Overview of SCALE 6.2


Oak Ridge National Laboratory

F. Havlůj
Nuclear Research Institute at Řež

S. E. Skutnik
University of Tennessee

K. J. Dugan
Texas A&M University

ANS NCSD 2013
Criticality Safety in the Modern Era: Raising the Bar
Wilmington, NC
SCALE 6.2 Preview

• Significant updates since SCALE 6.1 in June 2011
• Focus on improved fidelity of solutions

• Significant improvements in Monte Carlo capabilities
  – Comprehensive review and update of CE nuclear data, with orders of magnitude increase in testing for improved quality (sponsored by NRC)
  – CE TSUNAMI (sponsored by NCSP)
  – CE MAVRIC/Monaco (sponsored by NRC)
  – CE TRITON (other sponsor)
  – Hybrid source convergence tool

• Modular development, parallel computing, and integration with other code packages (NEAMS, CASL, external development)

• New sampling methods for uncertainty analysis and generation of experimental correlations (joint NCSP and DOE NE support)

• New nuclear data libraries in MG and CE

• Modernized resonance self-shielding tools
Monte Carlo Improvements for Criticality

- **Parallel KENO**
  - Significant speedups with MPI on Linux clusters

- **Improved CE efficiency**
  - Memory footprint reduced by 20-95%, depending on problem
  - Coding revised to provide improved consistency across platforms

- **Source Convergence**
  - Shannon Entropy test in KENO
  - Hybrid deterministic starting source methodology in Sourcerer for improved $k_{eff}$ reliability

- **Problem-Dependent Doppler broadening for CE calculations**

- **Doppler Broadened Rejection Correction**
  - Significant improvement in elevated temperature CE Monte Carlo
CE Monte Carlo Depletion

- Designed for high-fidelity analysis of full core reactors
- MG reaction and flux tallies from CE data
- Efficient memory management
- Coupling with ORIGEN

Graphite Reactor Benchmark Calculation
- 7,930 depletion zones
- ~10,000 units, ~32,000 regions
- 1.2GB memory
- 50M histories for ~1% standard deviation in fluxes
- Total problem time: 72 hours

<table>
<thead>
<tr>
<th></th>
<th>MG KENO</th>
<th>CE KENO</th>
</tr>
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<tbody>
<tr>
<td>U-234</td>
<td>3.0</td>
<td>3.2</td>
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<td>1.4</td>
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<td>-0.1</td>
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<td>-10.2</td>
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<td>Pu-239</td>
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<td>9.1</td>
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<tr>
<td>Pu-240</td>
<td>1.5</td>
<td>1.8</td>
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<tr>
<td>Pu-241</td>
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<tr>
<td>Pu-242</td>
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<td>Np-237</td>
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<td>3.1</td>
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<td>Am-241</td>
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<tr>
<td>Nd-150</td>
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<td>2.5</td>
</tr>
</tbody>
</table>
CE Sensitivity Analysis with TSUNAMI

CLUTCH and MG-TSUNAMI Sensitivity Profiles for an Infinitely-Reflected Fuel Pin Problem

Difficult convergence of MG adjoint

![Graph showing sensitivity profiles](image)

**Energy-Integrated Sensitivity Coefficient Comparison**

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Direct Pert.</th>
<th>MG-TSUNAMI</th>
<th>CLUTCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-235</td>
<td>0.1660</td>
<td>0.1595</td>
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<td>U-238</td>
<td>-0.2207</td>
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<td>H-1</td>
<td>0.0946</td>
<td>0.0785</td>
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<tr>
<td>O-16</td>
<td>-0.0147</td>
<td>-0.0250</td>
<td>-0.0139</td>
</tr>
</tbody>
</table>

**Runtime Parameter Comparison for the Fuel Pin Problem**

<table>
<thead>
<tr>
<th></th>
<th>CLUTCH</th>
<th>MG-TSUNAMI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Memory Increase over Eigenvvalue Calculation</td>
<td>2 MB</td>
<td>305 MB</td>
</tr>
<tr>
<td>Runtime</td>
<td>352.3 min</td>
<td>626.9 min</td>
</tr>
</tbody>
</table>

→ The CE-KENO + CLUTCH run was faster than the MG-KENO + TSUNAMI run and it had a small memory footprint!

**Energy-Integrated Sensitivity Coefficient Differences (in number of $\sigma_{\text{effective}}$)**

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>MG-TSUNAMI</th>
<th>CLUTCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-235</td>
<td>-0.79</td>
<td>-0.22</td>
</tr>
<tr>
<td>U-238</td>
<td>-0.64</td>
<td>0.91</td>
</tr>
<tr>
<td>H-1</td>
<td>-4.39</td>
<td>1.18</td>
</tr>
<tr>
<td>O-16</td>
<td>-7.49</td>
<td>0.51</td>
</tr>
</tbody>
</table>
CE Shielding with MAVRIC/Monaco

- All hybrid capabilities supported with CE fidelity
- SCALE Continuous-Energy Modular Physics Package (SCSEMPP)
  - Application Programmer Interface (API) for CE physics for next-generation Monte Carlo codes
- 6300 fixed-source transmission tests used in V&V

Flux results for iron sphere transmission experiment

Dose rate from $^{60}$Co source in transportation package
Modular ORIGEN

- ORIGEN restructured to provide Application Programmer Interface (API) and parallel capabilities
- New ORIGAMI tool developed to rapidly characterize spent fuel.

Front view

Top view

235 pins, 26 axial zones
6,110 depletion nodes

- ~50 hours runtime
- OpenMPI implementation with (near)-linear speed-up
Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

• **Sampler** provides uncertainty in any computed result from any SCALE sequence due to uncertainties in:
  – neutron cross sections
  – fission yield and decay data
  – geometry and composition

• **Sampler** propagates uncertainties through complex analysis sequences such depletion calculations

• **Correlations** between systems are also computed
New Data Libraries

- New CE cross-section data for neutron interactions, **gamma yield**, and **gamma interactions** (sponsored by NRC)
- New MG neutron libraries
  - Provides parameters for intermediate resonance approximation for rapid resonance self-shielding techniques
  - **252-group** energy structure (sponsored by NRC)
  - **56-group** energy structure (sponsored by NRC and DOE NE)
- Extensive test suite
  - 381 VALID benchmarks
  - 6300 transmission tests
  - 5000 infinite medium tests
- ENDF/B-VII.0 libraries released with SCALE 6.2 beta1
- ENDF/B-VII.1 libraries under QA review for release with SCALE 6.2 beta2
AMPX Processing Improvements Provide Improved C/E Especially for CE Calculations for MOX Benchmarks

Up to 1000 pcm improvement for burned fuel
## SCALE 6.2 beta1 Data Libraries

<table>
<thead>
<tr>
<th>Alphanumeric name</th>
<th>Primary data source/format</th>
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</thead>
<tbody>
<tr>
<td>v7-238</td>
<td>ENDF/B-VII.0 238-group neutron library</td>
</tr>
<tr>
<td>v7-252</td>
<td>ENDF/B-VII.0 252-group neutron library</td>
</tr>
<tr>
<td>v7-56</td>
<td>ENDF/B-VII.0 56-group neutron library</td>
</tr>
<tr>
<td>v7-200n47g</td>
<td>ENDF/B-VII.0 200 neutron/47 gamma library</td>
</tr>
<tr>
<td>v7-27n19g</td>
<td>ENDF/B-VII.0 27 neutron/19 gamma library</td>
</tr>
<tr>
<td>ce_v7_endfb</td>
<td>ENDF/B-VII.0 Continuous-energy neutron and gamma library</td>
</tr>
</tbody>
</table>
SCALE 6.1 Resonance Self-Shielding
(somewhat simplified view)

TRITON
- BONAMI Input Fuel Pins
- Worker Input Nuclides

CENTRM Input Fuel Pins
- CENTRM (compute pointwise flux in resolved resonance region)

Continuous-Energy XS
- 10s of GB distributed w/ SCALE

Pointwise Flux
- 100s of MB for each pin

Worker Input Nuclides
- PMC Input Fuel Pins

PMC (generate XS for resolved resonance region from pointwise flux and XS)
- PMC
- WORKER
  - (prepare all nuclide cross sections for use in transport calculation)

NEWT 2D Neutronics Solver
- combine nuclide cross section with material densities to produce material cross sections

Depletion (outside scope of current task)
- Depletion

Problem Independent MG XS by Isotope
- 100s of MG distributed w/ SCALE

Problem Dependent MG XS by Isotope for each pin
- 10s of MBs of reaction data needed for transport and depletion
- 10s of GBs of scattering data later consolidated in neutronics solver, but never independently used

Worker Input Nuclides
- Newt Input Fuel Assembly

Huge I/O and Memory use
- (10s–100s of GB)
SCALE 6.2 Resonance Self-Shielding

**Efficient operation**
- Small memory footprint
- Parallel calculations

**XSProc**
- (unresolved resonance treatment)
- (resolved resonance treatment)

**Problem Independent MG XS by Isotope**
- 100s of MG distributed w/ SCALE

**Continuous-Energy XS**
- 10s of GB distributed w/ SCALE

**Only save needed data**

**Fuel Pin Specifications**
- Parallel loop over each fuel pin

**Continuous-Energy XS**
- < 1 GB after initial I/O

**Pointwise Flux**
- Updated in memory for each pin

**NEWT Input Fuel Assembly**

**NEWT 2D Neutronics Solver**

**Depletion**
- (outside scope of current task)

**Key**
- Disk storage (slow)
- In-memory storage (fast)
Updated QA Program

- Designed for Compliance with:
  - ISO 9001-2008
  - DOE 414.1D
  - ORNL SBMS
  - Consistent with ASME NQA-1

- Capabilities are tracked with the Kanban process through the FogBugz electronic collaborative development environment

<table>
<thead>
<tr>
<th>Kanban Category</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed</td>
<td>Task has been proposed for management approval</td>
</tr>
<tr>
<td>Approved</td>
<td>Task has been approved by management and assigned to a developer for implementation</td>
</tr>
<tr>
<td>In Progress</td>
<td>Developer is actively working to implement the feature</td>
</tr>
<tr>
<td>Ready for Testing</td>
<td>Developer has completed the implementation and the feature is ready for comprehensive testing</td>
</tr>
<tr>
<td>Ready to Ship</td>
<td>Item has passed all tests and is a candidate feature for quality assurance implementation</td>
</tr>
<tr>
<td>Shipped</td>
<td>Feature is implemented in quality-assured version</td>
</tr>
</tbody>
</table>
Overview of SCALE 6.2

Improved SCALE V&V

• Routine Test Suite
  – Run dozens of times each day
  – 263 Sample Problems
  – 379 Regression Problems
  – ~1000 Unit Tests
  – 381 VALID Benchmarks

• Supported Platforms:
  – Linux, Mac, Windows
    • Intel Release
    • Intel Debug
    • GNU Release
    • GNU Debug
  – Suite repeated with MPI on Linux and Mac

Total of ~70,000 tests run every day
Conclusions

- SCALE 6.2 continues a 30-year legacy of nuclear systems modeling and simulation by providing comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity/uncertainty analysis.

- The new capabilities within SCALE 6.2 provide significant advances over previous versions
  - CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis,
  - Modularity for CE physics and depletion
  - Stochastic sampling with Sampler
  - Improved CE and MG data.
 SCALE 6.2 Tentative Schedule

- Beta1 – currently under limited release
- Beta2 – broader release expected by December 2013
- Beta3 – expected in Spring 2014
- Production release – expected in Summer 2014
Questions?

http://scale.ornl.gov
scalehelp@ornl.gov
Improved Collision Kinematics Processing in AMPX

Since primarily used for MG:

- **Y12** File 7 -> cosine moments
- **MONTEGO** cosine moments -> point-wise
- **JAMAICAN** point-wise -> probability distr.

Updated for CE library

- **Y12_GAM** File 7 -> point-wise
- **JAMAICAN** point-wise -> probability distr.

Refined energy grid is used → thinned to keep library size manageable

H₂O incident energy 0.1 eV
New 252-Group Library for SCALE

- 252 instead of 238 neutron groups, refined for LWRs
- Implements data needed for Intermediate Resonance approximation rapid self-shielding calculations with Bondarenko and Embedded Self-Shielding Methodology (SCALE and CASL)

- Weighted with CE flux for actinides and thermal H$_2$O
- Add Lambda-factors for all isotopes
- Add heterogeneous IR-factors for actinides
- Homogeneous IR-factors for other materials