Status of Recent Nodal Kinetics Advances in RELAP5-3D

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Presentation Outline

- History of Nodal Kinetics in RELAP5-3D
- Recent RELAP5-3D Nodal Kinetics Advances
  - Merged Data Structures for LSOR and Krylov
  - Merged Non-linear Solvers
  - Migrated Functionality from Krylov to LSOR
  - LSOR / Krylov Solver Switching Logic
- On-going Work
  - Sparse Direct Linear Solver

History of Nodal Kinetics

- The nodal kinetics model in RELAP5-3D originated with the NESTLE code developed by Paul Turinsky and colleagues at North Carolina State University (c.1993).
  - 2 or 4 group neutron diffusion equation
  - Cartesian or hexagonal geometry
  - 3-, 2-, or 1-dimensional models available
  - Symmetry options:
    - quarter, half, and full for Cartesian geometry
    - sixth, third, and full for hexagonal geometry
  - Boundary condition options:
    - Zero flux
    - Non-reentrant current
    - Reflective
    - Cyclic

History of Nodal Kinetics

- RELAP5-3D with NESTLE (cont'd)
  - Line Successive Over-Relaxation (LSOR) for linear solution
  - Higher-order non-linear solution using NEM
  - Fully implicit delayed neutron precursor equation
  - Thermal-hydraulic feedback incorporated into polynomial-based macroscopic cross sections

History of Nodal Kinetics

- 1996: PARCS Krylov solver based on BiCGStab added to the code.
  - Driven by need for high-fidelity, real-time simulation
  - Included shared-memory parallel programming
  - Through University Research Consortium with Purdue and NCSU
  - *Jerry Judd, Tom Downar, Han Gyu Joo, Doug Barber*
  - Initially for Cartesian, 2-group only
- 1997: Extended to hexagonal geometry
- 1998 – 2006: Minimal modifications to the NK solver in RELAP5-3D

History of Nodal Kinetics

- 2007: Addition of SS Krylov solver
- 2008: TPEN non-linear solver for hexagonal geometry
  Extension to 4 energy groups
  Reactivity feedback edits
- 2009: Control rod decusping
  Implement GMRES solver
- 2011: Modernize nodal kinetics data structure
- 2012: Asynchronous time advancement
- 2013: Face-dependent albedos
  Composition-dependent neutron velocity
  Automatic time step control for NK
- 2014: Shared-memory parallelization restored

All upgrades from 2007-2014 funded by Bettis

History of Nodal Kinetics (In Process)

- 2017: Merged Data Structures for LSOR and Krylov
- 2018 [*Completed*]:
  Merged Non-linear Solvers
  Migrated Functionality from Krylov to LSOR
  LSOR / Krylov Solver Switching Logic
- 2018 [*In Process*]:
  Sparse Direct Linear Solver

Current work funded by Bettis

Merged Data Structures

- Purpose: Merge repeated data structures used by LSOR and Krylov solvers.
  - Facilitate merging of NEM solvers and other functionality
  - Facilitate solver switching logic
    - Krylov-to-LSOR and vice-versa
    - Iterative-to-direct
  - May result in some memory inefficiency for the LSOR solver
- Status: Completed

Merged Data Structures

- Data Structures Merged:
  - Cross section arrays
  - Linear system coupling coefficient arrays
  - Solution arrays: flux, fission source, etc.
  - Neutron kinetics data: beta, lamda, etc.
  - Source terms
  - Geometry data
  - Boundary condition arrays
  - NEM arrays: nodal current, expansion terms, leakage terms

Merged Data Structures

- **Regression** testing produced mostly null differences
  - LSOR cases only had numerical differences due to order of operations changes
    - Flux errors on the order of 1.0E-08%
  - Some Krylov cases had significant differences
    - Maximum flux error: -4.068E-02%
    - Due to a bug that was uncovered and fixed during the merge process
- **Restart / Backup** testing produced null differences

Merged Non-linear Solvers

- Purpose: Use a consistent NEM solver for both LSOR and Krylov solvers
  - Allows seamless switching between LSOR and Krylov
  - Will facilitate switching to/from a direct solution
  - Results in some order of operation changes for both solvers
- Status: Completed

Merged Non-linear Solvers

LSOR	Krylov	Description
Cartesian Geometry		
nonnemc.F	nonnem.F	Driver for NEM
nonplmc.F	nonplm.F	Calculate leakage and expansion coefficients
nonnetc.F	nonnet.F	Calculate Net Currents
nononec.F	nonone.F	Solve One-node Problems
nontwoc.F	nontwo.F	Solve Two-node Problems
Hexagonal Geometry		
nonnemh.F	nonnemkh.F	Driver for NEM
nonplmh.F	nonplmkh.F	Calculate leakage and expansion coefficients
nonneth.F	nonnetkh.F	Calculate Net Currents
nononeh.F	nononekh.F	Solve One-node Problems
nontwoh.F	nontwokh.F	Solve Two-node Problems

Merged Non-linear Solvers

- **Regression** testing produced mostly null differences
  - LSOR and Krylov cases only had numerical differences due to order of operations changes
    - Flux errors on the order of 1.0E-06%
- **Restart / Backup** testing produced null differences

Migrated Functionality

- Purpose: Extend Krylov-only functionality to LSOR
  - TPEN solver
  - Reactivity feedback edits
  - Control rod decusping
  - Albedo boundary conditions, including face-dependent (In Process)
- Status: Completed, except albedo BCs

Migrated Functionality

- TPEN solver
  - Card 30000010, Word 16 can be selected for both solvers
    - 0 – NEM; 1 – TPEN
- Reactivity feedback edits
  - Card 30000010, Word 17 can be selected for both solvers
    - 0 – no edits; 1 – total reactivity; 2 – all feedback edits
- Control rod decusping
  - Card 30000010, Word 18 can be selected for both solvers
    - 0 – no decusping; 1 – homogeneous cross sections w/ intranode flux weighting; 2 – axial discontinuity factors used
- Albedo boundary conditions
  - Card 30000021 for group-wise albedos
  - Card 37IIJJKKF for face-dependent albedos

LSOR / Krylov Solver Switching Logic

- Purpose: Provide user control of which solver to use during the calculation
  - Utilizes the kinetics time step cards (2200-2299)
  - Allow the solver to switch between LSOR and Krylov
    - Steady-state
    - Transient
  - Allow switching for both hexagonal and Cartesian
  - Preserve CMFD / NEM / TPEN selection for both solvers
  - Provide for exact restarts, even when restarting during a solver switch
  - Solver selection included in minor edits
- Status: Completed

LSOR / Krylov Solver Switching Logic

- Modification to 2201-2299 cards - Add Word 4:

W4(I)	Nodal kinetics solver selection. A value of 0 indicates that the LSOR (line successive over-relaxation) solution algorithm is to be used. A value of 1 indicates that the Krylov solution algorithm is to be used. The value input here will overwrite the solver selection from Card 30000003, Word 17.

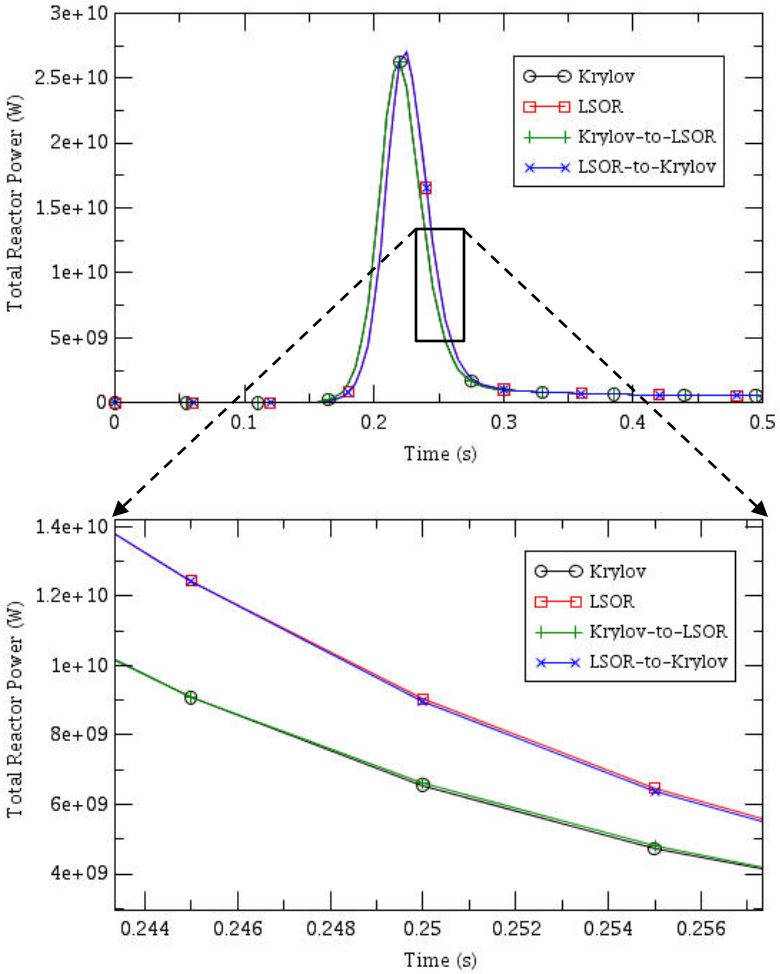
- Minor edit / plot variable added: rkosol
  - If rkosol is 0, then LSOR is being used
  - If rkosol is 1, then Krylov is being used

LSOR / Krylov Solver Switching Logic

- CMFD / NEM / TPEN selection on the 30000003 and 30000010 cards is preserved
  - LSOR to Krylov:
    - NEM update frequency for Krylov set to LSOR value if greater than 0
    - If NEM frequency for LSOR is 0 (CMFD-only), then the frequency for Krylov is also set to 0
    - TPEN selection is preserved when switching
  - Krylov to LSOR:
    - NEM update frequency for LSOR set to Krylov value if greater than 0
    - Ensure that frequency is greater than the Chebyshev extrapolation
    - If NEM frequency for Krylov is 0 (CMFD-only), then the frequency for LSOR is also set to 0
    - TPEN selection is preserved when switching

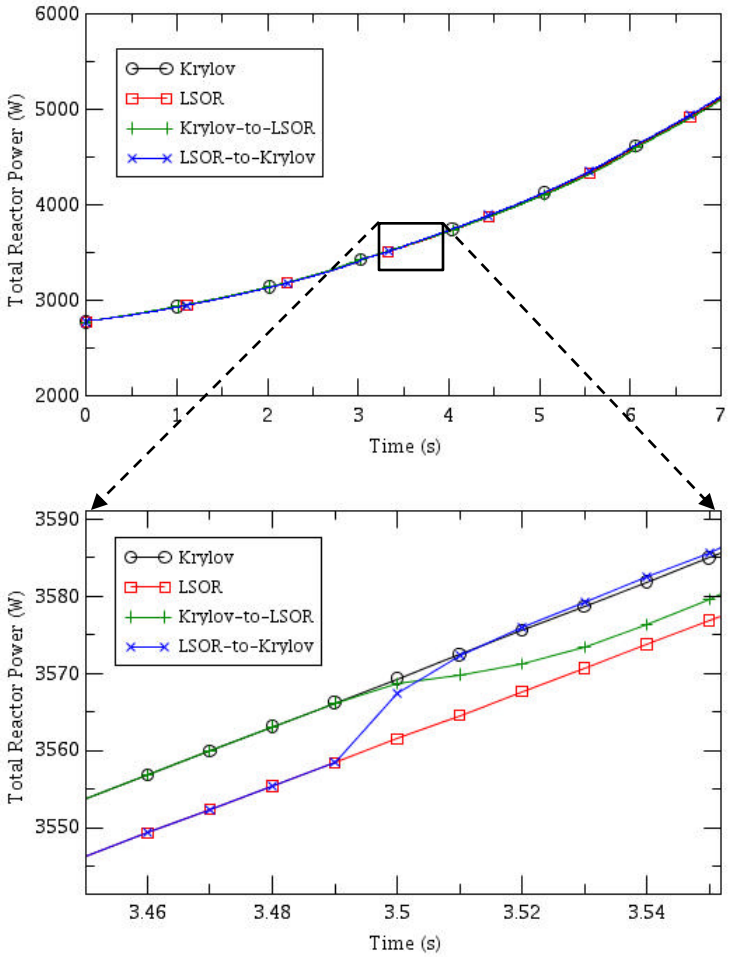
LSOR / Krylov Solver Switching Logic

- NEACRP C1 – Solver Switch at 0.25 sec



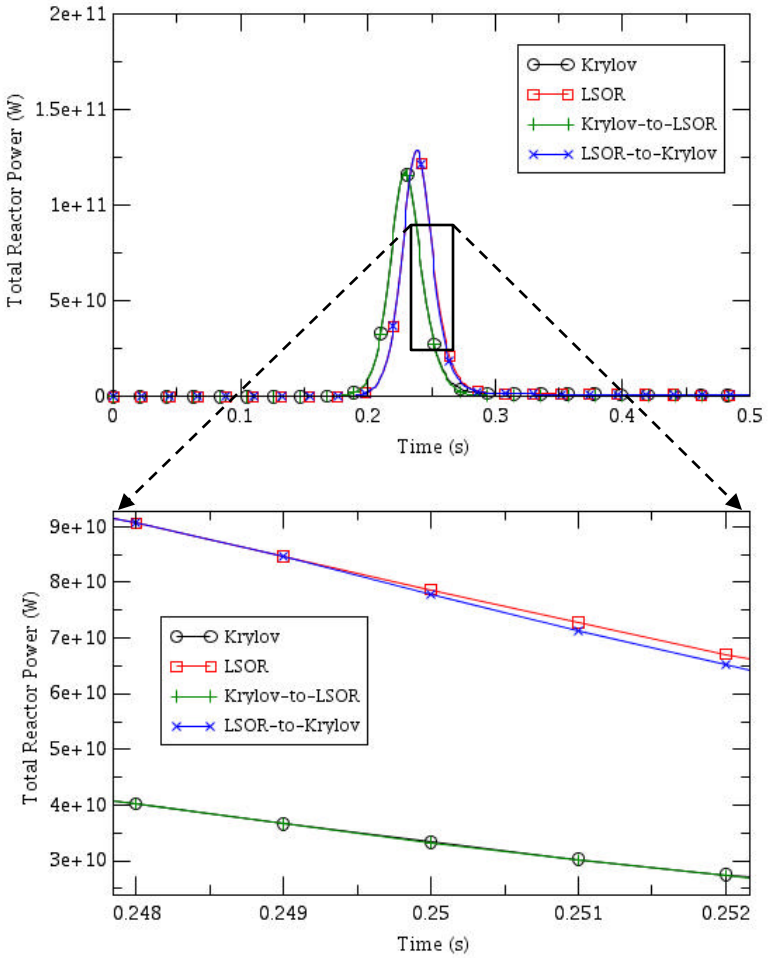
LSOR / Krylov Solver Switching Logic

- Rod Decusping Test – Solver Switch at 3.5 sec



LSOR / Krylov Solver Switching Logic

- Hexagonal TPEN Test – Solver Switch at 0.25 sec



On-going Work

- Sparse Direct Linear Solver
  - Investigate available packages
    - SuperLU (serial, unsymmetric)
    - SPARSPAK (serial, symmetric positive definite (SPD))
    - PARDISO (shared memory parallel, symmetric non-zero)
    - Cholesky (shared memory parallel, SPD, banded)
    - SuperLU_MT (shared memory parallel, unsymmetric)
    - With and without preconditioning
  - Prepare Software Requirements Specification
  - Implement / Document selected direct solver
- Verification and Validation
  - Utilizing the NUPAC Test Framework from Bettis
  - Using quantified metrics for testing
- Integrated Nodal Kinetics Testing

Summary

- Merged Data Structures for LSOR and Krylov
  - Code modifications completed August 2017
  - Testing completed March 2018
- Merged Non-linear Solvers
  Migrated Functionality from Krylov to LSOR
  LSOR / Krylov Solver Switching Logic
  - Code modifications (Rev. 0) completed December 2017
  - Code modifications (Rev. 1) completed April 2018
  - Testing completed April 2018
- Sparse Direct Linear Solver
  - Began April 2018
  - Expected completion (including testing) December 2018