VERA-CS
Development Progress

Presented by Scott Palmtag
Physics Integration (PHI)

CASL Industry Council Meeting
Greenville, SC
April 12-13, 2016
Overview

• VERA-CS Description
• Performance Improvements
• Thermal Expansion
• Library Validation
•Transient Development Status

• To be discussed in other presentations:
  – BWR Plans
  – Test Stands
  – VERAView Post-processing

Focus this year is to optimize performance (reduce run times) and make the code more robust.
Virtual Environment for Reactor Applications (VERA)

VERA is the "Environment"

Interoperability with External Components
- ANC
- STAR-CCM+
- RELAP5
- RELAP7
- Others TBD

Geometry / Mesh / Solution Transfer
- DTK
- libMesh

Solvers / Coupling / SA / UQ
- DAKOTA
- MOOSE
- Trilinos
- PETSc

Neutronics
- MPACT
- Shift
- ORIGEN

Thermal-Hydraulics
- CTF

Fuel Performance
- BISON

Chemistry

Common Input/Output and Visualization
- VeraIn/VeraOut
- VERAView

Software Tools
- ParaView
- VisIt
- MAMBA
- SCALE/AMPX

VERAView

CASL-U-2016-1082-000
VERA-CS is the subset of components needed to deplete the core over multiple cycles.
# Performance Improvements Milestone

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<th>Level</th>
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<td>L2.PHI</td>
<td>8/17</td>
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<td>• PHI Performance improvements in VERA-CS</td>
<td>L3.PHI</td>
<td>7/31</td>
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<td>• Restart File improvements for performance and coupling</td>
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<td>• Improve CTF Parallel Performance</td>
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<td>• Improvements to CMFD methodology</td>
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<td>Collins</td>
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<td>• MPACT Performance improvements in VERA-CS</td>
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<td>- Run time improvements to resonance methodology</td>
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<td>Liu</td>
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<td>- MOC Kernel optimization</td>
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<td>- Miscellaneous Hotspot Improvements</td>
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<td>- Port of MOC kernel to GPU/Intel MIC</td>
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DOE Reportable Milestone Due 8/17

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Example: Problem 5 Performance

- Test Problem: VERA Benchmark Problem 5
  - 3-D HZP Critical of Watts Bar Unit Cycle 1 with critical boron search
  - Quarter-Core problem, with **NO T/H feedback** and **NO depletion**

**Baseline (Total= 871 sec)**
- Meshing 6%
- Other 10%
- Subgroup 10%
- XS Calculation 30%
- MOC Sweep 17%
- CMFD Solve 27%

**Improved (Total= 287 sec)**
- Meshing 19%
- Other 31%
- Subgroup 9%
- XS Calculation 7%
- MOC Sweep 13%
- CMFD Solve 21%

3x Improvement!

All Cases run on Eos with 4234 Cores

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Problem 5 Improvements

• Major Accomplishments
  – Improvements to macroscopic cross section calculation
  – Stabilized CMFD (necessary for new MOC sweeper)
  – Jacobi-Inscatter Iteration based MOC Sweeper
  – Fast subgroup self-shielding kernel

• Work in progress
  – Space-dependent Wielandt Shift (SDWS)
  – Other misc. improvements to XS calculation
  – Post-corrector depletion
  – Advanced Eigenvalue Solvers
  – Improved CTF Parallelization
CTF Performance Improvements

- Increased domain decomposition parallelism from one core per assembly to 2x2 (or 3x3) cores per assembly
- 2x2 decomposition gives speedup of 3X
- Quarter-symmetry, pin-resolved simulation time dropped from 563 s (56 processors) to 193 s (193 processors)

Simulation time for ~15,000 channel full-core model reduced by factor of ~3X
Depletion Results

• Depletion cases use coupled CTF and the cross section processing takes a lot longer due to many more isotopes
• Watts Bar Milestone in June 2015
  – 21.9 hours to deplete a cycle (4307 cores, 37 statepoints per cycle)
• Initial cross section speedup in December
  – reduced time from 22 hours to 16 hours (1.37x)
• Recent Improvements
  – 3x speed up in MOC and CMFD
  – 3x speedup in CTF
  – 1.3x in cross sections
• Currently runtime at ~ 8 hours per cycle

Currently at 2.5x speedup!
Additional Planned Work

• Additional planned work to:
  – Improve predictor-corrector depletion to use “post corrector” method for a total speedup of 1.5x
  – Improve Krylov solvers in CMFD Solution
  – Speed up self-shielding calculation
  – Optimize depletion steps / substeps

• Conservatively expect another 2x speedup

• Roughly speaking, a cycle depletion will be:
  – 4 hours on 4000 cores, or
  – 16 hours on 1000 cores

1000 core target is achievable!
Thermal Expansion

- Initial Milestone Completed L3.PHI.VCS.P12.01 (February)
- Reviewed thermal expansion theory and determined a recommended set of thermal expansion coefficients
- Ran sensitivities on 2D and 3D assemblies by modifying input by hand
- MPACT Implementation Due in June 2016 (L3:PHI.VCS.P13.02)

S. Palmtag, “Investigation of Thermal Expansion Coefficients in MPACT,” CASL-U-2016-1015-000 (Feb 2016)
Thermal Expansion Effects

• Largest observed effect was the expansion of the core plate, which increases the assembly gap and amount of moderator
  – +150 pcm at 1300 boron, -50 at 0 boron
  – translates to potential -25 ppm trend in boron between BOC and EOC

• Smaller observed effect on the fuel pellet diameter
  – ±50 pcm, depends on enrichment and exposure
  – Fuel pellet diameter depends on more than thermal expansion

• Potential to increase ITC by about 0.5 pcm/°F
  – Current results tend to be low by about 0.8 pcm/°F

• Corner pin powers can increase 2.5%
Thermal Expansion Effect on Pin Power

### Absolute Pin Power Difference (TE – No TE %)

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<th>-0.64</th>
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Maximum pin power change +2.41% (corner)
Change in maximum pin power -0.47%
Library Validation by Comparing to Continuous-Energy Monte Carlo

• Previously had comparisons of 16 2-D assemblies from “Progression Problem 2”
• Extended this test suite to cover 1260 cases
  – 14 assembly geometries
  – Three U-235 enrichments (2.1%, 3.1%, and 4.1%)
  – Three hot coolant densities corresponding to typical inlet, average, and outlet conditions
  – Three hot fuel temperatures (600, 900, and 1200K)
  – One cold temperature and density
  – Three boron concentrations (0, 600, and 1300 ppm)
• 90 case “case matrix” for each geometry type
Assembly Geometries

- CE 16x16
- W 16x16
- B&W 15x15
- B&W 15x15 4 gad
- W 15x15
- W 17x17
- W 17x17 12 Pyrex
- W 17x17 24 Pyrex
- W 17x17 80 IFBA
- W 17x17 128 IFBA
- W 17x17 12 gad
- W 17x17 24 gad
- W 17x17 thermal expanded
- W 17x17 zoned enrichment
### Library Validation Results

#### Eigenvalue and Pin Power Comparisons (MPACT-MCNP)

<table>
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<tr>
<th></th>
<th>Ave (pcm)</th>
<th>Sdev (pcm)</th>
<th>Min (pcm)</th>
<th>Max (pcm)</th>
<th>AveRMS (%)</th>
<th>MaxPin (%)</th>
<th>Count</th>
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<td>-432.9</td>
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</table>

- Hot eigenvalues are reasonable, a good goal is to have all differences +/- 200 pcm
- Hot pin powers look very good, only a few cases (with high gad) with maximum difference > 0.5%
- Cold eigenvalues and pin powers need improvement
- No trends observed with enrichment, boron, density, or fuel temperature. Pyrex and Gad assemblies have larger differences

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**Test Suite Now Available to Measure Future Library Improvements!**

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Transient Development Status

1. Assessment of transient data in MPACT 51grp Cross Section Library (12/31/15)
2. Implementation of Control Rod Movement capability in VERAINT (1/31/16)
3. Testing of Direct Moderator Heating capability in MPACT for transient (2/29/16)
4. Implementation/Testing of Transient Control Rod Decusping capability in MPACT (3/31/16)
5. Completion of SPERT HZP and HFP tests (5/31/16)
6. Development of Watts Bar Transient Benchmark Problem (6/30/16)
7. Completion of Watts Bar Transient Benchmark (8/31/16)
8. Preparation/Submission of Milestone Report (9/30/16)

DOE Reportable Milestone L2:RTM.P13.03
3D SPERT Test 86

- Hot full power transient.
- 60 assemblies radially and 20 layers axially
- Initial core inlet temperature is at 502 °F ± 4 °F.
- Initial Power is 19 ± 1 MW.
- The transient rod worth $1.17 ± 0.05.
- Coupled with MPACT internal TH module.
- 1ms fixed time step.
- Execution time is 2 hrs with 2880 cores on ORNL Titan Computer.
3D SPERT Test 86 Result (HFP/Superprompt Critical $1.17)

Preliminary Results!
See Milestone for final results
Industry Methods vs. VERA-CS

- 2D infinite lattice physics in many energy groups
- Macroscopic cross section homogenization and parameterization
- 3D nodal diffusion in few energy groups
- Node average T/H quantities for feedback and depletion
- Pin power reconstruction
- Pin exposure reconstruction
- Spectral history corrections
- Approximate reflector models
- Fast runtime

VERA-CS

- Whole-core 3D transport
- 47 energy groups
- Explicit pin-by-pin powers with intra-pin distributions
- Explicit pin-by-pin depletion at local spectrum
- Explicit channel-by-channel two-phase T/H with cross-flow
- Simple pin-by-pin fuel temperatures by table-lookup
- Semi-explicit 3D reflector geometry
- Runs on 1000’s of cores over hours or days

VERA-CS is built for Accuracy at the Fuel Rod Level

CASL-U-2016-1082-000
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<th>Type</th>
<th>Ave (pcm)</th>
<th>Sdev (pcm)</th>
<th>Min (pcm)</th>
<th>Max (pcm)</th>
<th>AveRMS (%)</th>
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