## **Recent Developments in SCALE**

ANS Winter Meeting November 17-21, 2019 Washington DC

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#### 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

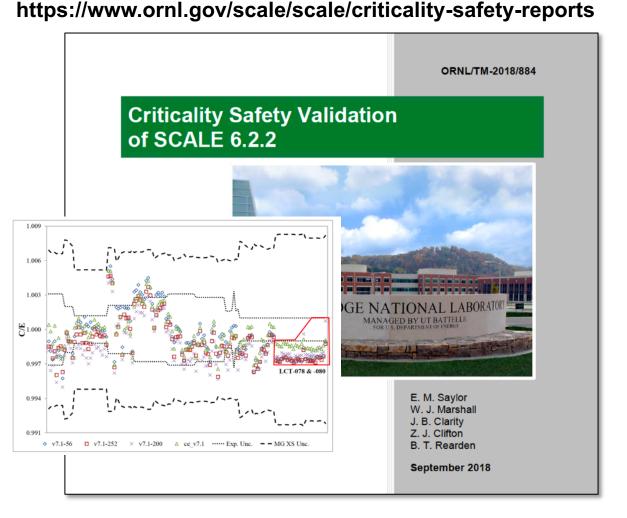
- 1. Sustain/improve SCALE NCS features through user-driven enhancements, software quality assurance (SQA) and V&V.
- 2. Assure adaptability to various computing platforms and compilers.
- 3. Improve user interfaces/documentation consistent with modern engineering software.
- **4. Support responsive 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.



**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



OAK RIDGE

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 autodeployment 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

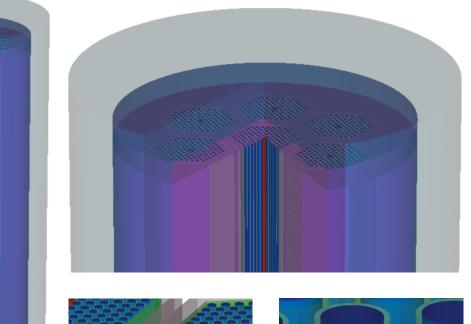
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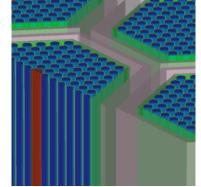
http://ci.ornl.gov/CDash/index.php?project=SCALE

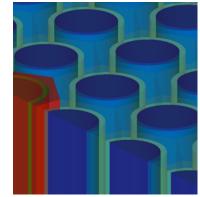
Improve user interfaces/documentation consistent with modern engineering software.

#### 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







Fulcrum 3D visualization



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

#### Highlights

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- Newsletters discussing 6.2.3

   updates
   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 <u>scalehelp@ornl.gov</u> 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)

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## Strategy for Shift integration into SCALE

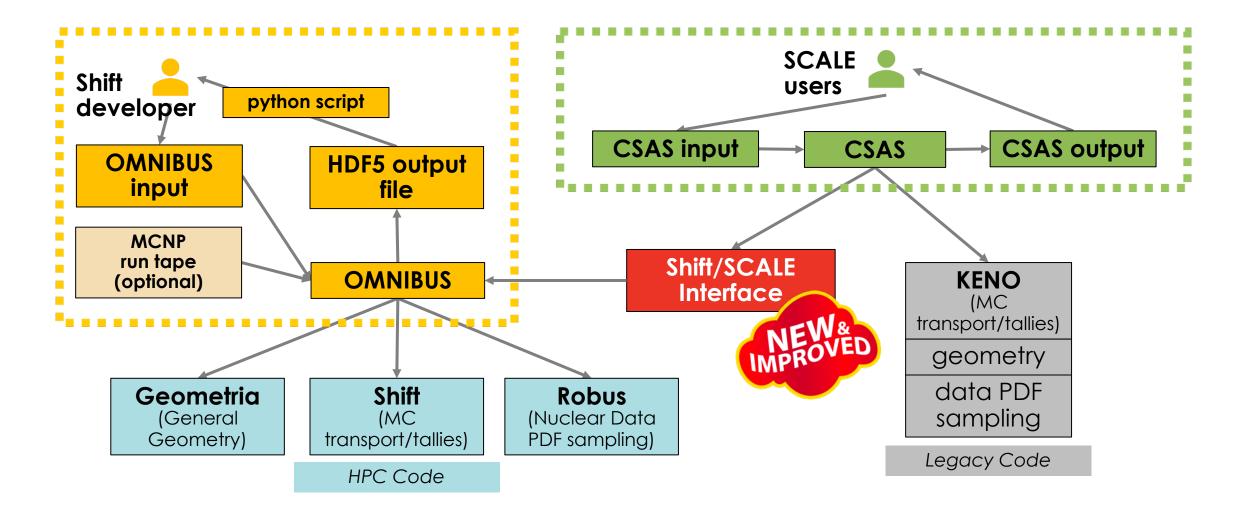
- The goal is to be as transparent to the user as possible
- Ultimately, the only input change that should be required is changing the sequence name; appending -shift to sequence name

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          1 0 0.000491995 300
                                end
u-235 1 0 0.0449996
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          1 0 0.002498
                          300
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read geometry
global unit 1
 sphere 1 1 8.741
end geometry
end data
end
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qodiva-k5
ce v7.1 endf
read composition
11-234
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u-235 1 0 0.0449996
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u-238
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end composition
read parameter
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read geometry
global unit 1
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end data
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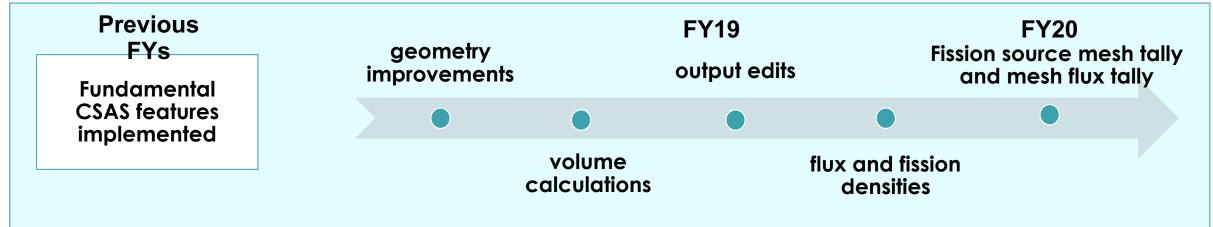


#### SCALE Monte Carlo Developments Simultaneously support **Shift HPC** users and **SCALE** users





## 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



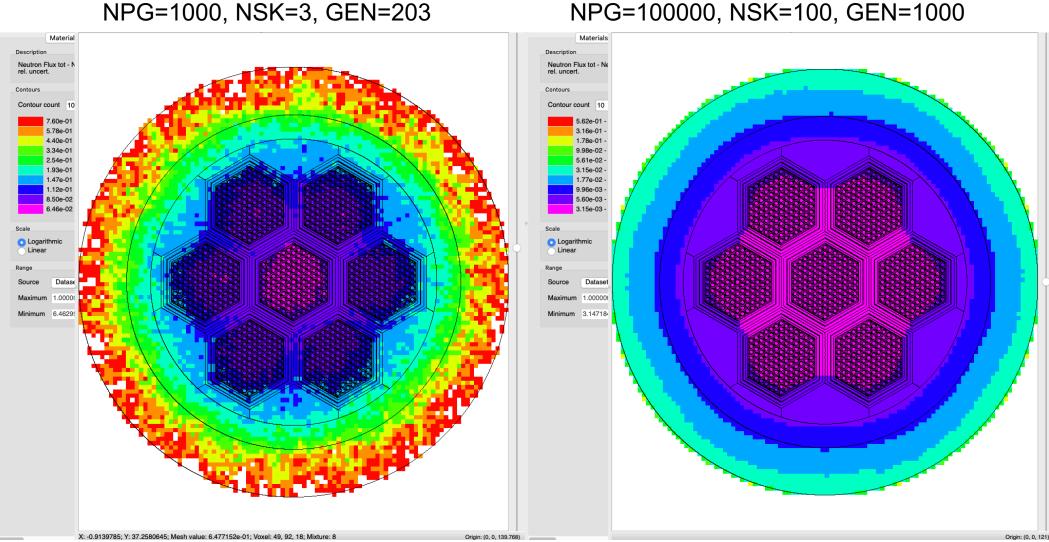
#### From October 2019 NRC Training Examine and Run the Castor model with defaults

- 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

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- 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



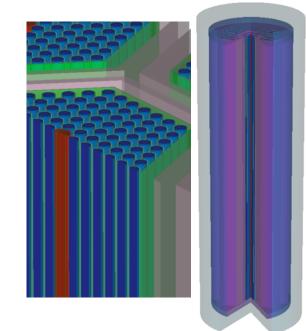
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# Summary

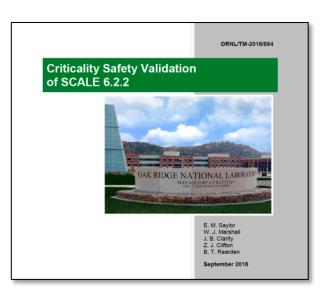
- Improved infrastructure
  - New software management on GitLab
  - Additional testing,
     esp. for Shift



- 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)

