Recent Developments in SCALE

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ORNL is managed by UT-Battelle, LLC for the US Department of Energy
US DOE Nuclear Criticality Safety Program
Five-Year Execution Plan for the Mission and Vision

ORNL-AM2

"Ongoing, approved task to provide SCALE/KENO/TSUNAMI maintenance and user support for performing Nuclear Criticality Safety (NCS) calculations with the SCALE package. Work tasks include: sustaining and continually improving SCALE NCS features through user-driven enhancements, software quality assurance (SQA) and V&V; assuring adaptability to various computing platforms and compilers; providing improved user interfaces and user documentation consistent with modern engineering software; supporting responsive communication to SCALE criticality safety users through SCALE Newsletters, email notices, and updates on the SCALE website. The task also includes support for modernizing the software infrastructure and capabilities to improve quality and reliability and to ensure long-term sustainability of the NCS capabilities."
US DOE Nuclear Criticality Safety Program
Five-Year Execution Plan for the Mission and Vision

ORNL-AM2

1. **Sustain/improve SCALE NCS features** through user-driven enhancements, software quality assurance (SQA) and V&V.

2. **Assure adaptability** to various computing platforms and compilers.

3. **Improve user interfaces/documentation** consistent with modern engineering software.

4. **Support responsive communication** to SCALE criticality safety users through SCALE Newsletters, email notices, and updates on the SCALE website.

5. **Modernize software infrastructure and capabilities** to improve quality and reliability and to ensure long-term sustainability of the NCS capabilities.
ORNL-AM2.1

Sustain/improve SCALE NCS features through user-driven enhancements, software quality assurance (SQA) and V&V.

**Highlights**

- Produced NCS Validation Report based on SCALE 6.2.2 KENO (provides important benchmark for SCALE 6.3 Shift)
- Deployed 6.2.3 update through RSICC
- Created and tested initial ENDF/B-VIII CE and MG nuclear data libraries

https://www.ornl.gov/scale/scale/criticality-safety-reports
Assure adaptability to various computing platforms and compilers.

**Highlights**

- Added "clang" compiler support to continuous testing
- **Added new Shift HPC tests**
- Investigated MPI version updates
  - OpenMPI (standard used in auto-deployment to ORNL clusters)
  - MPICH (anticipated support in FY19)
- Maintained testing support (through ORNL system updates/security patches, cluster upgrades)
  - platforms: Windows, Mac, Linux
  - compilers: Intel, GCC, new Clang

Platform/Compiler Test Result Dashboard

ORNL-AM2.3

Improve user interfaces/documentation consistent with modern engineering software.

**Highlights**

- Improved SCALE GUI (Fulcrum) robustness and speed for 6.2.3
- Added initial 3D visualization capability in Fulcrum for 6.3
  - uses new Geometria geometry package (from Shift integration)
  - transparency/cutplanes-with undo!
- Developed new documentation strategy for 6.3
  - based on reStructuredText
  - easy export to HTML & PDF
Support responsive communication to SCALE criticality safety users through SCALE Newsletters, email notices, and updates on the SCALE website.

**Highlights**

- Newsletters discussing 6.2.3 updates
  
  [https://www.ornl.gov/scale/newsletter](https://www.ornl.gov/scale/newsletter)  
  Upcoming newsletter will discuss "open" 6.3 beta and 6.2.4 maintenance update

- Supported user inquiries/reports through [scalehelp@ornl.gov](mailto:scalehelp@ornl.gov)  
  User-submitted criticality calculation defect resulted in rapid communication and resolution

- Continue to host Annual SCALE Users Group Workshop
Modernize software infrastructure and capabilities to improve quality and reliability and to ensure long-term sustainability of the NCS capabilities.

**Highlights**

- Migrated to new ORNL-hosted code management, GitLab
  - converted SQA record from *mercurial* version control to *git*
  - developed new processes and workflows consistent with SQA plan
  - began unifying data library, code, and validation suite storage in GitLab
- Continued CSAS-Shift effort (eventually to replace CSAS-KENO)

https://code-int.ornl.gov/msd/scale
Strategy for Shift integration into SCALE

• The goal is to be as transparent to the user as possible

• Ultimately, the only input change that should be required is changing the sequence name; appending `-shift` to sequence name

```plaintext
=csas5
  godiva-k5
  ce_v7.1_endf
read composition
  u-234  1 0 0.000491995 300 end
  u-235  1 0 0.0449996   300 end
  u-238  1 0 0.002498    300 end
end composition
read parameter
  htm=no
end parameter
read geometry
  global unit 1
  sphere 1 1  8.741
end geometry
end data
end

=csas5-shift
  godiva-k5
  ce_v7.1_endf
read composition
  u-234  1 0 0.000491995 300 end
  u-235  1 0 0.0449996   300 end
  u-238  1 0 0.002498    300 end
end composition
read parameter
  htm=no
end parameter
read geometry
  global unit 1
  sphere 1 1  8.741
end geometry
end data
end
```
SCALE Monte Carlo Developments
Simultaneously support **Shift HPC** users and **SCALE** users

- **OMNIBUS input**
  - python script
  - HDF5 output file
  - MCNP run tape (optional)
  - **OMNIBUS**
  - Geometria (General Geometry)
  - Shift (MC transport/tallies)
  - Robus (Nuclear Data PDF sampling)
  - **HPC Code**

- **SCALE users**
  - CSAS input
  - CSAS
  - CSAS output
  - **Shift/SCALE Interface**
    - KENO (MC transport/tallies)
    - geometry
    - data PDF sampling
    - Legacy Code

- **NEW & IMPROVED**

**OAK RIDGE National Laboratory**
CSAS-Shift Status Updates

- SCALE Criticality Validation Suite performance
  - FY18: 82%, FY19: 93%, remaining 7% is due to more precise Shift geometry
  - Shift vs. KENO: statistically identical results
- Volume calculations
  - KENO-VI geometry with parallel volume calculation with ray-tracer
  - KENO-V geometry allows for analytic volume calculation--enabled
- Flux and fission density tallies
- Tally fission source distribution and neutron flux on a mesh for visualization
Examine and Run the Castor model with defaults

• We test the convergence with Castor Cask model, run it in CSAS5-Shift with default parameters (GEN=203, NSK=3, NPG=1000)

• Then, we modify these parameters and rerun the modified input, and check the convergence

• We also tally fission source distribution on a mesh (CDS parameter) and visualize it to test the convergence

• Open and run castor_cask_default_parameters.inp
From October 2019 NRC Training
Comparison of Neutron Flux Std. Dev. at NPG=1000, 100000

NPG=1000, NSK=3, GEN=203

NPG=100000, NSK=100, GEN=1000
Summary

• Improved infrastructure
  – New software management on GitLab
  – Additional testing, esp. for Shift

• Developed future 6.3.0
  – 3D visualization of geometry
  – CSAS-Shift
  – open 6.3 beta for the Holidays

• Maintained existing 6.2.* series
  – Criticality validation report
  – 6.2.3 release
  – 6.2.4 ~1 month after open 6.3 beta
Questions?

SCALE 6.3 Dev Team Photo (from 2019 Users' Group)