FY13 Accomplishments for SCALE


Oak Ridge National Laboratory

Nuclear Criticality Safety Program
Technical Program Review
Los Alamos, NM, March 26, 2014
The SCALE Code System
Neutronics and Shielding Analysis
For Enabling Nuclear Technology Advancements
The SCALE Code System
Neutronics and Shielding Analysis
For Enabling Nuclear Technology Advancements

CASL
- Continuous-energy, high-fidelity reference solutions for reactor physics
- Cross-section data libraries
- Reactor fuel depletion
- Uncertainty quantification

DOE Used Fuel Disposition
- Radiation shielding
- Nuclear fuel depletion
- Used fuel source terms
- Criticality safety analysis
- Uncertainty quantification

DOE Nuclear Criticality Safety Program
- Criticality safety assessments
- Sensitivity and uncertainty analysis
- Advanced validation methods
- Experiment design
- Criticality accident alarm system analysis and design

Nuclear Regulatory Commission
- Supports licensing and regulatory research
- Original sponsors of SCALE – since 1976
- Reactor physics and source terms
- Criticality safety and shielding
- Cross section data libraries

Global Distribution
- 5600 users in 51 nations
- Regulators
- Industry
- Research and Development

Nuclear Nonproliferation and Safeguards
- Used fuel and radionuclide source terms
- Reactor depletion analysis
- Radiation transport
- Nuclear forensics

SCALE and AMPX Advancements to Support NCS Applications Applications
5600+ Users
51 Nations

Regulators
Industry
Utilities
Research Laboratories
Government Agencies
Universities

Distributed by RSICC (USA), NEA Data Bank (France) and RIST (Japan)
Outline

- Quality Assurance
- Advanced Features
- Modernization
# Evolution of SCALE – 1980–2011

Each era with differing tools and developers, same design and management strategy

<table>
<thead>
<tr>
<th>Lines of Code</th>
<th>Pages of Documentation</th>
<th>No. of Modules</th>
<th>Size of Data Libraries</th>
<th>No. of Data Libraries</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,000,000</td>
<td>8,900</td>
<td>80</td>
<td>22 GB</td>
<td>20</td>
</tr>
<tr>
<td>400,000</td>
<td>5,800</td>
<td>80</td>
<td>650 MB</td>
<td>12</td>
</tr>
<tr>
<td>250,000</td>
<td>4,300</td>
<td>55</td>
<td>110 MB</td>
<td>10</td>
</tr>
<tr>
<td>25,000</td>
<td>300</td>
<td>6</td>
<td>10 MB</td>
<td>4</td>
</tr>
</tbody>
</table>

**Diagram: SCALE Driver and TRITON**

- **Input**
  - BONAMI / NITAWL
  - BONAMI / CENTRM / PMC
- **YES**
  - ORIGEN-S
  - NEWT
  - COUPLE
- **NO**
  - All branches complete?
    - All mixtures complete?
      - All time steps done?
        - Output edits (repeat for all requested mixtures)
      - YES
      - ORIGEN-S
    - NO
      - OPUS

**World’s #1 Open Science Supercomputer**

Flagship accelerated computing system | 200-cabinet Cray XK7 supercomputer | 16,688 nodes (AMD 16-core Opteron + NVIDIA Tesla K20 GPU) | CPUs x GPUs working together - GPU accelerates 20+ Petaflops
SCALE MODULE REVISION REPORT

Part I - Change Request

Report No. MRR 00-001

Module/Unit Name: KENOVA
Version 4.2

Description: Changing PULL in MRR 00-003 requires minor changes to KENOVA. The changes made in generating angle x probabilities in perfume in MRR 99034 should also be incorporated in KENOVA.

Prepared by (Requestor): L.M. Petrie
Date: 1/4/00

Part II - Approval / Disapproval

Approved by: M. J. Bowman
Date: 1/4/00

Explanation (if not approved):

Fix made to file. Do after MRR 00-003

Part III - Documentation of Changes

Code Manager: L.M. Petrie

Attached are the following:
- Description of changes
- Verification report
- Test case inputs

Modified source modules and their location:
- KFEN
- XS.RD
- KAS.GR
- KAS.REP
- KAS.MARK

Location of our programs input:

Prepared for Software Coordinator:

Other SCALE Executable Modules affected:
- CSAS, modify 006009

Effect of change on previous calculations:
Should be none, although possibly the random sequence could change.

Prepared by (Code Manager): L.M. Petrie
Date: 1/5/00

2000 – Quality Assurance Document
Historical SCALE Testing and Defects

- During development SCALE was tested by running ~250 sample problems every six months to assess overall performance of all features and data.

- Preparation of final distribution generally required 6-9 months to synchronize all features and hand modify a specific version for Windows.

- Frustrated developers spent a large percentage of time fixing bugs and helping frustrated users.

- Corrective Actions Taken After Release
  - 2004 - SCALE 5.0
    - 7 patches
  - 2006 - SCALE 5.1
    - 8 patches
  - 2009 - SCALE 6.0
    - 10 patches
SCALE Development Hierarchy

- Advanced Methods
- Modern Framework
- Existing Capabilities and Data
- Build and Test Infrastructure
- Development Coordination
- Quality Assurance
What Developers Think They Want

- Advanced Methods
- Modern Framework
- Existing Capabilities and Data
- Build and Test Infrastructure
- Development Coordination
- Quality Assurance

Development
Maintenance
Communication and Coordination

• SCALE Leadership Team
  – SCALE manager, line managers, senior staff
  – Coordinates overall vision for SCALE
  – Sets priorities and reviews progress
  – Meets regularly to maintain close coordination

• SCALE Development & Applications Teams
  – Multiple teams meet frequently to discuss different technical areas
  – Promotes collaboration
    • Within and across technical areas
    • Between developers and users
    • Across organizational boundaries

• Friday Forum
  – Open discussions 2 hours each Friday
New Push for Quality

- Instilled culture of quality
- Migrated to electronic QA system
- Hired team of young computer scientists
- SCALE Testing Team
  - Five students tested SCALE 6.0 and SCALE 6.1-beta during summer of 2010
  - Worked directly with developers as mentors
  - Hundreds of previously unknown defects were identified spanning nearly every module
- Automated daily testing initiated using hundreds of student test cases
- All test results posted to internal website where anyone on the team can monitor outcomes
Infrastructure Investments

- 384 core, 4 Teraflop Linux cluster for SCALE development and testing

- Additional 30 Teraflop for capacity computing
SCALE 6.1 – July 2011

• New quality philosophy communicated through conference presentations and newsletter

• 2700 licenses issued through February 2014

• >1700 new users that had never used any previous version of SCALE (2500 total SCALE users in 2009)

• Record training attendance

• Many publications and license applications from other teams using SCALE for innovative analyses

• Only two patches issued

• Enhanced opportunities with cross-project collaboration, Ph.D. projects, etc.

• Rest and enjoy fruits of labor?
**FY13 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>
**Build and Test Infrastructure**

- **Electronic feature tracking system**
  - All developers can see all development all the time
  - Holistically review all features in development in 1 hour meeting

- **Testing fully automated and extended to ~70,000 tests/day**

- “Release candidate” prepared for distribution in 24 hours
Outline

• Quality Assurance
• Advanced Features
• Modernization
Monte Carlo Improvements for Criticality

- Parallel KENO Significant speedups with MPI on Linux clusters
- Problem-Dependent Doppler broadening for CE calculations for resolved and unresolved (probability table) energy ranges (PhD)
- Doppler Broadened Rejection Correction (PhD)
  - Significant improvement in elevated temperature CE Monte Carlo
## Memory Footprint

- Extensive rework of everything CE in SCALE and AMPX
- Introduction of efficient, XSProc module for MG calculations

### CE Memory Improvements for Each Material

<table>
<thead>
<tr>
<th>Improvement</th>
<th>% Reduction in Memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conversion of internal data storage from double- to single-precision</td>
<td>15–45</td>
</tr>
<tr>
<td>Redesign of 2D collision kinematics data</td>
<td>5–30</td>
</tr>
<tr>
<td>Optimize nuclide object (in memory access to data)</td>
<td>3–15</td>
</tr>
<tr>
<td>Optional within-nuclide unionized reaction energy grid</td>
<td>10–20</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>40–95</strong></td>
</tr>
</tbody>
</table>
CASL Application of Enhanced KENO-VI

- High-fidelity AP-1000 startup calculations in conjunction with Westinghouse
  - Each axial region of each pin is unique region for tallies
  - Reference solution for power dist.
  - Auto-generated 8,000,000 line input
  - 688,000 units
  - 5,000,000 particles/gen
  - 10,000 generations
  - 50 billion total particles
  - 180 cores on INL’s Fission
  - 10.3 days of wall time
  - 44,500 CPU-hours
  - 11 GB/core (2 TB total)
  - Max uncert. 3.4%
  - Credit: Andrew Godfrey
Continuous-Energy Sensitivity Analysis

- Two new methods integrated into TSUNAMI / KENO for CE Calculations
  - Iterated Fission Probability (similar to MCNP)
  - CLUTCH (Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization) – PhD topic

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>MG TSUNAMI</th>
<th>IFP</th>
<th>CLUTCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>0.06 GB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>U-238</td>
<td>13 GB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pu-239</td>
<td>11 GB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pu-240</td>
<td>0.06 GB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pu-241</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure of Merit (min⁻¹)

MIX-COMP-THERM-004 Critical Experiment
Convergence problems of NAC-UMS-TSC-24

- Difficult to capture most reactive regions
- Decoupling due to water and flux traps

\[ k_{\text{ref}} - k_{\text{calc}} = 7.7\sigma \]

30K neutron/cycle

Unaffordable computer and human resources required to ensure reliability of canister-specific calculations
Ibrahim et. al, "Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources," PHYSOR 2012
Reliability

Frequency of \textbf{not} calculating $k_{\text{eff}}$ inside confidence interval

$$k_{\text{ref}} - 3\sigma < k_{\text{calc}} < k_{\text{ref}} + 3\sigma$$

Reliability of uniform source is comparable with the reliability of deterministic source after skipping 350 cycles

- 30,000 Neutrons per cycle and 500 active cycles
- 100 independent (different random seed) calculations for each point
Efficiency $k_{\text{eff}}$ with 500 active generations

<table>
<thead>
<tr>
<th>Starting source</th>
<th>$k_{\text{eff}}$</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>$0.68977 \pm 0.00025$</td>
<td>1.00</td>
</tr>
<tr>
<td>Loose</td>
<td>$0.68944 \pm 0.00024$</td>
<td>1.71</td>
</tr>
<tr>
<td>Tight</td>
<td>$0.68900 \pm 0.00024$</td>
<td>1.36</td>
</tr>
</tbody>
</table>
Outline

• Quality Assurance
• Advanced Features
• Modernization
89 Independent Executable Modules in SCALE 6.1

- **Control Modules**
  - csas5
  - csas6
  - mavric
  - mcdancoff
  - sas1
  - smores
  - starbucks
  - triton
  - triton6
  - tsunami-1d
  - tsunami-3d_k5
  - tsunami-3d_k6

- **Resonance Self-Shielding**
  - bonami
  - bonamist
  - cajun
  - centrm
  - chops
  - crawdad
  - nitawl
  - nitawlst
  - worker

- **Transport**
  - keno_dancoff
  - kenova
  - kenovi
  - monaco
  - newt
  - newt-omp
  - qads
  - xkba
  - xdrn

- **Depletion**
  - arp
  - arplib
  - couple
  - opus
  - origen
  - prism
  - reorg
  - xseclist
  - tsunami-ip
  - tsurfer
  - xsdose

- **Post-Processing Analysis**
  - kmart5
  - kmart6
  - modify
  - sams5
  - sams6
  - swif
  - tsar
  - mim2wwinp
  - mt2ascii
  - mt2msm

- **Utility**
  - c5toc6
  - kmart5
  - kmart6
  - genwgts
  - gwas
  - legend
  - mal
  - mim2wwinp
  - mt2ascii
  - mt2msm

- **Utility (cont’d)**
  - c5toc6
  - kmart5
  - kmart6
  - genwgts
  - gwas
  - legend
  - mal
  - mim2wwinp
  - mt2ascii
  - mt2msm

- **Nuclear Data Tools**
  - aim
  - ajax
  - alpo
  - scalerte
  - shell

- **Runtime**
  - collect_output
  - scale
  - scalerte
  - shell
Hypothetical SCALE 6.1 Calculation

Graphical User Interface → User Input

- GUI Data
- SCALE Data

Intermediate Files

User Output

Visual Output/Plotting

Driver
- Read input A
- Write input B
- Write output
- Write control file
- Compute something
- Create input C
- Write input C
- Write output
- Write control

Sequence B
- Read input B
- Read control
- Read data A
- Read data B
- Compute something
- Read data C
- Compute something
- Write output
- Write control
- Quit

Module C
- Read input C
- Read control
- Read data C
- Compute something
- Write input D
- Write control
- Write output
- Write data D

Sequence B
- Read input D
- Read control
- Read data D
- Compute something
- Write input E
- Write control
- Write output
- Quit

Module D
- Read input E
- Read control
- Read data E
- Compute something
- Write output
- Write data E

Sequence B
- Read control
- Compute something
- Write output
- Write data D
- Quit
SCALE Modernization
New Framework, New Potential, New Motivation

Text Input
Interactive Input GUI
SNAP

Input Processor
Input Validator
Checks input and provides feedback

Sequences and Modules
Data Storage and I/O
Data D

Output Reporter

Data Visualizer
Data Plots (A,B,C,D,E)
Geometry Visualization

Data A,B,C
Data E
Text Output
HTML Output
XML Files
Database
Modular Interfaces

- SCALE Continuous-Energy Modular Physics Package (SCEMPP)
  - Coupled neutron/gamma physics
  - Application Programmer Interface (API) for CE physics for next-generation Monte Carlo codes
  - Implemented for shielding in Monaco
  - HPC Monte Carlo with Shift (125K processors)
- ORIGEN restructured to provide API and parallel capabilities
- New ORIGAMI tool developed to rapidly characterize spent fuel.
- MPI with (near)-linear speedup

• 6300 fixed-source transmission tests used in V&V
SCALE 5.0–6.1 Resonance Self-Shielding
(somewhat simplified view)

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

Efficient operation
Small memory footprint
Parallel calculations

- Only save needed data
- Parallel loop over each fuel pin
- Fuel Pin Specifications
- Continuous-Energy XS • < 1 GB after initial I/O
- Pointwise Flux • Updated in memory for each pin

XSPROC
(unresolved resonance treatment)
(resolved resonance treatment)

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

Continuous-Energy XS for Each Nuclide and Temperature
• 10s of GB

Problem Dependent MG XS by Material
• 100s of MB of data

Problem Dependent MG XS by Isotope
(for depletion)
• 100s of MB of data

NEWT 2D Neutronics Solver

OrigenLibraryBuilder
(create problem-dependent ORIGEN data)

NEWT Input Fuel Assembly

Neutron Spectrum

ORIGEN Input Nuclides, Power, Time

ORIGEN Data

ORIGEN (update nuclides for next depletion step)
Modernization Successes in SCALE 6.2beta

- Many calculations with 95% reduction in memory footprint
- Many calculations 3x faster, some calculations run 1800x faster
- Interfaces to physics capabilities provided to other high-profile projects and university R&D
The SCALE Code System
Neutronics and Shielding Analysis
For Enabling Nuclear Technology Advancements

**CASL**
- Continuous-energy, high-fidelity reference solutions for reactor physics
- Cross-section data libraries
- Reactor fuel depletion
- Uncertainty quantification

**DOE Used Fuel Disposition**
- Radiation shielding
- Nuclear fuel depletion
- Used fuel source terms
- Criticality safety analysis
- Uncertainty quantification

**DOE Nuclear Criticality Safety Program**
- Criticality safety assessments
- Sensitivity and uncertainty analysis
- Advanced validation methods
- Experiment design
- Criticality accident alarm system analysis and design

**Nuclear Regulatory Commission**
- Supports licensing and regulatory research
- Original sponsors of SCALE – since 1976
- Reactor physics and source terms
- Criticality safety and shielding
- Cross section data libraries

**Global Distribution**
- 5600 users in 51 nations
- Regulators
- Industry
- Research and Development

**Nuclear Nonproliferation and Safeguards**
- Used fuel and radionuclide source terms
- Reactor depletion analysis
- Radiation transport
- Nuclear forensics

SCALE and AMPX Advancements to Support NCS Applications
SCALE 6.2 Tentative Schedule

• Beta1 – August 2013
• Beta2 – broader release January 2014
• Beta3 – expected in Spring 2014
• Production release – expected in later in 2014
Questions?

http://scale.ornl.gov
scalehelp@ornl.gov