PARCS:
Parallel Advanced Reactor Core Simulator

U.S. NRC version 3.0

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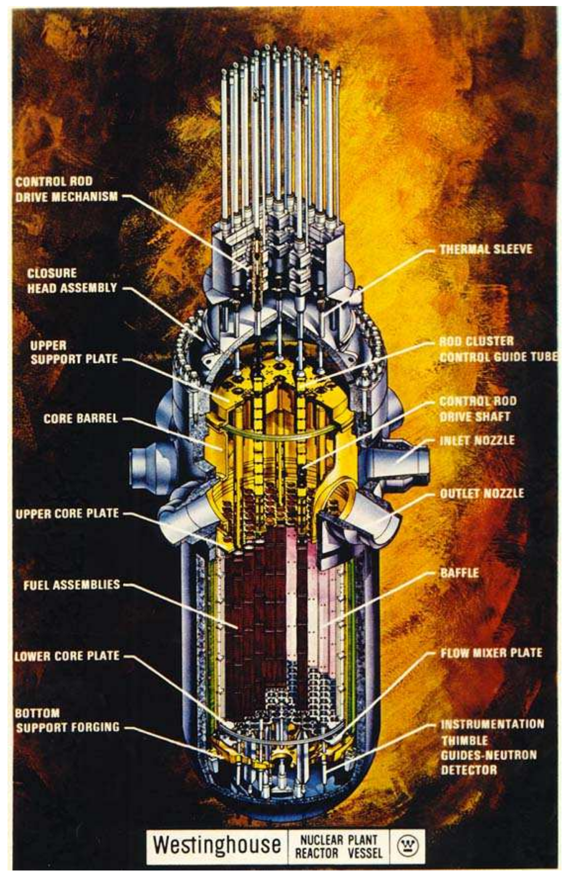
Coupled Neutron / Nuclide and Temperature/ Fluid Field Equations

- Neutron Transport Equation (Boltzmann)

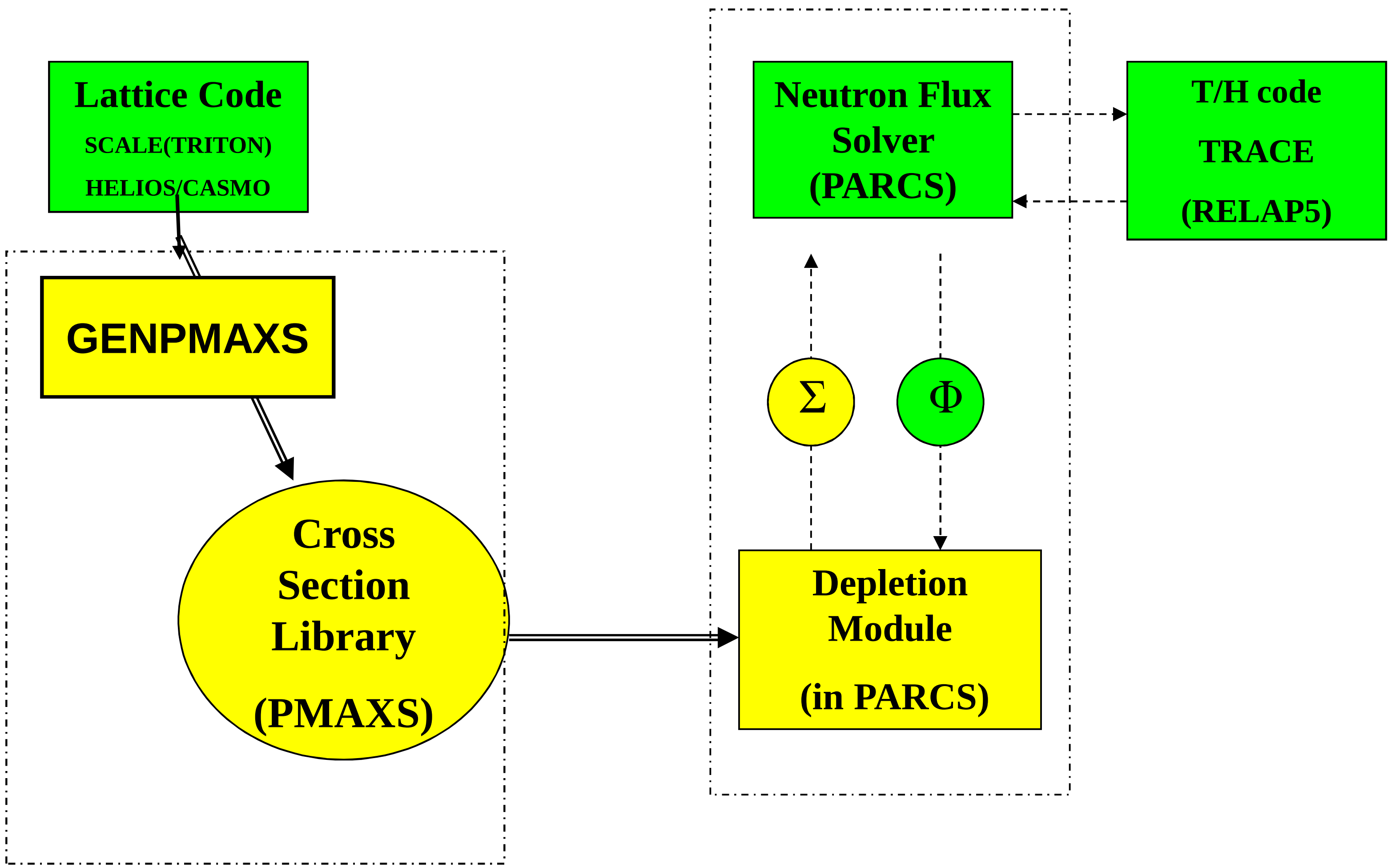
$$\frac{1}{v}\frac{\partial\phi}{\partial t}+\Omega\cdot\nabla\phi(r,E,\Omega,t)+\Sigma_t(r,E)\phi(r,E,\Omega,t)=\frac{1}{4\pi}S_f(r,E,t)$$
$$+\int_{\Omega'}\int_{E'}\Sigma_s(r,E'\to E,\Omega'\to\Omega)\phi(r,E',\Omega',t)\,dE'\,d\Omega'$$

- Nuclide depletion equation (Bateman)

$$\frac{dN_A(t)}{dt}=-(\sigma_A^a\phi+\lambda_A)N_A(t)+\sigma_C^\gamma\phi N_c(t)+\lambda_B N_B(t)$$



U.S. NRC Coupled Code System



Solution of Coupled Neutronics / Thermal-Hydraulics Field Equations

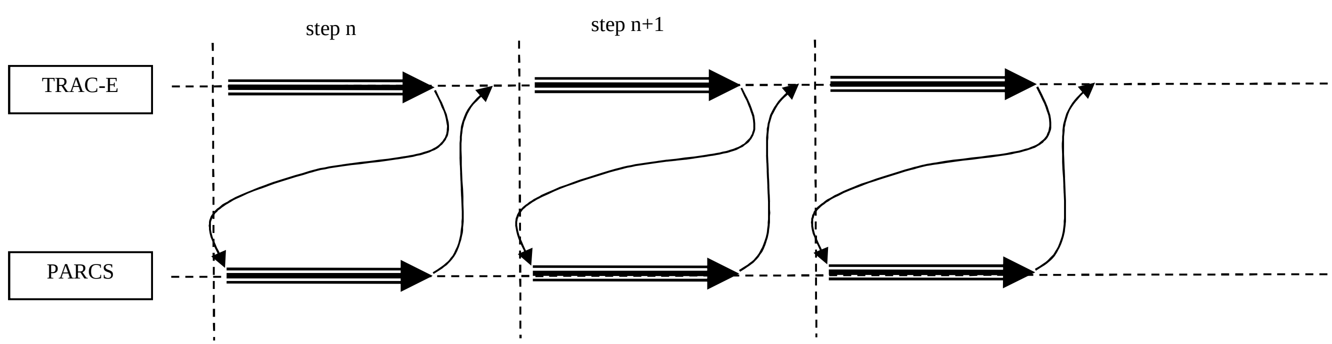
$$N(T)T = Q(\Phi)$$ Thermal-Hydraulic equation

$$M(T)\Phi = S$$ Neutronics spatial kinetic equation

$$T: the \quad vector \quad of \quad T/H \quad variables$$

$$\Phi: the \quad vector \quad of \quad Neutronics \quad variables$$

Current “Marching” Solution Method



Coupling of Neutronics and Thermal-Hydraulics

- Neutron Cross Section Model

$$\Sigma(\alpha, Tf, Tm, Dm, Sb) = \Sigma^r + \alpha\Delta\Sigma^{cr} + \frac{\partial\Sigma}{\partial\sqrt{Tf}}\Delta\sqrt{Tf} + \frac{\partial\Sigma}{\partial Tm}\Delta Tm + \frac{\partial\Sigma}{\partial Dm}\Delta Dm + \frac{\partial\Sigma}{\partial Sb}\Delta Sb + \frac{\partial^2\Sigma}{\partial Dm^2}(\Delta Dm)^2$$

$$\Delta\Sigma^{cr} = \Delta\Sigma^{cr}(BU, HIS1, HIS2)$$

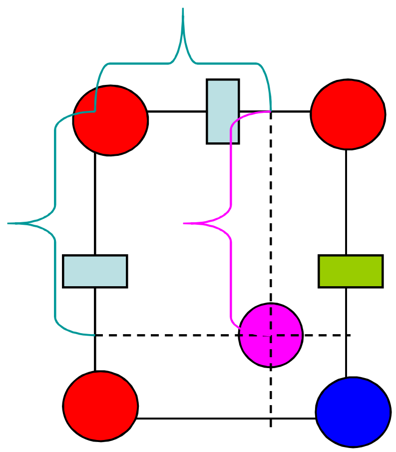
$$\frac{\partial\Sigma}{\partial\sqrt{Tf}} = \frac{\partial\Sigma}{\partial\sqrt{Tf}}(\sqrt{Tf}, BU, HIS1, HIS2)$$

$$\frac{\partial\Sigma}{\partial Dm} = \frac{\partial\Sigma}{\partial Dm}(Dm, BU, HIS1, HIS2)$$

$$\frac{\partial\Sigma}{\partial Sb} = \frac{\partial\Sigma}{\partial Sb}(Sb, BU, HIS1, HIS2)$$

$$\frac{\partial\Sigma}{\partial Tm} = \frac{\partial\Sigma}{\partial Tm}(Tm, BU, HIS1, HIS2)$$

$$\frac{\partial^2\Sigma}{\partial Dm^2} = \frac{\partial^2\Sigma}{\partial Dm^2}(Dm, BU, HIS1, HIS2)$$



- Partials obtained by piecewise linear interpolation
- Burnup and burnup “history” dependence

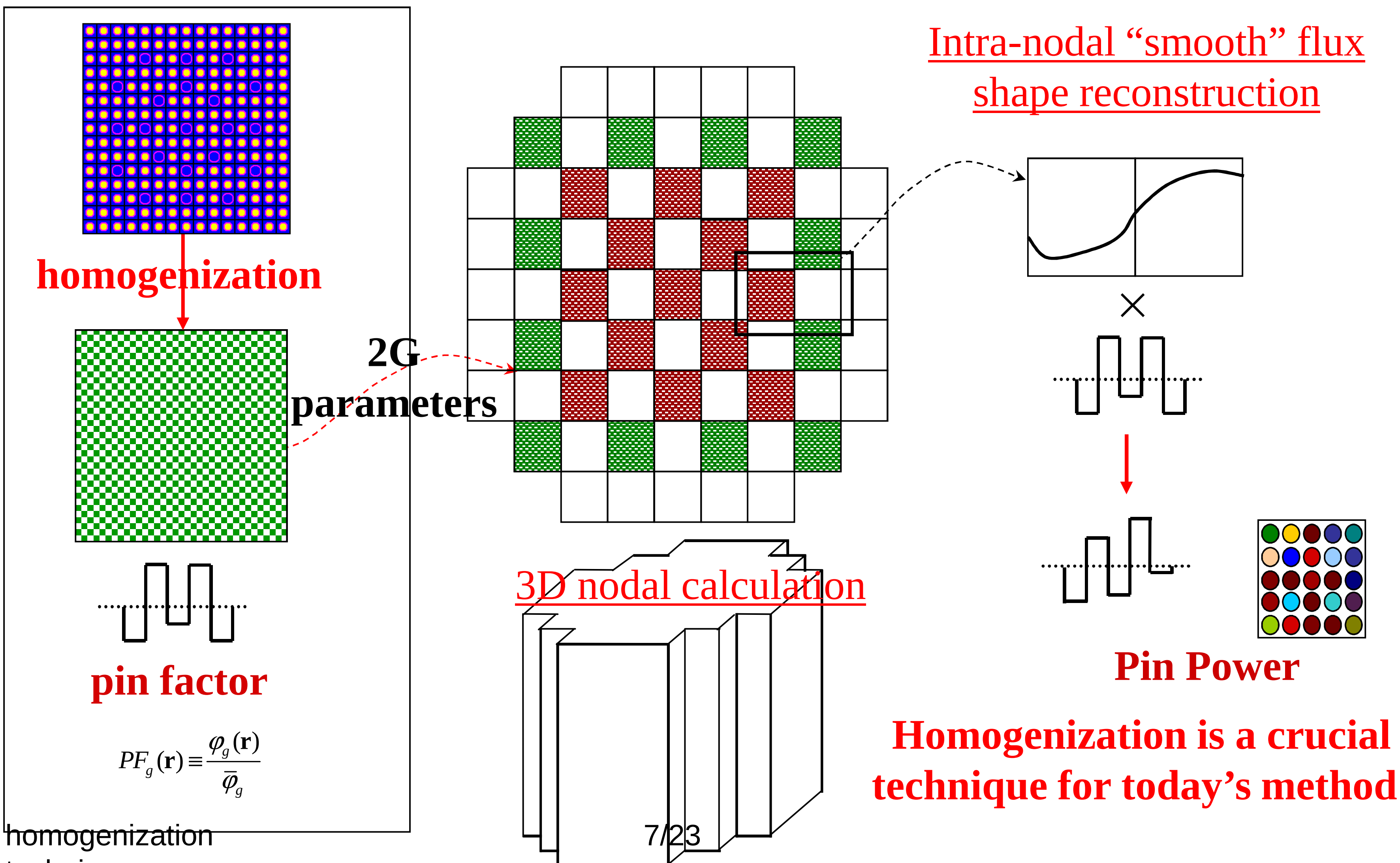
Primary Code Solution Features of PARCS

- Steady-state (Eigenvalues) and Transient Simulations
- Multigroup Nodal Diffusion for Rectangular/Hexagonal/Cylindrical Geometries
- CMFD Formulation with Krylov Subspace Linear Solver
- Consistent Pin Power Reconstruction
- Coupled to RELAP5 and TRACE
- Macroscopic Depletion for Fuel Cycle Analysis
- Pin-by-pin Multigroup FMFD or NEM Transport by SP_3
- Multidimensional Cross Section Table Functionalization

“Two-Step” Solution Method

1. Lattice calculation

2. Core calculation



Why don't we directly go to whole-core deterministic transport calculation without homogenization?

- **Scale of one single 3-D steady state problem:**
  - Number of fuel Assemblies ~200
  - Number of axial planes ~100
  - Number of pins per assembly ~300
  - Number of depletion regions per pin ~ 10
  - Number of angular directions ~100
  - Number of neutron energy groups ~100

  Total unknowns ~600 Billion

- At 100 FLOPS/unknown on 1 gigaflop machine = 16 CPU hours
  - Not yet tractable for full-scale LWR steady state core analysis, let alone transient or depletion calculation.

PARCS Neutronics Methods: Solution Kernels

Geometry Type	Kernel Name	Solution Method	Energy Treatment	Angle Treatment
Cartesian 3D	CMFD	FD	2G	Diffusion
	ANM	nodal	2G	Diffusion
	FMFD	FD	MG	SP3
	NEMMG	nodal	MG	SP_3
Hexagonal 3D	CMFD	FD	2G	Diffusion
	TPEN	nodal	MG	Diffusion
Cylindrical 3D	CMFD	FD	2G	Diffusion
	FMFD	FD	MG	Diffusion/ SP_3

CMFD = Coarse Mesh Finite Difference
ANM = Advanced Nodal Method
FMFD = Fine Mesh Finite Difference

NEM = Nodal Expansion Method
MG = Multigroup

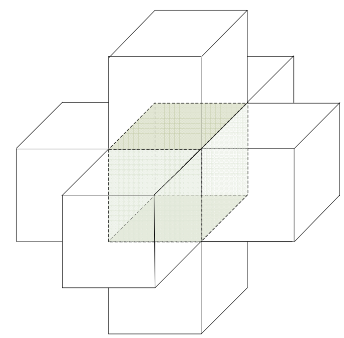
COARSE MESH NODAL METHODS

- 3-D Steady-State Multigroup Neutron Diffusion Equation

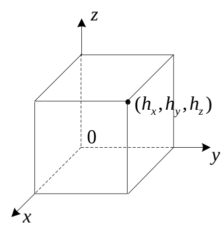
$$\nabla \cdot \vec{J}_g(\vec{r},E) + \Sigma_{rg}\phi_g(\vec{r},E) = \lambda\chi_g \sum_{g'=1}^{G} \nu\Sigma_{fg'}\phi_{g'}(\vec{r},E) + \sum_{g'=1}^{G} \Sigma_{sg'g}\phi_{g'}(\vec{r},E)$$

  - 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



- Property assumed constant within each homogenized node
  - FDM sufficiently accurate only if the node size is sufficiently small (~<10cm)
  - Nodal methods to achieve high accuracy with large nodes (20 cm)

Transverse Integrated One-Dimensional Neutron Diffusion Equation

- Transverse Integration of 3-D Neutron Diffusion Equation

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

- Define Transverse Leakage to Move to RHS

$$L_{gu}(\xi_x)=\frac{1}{h_u}\left(\bar{J}_{gur}(\xi_x)-\bar{J}_{gul}(\xi_x)\right)\quad,\quad u=y,z$$

- Transverse Integrated One-Dimensional Neutron Diffusion Equation (Final Form)

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

  – Diffusion Equivalent Group Constant

$$\Sigma_{Dg}^{x}=\frac{D}{h_x^2}$$

Transverse Integrated One-dimensional Neutron Diffusion Equations

- 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

    $\rightarrow$ Three 1-D Ordinary Differential Equations
  - Coupled through average transverse leakage term
    - Exact if the proper transverse 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

Nodal Expansion Method

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

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

  - Basis Functions

$$P_0(\xi) = 1$$

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

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

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

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

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

Response Matrix Equation

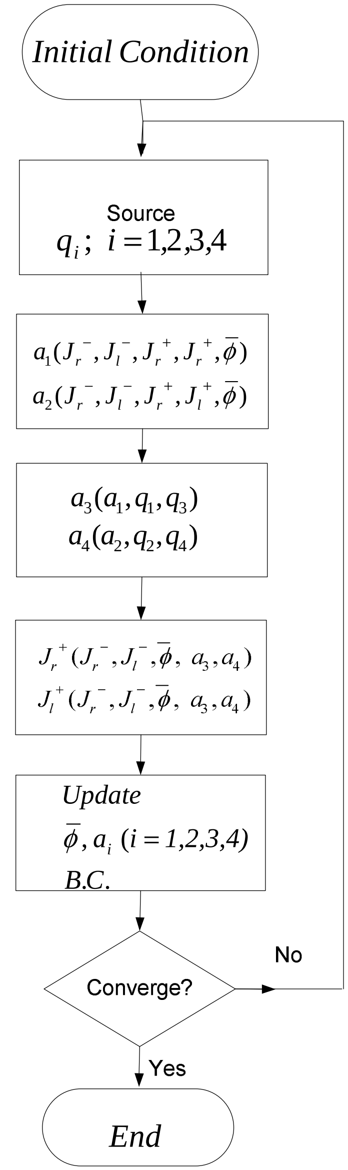
- Three-Directional Outgoing Currents Described Altogether

$$
\begin{bmatrix} J_{xl}^{+} \\ J_{xr}^{+} \\ J_{yl}^{+} \\ J_{yr}^{+} \\ J_{zl}^{+} \\ J_{zr}^{+} \end{bmatrix}
=
\begin{bmatrix}
c_2^x & c_3^x & & & & & c_1^x \\
c_3^x & c_2^x & & & & & c_1^x \\
& & c_2^y & c_3^y & & & c_1^y \\
& & c_3^y & c_2^y & & & c_1^y \\
& & & & c_2^z & c_3^z & c_1^z \\
& & & & c_3^z & c_2^z & c_1^z
\end{bmatrix}
\begin{bmatrix} J_{xl}^{-} \\ J_{xr}^{-} \\ J_{yl}^{-} \\ J_{yr}^{-} \\ J_{zl}^{-} \\ J_{zr}^{-} \\ \bar{\phi} \end{bmatrix}
+
\begin{bmatrix}
c_1^x a_4^x + c_4^x a_3^x \\
c_1^x a_4^x - c_4^x a_3^x \\
c_1^y a_4^y + c_4^y a_3^y \\
c_1^y a_4^y - c_4^y a_3^y \\
c_1^z a_4^z + c_4^z a_3^z \\
c_1^z a_4^z - c_4^z a_3^z
\end{bmatrix}
$$

  - a_3 and a_4 are treated as known by using a_1 and a_2 which are approximated by previously known surface fluxes
  - otherwise, to solve rigorously, need to solve for 13 unknowns including a_3 and a_4 for each direction simultaneously.

NEM Iterative Solution Sequence

- For a given group
  - Determine sequentially
    - Source expansion coeff.
    - a_1 and a_2 from previous surface fluxes
    - a_3 and a_4 using source moments and a_1 and a_2
    - node average flux
    - outgoing current
  - Move to next group
  - Move to next node once all groups are done
- Group sweep and node sweep can be reversed (node sweep then group sweep)
- Update eigenvalue



Analytic Nodal Method for 2-G Problem

- 1D, Two-Group Diffusion Equation

$$-D_1 \frac{d^2\phi_1(x)}{dx^2} + \Sigma_{r1}\phi_1(x) - \lambda\left(\nu\Sigma_{f1}\phi_1(x) + \nu\Sigma_{f2}\phi_2(x)\right) = -L_1(x)$$

$$-D_2 \frac{d^2\phi_2(x)}{dx^2} + \Sigma_{r2}\phi_2(x) \quad - \quad \Sigma_{12}\phi_1(x) \quad = -L_2(x)$$

  – All source terms except transverse leakage now on LHS

- Analytic Solution: Homogeneous + Particular Sol.

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

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

Determination of Buckling Eigenvalues

- Characteristic Equation $$\begin{bmatrix} D_1 B^2 + \Sigma_{r1} - \lambda\nu\Sigma_{f1} & -\lambda\nu\Sigma_{f1} \\ -\Sigma_{12} & D_2 B^2 + \Sigma_{r2} \end{bmatrix} \begin{bmatrix} \hat{\phi}_1^H \\ \hat{\phi}_2^H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

  – For Nontrivial Solution

$$Det(A) = 0 \quad \Rightarrow \quad (D_1 B^2 + \Sigma_{r1} - \lambda\nu\Sigma_{f1})(D_2 B^2 + \Sigma_{r2}) - \lambda\nu\Sigma_{f2}\Sigma_{12} = 0$$

$$\left(B^2\right)^2 + \left(\frac{\Sigma_{r1}}{D_1} + \frac{\Sigma_{r2}}{D_2} - \frac{\lambda\nu\Sigma_{f1}}{D_1}\right) B^2 + \left(1 - \frac{k_\infty}{k_{eff}}\right)\frac{\Sigma_{r1}}{D_1}\frac{\Sigma_{r2}}{D_2} = 0 \quad \Leftrightarrow \quad \left(B^2\right)^2 + 2b\, B^2 + c = 0$$

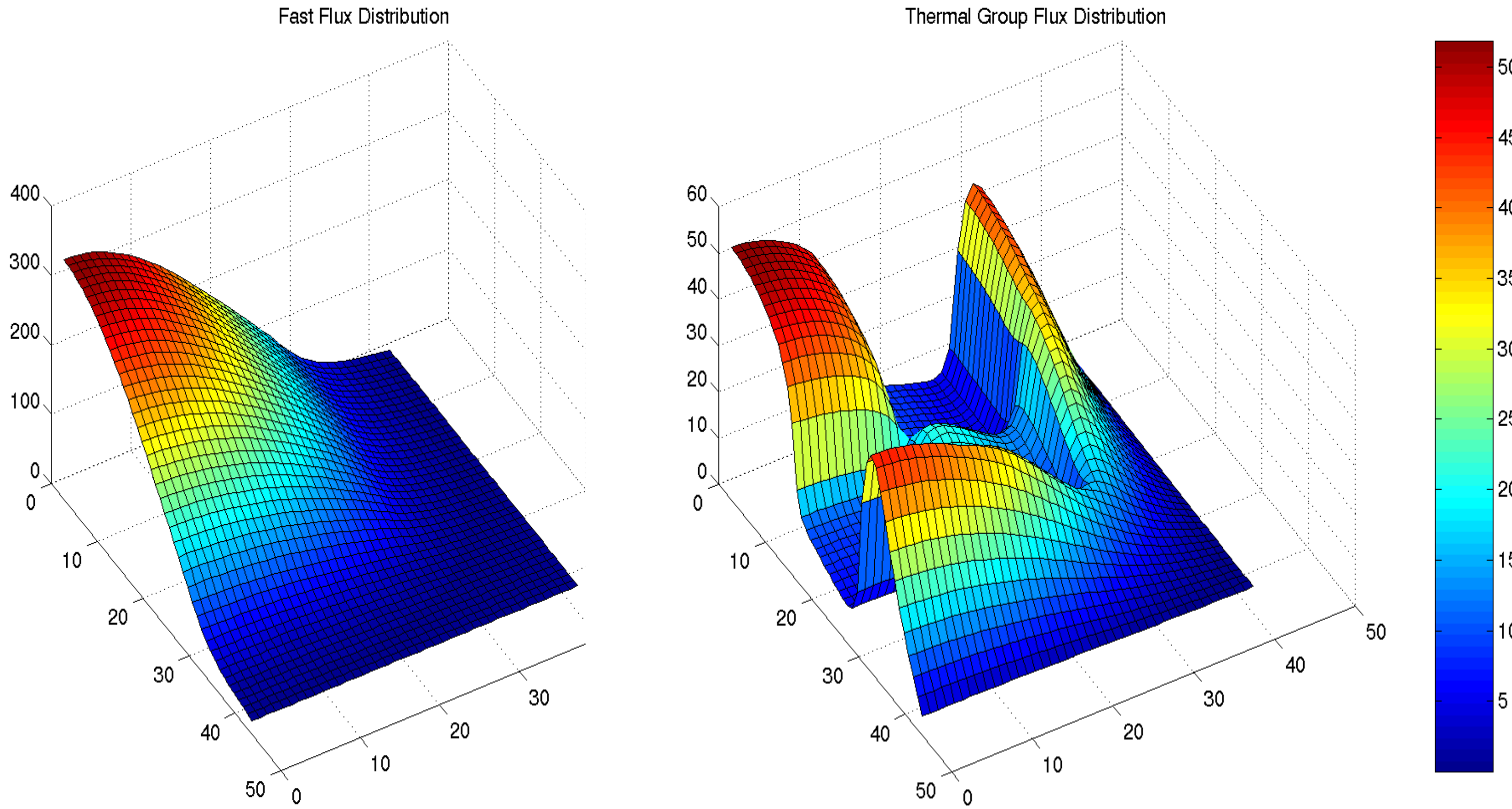
  – Solution $$B_1^2 = b\left(-1 + \sqrt{1 - \frac{c}{b^2}}\right) \begin{cases} > 0 \quad , & k_\infty > k_{eff} \\ < 0 \quad , & k_\infty < k_{eff} \end{cases}$$

$$\phi_{g1}^H(x) = \begin{cases} a_{g1} \sin(B_1 x) + a_{g2} \cos(B_1 x) \quad , & k_\infty > k_{eff} \\ a_{g1} \sinh(B_1 x) + a_{g2} \cosh(B_1 x) \quad , & k_\infty < k_{eff} \end{cases}$$

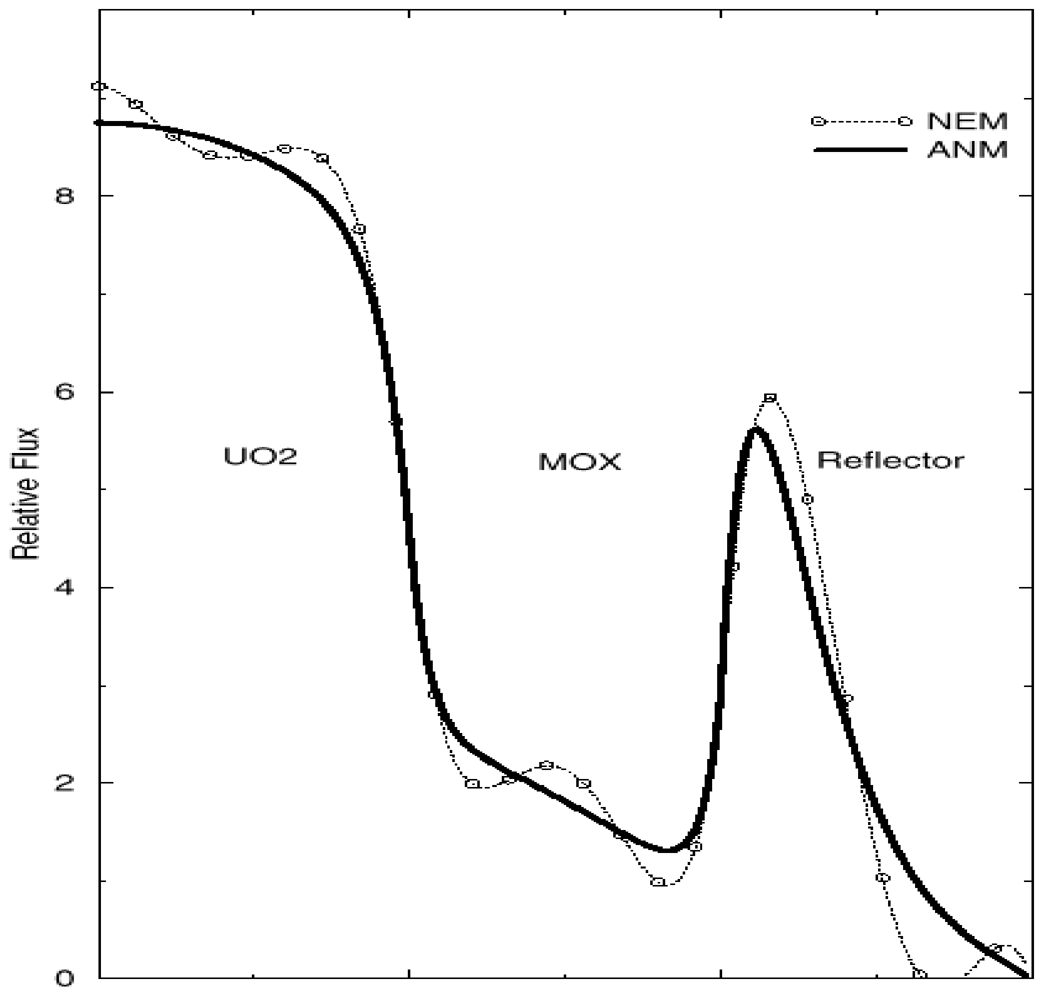
Two-Node ANM Solution

- Boundary Condition and Given Parameters
  - Quadratic Transverse Leakage for Two Nodes, k_{eff}
  - Node-Average Fluxes for Two Nodes
- 8 Unknown Coefficients
  - 4 per node x 2 nodes
- 8 Constraints $\rightarrow$ Unique Solution
  - 4 Node Average Fluxes (2 Groups x 2 Nodes)
  - 2 Flux Continuity at Interface (2 Groups)
  - 2 Current Continuity at Interface (2 Groups)
- Solution Sequence
  - Assume Node-Average Flux
  - Solve for Net Currents for each Direction from 2-Node
  - Update Node-Average Flux from Nodal Balance
  - Repeat

SS Cartesian: NEACRP L336 C5 problem, flux distribution



SS Cartesian: NEACRP L336 C5 problem, nodal flux shape



"HYBRID" ANM/NEM Method

- ANM is more accurate than NEM for many applications

- However, the ANM implementation is not stable for "just critical" nodes where a linear is required:

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

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

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

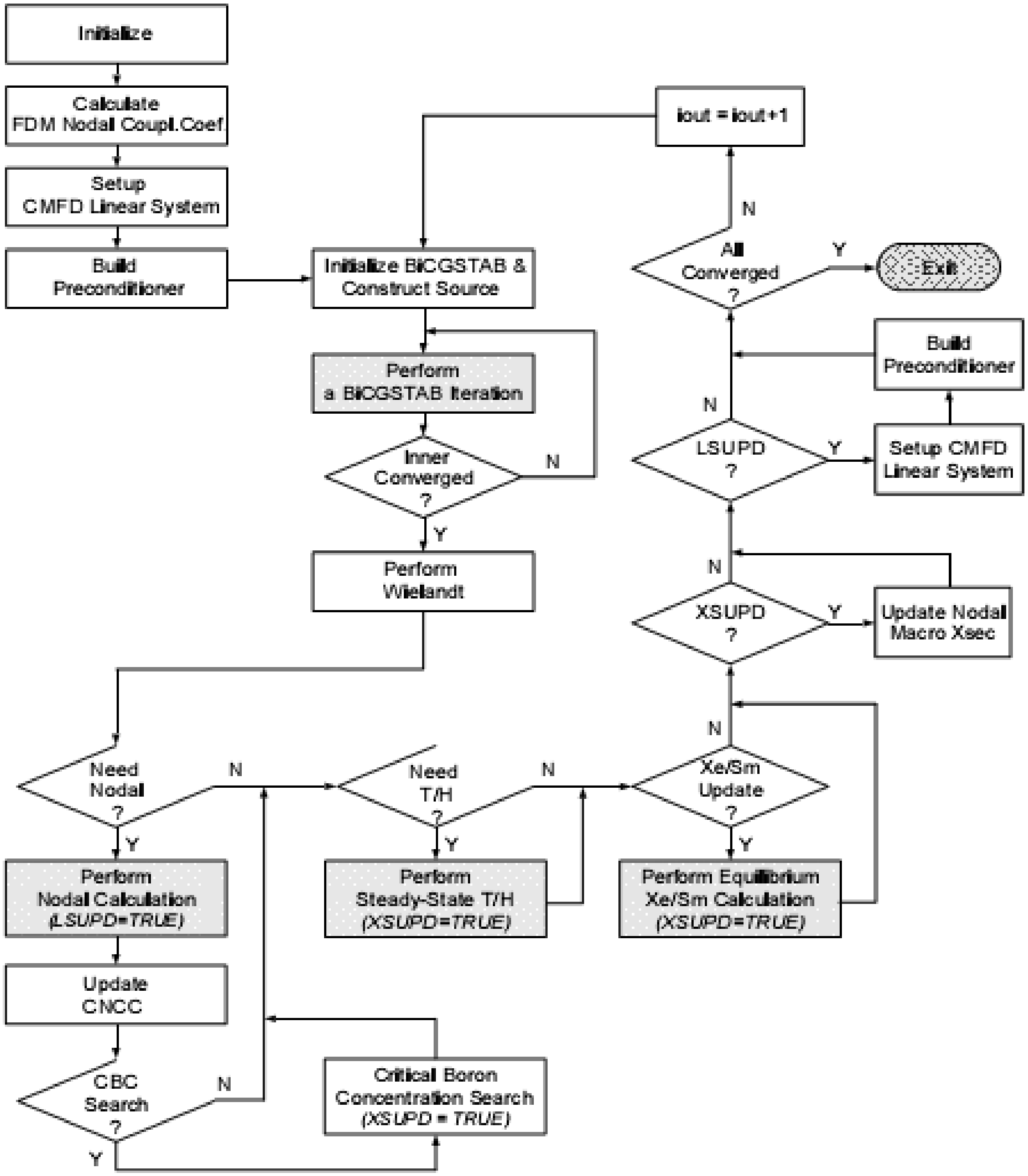


Figure 8.1: Eigenvalue Calculation Flow

Linear Solver: Krylov Method

$$Ax = b$$

- Traditional “Stationary” Methods (e.g. Successive Over Relaxation SOR)
  - Rate of convergence depends on spectral radius of iteration matrix

$$x^{n+1} = Gx^n + k$$

- Preconditioned Krylov Methods
  - “Three term recurrence relation”

$$x^{n+1} = G(n)x^n + G(n-1)x^{n-1} + k$$

  - Acceleration by Preconditioner

$$M^{-1}Ax = M^{-1}b$$

- PARCS uses BICGSTAB w/ BILU3D Preconditioner

Solving the Eigenvalue problem: the Power Method

- Eigenvalues of Matrix A $$Av_i = \lambda_i v_i$$

Assume: $\lambda_1 > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n|$ $\qquad \|v_i\|_2 = 1$ are unit eigenvectors

- Power method for finding maximum eigenvalue and its eigenvector

1. Given any initial guess of eigenvector
2. Power iteration

$$x_0 = \sum_{i=1}^{n} c_i v_i, \qquad c_1 \neq 0$$

$$x_k = \frac{Ax_{k-1}}{\|Ax_{k-1}\|_2} = \frac{A^k x_0}{\|A^k x_0\|_2}$$

$$A^k x_0 = \sum_{i=1}^{n} c_i A^k v_i = \sum_{i=1}^{n} c_i \lambda_i^k v_i = \lambda_1^k \left(c_1 v_1 + \sum_{i=2}^{n} c_i \left(\frac{\lambda_i}{\lambda_1} \right)^k v_i \right)$$

$$x_k = \left(c_1 v_1 + \sum_{i=2}^{n} c_i \left(\frac{\lambda_i}{\lambda_1} \right)^k v_i \right) \Bigg/ \left\| c_1 v_1 + \sum_{i=2}^{n} c_i \left(\frac{\lambda_i}{\lambda_1} \right)^k v_i \right\|_2$$

$$\lim_{k->\infty} x_k = \frac{c_1 v_1 + 0}{\|c_1 v_1 + 0\|_2} = \frac{c_1 v_1}{|c_1|} \qquad \lambda_1 = \lim_{k->\infty} \frac{\|Ax_k\|_2}{\|x_k\|_2}$$

Inverse Power Iteration with Wielandt Shift in PARCS

- Neutronic steady state problem (generalized eigenvalue-eigenvetor problem)

$$M\phi = \lambda F\phi \equiv \frac{1}{k_{eff}} F\phi$$

- Looking for minimum eigenvalue which is largest k_{eff}
- Let ϕ^0 be initial guess of flux solution, δk is user input parameter

$$k_{eff}^0 =< F\tilde{\phi}^0, u >$$

$$k_s^n = k_{eff}^n + \delta k \qquad S_f^n = \left(\frac{1}{k_{eff}^n} - \frac{1}{k_s^n} \right) F\phi^n = \left(\frac{\delta k}{k_{eff}^n k_s^n} \right) F\phi^n$$

$$\phi^{n+1} = \left(M - \frac{1}{k_s^n} F \right)^{-1} S_f^n \qquad k_{eff}^{n+1} = \left[\left(\frac{1}{k_{eff}^n} - \frac{1}{k_s^n} \right) \frac{< F\phi^n, u >}{< F\phi^{n+1}, u >} + \frac{1}{k_s^n} \right]^{-1}$$

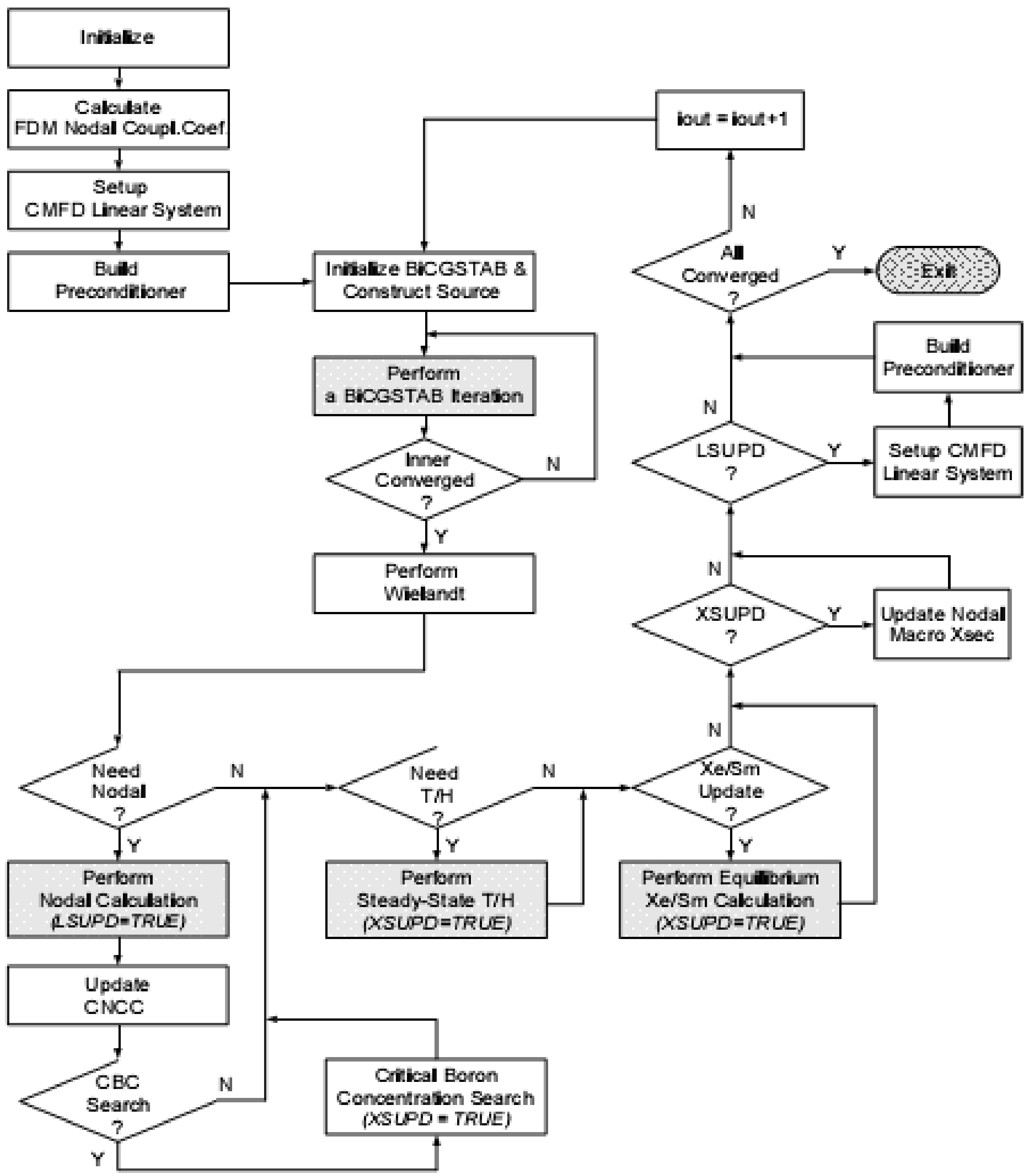


Figure 8.1: Eigenvalue Calculation Flow

PARCS Convergence

```
==============================================================================
          Executing Case l336C5
          by downar on NUCL112BPCLAP at 17:36:25, Oct.  8, 2006...
          Allocated Memory:      0.49 MBytes
==============================================================================
00:00.04  Input Processing Completed.
00:00.04  Performing Steady-State Eigenvalue Calculation...
 Itr Nin    k-eff        Global F.S.    Local F.S.   Dom. R     PPM
------------------------------------------------------------------------------
  1   1   0.9142296 F   9.1466E-01 F   3.2386E+00 F 10.0000      0.00
  2   3   0.9296559 F   2.5440E-01 F   3.7089E-01 F  0.2186      0.00
  3   3   0.9326269 T   4.8136E-02 F   7.9696E-02 F  0.2155      0.00
00:00.07  Nodal update...   1, NEM=    0, ANM=  288
  4   3   0.9377496 F   1.4679E-01 F   2.7124E-01 F  3.3320      0.00
  5   3   0.9373990 T   9.3391E-03 F   1.1604E-02 F  0.0679      0.00
  6   4   0.9373904 T   3.0558E-04 T   5.3557E-04 F  0.0326      0.00
00:00.09  Nodal update...   2, NEM=    0, ANM=  288
  7   3   0.9380279 T   1.7485E-02 F   3.7725E-02 F 10.0000      0.00
  8   3   0.9379567 T   1.9051E-03 F   2.4129E-03 F  0.1097      0.00
  9   4   0.9379550 T   6.2407E-05 T   1.1129E-04 T  0.0327      0.00
00:00.11  Nodal update...   3, NEM=    0, ANM=  288
 10   4   0.9381323 T   4.6583E-03 F   9.9657E-03 F 10.0000      0.00
 11   3   0.9381143 T   4.8244E-04 T   6.1868E-04 F  0.1038      0.00
 12   4   0.9381139 T   1.6327E-05 T   2.9306E-05 T  0.0338      0.00
00:00.14  Nodal update...   4, NEM=    0, ANM=  288
 13   4   0.9381586 T   1.1621E-03 F   2.5203E-03 F 10.0000      0.00
 14   3   0.9381542 T   1.1933E-04 T   1.5350E-04 T  0.1027      0.00
00:00.17  Nodal update...   5, NEM=    0, ANM=  288
 15   3   0.9381651 T   2.8123E-04 T   6.2931E-04 F  2.3569      0.00
 16   3   0.9381639 T   3.0126E-05 T   3.8955E-05 T  0.1071      0.00
00:00.17  Nodal update...   6, NEM=    0, ANM=  288
 17   3   0.9381666 T   6.8972E-05 T   1.5674E-04 T  2.2895      0.00
00:00.18  k-eff= 0.938167 , Tout=   0.00 , ppm=    0.00
Number of CMFD/Nodal/TH Updates/Inners and Sweeps:       17        6        0

 Time for Init.          0.020
          CMFD           0.140
          Nodal          0.020
          T/H            0.000
          Xsec           0.000
```

$$\delta_k = \left|k_{eff}^{n+1} - k_{eff}^{n}\right| , \quad \delta_{L2} = \frac{\left\|\psi_{n+1} - \psi_n\right\|_2}{\langle \psi_{n+1}, \psi_n \rangle^2} ,$$

$$\delta_{L\infty} = max\left|\frac{\psi_{n+1}^{m} - \psi_{n}^{m}}{\psi_{n+1}^{m}}\right| , \quad \delta_{Dop} = max\left|\frac{T_{D,t+1}^{m} - T_{D,t}^{m}}{T_{D,t+1}^{m}}\right|$$

```
CASEID l336C5                   L336  Case C5
!*****************************************************************************
CNTL
     PIN_POWER    F
     TH_FDBK      F
!                     input  iteration    planar                adj
!                      edit      table     power       pin     reac
      print_opt           T          T         T         T        F
!                      fdbk       flux    planar
!                       rho    precurs      flux        Xe      T/H
      print_opt           F          T         T         F        F


!*****************************************************************************
PARAM
! Basic Iteration Control Parameters
      n_iters    10 500                    !ninmax, noutmax

! Convergence Criteria
      conv_ss    5.e-3 5.e-4 5.e-4 0.1      !epseig,epsl2,epslinf,epstf!

! nodal_kern    nemmg
!       eps_anm  1.0E-15
!        eps_anm   5.0
!  nodal_kern    fmfd
!   nodal_kern    fdm
```

PARCS Neutronics Methods: Solution Kernels

Geometry Type	Kernel Name	Solution Method	Energy Treatment	Angle Treatment
Cartesian 3D	CMFD	FD	2G	Diffusion
	ANM	nodal	2G	Diffusion
	FMFD	FD	MG	**SP3**
	NEMMG	nodal	MG	**SP_3**
Hexagonal 3D	CMFD	FD	2G	Diffusion
	TPEN	nodal	MG	Diffusion
Cylindrical 3D	CMFD	FD	2G	Diffusion
	FMFD	FD	MG	Diffusion/ SP_3

CMFD = Coarse Mesh Finite Difference
ANM = Advanced Nodal Method
FMFD = Fine Mesh Finite Difference
NEM = Nodal Expansion Method
MG = Multigroup

Time-dependent SP_3 Equations

- Governing Equations

$$\frac{1}{v}\frac{\partial \phi_{0g}}{\partial t} + \nabla \cdot \phi_{1g} + \Sigma_{rg}\phi_{0g} = s_{0g}$$
$$\frac{1}{v}\frac{\partial \phi_{1g}}{\partial t} + \frac{2}{3}\nabla \phi_{2g} + \frac{1}{3}\nabla \phi_{0g} + \Sigma_{trg}\phi_{1g} = 0$$
$$\frac{1}{v}\frac{\partial \phi_{2g}}{\partial t} + \frac{3}{5}\nabla \cdot \phi_{3g} + \frac{2}{5}\nabla \cdot \phi_{1g} + \Sigma_{tg}\phi_{2g} = 0$$
$$\frac{1}{v}\frac{\partial \phi_{3g}}{\partial t} + \frac{3}{7}\nabla \phi_{2g} + \Sigma_{tg}\phi_{3g} = 0$$

$$\begin{cases} D_1^* \equiv \dfrac{1}{3\Sigma_{tr}^*} & \Sigma_\alpha^* = \Sigma_\alpha + \dfrac{1}{\upsilon \Delta t} \\ D_3^* \equiv \dfrac{3}{7\Sigma_t^*} & q_i^n = \dfrac{1}{\upsilon}\dfrac{\phi_i^n}{\Delta t} \end{cases}$$

- Second-order Differential Equations

$$\begin{bmatrix} -D_1^*\nabla^2 + \Sigma_r^* & -2D_1^*\nabla^2 \\ -\dfrac{2}{5}D_1^*\nabla^2 & -\left(\dfrac{3}{5}D_3^* + \dfrac{4}{5}D_1^*\right)\nabla^2 + \Sigma_t^* \end{bmatrix} \begin{bmatrix} \phi_0^{n+1} \\ \phi_2^{n+1} \end{bmatrix} = \begin{bmatrix} q_0^n - 3D_1^*\nabla \cdot q_1^n + S_{0t}^{n+1} \\ q_2^n - \dfrac{6}{5}D_1^*\nabla \cdot q_1^n - \dfrac{7}{5}D_3^*\nabla \cdot q_3^n \end{bmatrix}$$

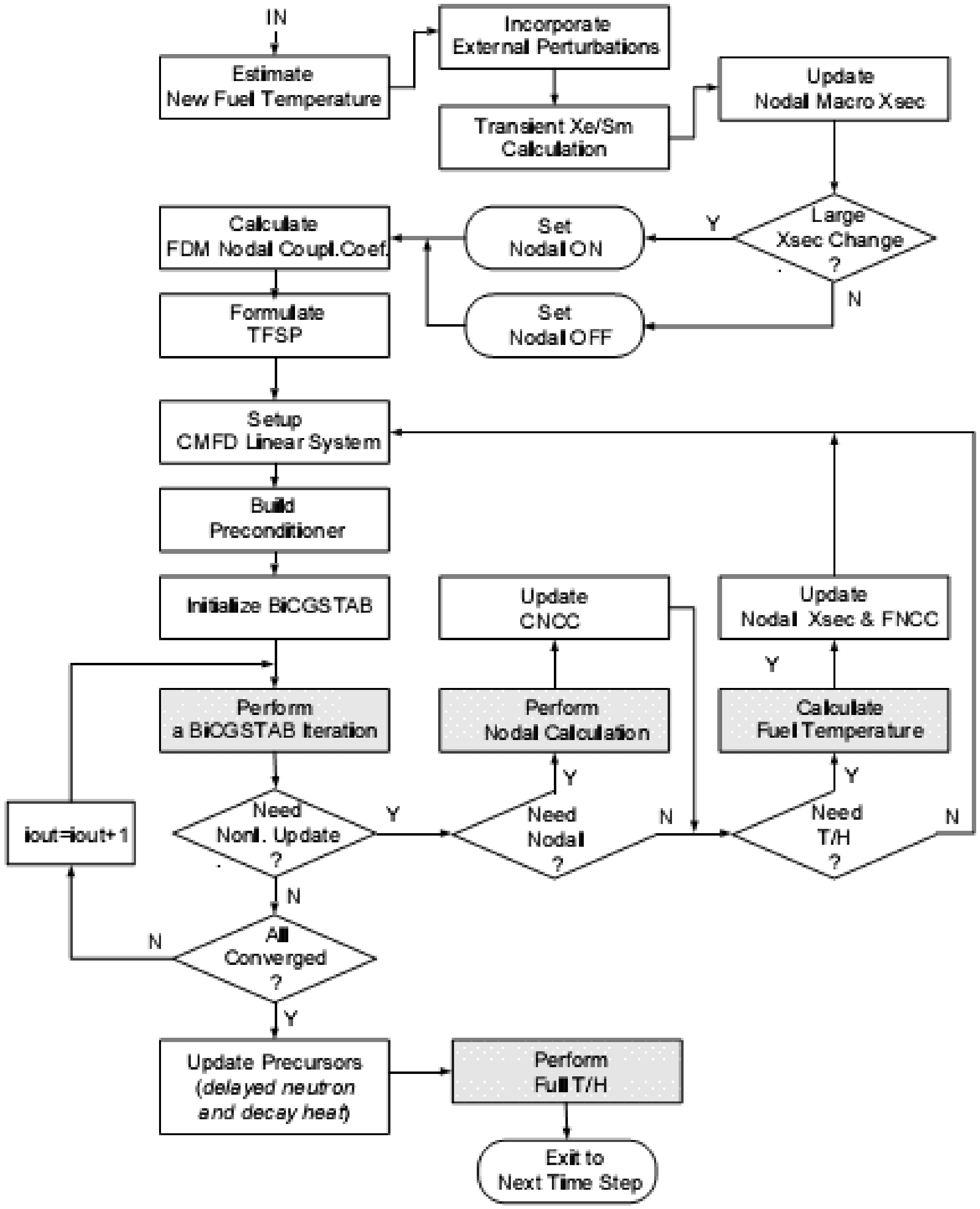
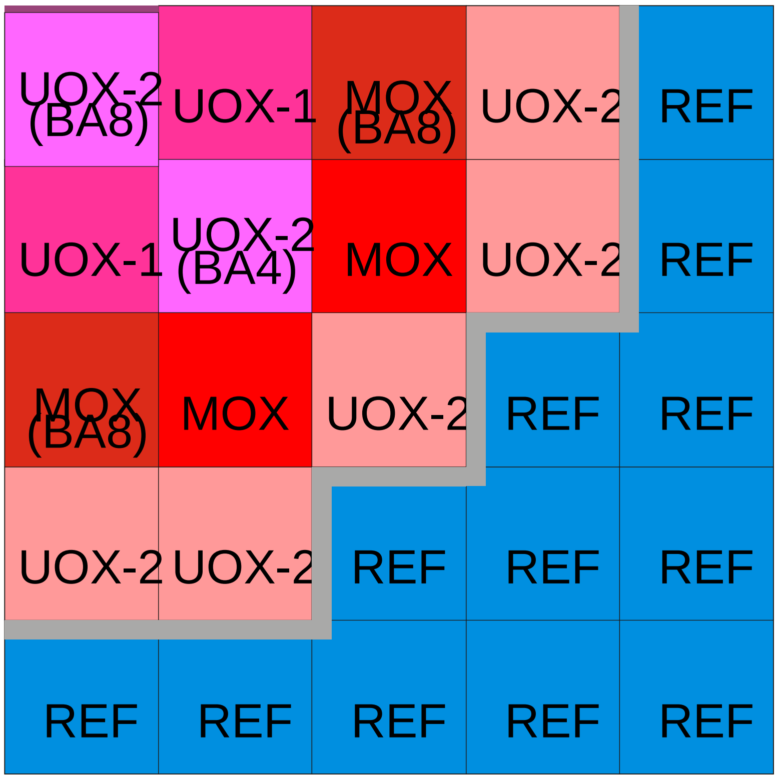
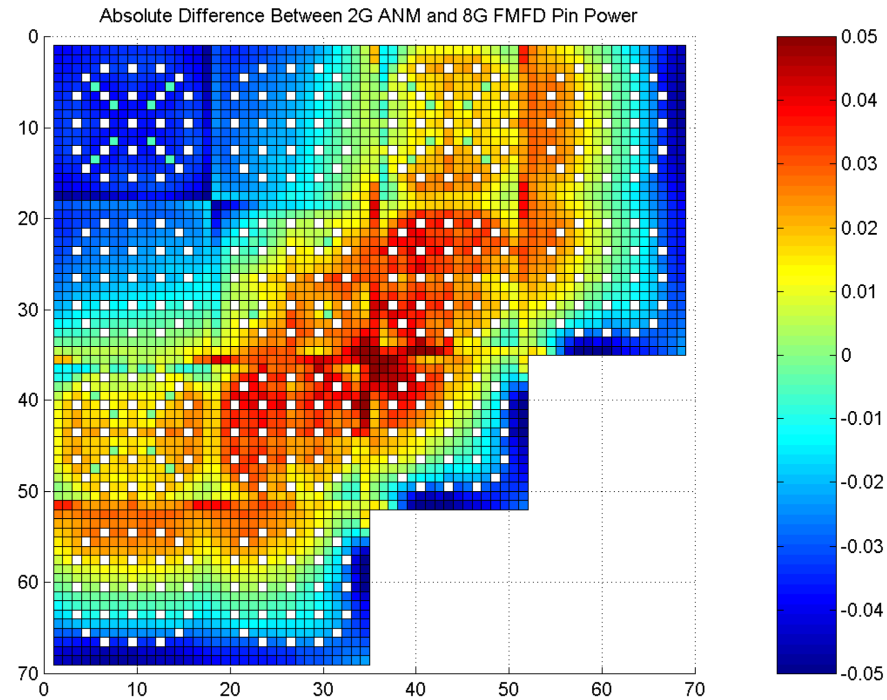


Figure 8.3: Transient Calculation Algorithm

MOX Core Loading

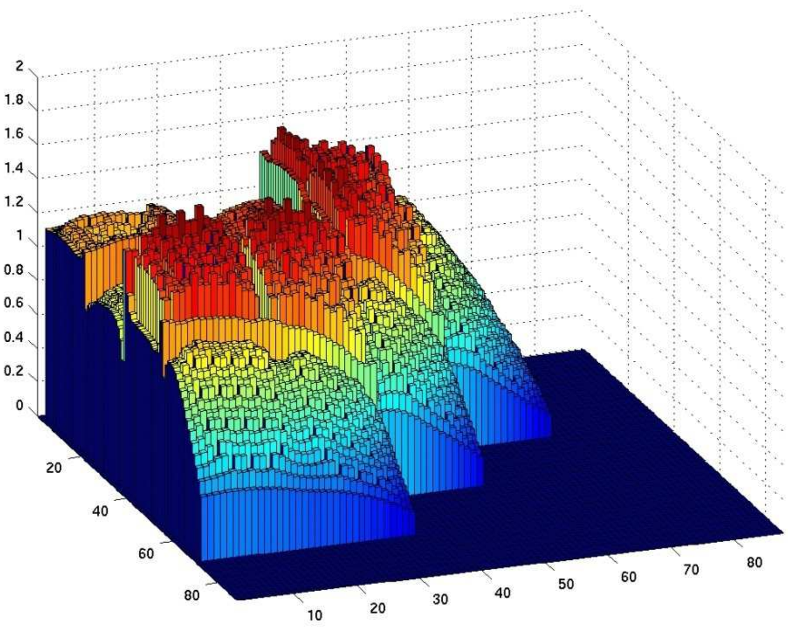




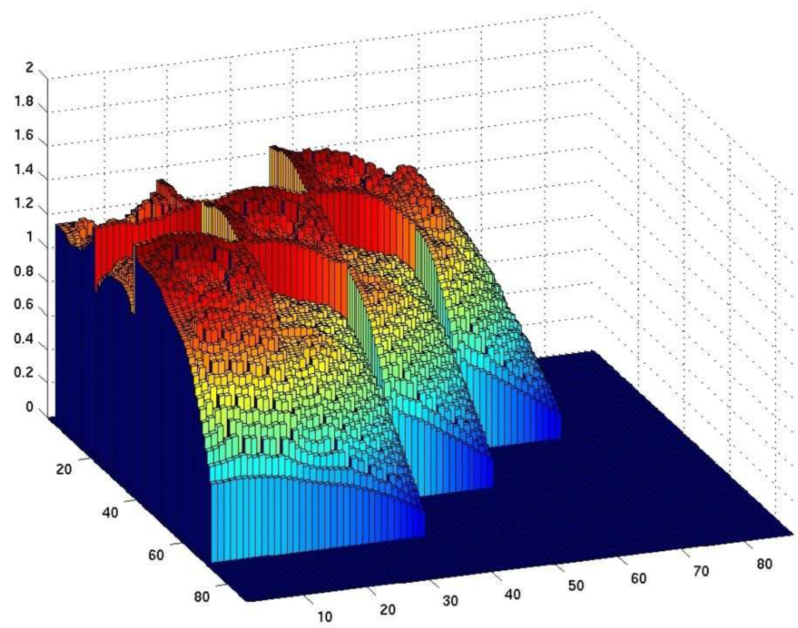
* Diff. = $(P_{2G\ Nodal} - P_{Refernce})$

Reference Results: Steady-State Power Distributions

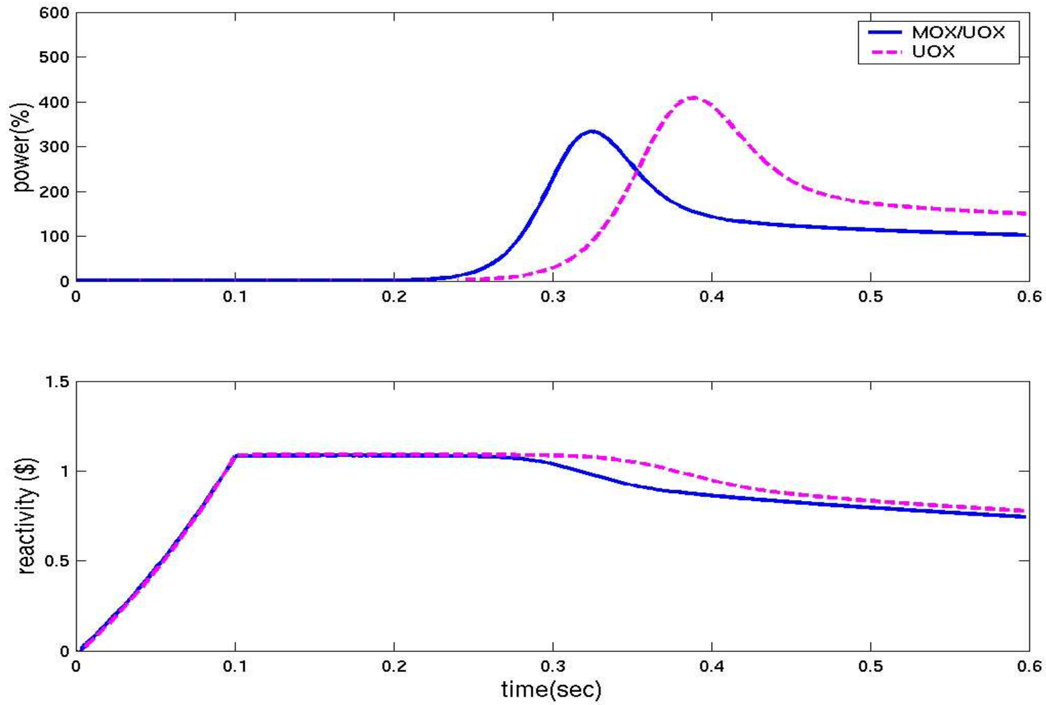
MOX/UOX



UOX



Core Power and Reactivity (MOX/UOX and UOX Cores)



" Analysis of Results for the OECD/NEA and U.S. NRC PWR MOX/UO2 Core Transient Benchmark, T. Kozlowski C. A. Cotton T. J. Downar, Reactor Physics ANS Topical Meeting, PHYSOR-04, April, 2004, Chicago, IL

Some Recent References

- Methods:
  - Multigroup SP3 Methods for Neutronics Analysis of MOX Fueled Cores," C. Lee and T. Downar, *Nuclear Science and Engineering,* Vol. 146, No.2, February, 2004.
  - "Convergence Analysis of the Nonlinear Coarse Mesh Finite Difference Method for One-dimensional Fixed Source Neutron Diffusion Problem," Deokjung Lee, Thomas J. Downar, and Yonghee Kim, *Nucl. Sci. Eng.*, Vol. 147, No.2, June, 2004.

- Applications
  - "Consistent Comparison of the Codes RELAP5/PARCS and TRAC-M/PARCS for the **OECD MSLB Coupled Code Benchmark,"** T. Kozlowski, R. Miller, T. Downar, H. Joo, D. Barber *Nuclear Technology,* Vol. 146, No. 1, April, 2004.

  - "Analysis of the **OECD/NRC Peach Bottom Turbine Trip Transient Benchmark** with the Coupled Neutronics and Thermal-hydraulics Code TRAC-M/PARCS," Deokjung Lee, Thomas J. Downar, Anthony Ulses, Bedirhan Akdeniz, Kostadin N. Ivanov, *Nucl. Sci. Eng*., Vol. 148, No.2, October, 2004.

Code Assessment

- Stand-alone Neutronics Tests
  - NEACRP-L336 Pin Benchmark
  - **NEACRP PWR Rod Ejection/Withdrawal Benchmarks**
  - VVER1000 Rod Ejection Benchmark
  - VENUS-2 Critical Benchmark
  - OECD MOX Core Transient Benchmark

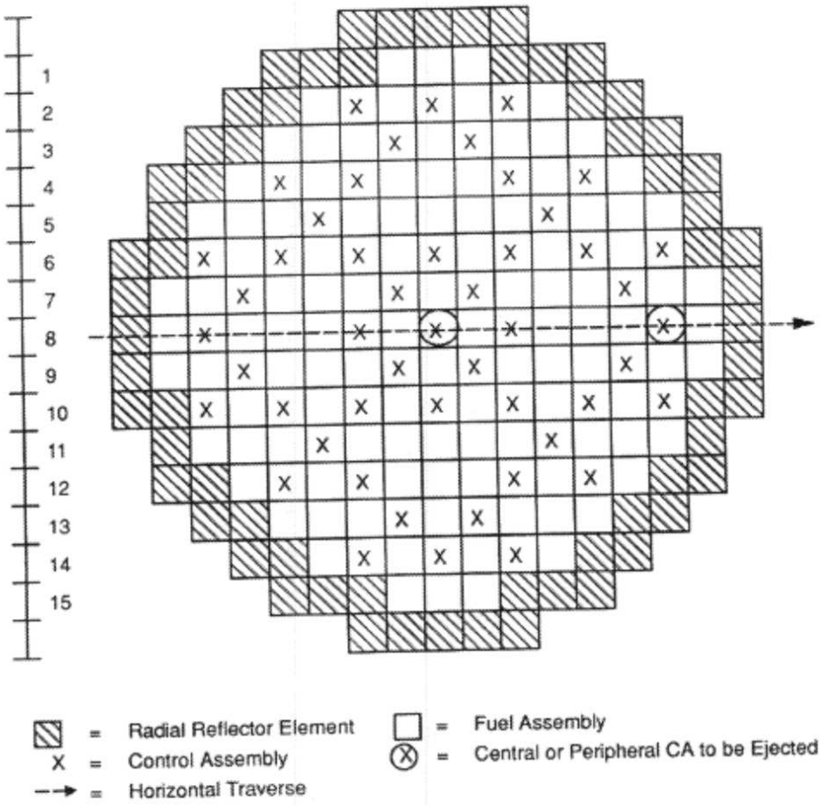
- Coupled Code Tests (TRACE/RELAP5/PARCS)
  - OECD PWR-MSLB Benchmark
  - OECD BWR PBTT BWR: Peach Bottom
  - BWR Ringhalls Stability
  - BWR: Peach Bottom Cycle 1 and 2 Depletion Benchmark

TR Cartesian: NEACRP L335 PWR rod ejection

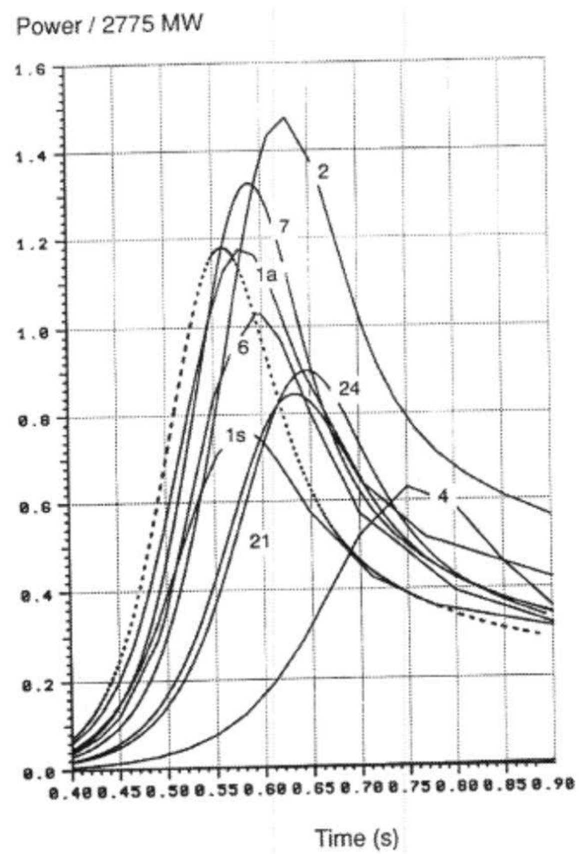
Table 2.1 PWR, Participants of the Benchmark Problems A1–C2

Part.No.	Organization	Country	Code		A1	A2	B1	B2	C1	C2
1	TRACTEBEL	Belgium	OKAPI	(s)	X	X	X	X	X	X
				(a)	X		X		X	
2	VTT	Finland	BOREAS,TRAB		X	X	X	X	X	X
4	FRAMATOME	France	CESAR		X	X	X	X	X	X
5	EDF	France	COCCINELLE					X	X	
6	SIEMENS	Germany	PANBOX		X	X	X	X	X	X
7	GRS	Germany	QUABOX–CUBBOX		X	X	X	X	X	X
10	ENEL	Italy	QUANDRY–EN				X		X	
13	JAERI	Japan	REFLA/TRAC		X					
14	JAERI	Japan	THYDE–NEU					X		
19	ECN	Netherl.	PRORIA		X	X			X	X
20	NV KEMA	Netherl.	LWRSIM		X	X	X	X	X	X
21	ETS	Spain	SIMTRAN		X	X	X	X	X	X
23	INER	Taiwan	ARROTTA						X	X
24	NE Ber Lab	UK	PANTHER		X	X	X	X	X	X
total number		14			10	9	9	9	12	11

TR Cartesian: NEACRP L335 PWR rod ejection



TR Cartesian: NEACRP L335 PWR rod ejection



PWR: Key to Figures 2.1–7.6

----	REFERENCE
1 s	OKAPI (s)
1 a	OKAPI (a)
2	TRAB
4	CESAR
5	COCCINELLE
6	PANBOX
7	QUABOX–CUBBOX
10	QUANDRY–EN
13	REFLA/TRAC
14	THYDE–NEU
19	PRORIA
20	LWRSIM
21	SIMTRAN
23	ARROTTA
24	PANTHER

Important items to remember about PARCS input

- Input was design to use as many default values as possible
  - Very short inputs are possible for 2G nodal PWR problems

- Input restrictions
  - Block names start in 1st column (CASEID, PARAM, CNTL, GEOM, TH, TRAN, PFF, ONEDK, PLOT)
  - Card names start in 2nd or later column
  - Card input can be in external files through “file” card
  - In general, block order is arbitrary (exception is FMFD, there FMFD block have to be before GEOM)
  - In general, cards order within a block can be in arbitrary order
  - BANG (!) is a comment
  - SLASH (/) is end of case
  - DOT (.) is end of input
  - Input is case insensitive
  - Multiple data on single card can be separated by space or TAB
  - Fortran style free format STAR (*) can be used for repeating data, 8*1.2 means repeat 1.2 eight times
  - Any empty lines are ignored

TR Cartesian: NEACRP L335 PWR rod ejection

```
Block 1:

CASEID A1                Neacrp Case A1
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 2:

```
CNTL
      core_power   0.0001 0.0  !in %
      bank_pos   0.0   0.   0. 228.   0.   0.   0. 228.
      ppm    561.26
      transient    T
!     search       ppm
!                    input  iteration     planar                  adj
!                     edit      table      power        pin       reac
      print_opt          F          F          F          F          T
!                     fdbk       flux     planar
!                      rho   precurs       flux         Xe        T/H
      print_opt          F          F          F          F          F
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 3:

```
PARAM
! no parameters are specified, all defaults
!      n_iters  100 10
```

TR Cartesian: NEACRP L335 PWR rod ejection

```
Block 4:
```

```
XSEC
      file ./xsec/XSEC_NEACRP
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 4 (external file):

```
 ref_cond   1200.2 306.6 0.7125 618.3 !ppm, Tm in C, rho in gm/cc, Tf in C
 comp_num   4    !fuel 1
!-------------------------------------------------------------------------------
 base_macro 2.221170e-01  8.717740e-03  4.982770e-03  6.111896e-14  1.824980e-02
            8.031400e-01  6.525500e-02  8.390260e-02  1.101520e-12
 dxs_dppm   3.478090e-08  1.285050e-07 -1.120990e-09 -1.761878e-20 -1.085900e-07
           -9.765100e-06  7.088070e-06 -2.430450e-06 -3.190845e-17
 dxs_dtm   -2.033100e-06  2.121910e-07  1.247090e-07  1.430354e-18  8.096760e-07
           -1.086740e-04 -3.155970e-05 -4.164390e-05 -5.467221e-16
 dxs_ddm    1.356650e-01  1.551850e-03  9.206940e-04  1.023919e-14  2.931950e-02
            9.926280e-01  2.526620e-02  2.477460e-02  3.252554e-13
 dxs_dtf   -3.091970e-05  3.497090e-05  6.401340e-07  7.154124e-18 -2.755360e-05
           -1.372920e-04 -3.718060e-05 -5.630370e-05 -7.391879e-16
 cdf        1.0069   0.9307   1.0034   0.9646   1.1040   1.4493   1.0096   1.1580

 delcr_comp 1   1 -5  7 -11  !compostions that this set applies
!-------------------------------------------------------------------------------
 delcr_base 3.732200e-03  2.477700e-03 -1.027860e-04 -1.214480e-15 -3.192530e-03
           -2.199260e-02  2.558750e-02 -2.823190e-03 -3.702378e-14

!Delayed Neutron Precurosor Data
!---------------------------------------------------------------------------------
 dnp_ngrp   6
 kin_comp   1  1 -11    !Compostions that this set applies
 dnp_lambda 0.0128  0.0318  0.119   0.3181  1.4027  3.9286 !decay constants
 dnp_beta   0.0002584 0.00152 0.0013908 0.0030704 0.001102 0.0002584 !beta
 neut_velo  2.8E7    4.4E5  ! Neutron Velocities (cm/sec)
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 5:

```
GEOM
      file ./xsec/GEOM_QC
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 5 (external file):

```
geo_dim   9 9 18              !nasyx,nasyy,nz
rad_conf
2 2 2 2 2 2 2 2 1
2 2 2 2 2 2 2 2 1
2 2 2 2 2 2 2 1 1
2 2 2 2 2 2 2 1 0
2 2 2 2 2 2 1 1 0
2 2 2 2 2 1 1 0 0
2 2 2 2 1 1 0 0 0
2 2 1 1 1 0 0 0 0
1 1 1 0 0 0 0 0 0
grid_x      10.803   8*21.606
neutmesh_x 1         8*2
grid_y      10.803   8*21.606
neutmesh_y 1         8*2
grid_z      30.  7.7  11.0  15.0  10*30.0  2*12.8  8.0  30.
boun_cond  0 1 0 1 1 1        !ibcw,ibce,ibcn,ibcs,ibcb,ibct
Planar_Reg 1
1  1  1  1  1  1  1  1  2
1  1  1  1  1  1  1  1  2
1  1  1  1  1  1  1  3  2
1  1  1  1  1  1  1  2
1  1  1  1  1  1  3  2
1  1  1  1  1  3  2
1  1  1  1  3  2
1  1  3  2  2
2  2  2
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 5 (external file):

```
Planar_Reg 3
 4  9  4  9  4  7  4  6  2
 9  4  8  4  8  4 11  6  2
 4  8  4  8  4  8  6  3  2
 9  4  8  4  8 10  6  2
 4  8  4  8  4  6  3  2
 7  4  8 10  6  3  2
 4 11  6  6  3  2
 6  6  3  2  2
 2  2  2
 PR_Assign  1   2   15*3   1
 cr_axinfo 37.7 1.5942237    !fully inserted position and step size
 bank_conf
 1  0  2  0  0  0  3  0  0
 0  4  0  0  0  6  0  0  0
 2  0  5  0  6  0  6  0  0
 0  0  0  4  0  0  0  0
 0  0  6  0  7  0  0  0
 0  6  0  0  0  0  0
 3  0  6  0  0  0
 0  0  0  0  0
 0  0  0
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 6:

```
TH
      file ./xsec/TH_QC
```

TR Cartesian: NEACRP L335 PWR rod ejection

Block 6 (external file):

```
n_pingt      264 25                     !npin,ngt
     fa_powpit    17.67516   21.606          !assembly power(Mw) and pitch(cm)
     pin_dim      4.1195 4.7585 0.571 6.1295 !pin radii, rs,rw,tw, and rgt in mm
     flow_cond    286.0 82.12102             !tin,cmfrfa(Kg/sec)
     gamma_frac   0.019                      !direc heating fraction
     hgap         10000.                     !hgap(w/M^2-C)
     n_ring       10                         !number of meshes in pellet
     thmesh_x     1   8*2                    !Number of T/H Nodes per FA in X-dir
     thmesh_y     1   8*2                    !Number of T/H Nodes per FA in y-dir
     thmesh_z     1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18  !junctions
```

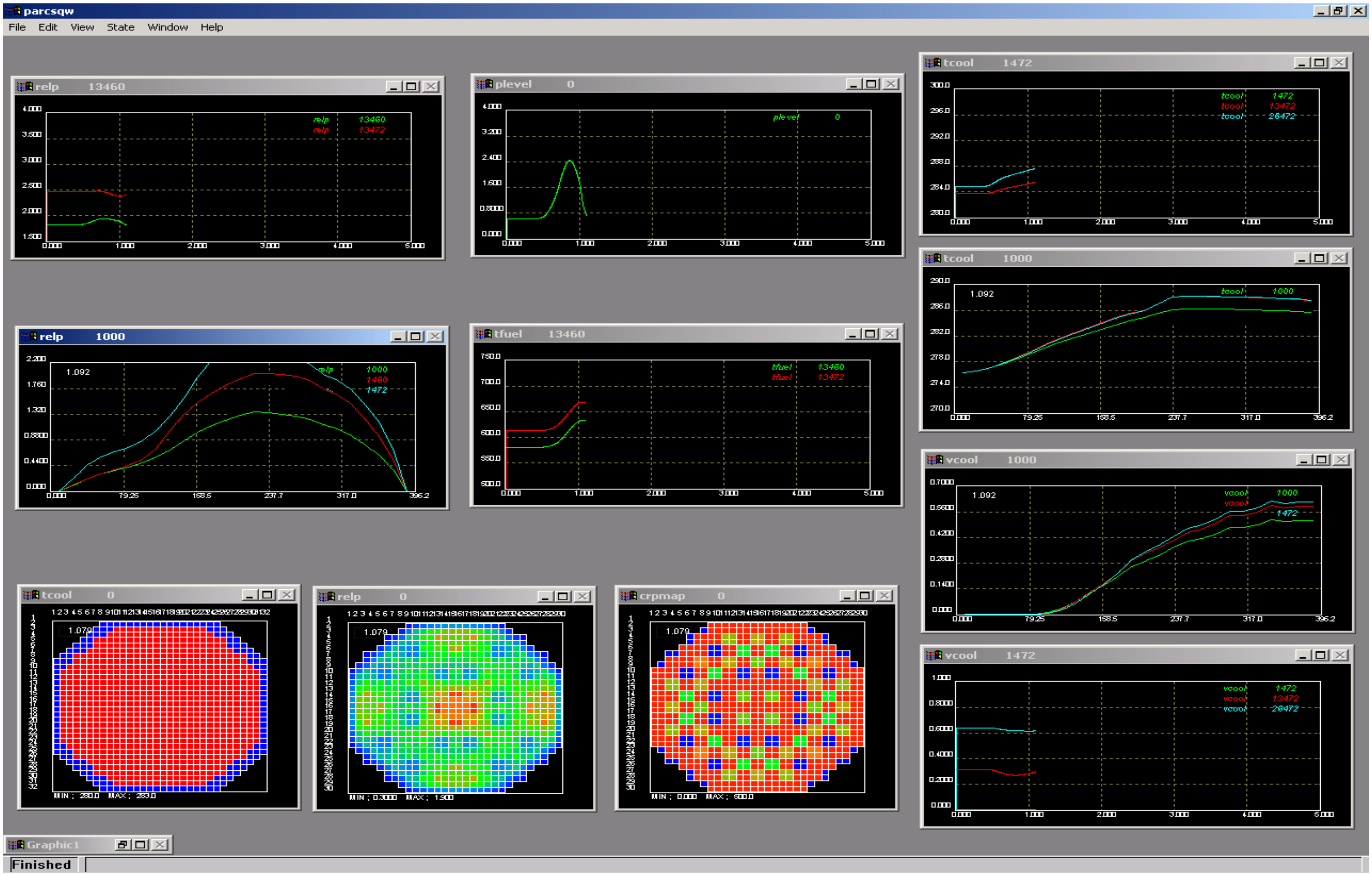
TR Cartesian: NEACRP L335 PWR rod ejection

Block 7:

```
TRAN
      time_step    5.00 0.01 1.0  10.0  !tend,delt0,tswitch,texpand
      move_bank    1  0.0 0.0   0.1 228.0
      conv_tr      0.0001             !eps_r2
!     sum_step     1.0  10  5.0 2
!
!                       rho        % power    peaking     temp
!     plot_cntl    T -0.3 1.2      0. 130.     1. 7.     280. 560.

.
```

PARCS GUI



parcsqw
File Edit View State Window Help
relp 13460
plevel 0
tcool 1472
tcool 1000
relp 1000
tfuel 13460
vcool 1000
vcool 1472
tcool 0
relp 0
crpmap 0
Graphic1
Finished