Nodal Kinetics Upgrades to RELAP5-3D

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Introduction

- Kinetics Upgrades in RELAP5-3D:
  - Installed Krylov solver for SS
  - Extended Krylov solver to 4 energy groups
  - Installed TPEN nodal solver for Hex
  - Installed GMRES option for Krylov solver
  - Implement rod cusping correction (for TPEN only)
  - Implemented reactivity feedback calculation

Krylov SS Solver

- BiCGSTAB implemented for transients (1996)
  - Used LSOR SS solution for initial condition
  - Caused complications in data mapping between two solvers
- BiCGSTAB solver now extended to steady-state
  - Simplifies database.
  - Provides better consistency between steady-state and transient solution
- Weilandt Shift is used to accelerate eigenvalue calculation (replaces Chebyshev)

4 Energy Groups

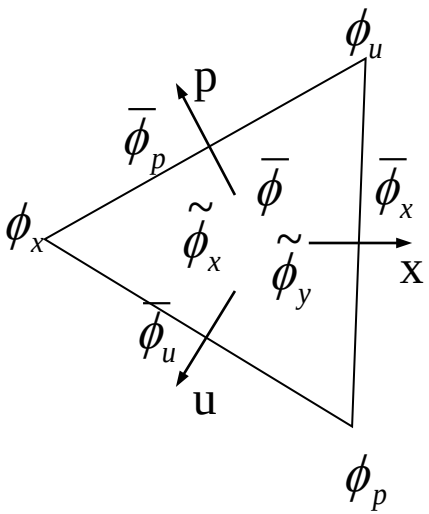
- LSOR solver handles up to 4 energy groups
- Krylov solver only handled up to 2 energy groups
- All Krylov solver logic has now been extended
  - Coarse mesh problem
  - Nodal solution (NEM, TPEN)
  - Cross section evaluation
    - Up- and Down- scatter both treated
  - Ancillary routines

TPEN Nodal Solver

- Tri-angular Polynomial Expansion Nodal (TPEN)
  - For Hexagonal geometries
  - Replaces Nodal Expansion Method (NEM) in the radial direction
  - NEM still used in the axial direction
- Purpose:
  - Obtain higher-order intra-nodal flux distribution
  - Provide more accurate current at the boundaries
- Design
  - Divide hexagon node into 6 triangles
  - Solve for surface and corner fluxes
  - Update Coarse-mesh solution with refined current across hex boundaries

TPEN Nodal Solver

- Unknowns Selected for a Triangle (9 in total per Group)



  - Fluxes at three Corners, $\phi_d = \phi\ (r_d)$
  - Surface average fluxes at three surfaces

$$\bar{\phi}_x = \frac{1}{h}\int \phi\ (x,y)\, dy$$

  - Moments

$$\tilde{\phi}_x = \frac{2\sqrt{3}}{3h}\frac{1}{V}\iint x\phi\ (x,y)\, dydx \qquad \tilde{\phi}_y = \frac{2}{h}\frac{1}{V}\iint y\phi\ (x,y)\, dydx$$

  - Nodal Volume Average Flux, $\bar{\phi} = \frac{1}{V}\iint \phi\ (x,y)\, dydx$

- Flux Expansion for a Triangle

$$\phi\ (x,y) = c_0 + a_x x + a_y y + b_x x^2 + b_u u^2 + b_p p^2 + c_x x^3 + c_u u^3 + c_p p^3$$

GMRES Solver

- GMRES is the most reliable Krylov subspace method for solving asymmetric linear system $Ax=b$.
- At each step of the iteration m, GMRES finds the solution in Krylov subspace $K_m = \text{span}\{r_0, Ar_0, A^2r_0, \ldots A^{m-1}r_0\}$, which minimizes the L2-norm of the residual. Where $r_0=b-Ax_0$.
- If V_m is the orthonormal base of K_m , then the mth step GMRES solution is $x_m=x_0+V_m y_m$, where $y_m = \text{argmin}_y \| b- A(x_0+v_m y)\|_2$
- The L2-norm of residual is guaranteed to decrease monotonically during the GMRES iteration (unlike other Krylov methods).
- The exact solution can be obtained with no more than n iterations, where n is the dimension of linear system.

Preconditioned GMRES

- The convergence rate of GMRES relies on the condition number of matrix A. If the condition number of A is too large, then large a number of GMRES iterations will be needed to achieve acceptable convergence.
- If a matrix M which is similar to matrix A and is easier to be inverted, then M can be used as preconditioner. A solution z can be obtained from linear system: $(AM^{-1})\ z=b$, the final solution is then obtained as $x=M^{-1}\ z$.
- As M is similar to A, the condition number of (AM^{-1}) is normally much smaller than condition number of A, z can be obtained with many fewer iterations of GMRES than would be required to solve x directly with the unconditioned GMRES method.

Restarted GMRES

- In GMRES, the vectors in V_m, the orthonormal basis of K_m should be stored. The number of vectors, m, is the same as the number of iterations. The GMRES algorithm can become computationally impractical when m is large because of the growth of memory and computational requirements as m increases.

- One way to reduce the memory requirement is Restarted GMRES in which only a fixed number of vectors are stored. When the number of iteration reaches the specified number of vectors, the GMRES solution at this step will be used as initial solution guess for a new restarted GMRES iteration. This method is implemented in RELAP3D.

GMRES Implementation

- As the Matrix-vector production (Axb) and the preconditioning (minv) of the Block Incomplete LU factorization (BILU) have already been developed for previous Krylov solver BiCGstab, the major task of implementing GMRES was coding the GMRES algorithm.

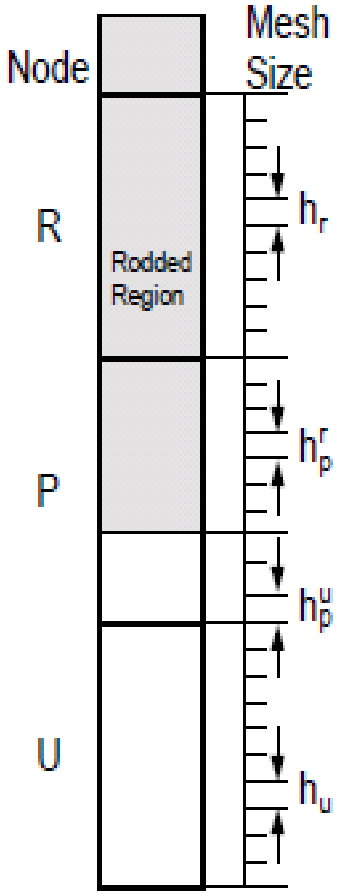
- This consisted of two major parts:
  - Orthogonalization with Modified Gram-Schmidt method
  - Solving the linear system with Hessenberg matrix by *QR factrization with Givens rotation*

GMRES Solver

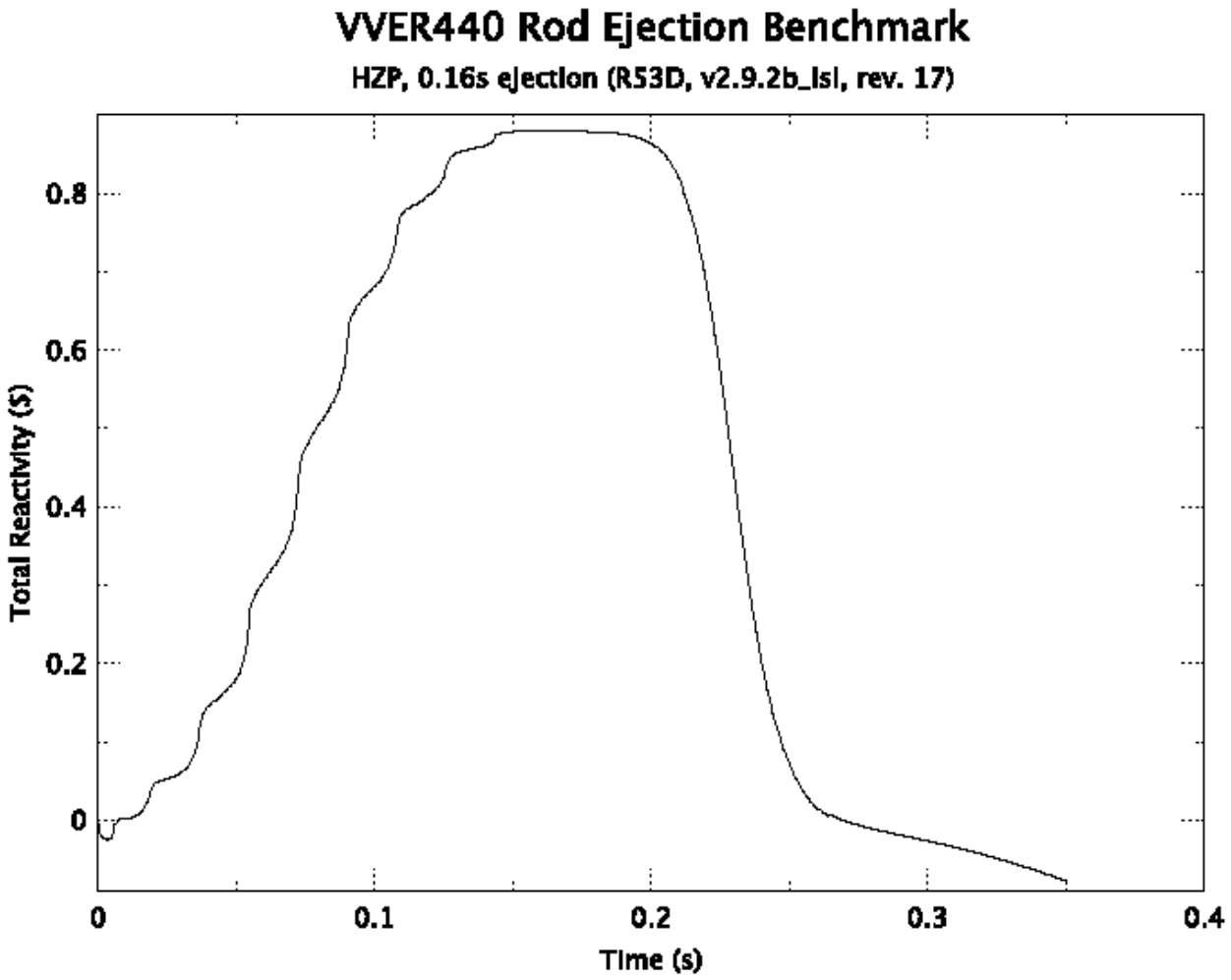
- The convergence rates of both GMRES and BiCGstab rely on the condition number of matrix.
- If the condition number of the matrix is small, the performances of GMRES and BiCGstab are comparable.
- If the condition number of matrix is very large, GMRES is more reliable than BiCGstab. BiCGstab may not converge for some matrices, but in these cases GMRES will converge.
- The condition numbers of matrices at steady state and transient can be effected by user input.
  - For transients, the condition number reduces when time step size decreases.
  - For steady state, Wielandt shift is often used to accelerate eigenvalue, but at the same time, it also makes the linear system ill-conditioned. So, when the linear system is ill-conditioned, Wielandt shift should be turned off. GMRES instead of BiCGstab should be used to solve the linear sytem.

Rod Cusping Effect

- When the control rod is partially inserted into a node, the intranodal flux distribution is distorted due to the presence of the strong thermal absorber. In such cases, the volume weighting scheme to obtain the homogenized nodal cross section can introduce significant errors in the core calculation.
- The detailed intranodal flux variation is required to flux/volume weight the cross sections and to preserve the reaction rate when computing the homogenized cross section. The intranodal flux shape is not known “a priori” and the volume weighting introduces the so-called "rod cusping" effect for partially inserted control rods.
- The typical rod cusping effect occurs in eigenvalue calculations in such a way that the core keff varies in a cusp (or wavy) shape as the control rod insertion depth changes. The rod cusping effect is also observed in core power variation during a transient that involves slow control rod motion.

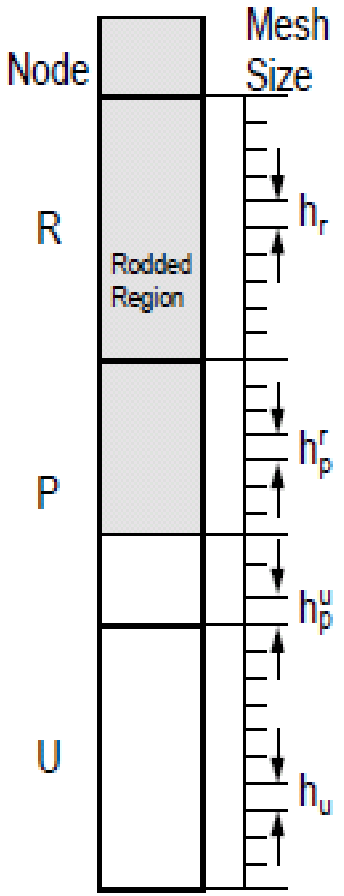


Rod Cusping Effect



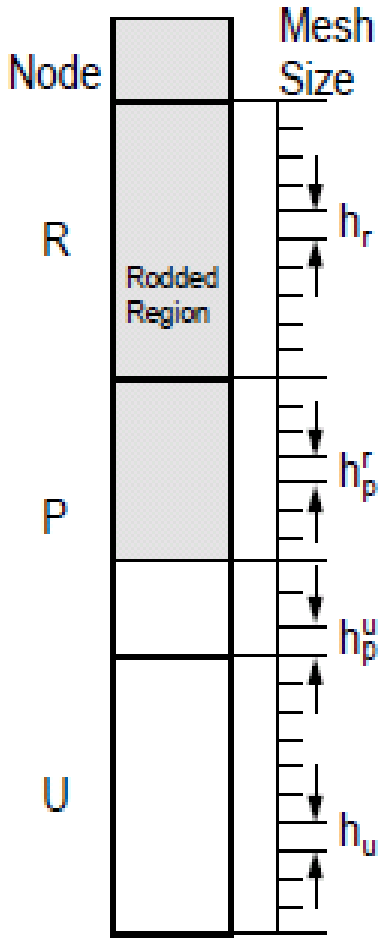
Rod Cusping Correction Method

- To correct for the rod cusping effect, the detailed axial flux distribution needs to be calculated prior
- The intranodal flux distribution in a partially rodded node is obtained by solving a three node problem by the fine mesh finite difference scheme. The flux weighting factor can be readily obtained from the intranodal flux solution.
- To insure the consistency of the nodal solution with the homogenized nodal cross sections and the fine mesh solution, discontinuity factors are defined at both surfaces of partially rodded node.



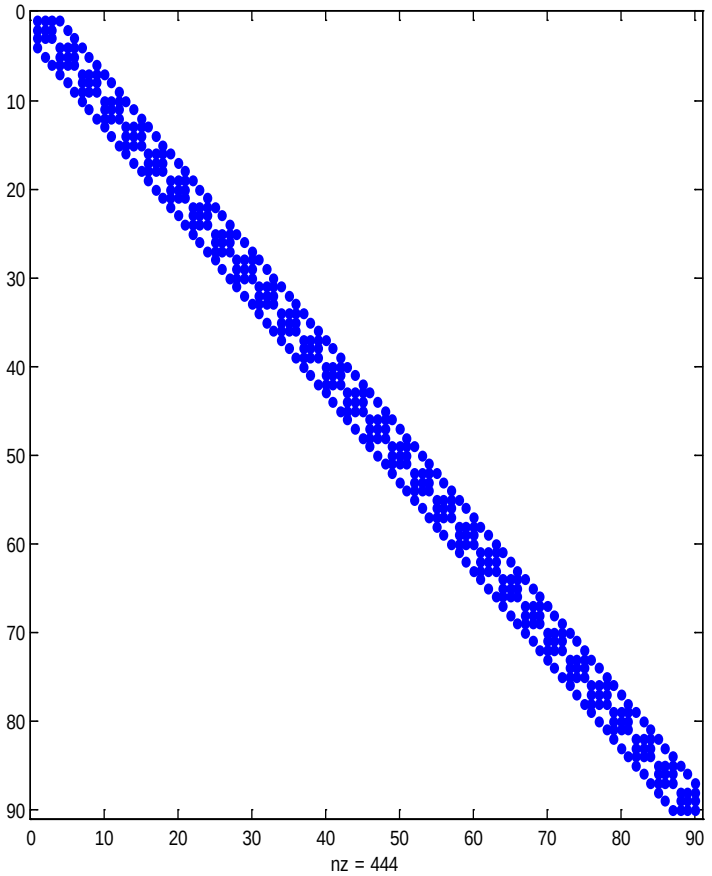
“Three Node” Problem

- The middle node is partially rodded and it is adjacent to a fully rodded and an unrodded node. For the three-node problem, a transverse-integrated neutron balance equation can be obtained in the same way as the two-node nodal problem.
- There are 30 fine mesh in the three node problem with 10 mesh in each node. The mesh are uniform within each of the 4 regions and the rod tip is set at interface of the mesh.
- The three node problem is solved using the finite difference method.

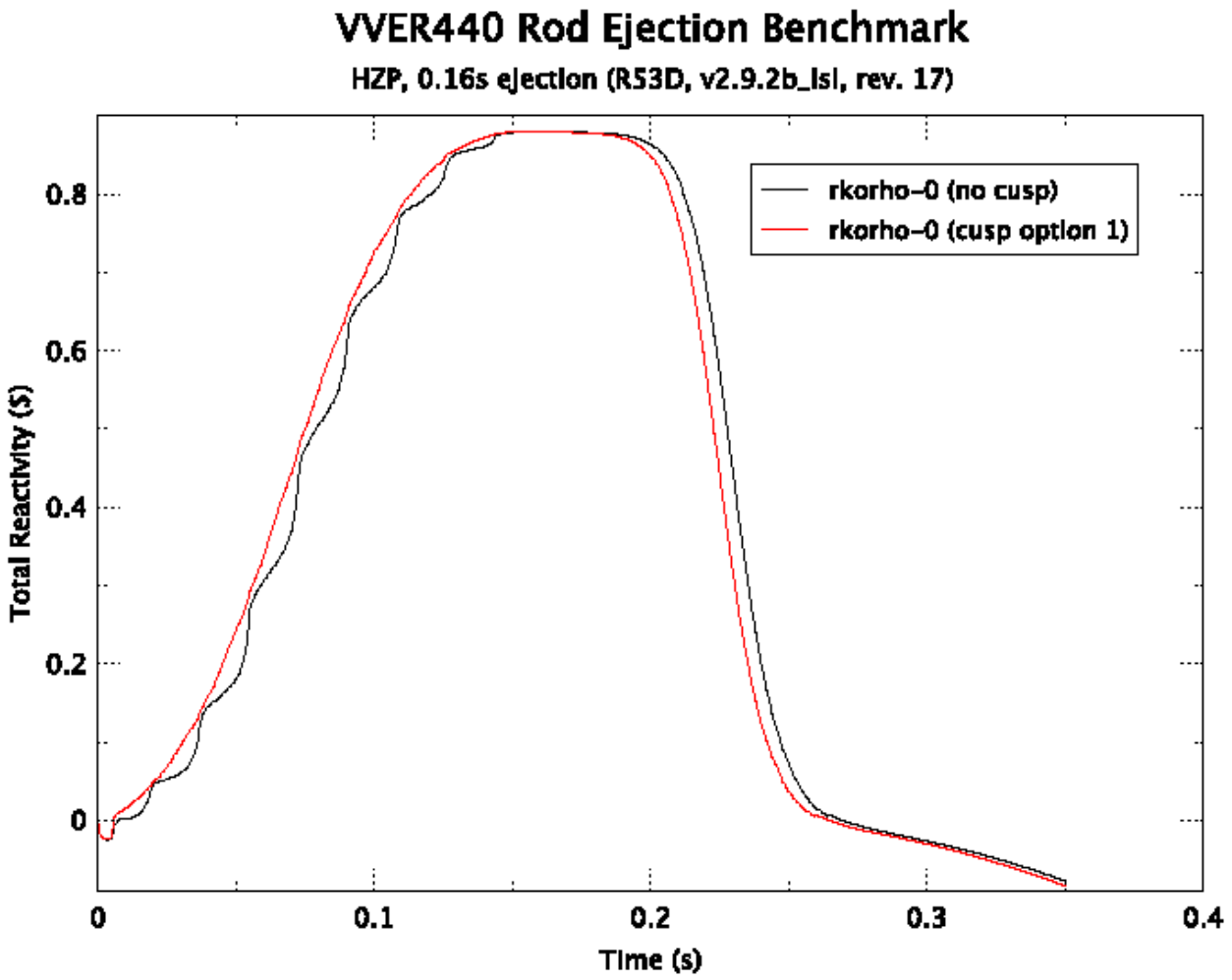


Matrix Structure of Three Node Problem

- The average fluxes of the rodded and unrodded nodes are used as constraints in the solution and the incoming currents at both ends of three nodes model are used as boundary conditions.
- This results in a sparse matrix with a bandwidth equal to the number of neutron groups.
- This problem is solved by Gauss Elimination (or LU factorization).



Rod Cusping Effect



Rod Cusping Implementation

- Currently only used with TPEN
  - Complications in implementing for 4-groups
  - Two options available
    - Homogenous cross sections with intra-nodal flux weight
    - Use axial discontinuity factors for correction
- Future work:
  - Expand for use with NEM (hexagonal and cartesian)
  - Expand for use with CMFD-only

Reactivity Feedback Edits

- Partial reactivity due to feedback mechanisms
  - Control rods
  - Doppler temperature
  - Moderator temperature
  - Moderator density
  - Boron concentration
  - Xe/Sm concentration
- Calculated based on initial adjoint solution

Reactivity Feedback Edits

- Dynamic reactivity

$$\rho = \frac{\left\langle \phi_0^*, A\phi \right\rangle}{\left\langle \phi_0^*, F\phi \right\rangle}$$

- Changes expressed as perturbations

$$A = A_0 + \Delta A$$

$$\Delta A = \Delta A_{CR} + \Delta A_{PPM} + \Delta A_{TDOPL} + \Delta A_{TMOD} + \Delta A_{DENS} + \Delta A_{XESM} + \Delta A_{NL}$$

- Reactivity components

$$\rho_X = \frac{\left\langle \phi_0^*, A_X\phi \right\rangle}{\left\langle \phi_0^*, F\phi \right\rangle} - \frac{\left\langle \phi_0^*, A_0\phi \right\rangle}{\left\langle \phi_0^*, F\phi \right\rangle}$$

$$X \in \{CR, PPM, TDOPL, TMOD, DENS, XESM, NL\}$$

Reactivity Feedback Edits

- Total Reactivity

$$\rho_{TOT} = \rho_{CR} + \rho_{PPM} + \rho_{TDOPL} + \rho_{TMOD} + \rho_{DENS} + \rho_{XESM} + \rho_{NL} + \rho_{NULL}$$

$$\rho_{NULL} = \frac{\left\langle \phi_0^*, A_0 \phi \right\rangle}{\left\langle \phi_0^*, F \phi \right\rangle}$$

- Caveats
  - Null reactivity should be zero (by definition)
  - It is nonzero in most cases due to numerics (negligible)
  - Nodal Leakage component is an abstract term
    - Should be lumped with the parameter causing the biggest change
    - Usually this is control rods
    - Left to user to decide how to treat this term

Summary

- Krylov solver is recommended over LSOR
  - Card 30000003, Word 17 (set to 1)
- New features include
  - Full steady-state & transient solution (with restart)
  - 4 Energy group representation (up- and down-scatter)
  - TPEN nodal solution
    - Slower, but higher accuracy over NEM
    - Useful for problems with steep flux gradients
  - GMRES solver added as compliment to BiCGSTAB
    - Better performance for poorly-conditioned linear systems
  - Rod Decusping Logic (TPEN only)
  - Reactivity feedback edits

Summary

- Future work
  - Extend rod decusping logic
    - CMFD-only
    - NEM (hexagonal and cartesian)
  - Improve CPU performance
    - Real-time computing
    - Clean up existing parallel logic in source code