Neutronics Code Development at Argonne National Laboratory

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Fast Reactor Modeling and Simulation Challenges

- Detailed energy modeling
  - Lack of a 1/E spectrum as a basis for resonance absorption calculation
  - Inelastic, (n,2n), anisotropic scattering are of great importance
- Long neutron mean free paths
  - Neutron leakage is enhanced, 25% at moderate sizes
  - Local reactivity effects impact entire core
- High leakage and heterogeneous core configurations challenge design methods
  - Transport effects are magnified
  - Spectral and directional transitions at the core and reflector interface are hard to model
  - Core reactivity is sensitive to minor geometric changes
    - Integration with thermal-hydraulics and structural mechanics analyses to account for reactivity feedbacks due to geometry deformation accurately
High Fidelity Modeling, What is the point?

- The existing approach: Homogenized assembly
  - Vast reduction of space-angle-energy dofs
  - Focused on producing the global gradient
  - Reconstruct: local and global solution must be merged

- Explicit geometry core calculations?
  - \( >10^{10} \) degrees of freedom requires some parallelism
  - Few large problems have been attempted

- Can we improve the existing calculation accuracy?
  - Not really concerned about depletion in short term
    - Errors in cross section data? Multi-group processing?
  - Material loading uncertainties
    - Are we solving a contrived problem; i.e. predicting the weather?
    - Not the case for ZPR and other similar benchmarks. Production reactors?

- Safety analysis was identified as one area of weakness that can be improved
  - Radial thermal expansion is generally treated poorly in neutronics
  - Above core mixing (thermal induced stress) is poor in CFD
  - Modeling of seismic event impacts on core and plant?

- Considerable development lead time before significant results can be achieved
“Allow the existing reactor analysis work to transition smoothly from assembly level homogenization to less crude homogenization and eventually to fully heterogeneous descriptions”

- Diffusion theory structured geometry solver (NODAL)
  - Reproduce nodal diffusion capability in existing tools
  - Can be extended to 1st order $S_N$ or VARIANT
- Even-parity transport equation with spherical harmonics (PN2ND)
  - Immediate use on problems with significant homogenization
- Method of Characteristics (MOCFE)
  - Long term deployment and use on problems without homogenization
- Even-parity transport equation with discrete ordinate (SN2ND)
  - Modeling transition region between PN2ND and MOCFE solvers
  - Still has the second-order limitations (voids?)
  - We still prefer to homogenize similar regions

- $MC^2$-3 module for in-line multi-group cross section generation
  - Hyperfine (~400,000) group transport capability for homogeneous mixture and 1-D slab and cylindrical geometries. Started 2-D work.
Parallelism in UNIC

- Novel?
  - Parallel transport studied for well over a decade
    - LANL, Sandia, French, Japanese,…
  - Production tools?
    - Unstructured mesh capabilities?
    - Parallel capabilities?

- Lessons learned at ANL
  - Parallelization in space-angle-energy is necessary
  - There are small, medium, and large parallel machines
    - Spatial domain decomposition is not best for all
    - Angle decomposition for S_N is generally good up to a limit
    - We have not studied energy decomposition at this point
  - Focused parallelization of L is not necessarily best idea

\[
\begin{pmatrix}
  A_l & 0 & 0 \\
  \vdots & \ddots & 0 \\
  W_{l \rightarrow G} & \cdots & A_G
\end{pmatrix}
\begin{pmatrix}
  W_{l \rightarrow l} & \cdots & W_{G \rightarrow l} \\
  \vdots & \ddots & \vdots \\
  W_{l \rightarrow G} & \cdots & W_{G \rightarrow G}
\end{pmatrix}
\begin{pmatrix}
  \Psi_1 \\
  \vdots \\
  \Psi_G
\end{pmatrix}
= 
\begin{pmatrix}
  S_l \\
  \vdots \\
  S_G
\end{pmatrix}
\]

- Capabilities
  - PN2ND: 500-3,000 processors (2007)
  - SN2ND: 1,000-300,000+ processors
  - MOCFE and NODAL: unknown
Existing Approach (Assembly Homogenization)

- Typical approach used in fast reactor physics today
  - VARIANT residual error is due to $P_N$ order and source approximation
    - Used 4th order source, 8th order flux, and 3rd order leakage
  - PN2ND residual error is due to $P_N$ order and spatial mesh refinement
    - Used 109,740 hexahedral elements with 461,219 vertices
  - SN2ND residual error is due to spatial mesh refinement
    - Used Carlson even-moment (level symmetric) cubature

ABTR 33 group (120 periodic)

<table>
<thead>
<tr>
<th>Angular Resolution</th>
<th>VARIANT</th>
<th>PN2ND</th>
<th>SN2ND</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1588</td>
<td>-1594</td>
<td>-192</td>
</tr>
<tr>
<td>2</td>
<td>-237</td>
<td>-249</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
<td>-91</td>
<td>-109</td>
<td>-69</td>
</tr>
<tr>
<td>4</td>
<td>-47</td>
<td>-70</td>
<td>-47</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>-55</td>
<td>-51</td>
</tr>
</tbody>
</table>
Assembly Level Homogenization (cont…)

- VARIANT can easily out perform PN2ND and SN2ND
  - Uses hybrid finite element (nodal) combined with spherical harmonics
    - Spatial approximation includes discontinuities in even- and odd-parity flux
    - Defines much fewer degrees of freedom in assembly homogenized problems
  - Not currently ideal for all problems
    - 1/6 hexagonal ABTR with P5-S5 requires 14 hours of cpu time (5⋅10^8 dofs)
    - ZPR drawer homogenized problems have convergence problems
    - Cannot treat void or pure scattering regions

- PN2ND uses UFE combined with spherical harmonics
  - Even-parity unstructured mesh treatment assumes continuous even-parity flux
    - Requires careful boundary layer meshing (key weakness of method)
    - Increased memory storage relative to VARIANT and bandwidth limited flop rate
  - Uses a parallel CG operation on the WG space-angle system
    - Preconditioner is just diagonal angular sub-system
    - Use SSOR in parallel CG solver from PETSc on each angular sub-system

- SN2ND uses UFE combined with discrete ordinates
  - Mesh related problems are identical to PN2ND
  - Uses a scattering source iteration on WG space-angle system (CG on L^-1)
    - Uses diagonal angular sub-system preconditioner
    - Uses SSOR via parallel CG solver in PETSc
    - Started development of multi-level h multi-grid preconditioner
Over a period of 30 years, more than a hundred ZPR critical assemblies were constructed at Argonne National Laboratory: ZPR-3, ZPR-6, ZPR-9 and ZPPR.

- The geometrical information for selected loadings is now widely available (ICSBEP)
- Materials are very well known compared with existing production reactors.
- In addition to experimental validation we can compare with CE MCNP/VIM solutions
- No concerns for multi-physics coupling
Standard Homogenized Approach

- Used 1-D “equivalent” lattice cell calculation to generate cross sections in MC2-3
  - Homogeneous solution only gives the global gradient
  - Done to capture foil reaction rates and compare other reactor physics parameters
  - Need to combine global gradient with lattice cell calculation to extract solution
- Reference solution is experiment (i.e. critical)
  - SN2ND: 0.99966  VIM: CE 0.99981±0.00025
  - Ignoring plate heterogeneity
    - SN2ND: 0.99344  VIM CE: 0.99400±0.00020
- We have obtained similar results on ZPR 6/7 and ZPPR-15
- We are focused on using 2-D MOC for future cross section generation
Plate-by-Plate ZPR6 Assembly 6A

- SN2ND cannot handle explicit voids
  - Not really an issue for this problem
  - Development: $2 \cdot 10^6 \rightarrow +50 \cdot 10^6$ vertex mesh
  - 33 group calculation requires ~40 minutes on full parallel machine (~700 billion dof)

- Cross sections generated with 1-D lattice cell
  - The implementation of these cross sections in the explicit geometry model is not consistent.
  - The cross section data representation is inaccurate
- Maximum of 116 group with $P_5$ scattering (9, 33, 70, 116)
- Maximum 50,000,000 vertex mesh (cubic hexahedrons)
- Maximum $S_{28}$, (LT or DLT)
Flux Solution for ZPR6 Assembly 6A Experiments

- Local gradients on drawers exhibit global gradient
- Resolved spatial gradients should result in better foil reaction rates
SN2ND Parallel Performance

- Strong spatial scaling of 94% on BlueGene/P-ANL

<table>
<thead>
<tr>
<th>Total Cores</th>
<th>Vertices/Process</th>
<th>Total Time (seconds)</th>
<th>Parallel Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>8,192</td>
<td>7,324</td>
<td>2,402</td>
<td>100%</td>
</tr>
<tr>
<td>16,384</td>
<td>3,662</td>
<td>1,312</td>
<td>92%</td>
</tr>
<tr>
<td>24,576</td>
<td>2,441</td>
<td>873</td>
<td>92%</td>
</tr>
<tr>
<td>32,768</td>
<td>1,831</td>
<td>637</td>
<td>94%</td>
</tr>
</tbody>
</table>

- Weak angle scaling of 75% on XT5. 76% on BlueGene/P 294,912 cores JSC

<table>
<thead>
<tr>
<th>Total Cores</th>
<th>4π Angles</th>
<th>Total Time (seconds)</th>
<th>Weak Scaling</th>
</tr>
</thead>
<tbody>
<tr>
<td>16,512</td>
<td>32</td>
<td>1891</td>
<td>100%</td>
</tr>
<tr>
<td>37,152</td>
<td>72</td>
<td>1901</td>
<td>99%</td>
</tr>
<tr>
<td>66,048</td>
<td>128</td>
<td>1829</td>
<td>103%</td>
</tr>
<tr>
<td>103,200</td>
<td>200</td>
<td>2050</td>
<td>92%</td>
</tr>
<tr>
<td>148,608</td>
<td>288</td>
<td>2298</td>
<td>82%</td>
</tr>
<tr>
<td>222,912</td>
<td>432</td>
<td>2517</td>
<td>75%</td>
</tr>
</tbody>
</table>

Mainly measurement of PETSc

- Strong scaling in angle is <75%

Diffusion equation needs further partitioning

Weak scaling in space means mesh refinement for us

This can be good and bad. Refinement of bad aspect ratio elements produced >95%
Lessons Learned from ZPR

- Cross sections are not sufficiently accurate
  - 1-D model is appropriate and proves to be accurate for drawer average cross sections
  - Equivalence theory used to generate self-shielded ultrafine group cross sections is approximate
    - A hyperfine group (i.e., pointwise) calculation can help
  - Plate-by-plate cross sections may reduce the error, but the fundamental issue is that the global gradient is not seen in the cell lattice problem (either 1-D slab or 2-D MOC)

- New approach: Improve accuracy of legacy methodology
  - Incorporate global and local gradients via a 2-D MOC solution
    - Generate drawer homogenized cross sections
    - Use SN2ND or improved VARIANT to solve global homogenized problem
  - With new capability we will research using plate-dependent cross sections in the radial plane
The Future for Fast Reactor Cross Sections?

- In 2007 we researched a 3-D MOC for fine level solution
  - 10,000 to 1 element comparison with SN2ND
  - Parallel algorithm is relatively immature; ours was not scaling

- In 2009 we rebuilt 2D and 3D MOCFE solver
  - Easier to modify/maintain/develop
  - Faster ray tracing, exact domain surface discretization
  - Assumed a Krylov subspace method for spatial decomposition
    - More appropriate path for large scale parallelism
    - Assumes trajectory splitting and communication of trajectory flux
    - Needs research into good preconditioner (synthetic diffusion?)
MOCFE continued

- New version is >10 times faster than old version
- Validated “accuracy” on C5G7, CANDU, ABTR geometries
- Working on PWR, BWR, VHTR, and ZPR geometries
- Haven’t tested out any parallel options
- Haven’t tested out the Krylov solver options
- Have no clue how well it compares to other MOC solvers
Future Work and Key Issues

- **SN2ND**
  - Implement multi-level h-multigrid preconditioner scheme
  - Implement error estimator for intelligent mesh refinement and accuracy assessment
  - Investigate parallel decomposition of energy with Krylov subspace methodology
  - Even with ~300,000 cores, direct whole core transport calculations are not practical yet

- **Cross Section Generation**
  - Optimize MC\(^2\)-3 code for speed and investigate parallel execution of work
  - Fully validate 1-D, 2-D, and 3-D MOCFE for parallel execution of space-angle-energy
  - Investigate option to use localized hyperfine-group spectrum calculation with fine-group whole core transport calculation

- **“Intermediate” fidelity methods to perform routine design calculations (<<1000 processors)**
  - 2D MOC calculation for cross section generation
    - New homogenization and group collapsing schemes
  - PN2ND or SN2ND calculation with homogenized pin-cell
  - Improved NODAL based code with assembly homogenization
    - Is there a potential for 2D/1D coupled schemes like DeCART?