Information Systems Laboratories, Inc.

Status of Recent Nodal Kinetics Upgrades in RELAP5-3D

2014 International RELAP5 Users Group Meeting

Idaho Falls, Idaho

September 11-12, 2014

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- RELAP5-3D Nodal Kinetics Upgrades
 - Asynchronous Nodal Advancement
 - <u>Purpose</u>: Provide automatic time step control for the nodal kinetics.
 - Parallel Processing with Domain Decomp
 - <u>Purpose</u>: Resurrect parallel domain decomposition logic for the nodal kinetics.

- <u>Purpose</u>:
 - Nodal kinetics solution can be computationally intensive
 - Need dynamic time step control
 - Use small time steps when conditions are changing
 - Use large time steps when conditions are quasi-steady
 - Implement automatic time step prediction based on change in:
 - Absorption + removal cross section
 - Neutron flux
- Status: Completed

- <u>Approach</u>:
 - Use dynamic time scale^[1]
 - Determine the linear rate of change
- Apply user-defined fractional allowable change

$$\tau_{\theta} = \frac{1}{\left|\frac{1}{\theta}\frac{\partial\theta}{\partial t}\right|}$$

$$\Delta t_{\theta}^{n} = \eta_{dyn} \left[\min \tau_{\theta,i,j}^{n} \right]$$

- Ratio of kinetics and T/H time step size is restricted to be a rational number
- Take the minimum linear rate of change across all nodes and all parameters (cross section and flux)
- Option for using extrapolation when kinetics is supercycling T/H
- Potentially unstable
 - Synchronization will be key
 - User input min/max kinetics time step size will help

[1] Pope, Michael A. and Mousseau, Vincent A., "Accuracy and Efficiency of a Coupled Neutronics and Thermal Hydraulics Model," Nuclear Engineering and Technology, Vol. 47 No. 7, September 2009.

- NEACRP C1 Rod Eject Benchmark
 - Peripheral Rod Ejection
 - 0.1s ejection
 - Peak Power @ 0.22s



- Time step analysis
 - Expected dt=0.001s during ejection
 - dt=0.100s 0.250s during asymptotic phase

NEACRP C1 Rod Eject Benchmark

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• NEACRP C1 Rod Eject Benchmark



- Time step size prediction reaches 0.250 s (kinetics max.) at 1.2 s
- A slight CPU increase observed up to about 0.4 s.
 - Due to predicted time step size less than 0.001 s during initial phase
 - Kinetics minimum time step size was 1.0E-7 s.
- Roughly 50% reduction in CPU time over the entire transient simulation

- <u>Purpose</u>:
 - Nodal kinetics solution is largely parallelizable.
 - This work was done 15 years ago, but coding has not been maintained
 - Resurrect parallel processing logic for the nodal kinetics.
 - Utilize axial domain decomposition.
 - Maximum of 4 axial subdomains solved in parallel.
 - Expect near 100% efficiency for 2 processors and slightly less for 4 processors.
- <u>Status</u>: Completed

- Parallel Coarse Mesh Finite Difference (CMFD)
 - Requires extra solution at the interface
 - Incomplete Domain Decomposition (IDD) Preconditioner is utilized
 - Near 100% efficiency is possible
- Parallel Nonlinear Nodal Solver
 - Two-node solutions are perfectly parallelizable
 - Super-speedups are expected since memory fetch times are reduced (more on-chip storage per domain)
- Support Calculations
 - e.g., cross section evaluation, linear system setup, etc.
 - Inherently parallel
 - Should see 100% efficiency

- Diagonal Incomplete Domain Decomposition (DIDD)
 - $\begin{bmatrix} \boldsymbol{P}_1 & \boldsymbol{U} \\ \boldsymbol{L} & \boldsymbol{P}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{b}_1 \\ \boldsymbol{b}_2 \end{bmatrix} \quad (\boldsymbol{x}_1, \boldsymbol{x}_2) \in \mathbb{R}^{N/2}$
- Costly to invert, so approx.
 - Solve 2-plane linear system
 - Only use block diagonals

$$\begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} = \begin{bmatrix} \Gamma_1^{-1} & \\ & \Gamma_2^{-1} \end{bmatrix} \begin{bmatrix} \boldsymbol{b}_1 \\ \boldsymbol{b}_2 \end{bmatrix} \quad (\tilde{x}_1, \tilde{x}_2) \in \mathbb{R}^{N/k}$$

• Substituting yields:

$$\boldsymbol{P} = \begin{bmatrix} \boldsymbol{I}_{1} & & & \\ & \ddots & & \\ & & \boldsymbol{I}_{k/2} & -\boldsymbol{U}_{k/2}\Gamma_{2}^{-1} & & \\ & & -\boldsymbol{L}_{k/2+1}\Gamma_{1}^{-1} & \boldsymbol{I}_{k/2+1} & & \\ & & & \ddots & & \boldsymbol{I}_{k} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{P}_{1} & \boldsymbol{U}_{1} \\ \boldsymbol{L}_{2} & \ddots & \ddots \\ & \ddots & \ddots & \boldsymbol{U}_{k/2-1} \\ & & \boldsymbol{L}_{k/2} & \boldsymbol{P}_{k/2} \\ & & & \boldsymbol{P}_{k/2+1} & \boldsymbol{U}_{k/2+1} \\ & & & \boldsymbol{L}_{k/2-2} & \ddots & \ddots \\ & & & \ddots & \ddots & \boldsymbol{U}_{k-1} \\ & & & & \boldsymbol{L}_{k} & \boldsymbol{P}_{k} \end{bmatrix}$$



- Comparison of 3 IDD Preconditioners
 - Block Diagonal (BD)
 - Diagonal IDD (DIDD)
 - Planar IDD (PIDD)



Comparison of 3 IDD Preconditioners



- PIDD generally shows the best residual performance
- DIDD has similar performance but is easier to construct



- Critical Characteristics (Expectations)
 - Solution Results
 - Identical results are obtained compared to the base code when the entire solution, except for the coarse-mesh finite difference (CMFD) solver, is run in parallel mode.
 - Identical results are obtained when the nonlinear nodal solver (NEM, TPEN) is run in parallel and serial mode.
 - Differences in the CMFD solution for single-threaded and multi-threaded runs should be relatively small.
 - Using 2 CPUs and 4 CPUs, each test case should generate five identical results when run five times.
 - Solution Performance
 - Speedup efficiencies of near 100% are obtained for just the nonlinear nodal solver (NEM, TPEN).
 - Speedup efficiencies of near 100% are obtained for all other nodal kinetics functions, except the CMFD solver.
 - Speedup efficiencies greater than 75% on 2 CPUs and 50% on 4 CPUs are obtained for the CMFD solver.

- Verification Testing
 - Following runs were made:
 - 1. Base code
 - 2. Modified code (regression mode), 1 thread
 - 3. Modified code (regression mode), 2 threads, 5 times
 - 4. Modified code (regression mode), 4 threads, 5 times
 - 5. Modified code (standard mode), 1 thread
 - 6. Modified code (standard mode), 2 threads, 5 times
 - 7. Modified code (standard mode), 4 threads, 5 times
 - Expectations:
 - Runs 1, 2 and 5 should be identical except for TPEN
 - Runs 3 and 4 should be identical to 2
 - Runs 6 and 7 should be different compared to Run 5
 - All 5 executions for Runs 6 & 7 should be identical



- Verification Testing (Solution Results)
 - Regression Testing
 - Single-threaded results for base code and modified code (both regression and standard mode) were identical for most cases.
 - Exception was for cases that used the TPEN solver, which was expected
 - 2-threaded results with the modified code (regression mode) were identical to single-threaded results
 - All 5 executions were identical
 - 4-threaded results with the modified code (regression mode) were identical to single-threaded results
 - All 5 executions were identical
 - 2- and 4-threaded results with the modified code (standard mode) were different compared to single-threaded results
 - Differences were small and expected, but the accuracy of the solution was not impacted

Verification Testing (Performance Results)
– Effective efficiency for Krylov Solver (%)

NK Case	1 Thread	2 Thr (avg)	4 Thr (avg)	4 Thr (max)
neacrp-c1-4node-krlv-nem ^[1]	117.4	99.3	78.4	82.1
smart330-c1g4-tr-krlv-cmfd ^[1]	140.1	96.3	50.6	84.5
smart330-c1g4-tr-krlv-nem ^[1]	128.2	99.7	57.7	75.9
smart330-c1g4-tr-krlv-tpen ^[1]	123.2	96.6	79.9	84.0
vver440-tr-hzp-krlv-cmfd	104.6	100.3	83.7	98.9
vver440-tr-hzp-krlv-nem	100.3	100.5	93.5	98.4
vver440-tr-hzp-krlv-tpen	102.7	98.0	95.8	98.9

[1] Load imbalance on 4 threads

Verification Testing (Performance Results)
– Effective efficiency for Nonlinear Nodal Solver (%)

NK Case	1 Thread	2 Thr (avg)	4 Thr (avg)	4 Thr (max)
neacrp-c1-4node-krlv-nem ^[1]	97.7	95.6	77.0	83.0
smart330-c1g4-tr-krlv-cmfd ^[1]	N/A			
smart330-c1g4-tr-krlv-nem ^[1]	113.6	96.1	81.2	84.0
smart330-c1g4-tr-krlv-tpen ^[1]	91.3	99.8	84.6	86.7
vver440-tr-hzp-krlv-cmfd	N/A			
vver440-tr-hzp-krlv-nem	97.3	94.9	90.8	92.6
vver440-tr-hzp-krlv-tpen	88.5	98.5	93.5	95.8

[1] Load imbalance on 4 threads

Verification Testing (Performance Results)
– Overall "Realized" Performance Efficiency (%)

1 Thread	2 Thr (avg)	4 Thr (avg)	4 Thr (max)
105.9	97.7	68.5	71.2
117.0	105.9	57.1	80.7
118.5	112.5	64.4	69.6
168.8	164.8	124.8	127.9
104.3	94.7	68.0	78.0
101.0	92.9	80.0	82.9
94.3	88.2	78.7	81.1
	1 Thread 105.9 117.0 118.5 168.8 104.3 101.0 94.3	1 Thread2 Thr (avg)105.997.7117.0105.9117.0105.9118.5112.5168.8164.8104.394.7101.092.994.388.2	1 Thread2 Thr (avg)4 Thr (avg)105.997.768.5117.0105.957.1118.5112.564.4168.8164.8124.8104.394.768.0101.092.980.094.388.278.7

[1] Load imbalance on 4 threads

- Summary
 - Entire Nodal Kinetics solver has been parallelized (for Krylov)
 - Regression testing yielded expected results
 - Multiple multi-threaded runs showed no variability in results
 - Parallel performance was better than expected
 - Parallel efficiency for Krylov solver on 2 and 4 threads was over 95% for cases with load balance
 - Parallel efficiency for NEM solver on 2 and 4 threads was over 95% for cases with load balance
 - Parallel efficiency for TPEN solver on 2 and 4 threads was 95% and 90%, respectively
 - TPEN solver display unstable error reduction
 - Overall performance improvement was very good
 - Between 90% and 100% on 2 threads
 - Greater than 80% on 4 threads (CPU utilization issues)



- Automatic Nodal Kinetics Time Step Control
 - Completed December 2013
- Parallel Nodal Kinetics (Krylov-based)
 - Completed June 2014
- Both updates will be included in a post-4.2.1 version