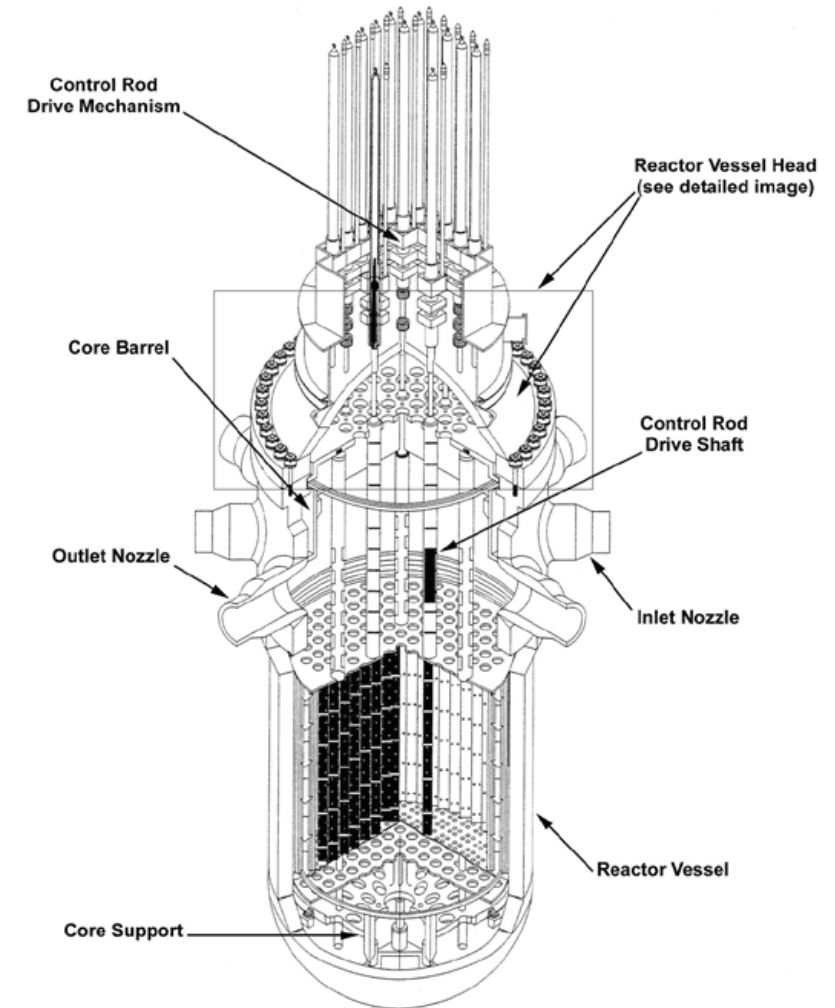
- Neutron transport equation (Boltzman)

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi(r, E, \Omega, t) + \Sigma_t(r, E) \phi(r, E, \Omega, t) = \frac{1}{4\pi} S_f(r, E, t) + \int \int_{\Omega' E'} \Sigma_s(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(r, E', \Omega', t) dE' d\Omega'$$

- Nuclide depletion equation (Bateman)

$$\frac{dN_i}{dt} = \sum_{j=1}^m l_{ij} \lambda_j N_j + \bar{\Phi} \sum_{k=1}^m f_{ik} \sigma_k N_k - (\lambda_i + \bar{\Phi} \sigma_i) N_i \quad (i = 1, \dots, m)$$

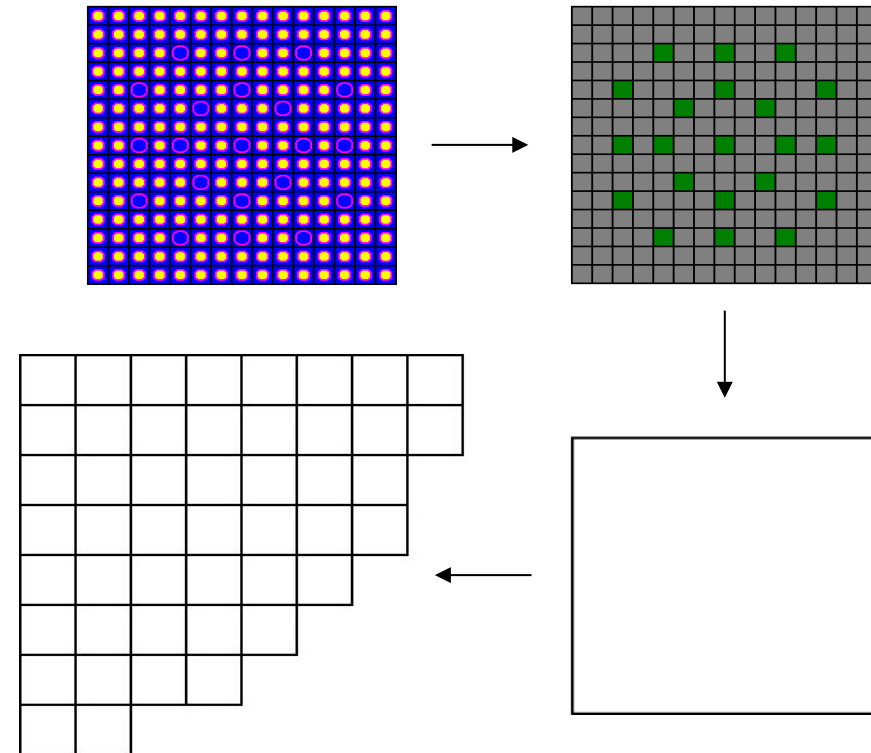
Typical Pressurized Water Reactor



<https://www.nrc.gov/reactors/operating/ops-experience/vessel-head-degradation/vessel-head-degradation-files/pwr-rx-vessel.html>

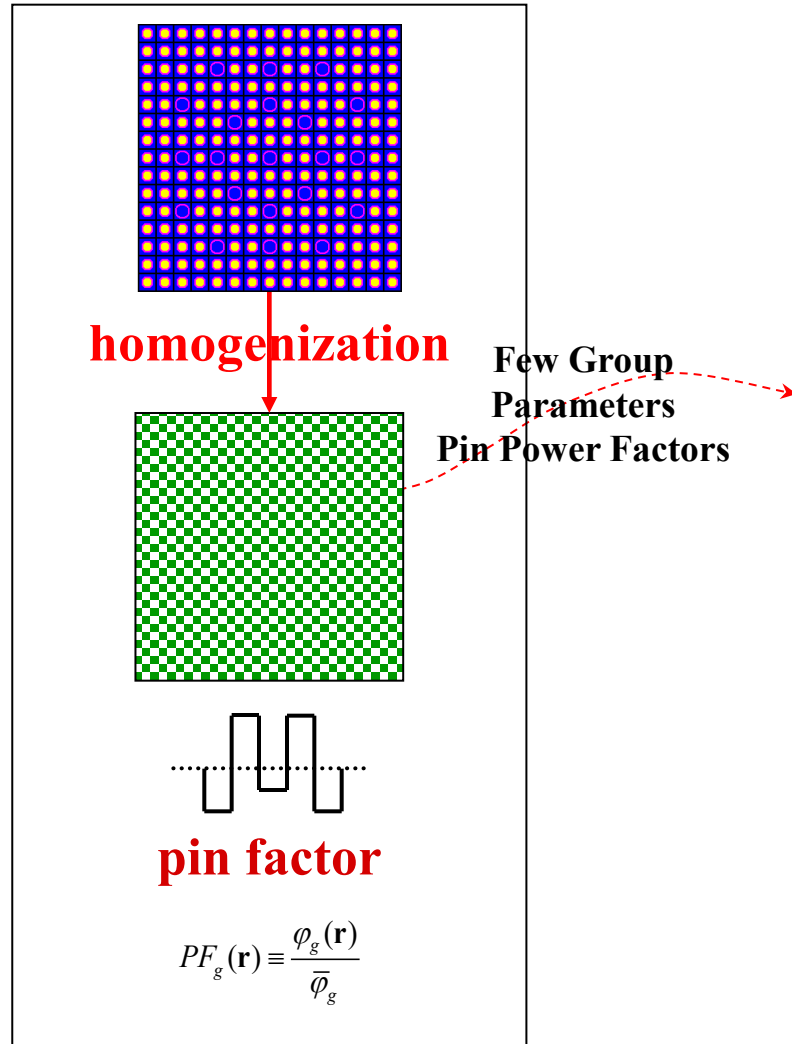
Current Methods for Boltzmann Neutron Flux Solution in a Power Reactor

- “Two-Step Procedure”
 - Pre-generate homogenized coefficients w/ High Order Solution for fuel assembly
 - Diffusion Approximation for Core Calculation
- First step can be done one time
 - More computational expense
- Second step can be repeated over and over
 - Computational expense is small compared to step 1



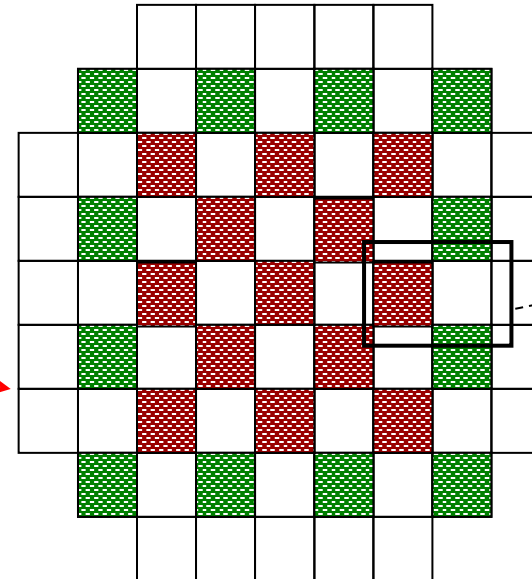
Two-Step Solution

Step 1: Lattice Calculation

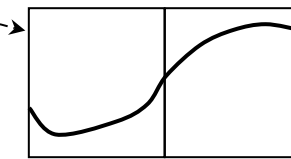


Step 2: Core Calculation

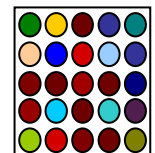
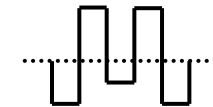
3D nodal calculation



Intra-nodal “smooth” flux shape reconstruction



×



Pin Power

Coarse Mesh Nodal Methods

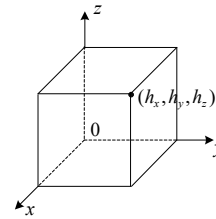
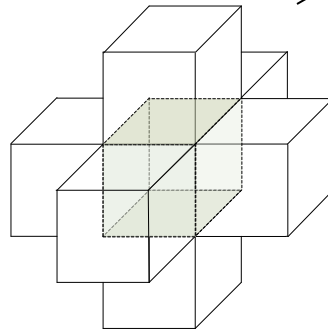
- 3-D Steady-State Multigroup Neutron Diffusion Equation

$$\nabla \cdot \vec{J}_g(\vec{r}, E) + \Sigma_{rg} \phi_g(\vec{r}, E) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \phi_{g'}(\vec{r}, E) + \sum_{g'=1}^G \Sigma_{sg'g} \phi_{g'}(\vec{r}, E)$$

- Fick's Law of Diffusion for Current out of Flux

$$\vec{J}_g(\vec{r}, E) = -D_g(\vec{r}, E) \nabla \phi_g(\vec{r}, E)$$

- Computational Node in 3-D Space



PWR Mesh: ~21cm
BWR Mesh: ~15cm

Transverse Integration of Neutron Balance Equation

- Transverse Integration of Leakage Term

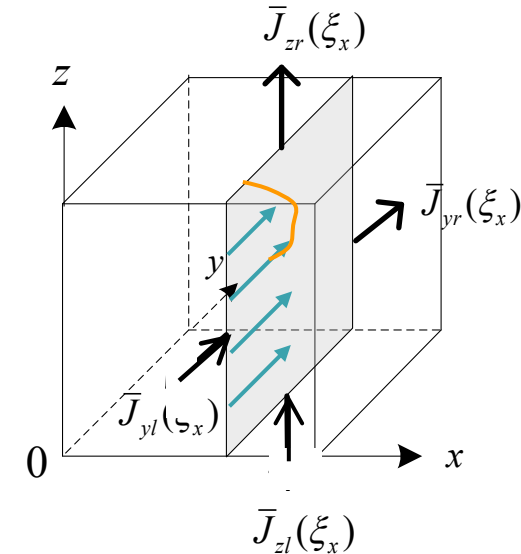
$$\int_0^1 \int_0^1 \nabla \cdot \vec{J} d\xi_y d\xi_z = -\frac{D_g}{h_x^2} \frac{\partial \bar{\phi}_x(\xi_x)}{\partial \xi_x^2} + \frac{\bar{J}_{yr}(\xi_x) - \bar{J}_{yl}(\xi_x)}{h_y} + \frac{\bar{J}_{zr}(\xi_x) - \bar{J}_{zl}(\xi_x)}{h_z}$$

where

$$\bar{\phi}_x(\xi_x) = \int_0^1 \int_0^1 \phi(\xi_x, \xi_y, \xi_z) d\xi_y d\xi_z : \text{Plane Averaged Flux}$$

$$\bar{J}_{yr}(\xi_x) = \int_0^l J_y(\xi_x, 1, \xi_z) d\xi_z, \quad \bar{J}_{yl}(\xi_x) = \int_0^l J_y(\xi_x, 0, \xi_z) d\xi_z$$

Line averaged currents



- 1-Dimensional Balance Equation

$$\sum_{u=y,z} \frac{\bar{J}_{gur}(\xi_x) - \bar{J}_{gul}(\xi_x)}{h_u} - \frac{D}{h_x^2} \frac{d^2}{d\xi_x^2} \bar{\phi}_{gx}(\xi_x) + \Sigma_{rg} \bar{\phi}_{gx}(\xi_x) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'x}(\xi_x) + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'x}(\xi_x)$$

- Iterative Treatment of Transverse Leakage Source

$$-\Sigma_{Dg}^x \frac{d^2}{d\xi_x^2} \bar{\phi}_{gx}(\xi_x) + \Sigma_{rg} \bar{\phi}_{gx}(\xi_x) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'x}(\xi_x) + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'x}(\xi_x) - L_{gy}(\xi_x) - L_{gz}(\xi_x)$$

Transverse Integrated 1-D Diff Eq.

- Set of 3 Directional 1-D Neutron Diffusion Equations

$$-\Sigma_{Dg}^x \frac{d^2}{d\xi_x^2} \bar{\phi}_{gx}(\xi_x) + \Sigma_{rg} \bar{\phi}_{gx}(\xi_x) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'x}(\xi_x) + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'x}(\xi_x) - L_{gy}(\xi_x) - L_{gz}(\xi_x)$$

$$-\Sigma_{Dg}^y \frac{d^2}{d\xi_y^2} \bar{\phi}_{gy}(\xi_y) + \Sigma_{rg} \bar{\phi}_{gy}(\xi_y) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'y}(\xi_y) + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'y}(\xi_y) - L_{gz}(\xi_y) - L_{gx}(\xi_y)$$

$$-\Sigma_{Dg}^z \frac{d^2}{d\xi_z^2} \bar{\phi}_{gz}(\xi_z) + \Sigma_{rg} \bar{\phi}_{gz}(\xi_z) = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'z}(\xi_z) + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'z}(\xi_z) - L_{gx}(\xi_z) - L_{gy}(\xi_z)$$

- 3-D Partial Differential Equation → Three 1-D Orid. Diff Eqs.
- Coupled through average transvers leakage term
 - → EXACT if the proper leakages are used
- Approximation on Transverse Leakage
 - Quadratic Shape (2nd order polynomial)
 - based on observation that change of flux distribution is not sensitive to change of transverse leakage
 - Iteratively update transverse leakage

PARCS Neutronics Methods: Solution Kernels

Kernel	Geometry	Method	Form	Energy	CMFD	Angular
ANM	Cartesian	Nodal	2-Node	2G	2G	Diffusion
NEM	Cartesian	Nodal	2-Node	2G	2G	Diffusion
FD-Only	Cartesian	Finite Diff.	N/A	2G	2G	Diffusion
NEMSPN	Cartesian	Nodal	1-Node	MG	2G	Diff/Sp3
FMFD	Cartesian	Finite Diff.	N/A	MG	2G	Diff/Sp3
NEMMG	Cartesian	Nodal	2-Node	MG	MG	Diffusion
SENM	Cartesian	Nodal	2-Node	MG	MG	Diffusion
TPEN	Hexagonal	Nodal	1-N / CPB	MG	2G	Diffusion
TriPEN*	Triangular	Nodal	2-Node	MG	MG	Diffusion

CMFD: Coarse Mesh Finite Difference
ANM: Analytic Nodal Method
FMFD: Fine Mesh Finite Difference
NEMMG: Multi-level NEM + Edd. Factors
TriPEN: Triangular Poly. Exp Method

MG: Multigroup
NEM: Nodal Expansion Method
SENM: Source Expansion Nodal Method
TPEN: Triangular Poly. Exp. Nodal Method
NEMPSN: NEM with optional SP3

*TriPEN is working but not yet released

Nodal Expansion Method

- Intranodal Flux Expansion of 1-D Flux
 - Approximate 1-D Flux by 4th Order Polynomial

$$\bar{\phi}(\xi) = \sum_{i=0}^4 a_i P_i(\xi)$$

- Basis Functions

$$P_0(\xi) = 1$$

$$P_1(\xi) = 2\xi - 1$$

$$P_2(\xi) = 6\xi(1 - \xi) - 1$$

$$P_3(\xi) = 6\xi(1 - \xi)(2\xi - 1)$$

$$P_4(\xi) = 6\xi(1 - \xi)(5\xi^2 - 5\xi + 1)$$

$$L(\xi) = \sum_{i=0}^2 l_i P_i(\xi)$$

Analytical Nodal Method (2G)

- 1D, 2 Group Diffusion Equation
 - All source terms except transverse leakage moved to LHS

$$\begin{aligned} -D_1 \frac{d^2 \phi_1(x)}{dx^2} + \Sigma_{r1} \phi_1(x) - \lambda (\nu \Sigma_{f1} \phi_1(x) + \nu \Sigma_{f2} \phi_2(x)) &= -L_1(x) \\ -D_2 \frac{d^2 \phi_2(x)}{dx^2} + \Sigma_{r2} \phi_2(x) - \Sigma_{12} \phi_1(x) &= -L_2(x) \end{aligned}$$

- Analytic Solution: Homogeneous + Particular Sol.

$$\phi_g(x) = \phi_g^H(x) + \phi_g^P(x)$$

$$\phi_g^H(x) = \hat{\phi}_g^H \exp(iBx)$$

“Hybrid” ANM / NEM Method

- ANM is more accurate than NEM for many applications

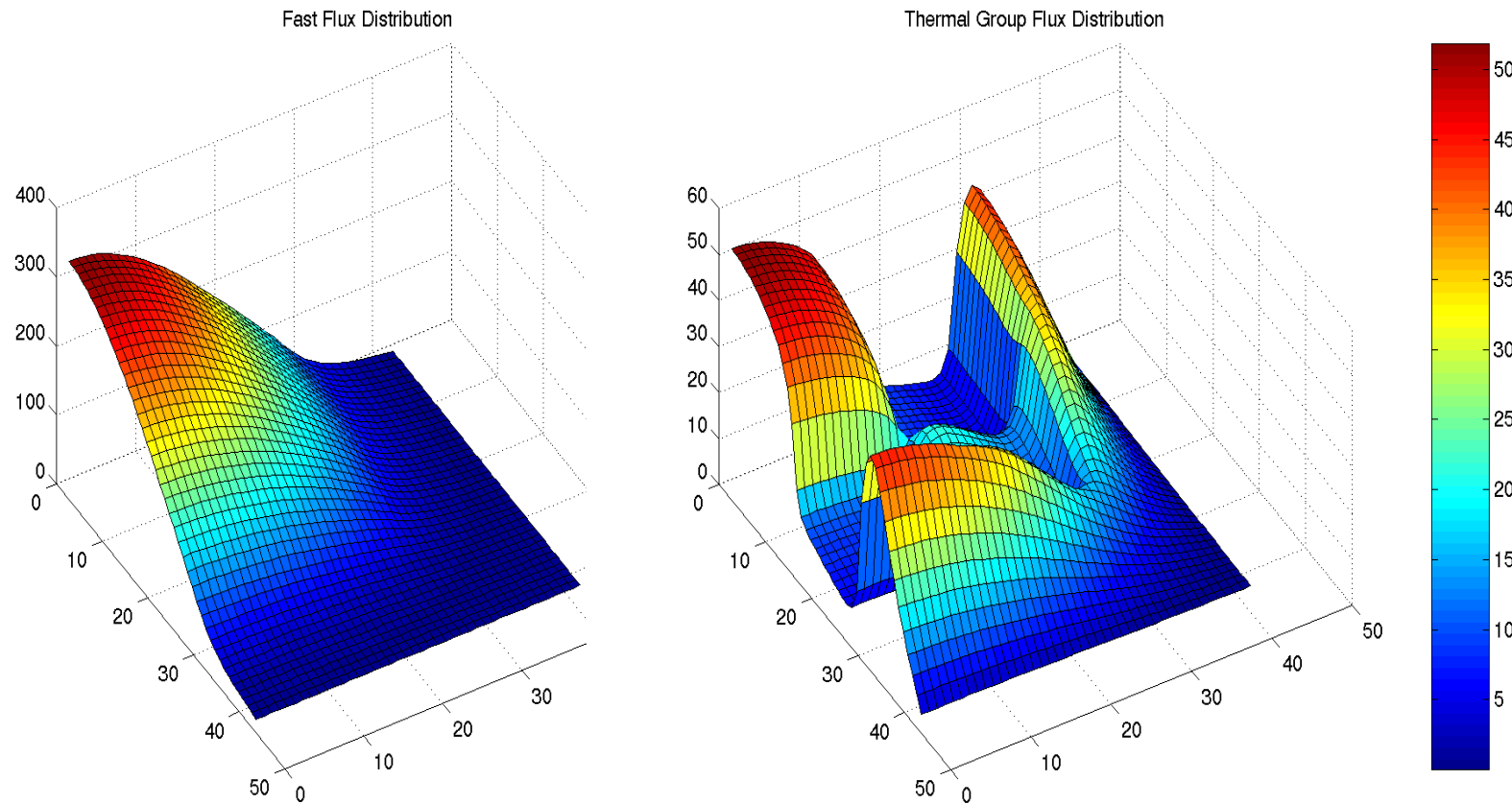
$$\phi_{\varepsilon}^H(x) \in \begin{cases} \{\sin(\kappa x), \cos(\kappa x), \sinh(\mu x), \cosh(\mu x)\} & , \quad k_{\infty} > k_{eff} \\ \{x, 1, \sinh(\mu x), \cosh(\mu x)\} & , \quad k_{\infty} = k_{eff} \\ \{\sinh(\kappa x), \cosh(\kappa x), \sinh(\mu x), \cosh(\mu x)\} & , \quad k_{\infty} < k_{eff} \end{cases}$$

- However, the ANM implementation is not stable for “just critical” nodes where a linear stopping criteria is required:

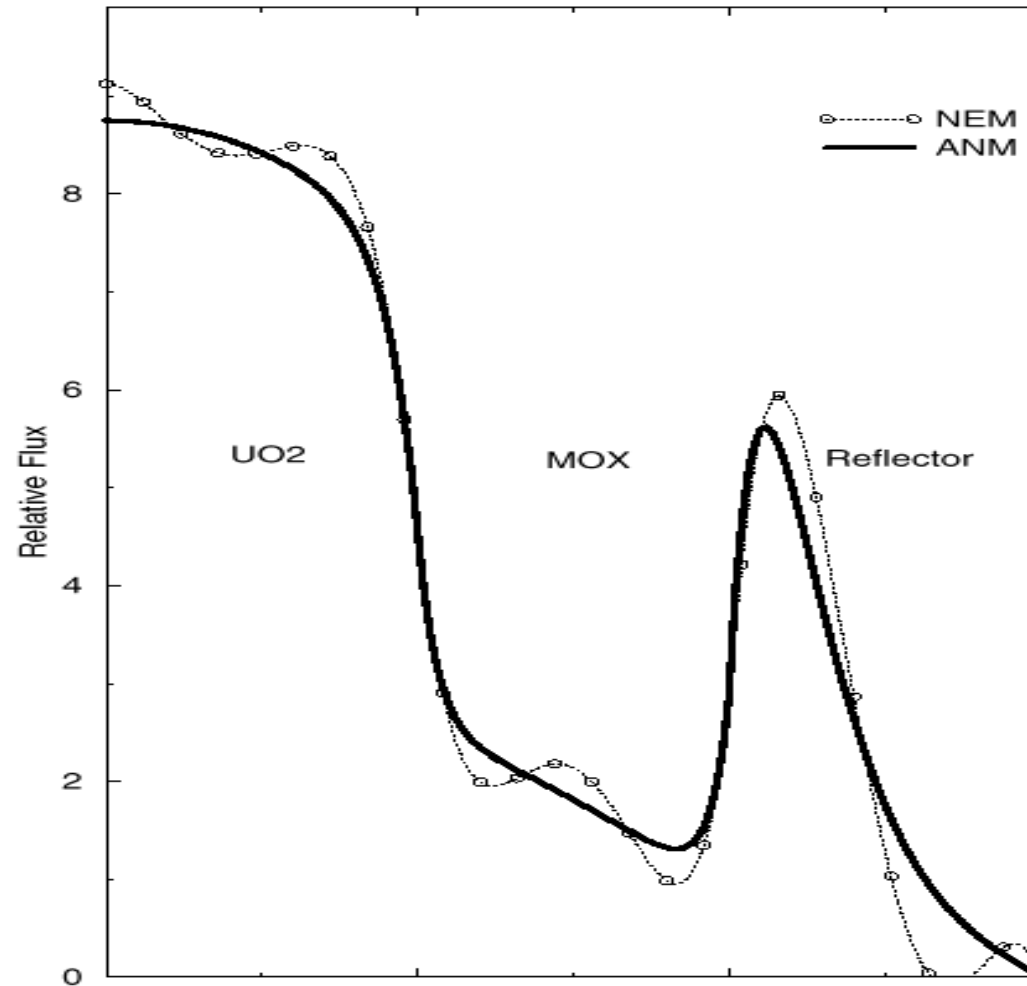
$$\delta = \left| \frac{k_{\infty}}{k_{keff}} - 1 \right| < \varepsilon$$

- Therefore a “hybrid” was implemented in which ANM is the base solution and NEM is invoked whenever the node k-inf approaches unity.

SS Cartesian: NEACRP L336 C5 problem, flux distribution



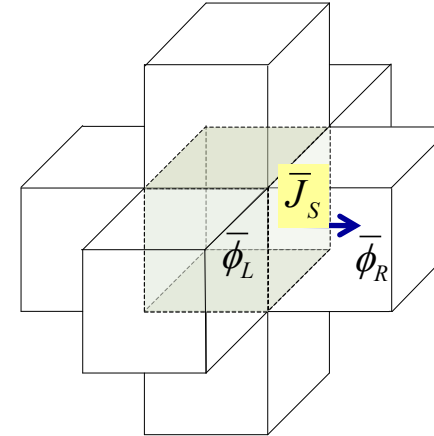
SS Cartesian: NEACRP L336 C5 problem, nodal flux shape



Acceleration Methods: CMFD

- Neutron Balance Equation

$$\sum_{u=x,y,z} \frac{\bar{J}_{gur} - \bar{J}_{gul}}{h_u} + \Sigma_{rg} \bar{\phi}_g = \lambda \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'} \bar{\phi}_{g'} + \sum_{g'=1}^G \Sigma_{sg'g} \bar{\phi}_{g'}$$



- Coarse Mesh Finite Difference (CMFD)
 - Introduce a special current vs. flux relation

$$\bar{J}_S = -D_S \frac{\bar{\phi}_R - \bar{\phi}_L}{h} = -\tilde{D}_S (\bar{\phi}_R - \bar{\phi}_L) \text{ where } \tilde{D}_S = \frac{2D_R D_L}{h_L D_R + h_R D_L} \rightarrow \bar{J}_S = -\tilde{D}_S (\bar{\phi}_R - \bar{\phi}_L) + \hat{D}_S (\bar{\phi}_R + \bar{\phi}_L)$$

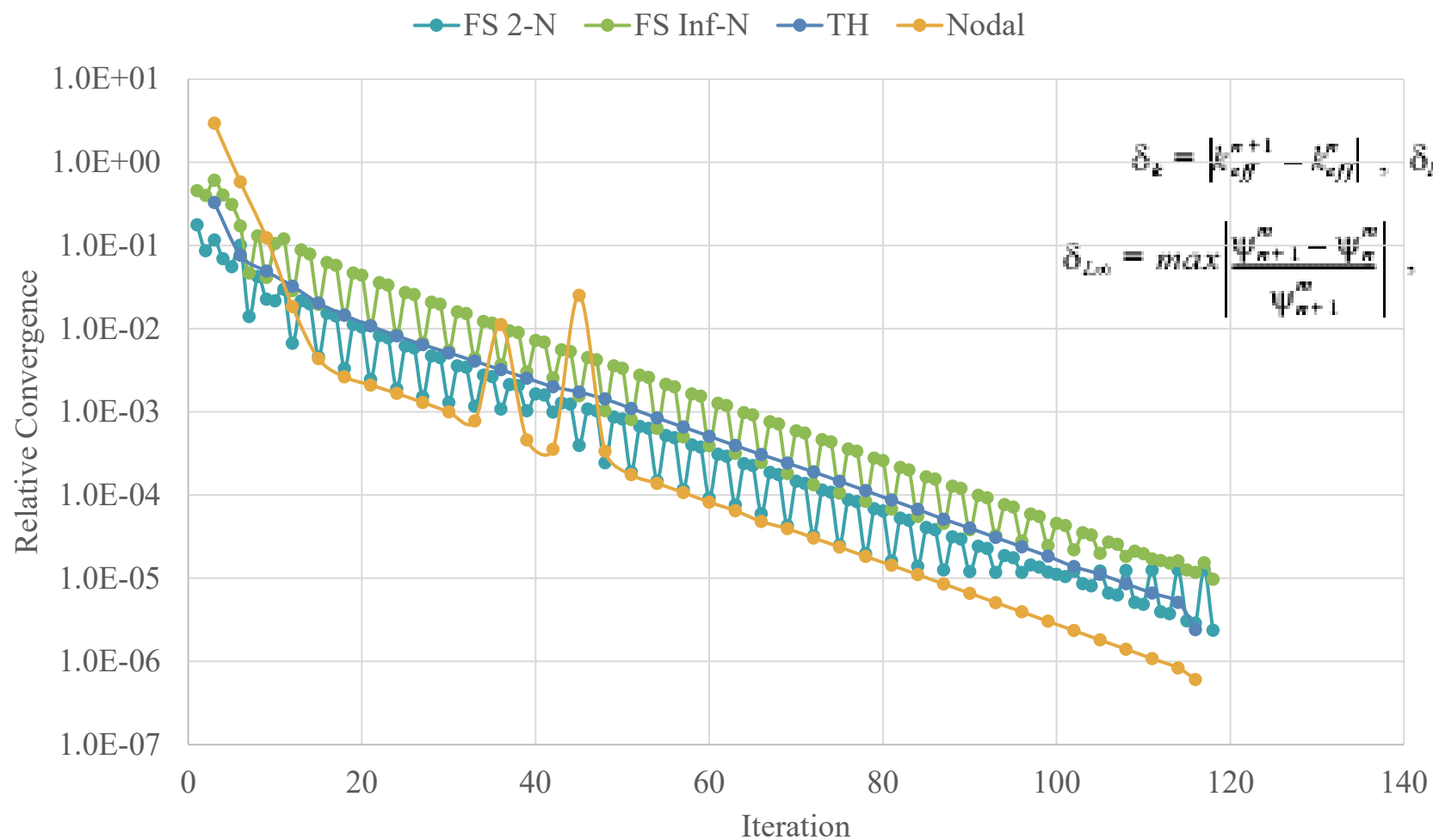
- Build a system of nodal balance equations for the entire core to form the 3D CMFD linear system

$$\mathbf{M}\phi = \lambda \mathbf{F}\phi$$

- Iteratively determine D-hat using partially converged solution of 3D CMFD problem and a [higher order method for local problems](#)

Kord Smith, "Nodal Method Storage Reduction by Nonlinear Iteration," Trans. Am. Nucl. Soc., 44, 265 (1983)

PARCS Convergence



Solution of Coupled Neutronics / Thermal-Hydraulics Field Equations

$$N(T)T = Q(\Phi)$$

Thermal-Hydraulic equation

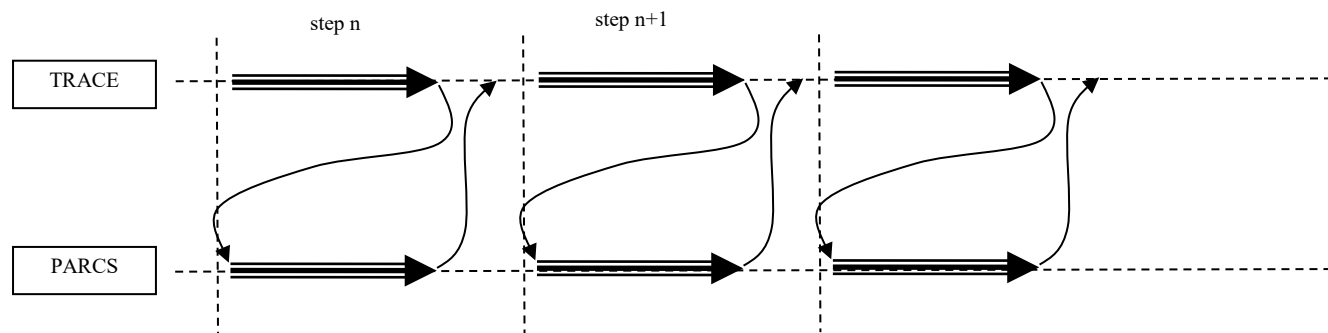
$$M(T)\Phi = S$$

Neutronics spatial kinetic equation

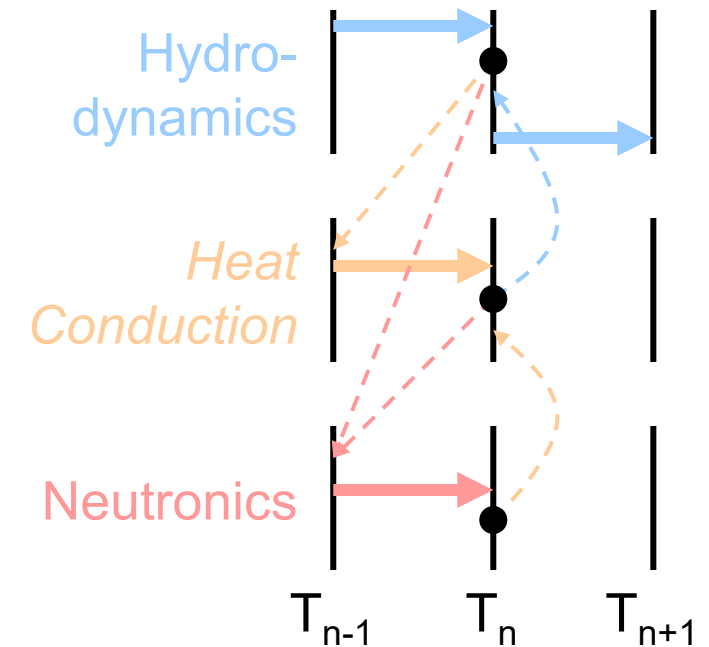
T : the vector of T/H variables

Φ : the vector of Neutronics variables

Current “Marching” Solution Method



TRACE / PARCS



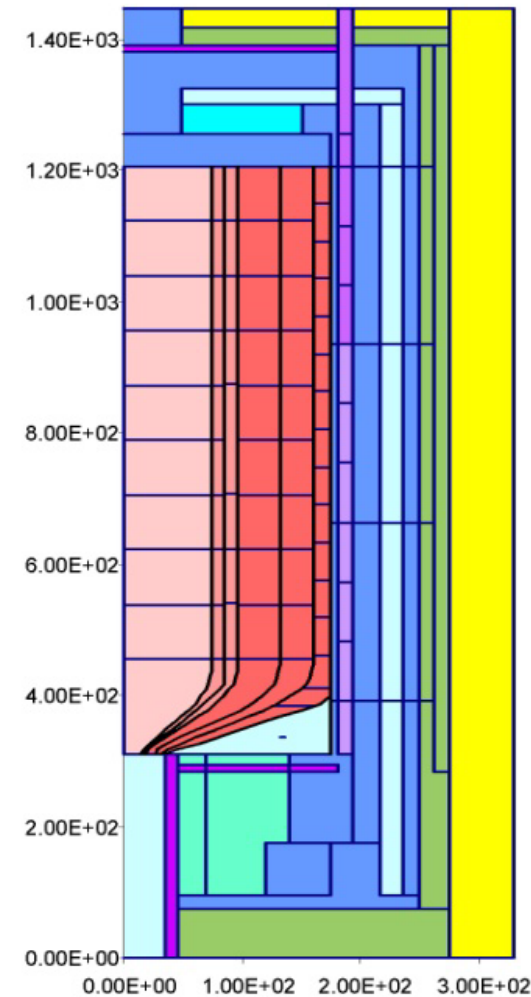
Advantage: $\tau_{\text{hydro}} > \tau_{\text{heat}} > \tau_{\text{neut}}$

Application & Assessment

- Light Water Reactors
 - 60+ International Users
 - PWR: Watts Bar 2, BEAVRS, Three Mile Island, MOX Benchmark, MSLB, Surry, APR-1400 Bench, Turkey Point
 - BWR: Peach Bottom, Hatch, Quad Cities, Oskarshamn, Ringhals, Cofrentes, PB Turbine Trip, PB Low Flow
 - VVER: Metsamor (Armenia)
 - Misc: VENUS, SPERT
- Criticals
 - Otto Hahn, DIMPLE, CROCUS

Application & Assessment

- Heavy Water Reactors
 - Atucha (Argentina), CANDU
- High Temperature Reactors
 - Pebble Bed Modular Reactor
 - Prismatic Gas Reactor
- Fast Reactors
 - EBR-2
 - SFR (PSI), FFTF (HZDR, Germany)



Acknowledgments

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