

# SCALE in 2021 and Beyond

SCALE Users' Group Workshop July 27, 2020

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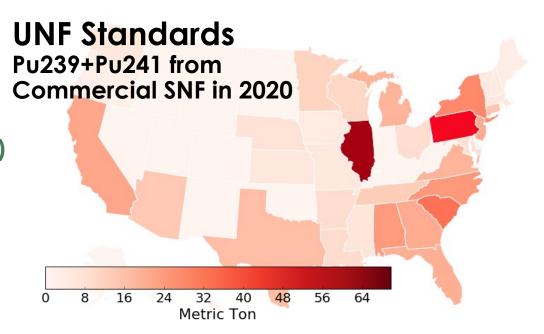
## Overview

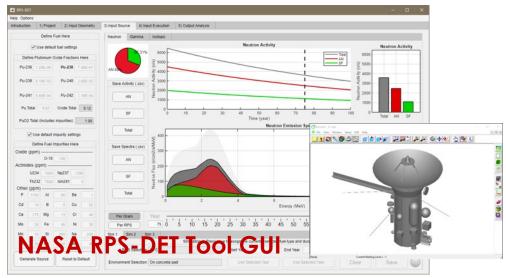
- Near term activities
  - Support
  - Optimize
  - Innovate
- Vision for SCALE in 2021 and beyond
  - Release schedule
  - Key features



## Users of SCALE

- Conventional users (2004 to Jan 2020)
  - ~15000 copies of SCALE
  - ~9500 unique users in 61 nations
  - ~5000 6.2.\* users (6.2.4 is last production release)
- ORNL UNF Standards Project
- DOE CASL VERA Core Simulator
- DOE Exascale Computing Project (ECP)
- X-Energy DoD Micro Reactor Shielding Design
- NASA The Radioisotope Power System Dose Estimation Tool (RPS-DET)
- IAEA RADAR Safeguards System
- ORNL Transformational Challenge Reactor (TCR)





## SCALE 6.3 Team

#### **Director**

**Direction Team** 

Will Wieselquist

**Production Coordinator** 

Rob Lefebvre

**User Support Coordinator** 

Germina Ilas

**Technology Coordinator** 

Seth Johnson

**Quality Assurance Coordinator** 

Marsha Henley

**NCSP** Representative

B.J. Marshall

NRC Representative

Matt Jessee

Radiation Transport Group Leader

**Bob Grove** 

Nuclear Data and Criticality Safety

Group Leader

Doug Bowen

### OAK RIDGE National Laboratory

#### **Product Owners**

**AMPX** Doro Wiarda

**CSAS** Kursat Bekar

**DATA** Andrew Holcomb

FULCRUM Rob Lefebvre

MAVRIC Cihangir Celik

**OMNIBUS** Seth Johnson

**ORIGAMI** Steve Skutnik

**ORIGEN** Will Wieselquist\*

**POLARIS** Matt Jessee

**SAMPLER** Ugur Mertyurek

**STDCOMP** Rob Lefebvre\*

**TRITON** Rike Bostelmann

**TSUNAMI** Will Wieselquist\*

**VADER** Shane Hart

**XSPROC** Kang Seog Kim

\*Interim owner

### Dev/Testing/Analysis

Brian Ade Steven Hamilton

Mark Baird Briana Hiscox

Kaushik Banerjee Israel Huff

Ben Betzler Jianwei Hu

Elliot Biondo Brandon Langley

Jesse Brown Jordan McDonnell

Joey Burns Paul Miller

Chris Chapman Tara Pandya

Justin Clarity Douglas Peplow

Riley Cumberland Marco Pigni

Gregory Davidson Georgeta Radalescu

Mathieu Dupont

Tom Evans Kat Royston

Cole Gentry

Tarek Ghaddar

Travis Greene

Bob Hall

Jose Perez Ellen Saylor

Joel Risner

Ryan Sweet

Erik Walker

#### NRC Projects Office

Program Manager

Bruce Bevard

**Business Ops Manager** 

Linsey Aloisi

#### NCSP Execution Manager

Doug Bowen

**Business Systems** 

Marsha Henley

## **Support** sponsors and users

- Newsletter 52, thanks to User Support Coordinator, Germina Ilas
- New releases, thanks to Production Coordinator, Rob Lefebvre
  - 6.2.4 maintenance update for production series
  - two 6.3 beta releases per quarter

Table 1. SCALE version support and end-of-life dates

Version	0,1,2,3,44.4a	5.0	5.1	6.0	6.1	6.2	6.3
Customer support	No	No	Limited	Limited	Limited	Yes	Yes
Technical support	No	No	No	No	No	Yes	Yes
Release date	2000	2004	2006	2009	2011	2016	~2020
End-of-life date	NA	NA	2019	2019	2020	~2023	~2026

**customer support**: installation, compatibility with OS **technical support**: help using the code

 Virtual Users' Group Workshop and Training, thanks to Sandra Poarch, Germina Ilas, Marsha Henley

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https://www.ornl.gov/file/spring-2020-scale-newsletter/display

- 4-volume SCALE validation report 2020
  - vol 1: Summary
  - vol 2: Criticality Safety
  - vol 3: Reactor Physics
  - vol 4: Shielding



## **Optimize** capabilities and processes

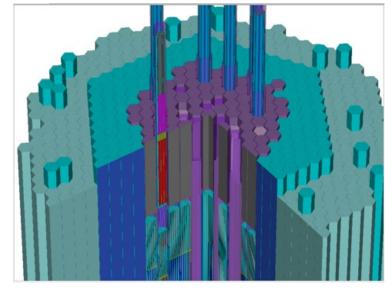
- Communication via website
  - gather SCALE publications in one place with OSTI download link
  - QA & release info (in progress)
    - "known discrepancies" tracked on webpage for each production release
    - beta release page with official SQA feature descriptions
    - online documentation for each beta release
- SCALE code repository is home to 3 major projects
  - HPC-focused (Exnihilo): Denovo, Shift
  - Nuclear data processing: AMPX
  - "Traditional" sequences: ORIGEN, MAVRIC, TRITON, CSAS, Polaris, ORIGAMI, Sampler, etc.

- Software usage
  - Traditional end-users of "sequences"
    - SCALE should be a one-stop shop for input setup/job launch/analysis
  - Application builders
    - API users linking to SCALE for capabilities
    - Driving SCALE input/processing output
  - Methods R&D
    - Benchmark implementation
    - Realistic test bed
- Development processes
  - Open source and export-controlled code in same repo, under same QA plan
  - Feedback loop
     Request→Plan→Feature→Release→Feedback



## **Innovate** with new methods and data

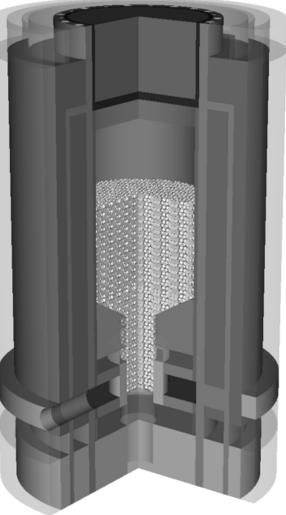
- CE and MG method improvements
  - Fast reactor MG library
  - Improved HTGR performance
- Shift integrations
  - parallel MAVRIC-Shift
  - nodal methods in TRITON-Shift
- Sensitivity indices in Sampler
- Sensitivity methods in ORIGEN
- 3D Visualization in Fulcrum



**SCALE Model of EBR-II** 

- Modernization of trend analysis code (USLSTATS→VADER)
- ENDF/B-VIII data with new scattering kernels





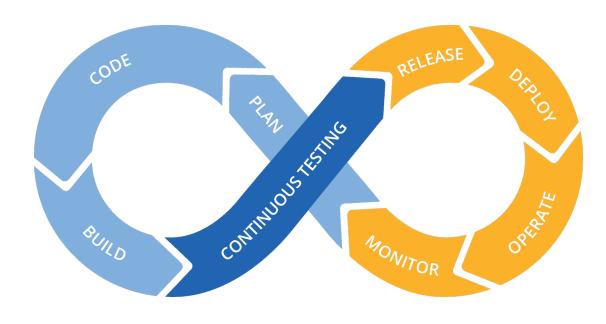
# Looking forward: important releases

- No more maintenance releases for the 6.2 series (6.2.4 was last)
- September 2020: SCALE 6.2.4 validation report
- Dec 2020: first in the 6.3 series. 6.3.0
  - maintenance releases (6.3.1, 6.3.2, ...) as needed
  - September 2021: SCALE 6.3 validation report
- Mid 2021: 7.0 beta1
- Dec 2023: 7.0 series release (7.0.0)
  - no more technical support for 6.2

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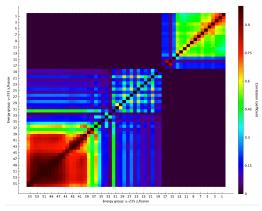
# Vision for SCALE 7.0 betas (2021-2023) INFRASTRUCTURE

- Installation and verification is trivial ©
  - Fulcrum-guided installation asks which codes to install and knows which data sources those depend on--only that data is downloaded
  - Users run test suites from Fulcrum or command line
    - fast-running installation tests
    - code-specific verification & validation suites
    - user-created test suites
- Linking external applications to SCALE
  - Non-export controlled parts of SCALE are openly available
  - High-quality, easy-to-use APIs with online documentation targeting ORIGEN and XSPROC
  - C++ based with Python and Fortran interfaces
  - Standard data formats let's users easily load their own data

# Vision for SCALE 7.0 betas (2021-2023)

#### DATA UNCERTAINTY AND SENSITIVITY

- New uncertainty data
  - delayed neutron
  - thermal scattering
  - energy release/deposition



- Cross-correlations
  - correlations can exist between any data (delayed neutron fraction and decay constant)

correlations can be added by validation/data assimilation processes

## Sampling

- random samples (realizations) of data can be made on-the-fly
- realizations are traceable and reproducible across platforms

## Sensitivity

- SDF format is generalized
- can store sensitivity of any response to any nuclear data



# Vision for SCALE 7.0 betas (2021-2023) CAPABILITIES

- Shift-based reactor physics is a complete non-LWR reference solution
  - flexible and performant geometry (MCNP-style, KENOstyle, randomized, some CAD capability?)
  - robust source convergence monitoring
  - fuel flow models (HTGR/MSR)
- Polaris
  - significantly faster runtime

- non-LWR lattice physics capability
- Search and optimization
  - any SCALE model can define parameters for search/optimization
- ORIGEN reactor libraries
  - rapid isotopics generation for HALEU, HBU, ATF, and non-LWR systems
  - stable interfaces to severe accident analysis, inventory management and fuel cycle



# Vision for SCALE 7.0 betas (2021-2023) **DOCUMENTATION**

- Website
  - Recent journal papers/TMs
     (~weekly updates) with inputs
  - 7.0 Beta release notes
  - 6.3.\* Production release "known discrepancies" page
- Validation Reports
  - Annual validation report for the current production version of SCALE
  - Validation suites available to users, automated run and post-

processing

- Add to suite annually based on current priorities
- Manual
  - Web HTML and PDF versions
  - Updated each beta release
- New Primers
  - CSAS in the works
  - Others to follow



# Summary

- Upcoming SCALE 6.3.0 features will be discussed at this Workshop--current beta used in some tutorials
- Version 7.0 next @ (betas to start in 2021)
  - increase installation ease and verification robustness
  - add/refine sensitivity and uncertainty (with better connection to validation for non-keff responses)
  - best in world Monte Carlo reactor physics with Shift
  - generalize sensitivity storage, search and optimization
  - provide online manual, validation report, primers, window into our SQA

#### **Acknowledgements**

Thanks to our DOE, NCSP, NRC sponsors and GAIN for their support for this meeting!

Thanks to Sandra Poarch and Germina Ilas for planning this meeting!

Thanks to our speakers and tutorial leaders and all other participants!

