OAK RIDGE National Laboratory

Recent Developments in SCALE

ANS Winter Meeting
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Washington DC

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U.S. 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.

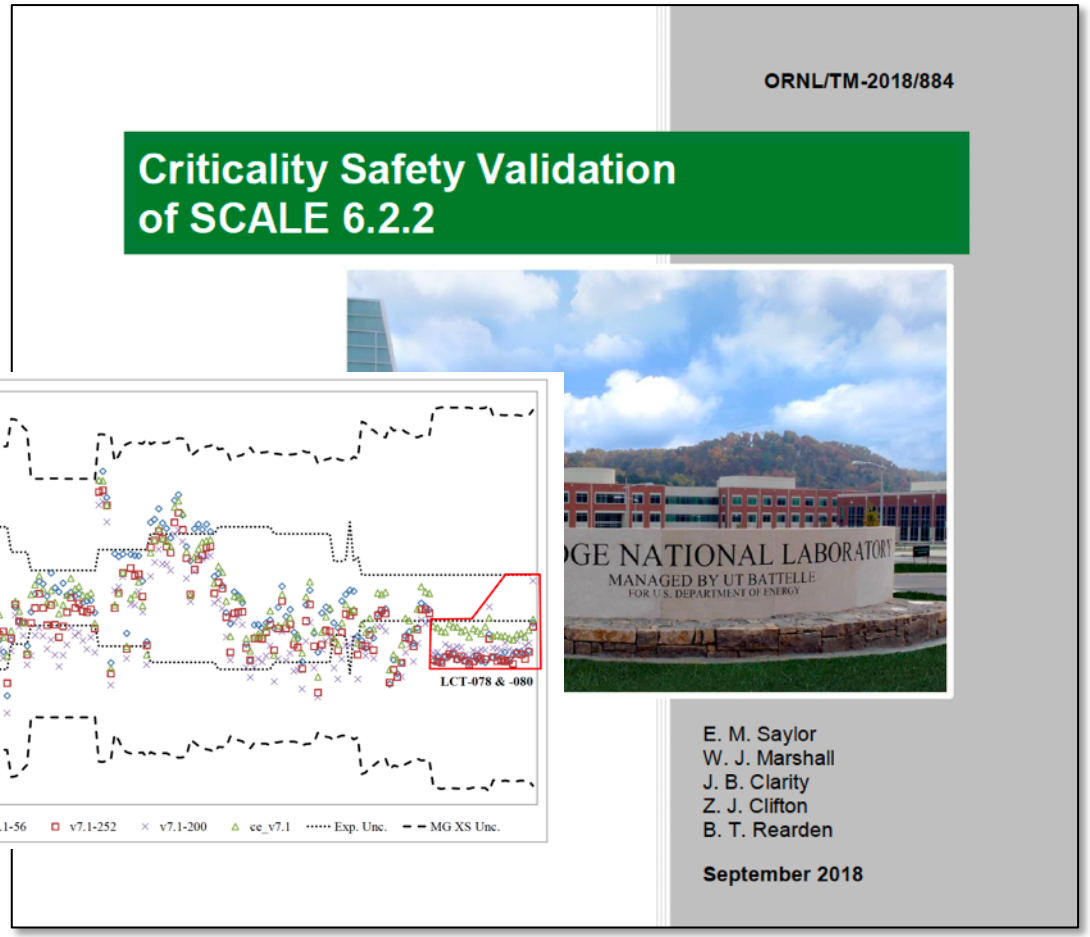
ORNL-AM2.1

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



ORNL-AM2.2

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

Linux

Build Name	Update	Configure		Build		Test		
	Files	Error	Warn	Error	Warn	Not Run	Fail	Pass
master-linux-gcc-ampx		0	1	0	21 +6 -6	0	0	207
master-linux-gcc-bundle		0	1	0	41 +6 -6			
master-linux-gcc-mpi		0	0	0	200			
master-linux-gcc-mpi-all-packages		0	1	0	200	0	0	2667 +1 -28
master-linux-gcc-regression-sample		0	1	0	27	0	0	1193 +1 -52
master-linux-gcc-static		0	1	0	7	0	0	355 +18 -1
master-linux-gcc-unit-debug		0	1	0	36	0	0	1628 +2 -11
master-linux-intel-ampx		0	1	0	198	0	0	207
master-linux-intel-mpi		0	1	0	200	0	0	2350 +1 -27

Darwin

Build Name	Update	Configure		Build		Test		
	Files	Error	Warn	Error	Warn	Not Run	Fail	Pass
master-mac-clang-unit		0	5	0	200 +3	0	0	1106 -12
master-mac-gcc-bundle		0	3	0	200			
master-mac-gcc-regression-sample		0	5	0	200	0	0	1195
master-mac-gcc-unit		0	5	0	200	0	0	1106
master-mac-gcc-unit-debug		0	5	0	200 +4	0	0	1106

Windows

Build Name	Update	Configure		Build		Test		
	Files	Error	Warn	Error	Warn	Not Run	Fail	Pass
master-windows-intel-ampx		0	22	0	200 +32 -114	0	0	200 +31
master-windows-intel-bundle		0	21	0	200 +199 -199			
master-windows-intel-regression-sample		0	21	0	200	0	0	1186 -52
master-windows-intel-unit		0	21	0	200 +3	0	0	1088 -12

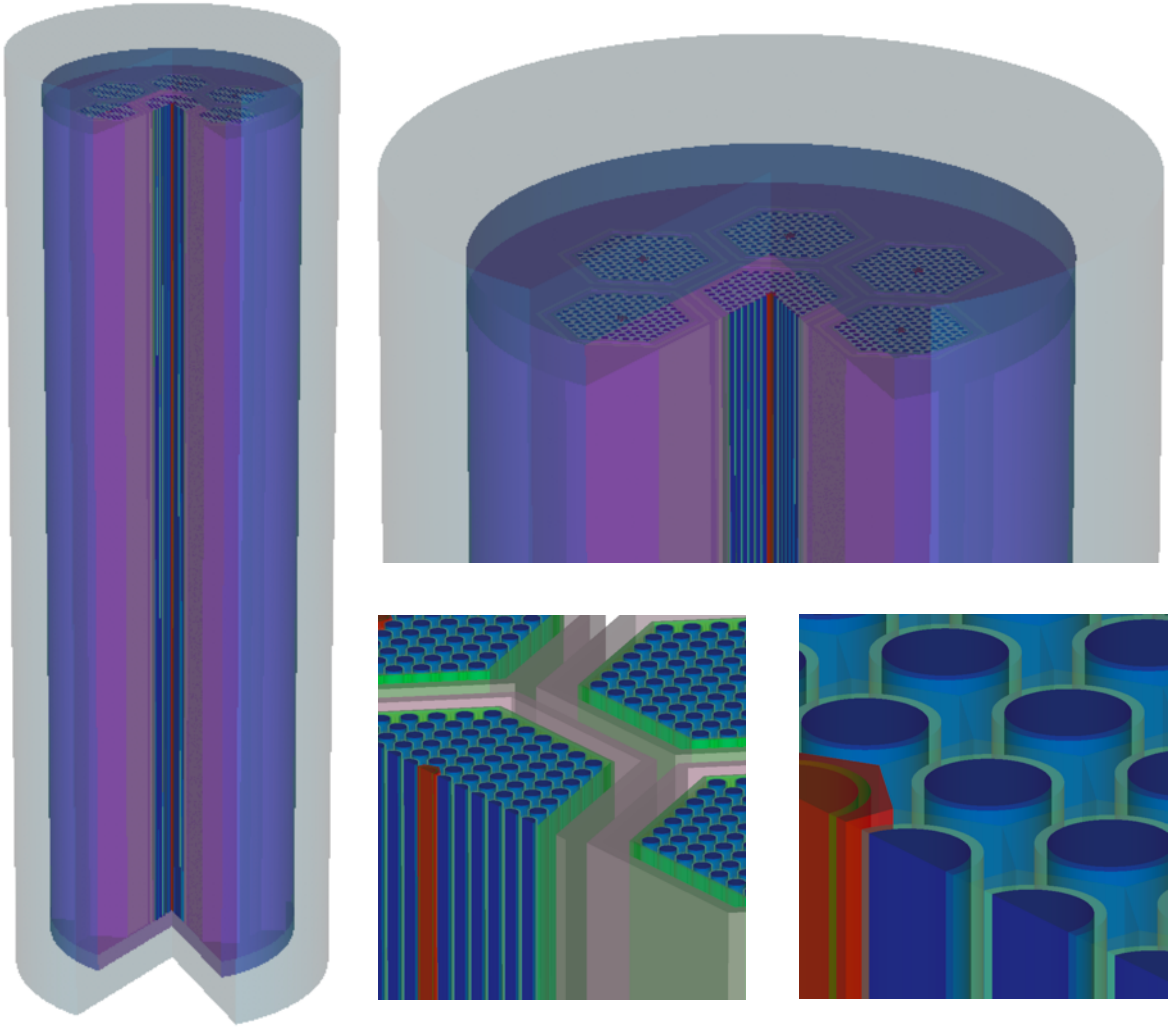
http://ci.ornl.gov/CDash/index.php?project=SCALE

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



Fulcrum 3D visualization

ORNL-AM2.4

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
  upcoming newsletter will discuss "open" 6.3 beta and 6.2.4 maintenance update

- Supported user inquiries/reports through scalehelp@ornl.gov
  User-submitted criticality calculation defect resulted in rapid communication and resolution

- Continue to host Annual SCALE Users Group Workshop

ORNL-AM2.5

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/rnsd/scale

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Strategy for Shift integration into SCALE

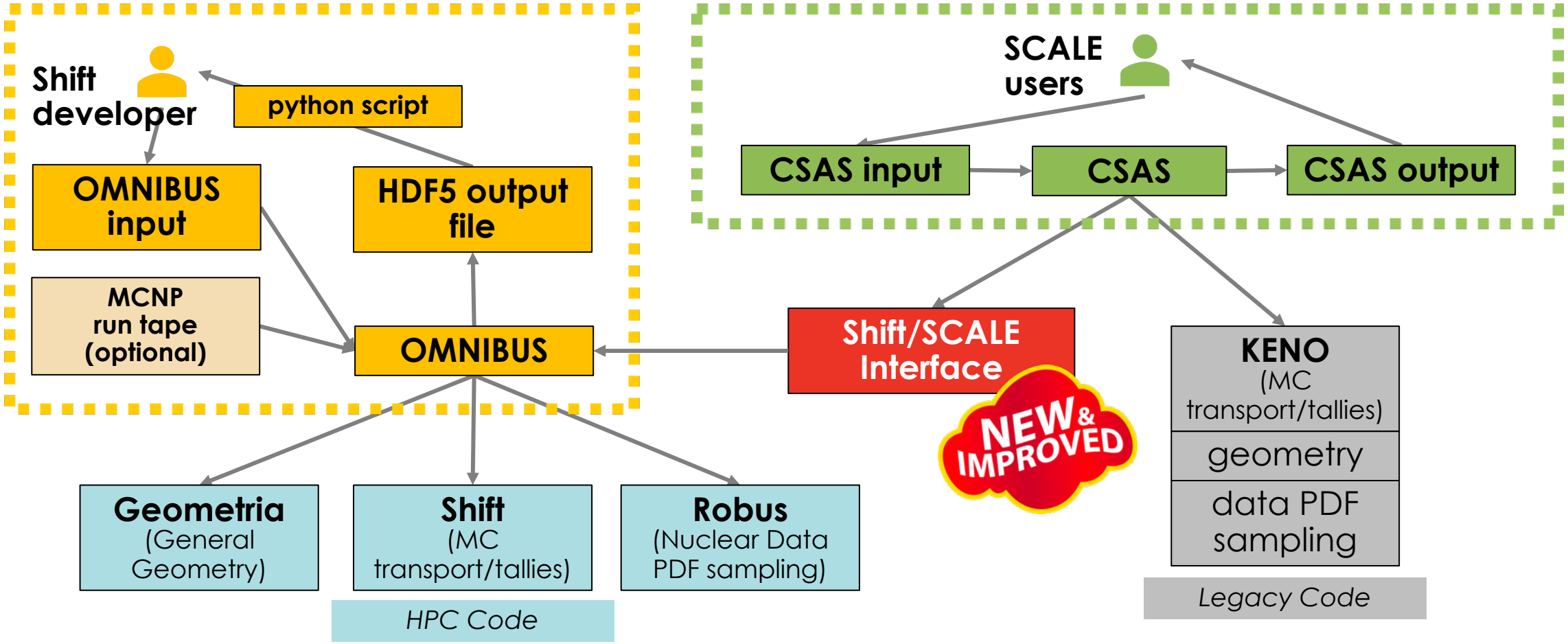
- The goal is to be as transparent to the user as possible
- Ultimately, the only input change that should be required is changing the sequence name; appending **–shift** to sequence name

```
=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
```

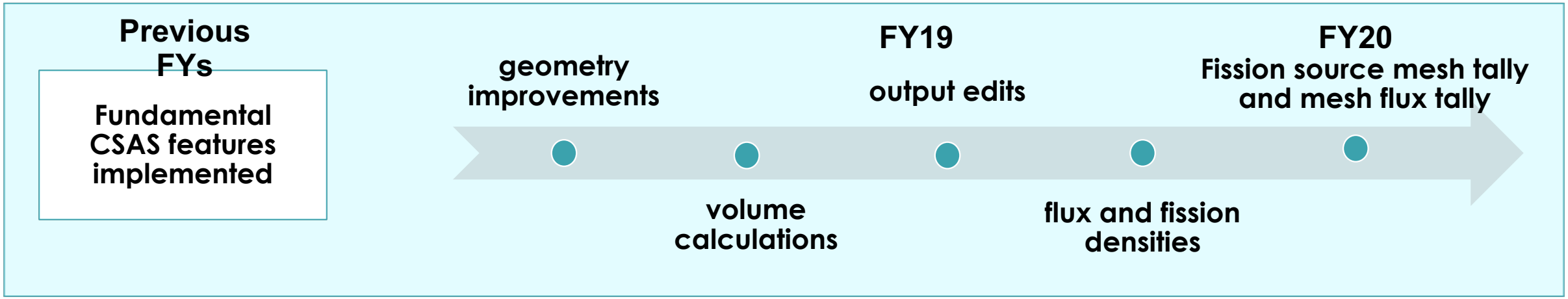
```
=csas5-shift
godiva-k5
ce_v7.1_endf
read composition
 u-234      1 0 0.000491995 300    end
 u-235      1 0 0.0449996   300    end
 u-238      1 0 0.002498    300    end
end composition
read parameter
 htm=no
end parameter
read geometry
global unit 1
 sphere 1 1    8.741
end geometry
end data
end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

SCALE Monte Carlo Developments

Simultaneously support **Shift HPC** users and **SCALE** users



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**

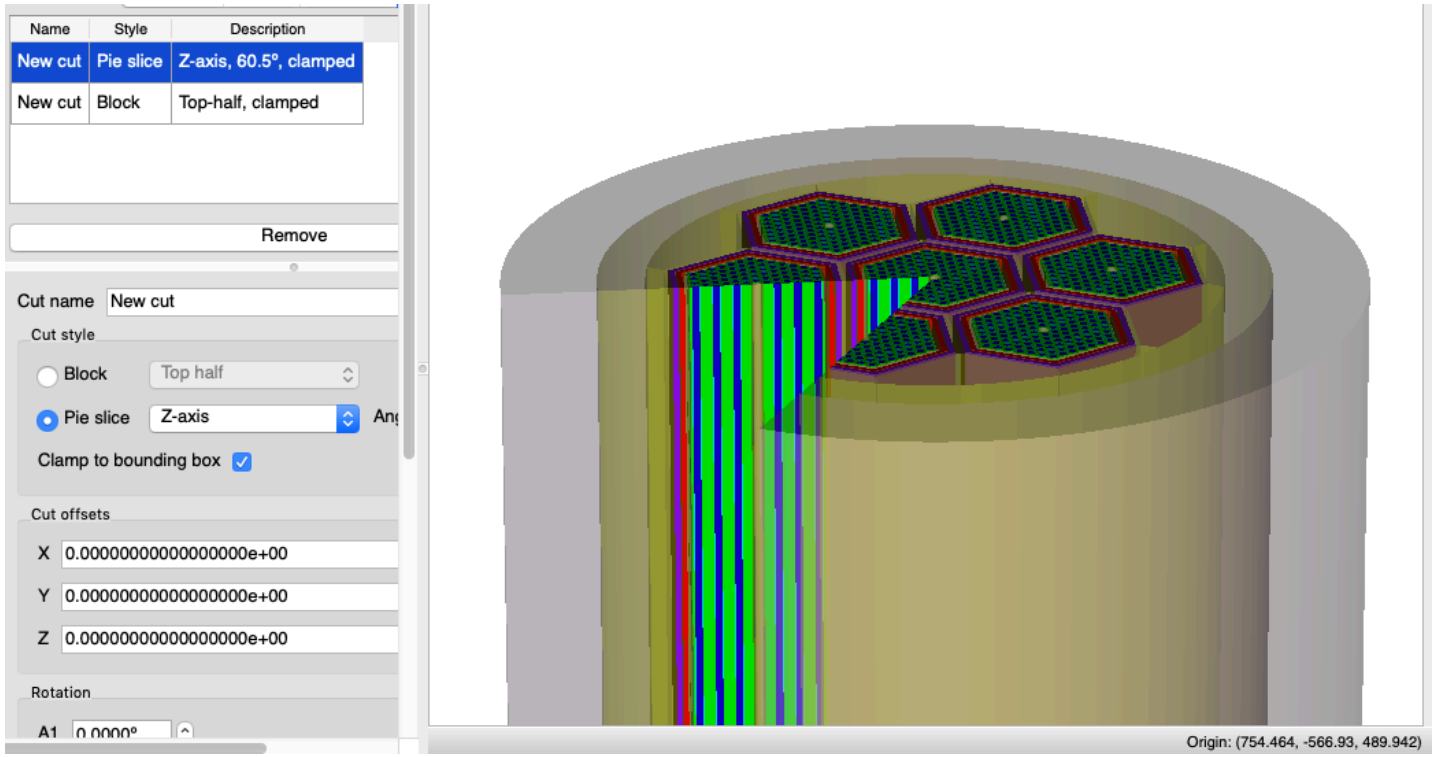
- Volume calculations
  - KENO-VI geometry with parallel volume calculation with ray-tracer
  - KENO-V geometry allows for analytic volume calculation--enabled

- **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

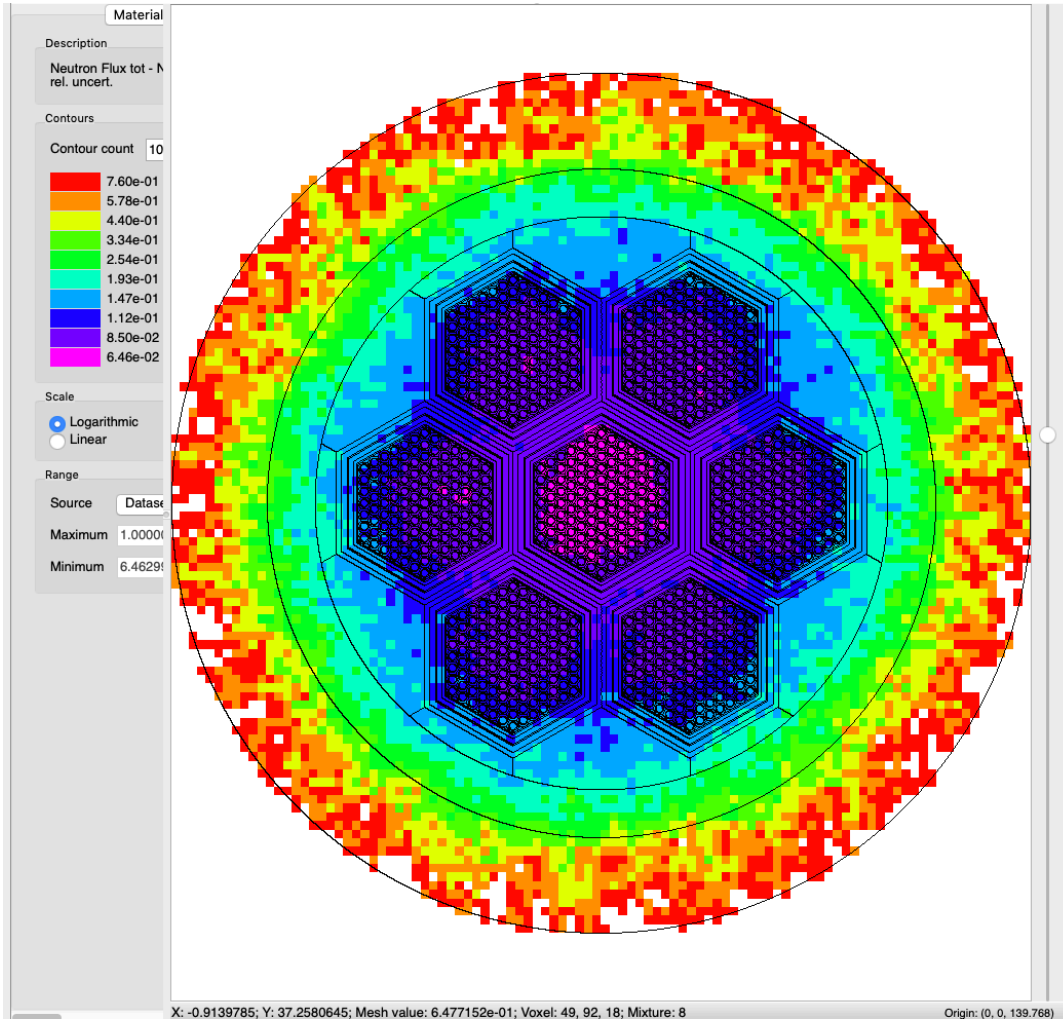


- We also tally fission source distribution on a mesh (CDS parameter) and visualize it to test the convergence
- Open and run *castor_cask_default_parameters.inp*

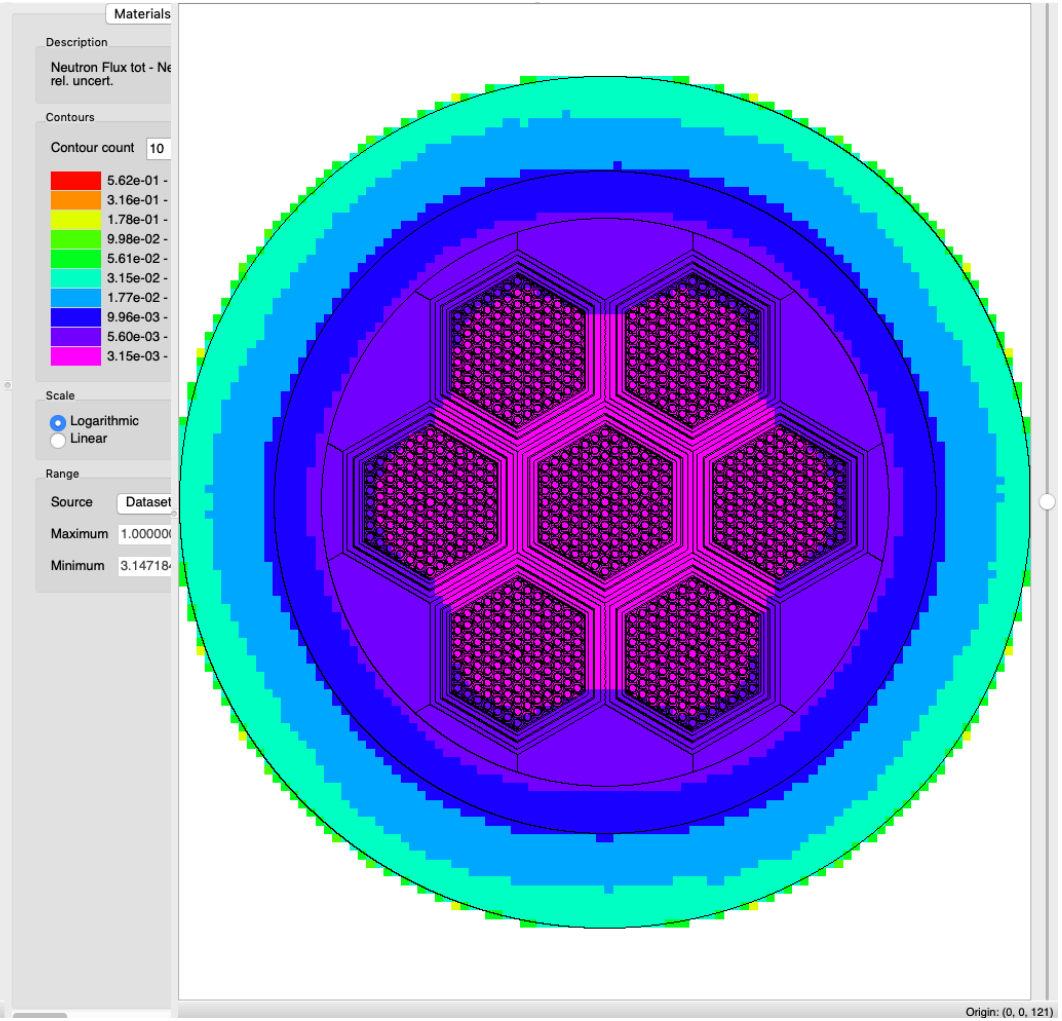
From October 2019 NRC Training

Comparison of Neutron Flux Std. Dev. at NPG=1000,100000

NPG=1000, NSK=3, GEN=203



NPG=100000, NSK=100, GEN=1000



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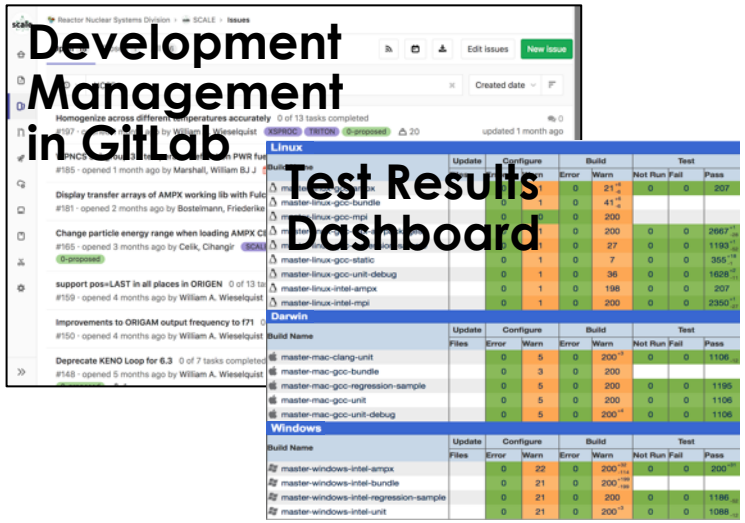
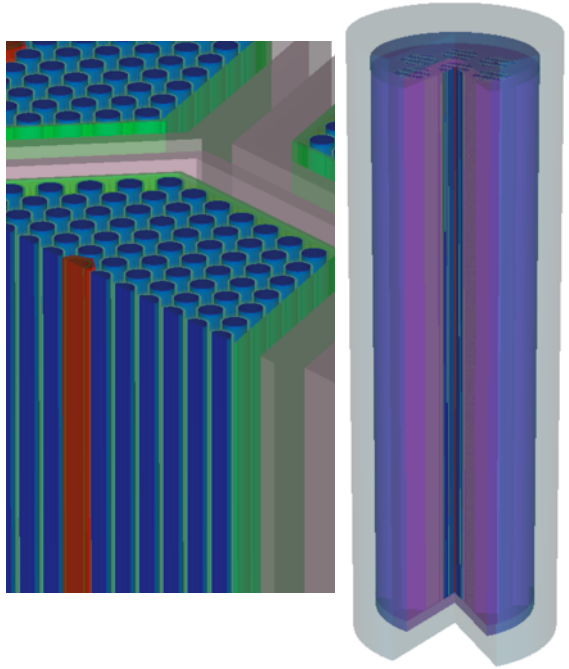
Summary

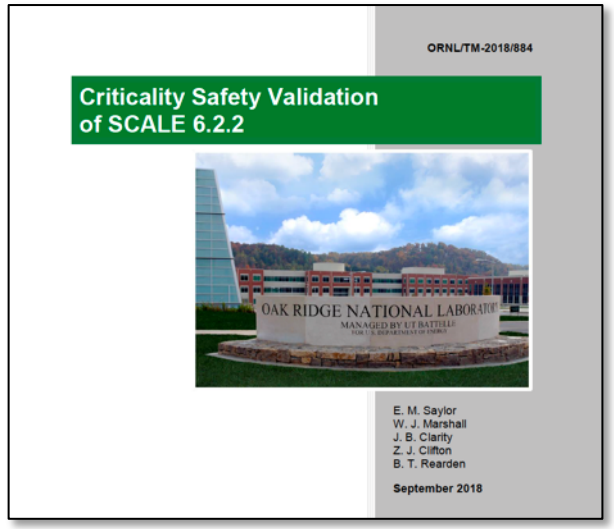
- Improved infrastructure
  - New software management on GitLab
  - Additional testing, **esp. for Shift**



- 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**



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Questions?