

Emerging Initiatives in SCALE

Presented to:

2018 SCALE Users' Group Workshop

Presented by:

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August 27, 2018

ORNL is managed by UT-Battelle, LLC for the US Department of Energy





SCALE Evolution (1976 – present)



SCALE 0.0 - SCALE 4.4a

1980 - 2000

Established for Nuclear Regulatory Commission

Provides an independent rigorous nuclear safety analysis capability for out-of-reactor license reviews

Key Capabilities

Criticality safety

Radiation source term characterization

Radiation shielding

Heat transfer

SCALE 5.0 – SCALE 6.1

2004 - 2011

Expanded Capabilities to Address a Broader Classes of Analysis

Reactor physics for LWR, MOX, HTGR, CANDU, FHR, and high-burnup fuels

Shielding analysis for large, complex systems with automated variance reduction

Sensitivity and uncertainty analysis, especially for validation and gap analysis

High-fidelity criticality safety in continuous energy

Graphical user interfaces and visualization tools

Expanded impact

Used in 56 nations by regulators, industry, utilities, and researchers

SCALE 6.2

2016 - 2018

Increased Fidelity, Infrastructure Modernization, Parallelization, Enhanced Quality Assurance

Solutions for extremely complex systems

High-fidelity shielding, depletion and sensitivity analysis in continuous energy

Simplified and efficient lattice physics

Unified user interface

Modern, modular software design integrated with QA

Expanded Use

9,000 users

Tools leveraged by many projects

SCALE 6.3 – SCALE 7.0

2018 -

High-performance Monte Carlo, Capabilities for Advanced Reactors and Advanced Fuels, Integration with Many other Tools

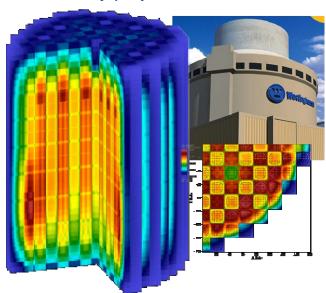
Focused capabilities for ATF and nonLWR

High-fidelity, highly parallelized criticality shielding, depletion and sensitivity analysis in continuous energy

Extended modern, modular software design

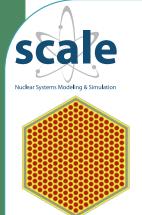
Expanded Integration

Tools directly integrated with many projects





SCALE is part of the NRC's reactor licensing path



ENDF

Physics data
Thermal scattering law,
resonance data,
energy distributions,
fission yields, decay
constants, etc.

AMPX

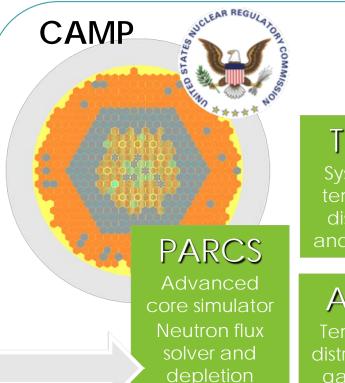
Validated cross section libraries in multigroup (O(100g)) or continuous-energy (O(100,000g); depletion and decay data

TRITON / Polaris

Transport and depletion in 1D, 2D, and 3D for LWR, ATF, and nonLWR

ORIGEN / ORIGAMI

Depletion, activation and decay Reactor-specific radioactive source term characterization



FAST

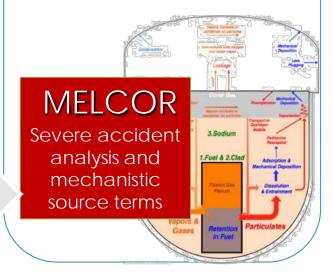
Fuel performance

TRACE System level temperature distributions and feedback

AGREE

Temperature distributions for gas reactors

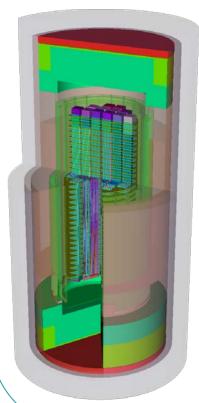






SCALE is part of NRC's transportation and storage licensing path





UNF-ST&DARDS

Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data System

ENDF

Physics data
Thermal scattering law,
resonance data,
energy distributions,
fission yields, decay
constants, etc.

AMPX

Validated cross section libraries in multigroup (O(100g)) or continuous-energy (O(100,000g); depletion and decay data

TRITON / Polaris

Transport and depletion in 1D, 2D, and 3D for LWR, ATF, and nonLWR

CSAS / KENO

3D criticality safety analysis

MAVRIC / Monaco

3D shielding and dose rate analysis

TSUNAMI

Sensitivity and uncertainty analysis and validation applicability

ORIGEN / ORIGAMI

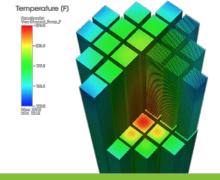
Depletion, activation and decay Reactor-specific radioactive source term characterization

Structural analysis

ANSYS / LS-DYNA

Commercial finite element analysis

Thermal analysis

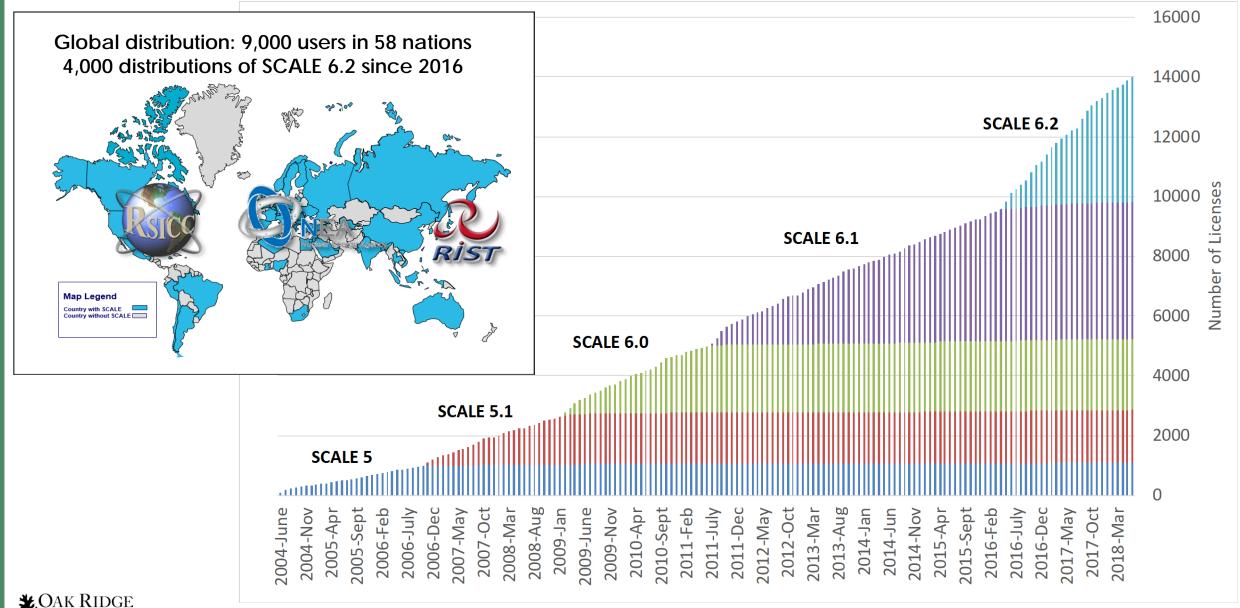


STAR-CCM+ / FLUENT

Commercial computational fluid dynamics codes



SCALE licenses by version



SCALE training courses are routinely provided to the user community

Public courses at ORNL and NEA Application-specific training provided at NRC and user facilities

Sensitivity and Uncertainty Analysis for Criticality Safety October 15-19 Assessment and Validation

October 22-26 SCALE/TRITON Lattice Physics and Depletion

SCALE/ORIGEN Standalone Fuel Depletion, Activation, October 29 -November 2 and Source Term Analysis

November 5 – 9 SCALE Criticality Safety and Radiation Shielding











Collaboration with other projects:

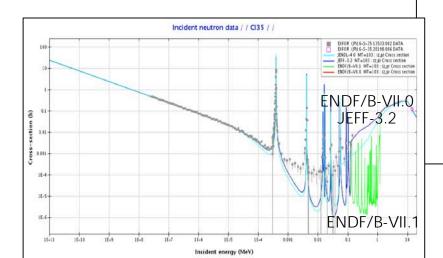
- DOE Nuclear Data and Benchmarking (ND/B) Program
- NNSA Nuclear Criticality Safety Program
- DOE Used Fuel Disposition (UFD) R&D Program
- High performance computing:
 - DOE-NE Consortium for the Advanced Simulation of LWRs (CASL)
 - Exascale Computing Project

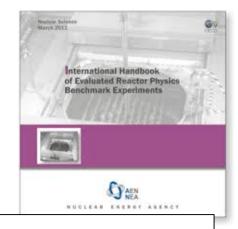


Nuclear Data and Benchmarking Program



- New Nuclear Energy Enabling Technology (NEET) Crosscutting Program
- Partner with industry, NRC, and other programs to:
 - Identify priority needs for nuclear data and benchmarking
 - Perform new data measurements and evaluations
 - Support integral experiments and handbooks
 - Participate in application benchmark studies





PROGRAM ANNOUNCEMENT TO DOE NATIONAL LABORATORIES



U. S. Department of Energy Office of Science Nuclear Physics

Nuclear Data Interagency Working Group / Research Program

OE National Laboratory Announcement Number: LAB 17-1763
Announcement Type: Initial

ie Date: 04/26

er of Intent Due Date: 05/12/2017 at 5 PM Eastern Tim

ourage/Discourage Date: 05/26/2017 at 5 PM Eastern T

ation Due Date: 07/21/2017 at 5 PM Eastern Time

USE OF SENSITIVITY AND UNCERTAINTY ANALYSIS IN THE DESIGN OF REACTOR PHYSICS AND CRITICALITY BENCHMARK EXPERIMENTS FOR ADVANCED NUCLEAR FUEL

REYWORDS: sensitivity and i certainty analysis, experiment sign, highly enriched fuel

B. T. REARDEN Oak Ridge National Laboratory, P.O. Box 2008 Oak Ridge, Tenneysee, 37831-6170

W. J. ANDERSON Framatome ANP, Inc., P.O. Box 10935, 3315 Old Forest Road Lynchburg. Virginia 24506,0935

G. A. HARMS Sandia National Laboratories, P.O. Box 5800

Received June 4, 2004

Franatome ANP, Sendia National Laboratories: SNL), On Ridge National Laboratory (ORNL), and the University of Florida are cooperating on the U.S. Department of Deray National Energy Research Initiative (NER), project 2001–0124 to design, assemble, execute, analyze, project 2001–0124 to design, assemble, execute, analyze, reactor physics and criticality safety codes for the analysist of commercial power reactor physics and criticality safety codes for the analysist of commercial power reactor playsic constitute of U.O. with 2012 enrichments 25 vrffs. The experiments will be conducted at the XIV. Plant of Research Excition.

Framatome ANP and SNL produced two series of conceptual experiment designs based on typical paramters, near as just-to-mosteriable ratios, that indeed the regularities and the control of this project within the glore growth and the control of the project within the glore seed the Dods for Sensitivity and Uncertainty Analysis fethodology indepensation (TSUMM) to assess, from detailed physics-based perspective, the similarity of the experiment designs to the commercial systems tive restanted to validate. Based on the results of the TSU-MM analysis, one series of experiment was found in sew data for the validation of reactor physics and critiulty suffer colors.

I. INTRODUCTION

Framatome ANP, Sandia National Laboratories (SNL), Oak Rége National Laboratory (ORNL), and the University of Florind (UP) are collaborating on the US. Department of Energy Nuclear Energy Research Initiative (NIRI) project 2001-1072 to design, assemble, analyze, and document as series of critical experiments to the experiments to the control of the Computer of the

.

(PWR) and boiling water reactor (BWR) UO₂ fuels with ²³⁵U enrichments ≥5 wt%.

At the inception of this project, a supply of nuclear help, originally manufactured for the PATHFINDER system intended for assembly at The Pennsylvanis State (ulversity) (Penn State) in the 1960s, was identified for use in the experiments. The PATHFINDER program was ventually succeeded, the full was never irradiated and current project, the PATHFINDER fuel has been shipped to SNL, for disastembly, Disassembly is necessary be-





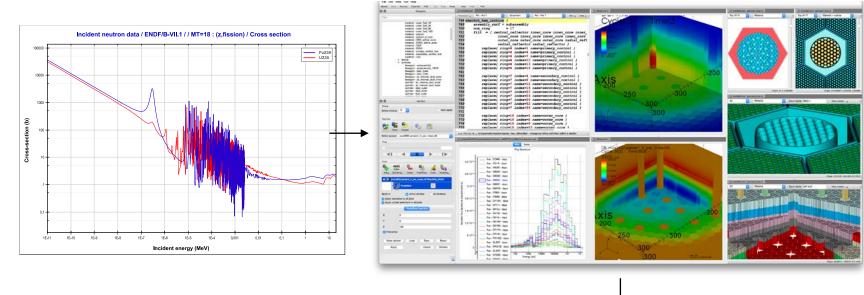
Nuclear data is necessary for reliable modeling and simulation of the next generation of nuclear reactors because of limited experimental data

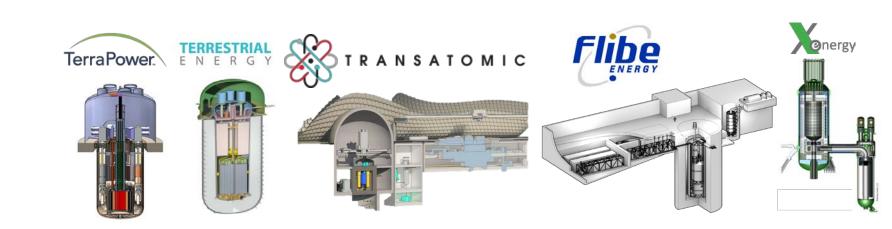
SCALE/AMPX

 assessment of nuclear data needs

• TSUNAMI/Sampler

- uncertainty quantification
- validation assessment
- experiment design









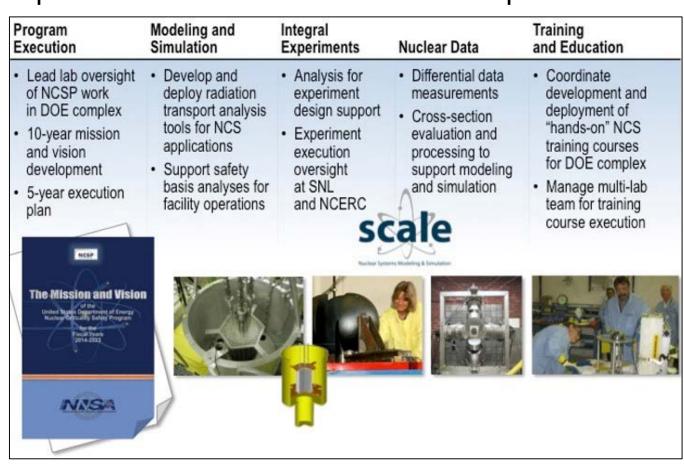
Collaboration with other projects:

- DOE Nuclear Data and Benchmarking (ND/B) Program
- NNSA Nuclear Criticality Safety Program
- DOE Used Fuel Disposition (UFD) R&D Program
- High performance computing:
 - DOE-NE Consortium for the Advanced Simulation of LWRs (CASL)
 - Exascale Computing Project



NNSA Nuclear Criticality Safety Program

- Technology infrastructure needed to enable sites to perform safe, efficient fissionable material operations in the DOE Complex
 - Nuclear data generation and testing
 - SAMMY, AMPX
 - Criticality safety assessments
 - AMPX, KENO
 - Criticality accident alarm system analysis
 - KENO, ORIGEN, MAVRIC
 - Validation and uncertainty quantification
 - TSUNAMI, Sampler
 - Nuclear criticality and shielding experiment design
 - TSUNAMI, MAVRIC



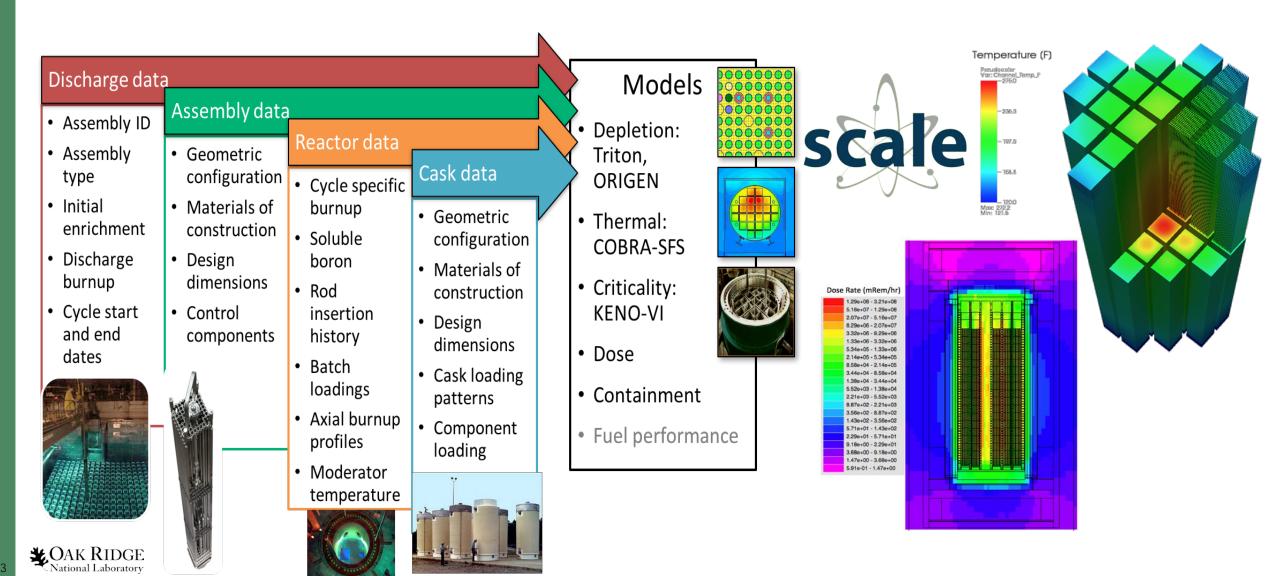


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UNF-ST&DARDS integrates data with analysis capabilities to simplify UNF characterization process





Collaboration with other projects:

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VERA Core Simulator

Virtual Environment for Reactor Applications Flexible multiphysics framework

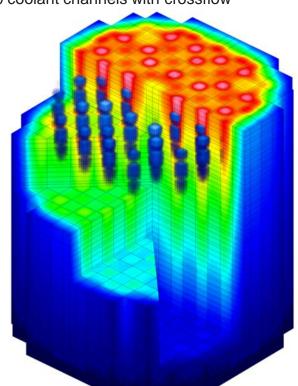
MPACT or Shift

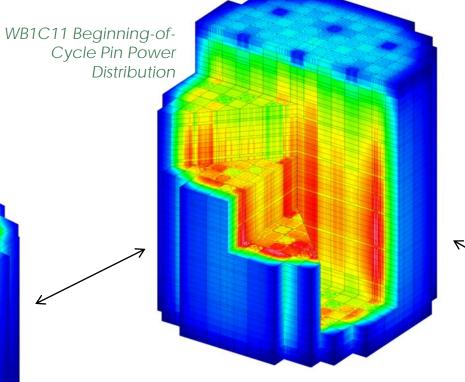
Advanced pin-resolved 3-D whole-core deterministic neutron transport in 51 energy group or continuous energy SCALE/AMPX nuclear data library

Mesh / Solution Transfer PETSC MPACT ORIGEN Thermal-Hydraulics COBRA-TF Common I/O & Visualization Veraln/Out VERAView

<u>CTF</u>

Subchannel thermal-hydraulics with transient two-fluid, three-field solutions in 14,000 coolant channels with crossflow



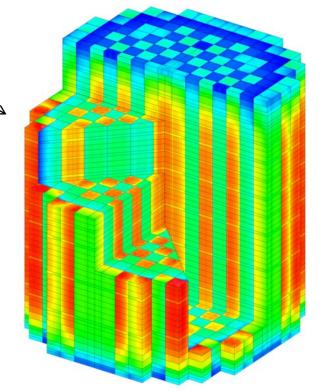


WB1C11 Middle-of-Cycle Coolant Density Distribution

WB1C11 End-of-Cycle Pin Exposure Distribution

SCALE/ORIGEN

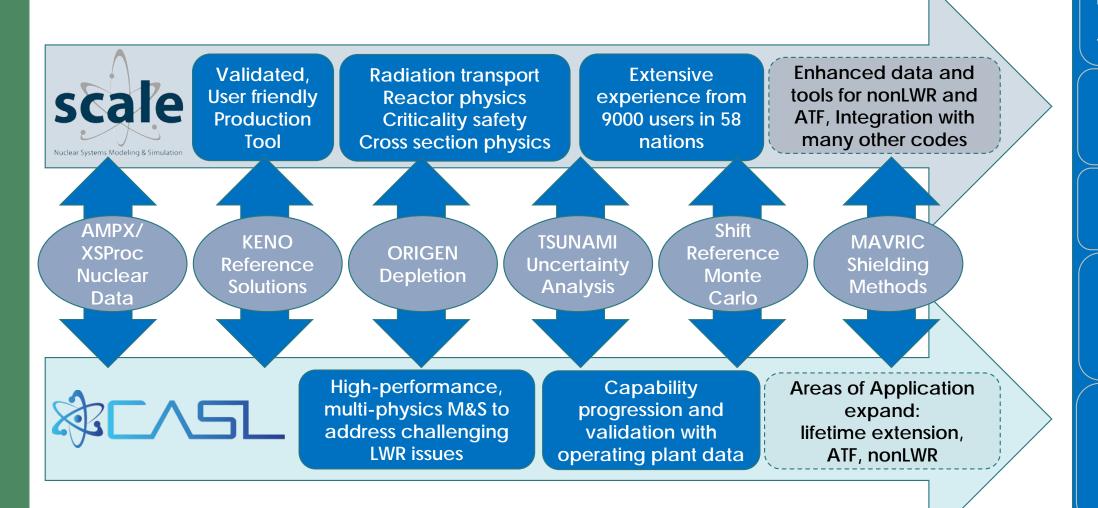
Isotopic depletion and decay in >2M regions tracking 263 isotopes in 2.5 million depletion regions





SCALE and CASL:

Meeting user needs while transforming the state-of-the-art



Wide range of integrated tools with strong validation basis

Versioned releases through RSICC

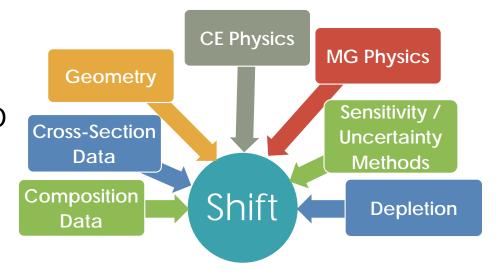
Attractive for capacity computing

Scalable from design scenarios to challenge problems

Flexible multiphysics framework for expansion to other nuclear applications

Shift Monte Carlo code system

- Flexible, high-performance Monte Carlo radiation transport framework
- Shift is physics agnostic
 - SCALE CE physics
 - SCALE MG physics
- Shift is geometry agnostic
 - SCALE geometry
 - Exnihilo RTK geometry
 - MCNP geometry
 - DagMC-CUBIT CAD geometry •

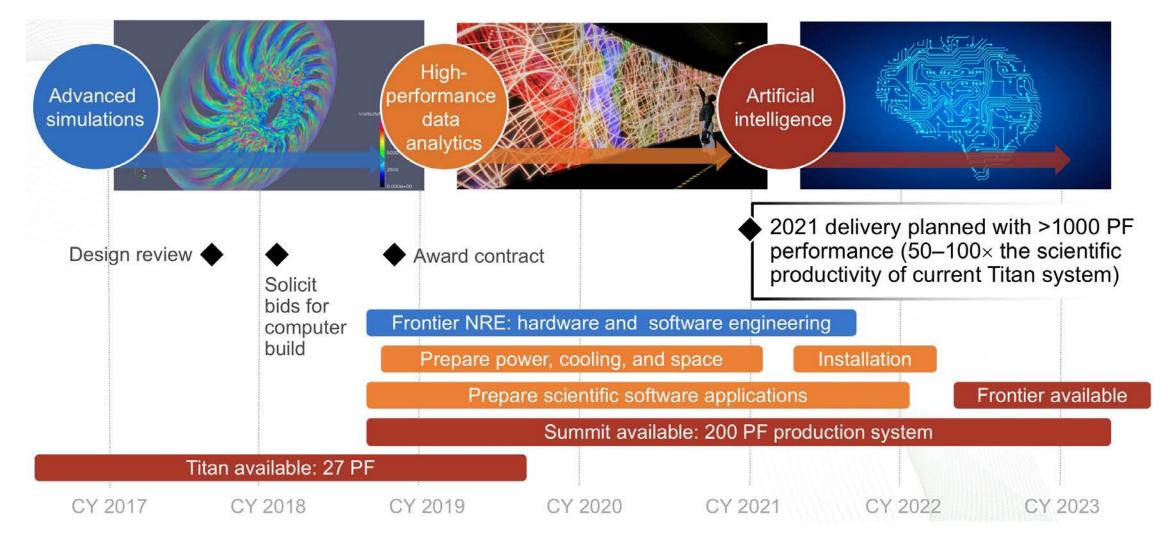


- Fixed-source and eigenvalue solvers
- Integrated with Denovo for hybrid methods
- Multiple parallel decompositions and concurrency models
- Shift is designed to scale from supercomputers to laptops

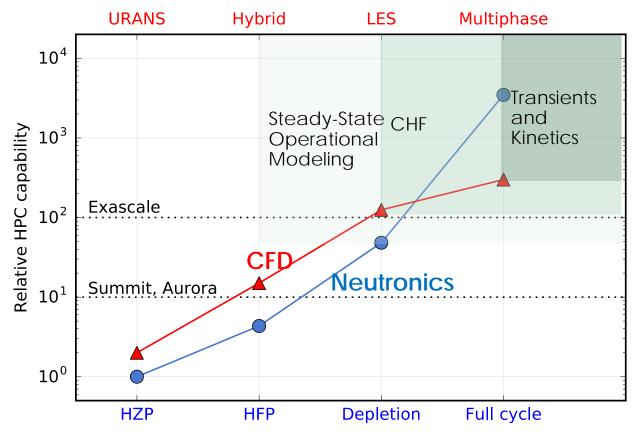


Shift is being extended for operation on GPUs as part of the \$2B Exascale Computing Project EXASCALE COMPUTING PROJECT

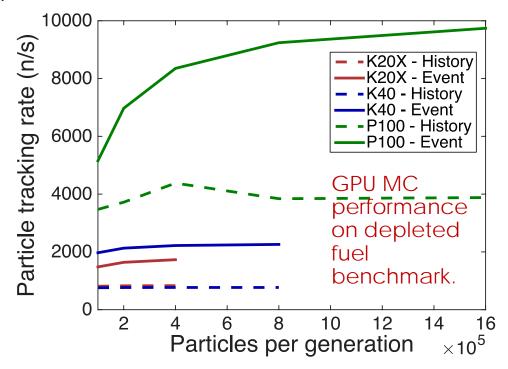




Application project: ExaSMR



- Improved Monte Carlo particle tracking rate allows reduction in statistical errors
- Cost of tallies and data access is implicit in this measure
- Improved device performance yields better results – Algorithms are tracking hardware improvements





SCALE 6.3

- Motivation Advanced Systems
- Nuclear data libraries
- Shift Monte Carlo Code
- Beta release



Abbreviated advanced reactor technology matrix (1/2)

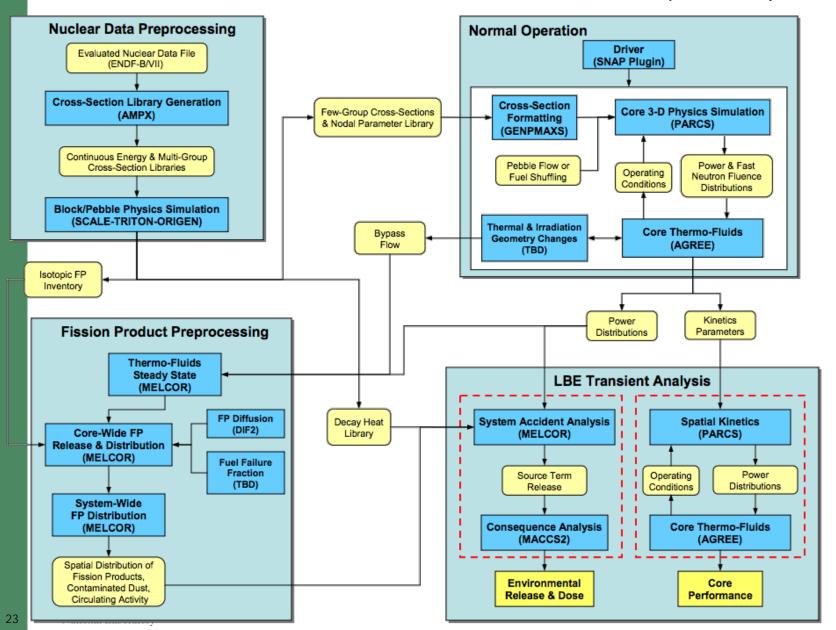
Reactor Type	Companies	Licensing action expected	Fuel / Enrichment	Thermal spectrum	Fast Spectrum	Coolant	Radial core expansion	Flowing Fuel	Fuel Form	Control elements
	Oklo	2019	~20%		✓	Sodium heat pipes	✓		Metallic Castings	External drums
HPR	Westinghouse (eVinci)	2019	19.75%	Thermal/ Epithermal		Sodium heat pipes (dual condenser)			Oxide	External drums
SFR	TerraPower (TWR)		~20%		✓	Sodium	✓		Metallic Rods	Internal rods
	GE PRISM		~20%		✓	Sodium	✓		Metallic Rods	Internal rods
LFR	Westinghouse		15-20%		✓	Lead	✓		Oxide/ Nitride	Internal rods
HTGR	X-energy (Xe-100)	2020s	15.5%	✓		Helium		Pebbles	TRISO	External rods
	Areva (SC-HTGR)		~20%	✓		Helium			TRISO	Internal rods
FHR	Kairos	2020s	~17%	✓		FLiBe		Pebbles	TRISO	External rods



Abbreviated advanced reactor technology matrix (2/2)

Reactor Type	Companies	Licensing action expected	Fuel / Enrichment	Thermal spectrum	Fast Spectrum	Coolant	Radial core expansion	Flowing Fuel	Fuel Form	Control elements
MSR	Terrestrial Energy (IMSR)	2019	~5%	√		Proprietary		Salt	Molten Salt	Internal rod
	Transatomic	2020s	~5%	Thermal/ Epithermal		FLiBe		Salt	Molten Salt	Internal ZrH moderating rods
	TerraPower (MCFR)	2020s	~20%		✓	Chloride salt		Salt	Molten Salt	External rods?
	Elysium		~20%		✓	Chloride salt		Salt	Molten Salt	
	FLiBe Energy		Thorium	√		FLiBe		Salt	Molten Salt	Internal rods

NRC NGNP Evaluation Model (2008)





NRC Evaluation Model Development

RIC 2010

Next Generation Nuclear Plant (NGNP) Research

J.M. Kelly USNRC Research March 11, 2010

Department of Energy

DOE, NRC Issue Licensing Roadmap For Next-Generation Nuclear Plant

AUGUST 15, 2008

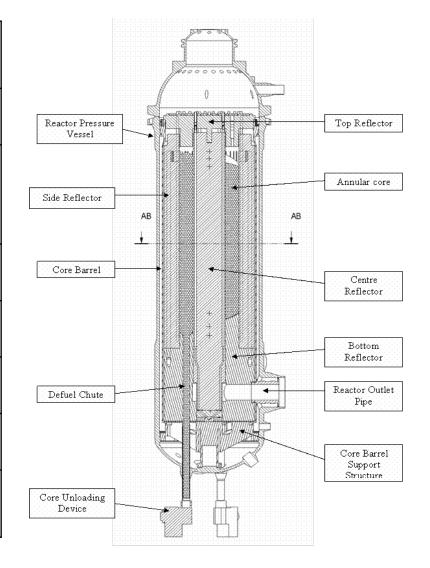
Home » DOE, NRC Issue Licensing Roadmap For Next-Generation Nuclear Plant

WASHINGTON, DC -The U.S. Department of Energy (DOE) and the U.S. Nuclear Regulatory

"The NRC's new reactor licensing process is currently focused on light-water reactors, and the staff is confident this basic framework can also support an NGNP review," said NRC Chairman Dale Klein. "We will work with DOE to supplement that framework with NGNP-specific items."

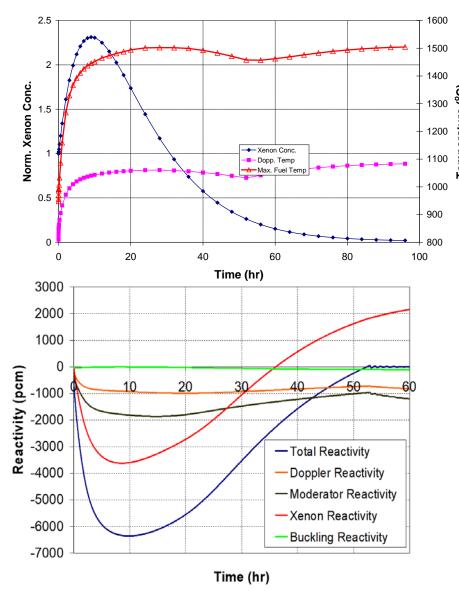
OECD/NEA PBMR-400 Benchmark

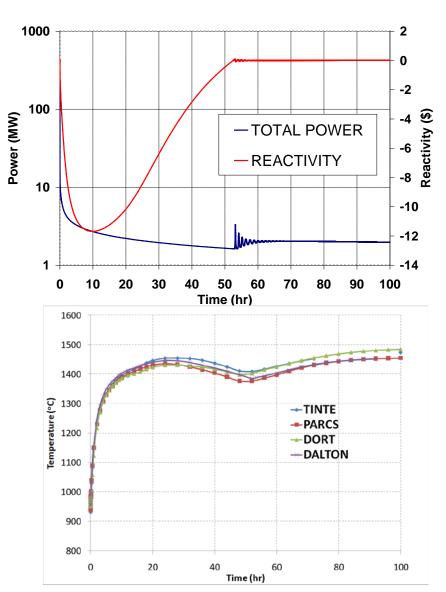
PBMR Characteristic	Value				
Thermal Power	400 MW				
Core configuration	Vertical with fixed centre graphite reflector				
Outer diameter	3.7 m				
Core Height	11 m				
Reactor pressure	9МРа				
Mass flow rate	192.5 kg/s				
Core inlet temperature	500°C.				



SCALE/PARCS/AGREE CASE T-1: Depressurised Loss of Forced Cooling (DLOFC) without SCRAM

XENON Concentration / FUEL Temperatures

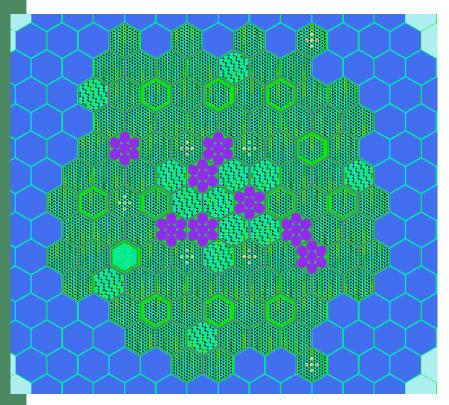


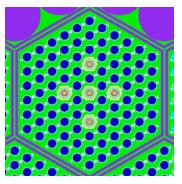




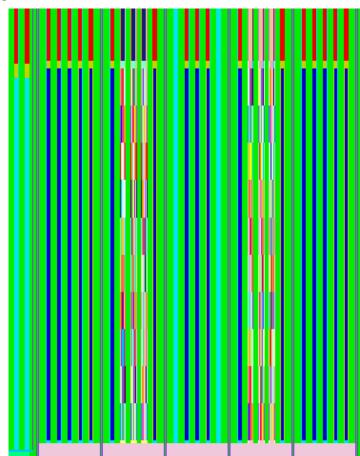
Sodium fast reactors: EBR-II Model with TRITON / Shift

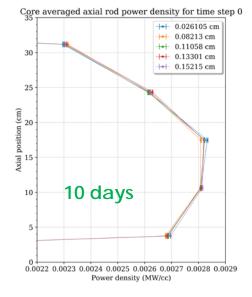
 Hi fidelity Monte Carlo neutronics with depletion for with coupling to NRC's FAST fuel performance code

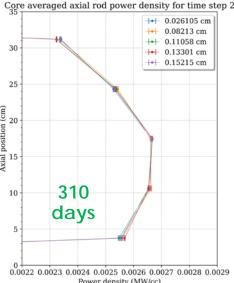






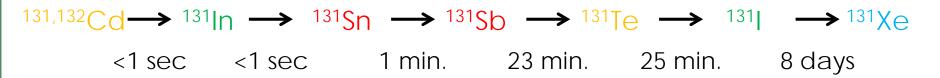


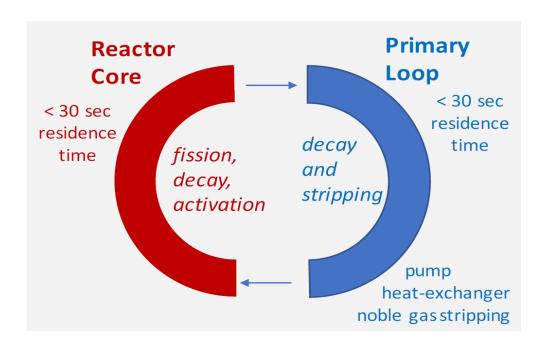




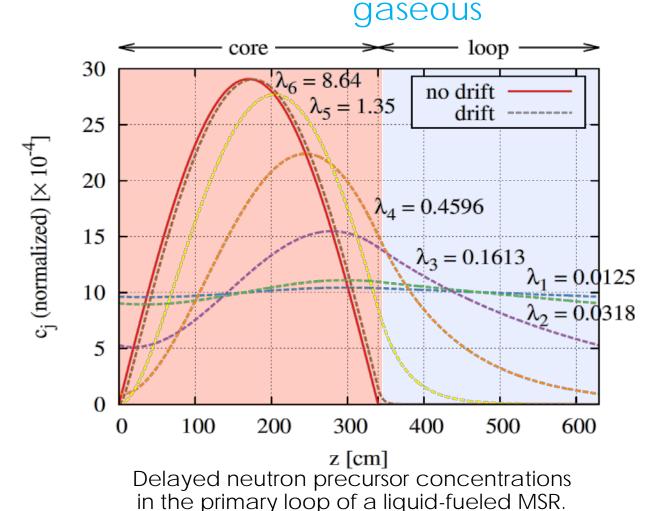


TRITON for MSR neutronics (a.k.a. ChemTRITON)





- Delayed neutron precursor drift
- Material removal and feed



soluble

insoluble

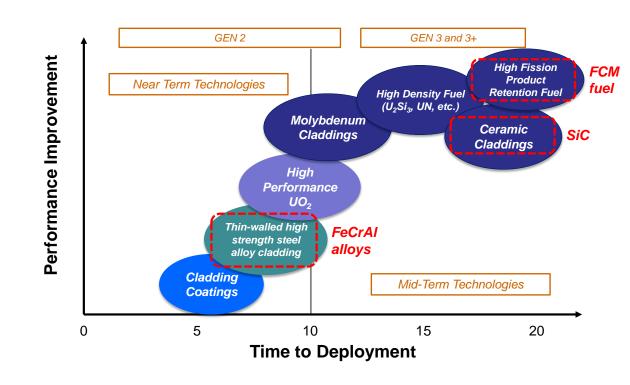
sometimes soluble

Demonstration of VERA-MSR for integrated multiphysics analysis of Molten Salt Reactor Experiment (MSRE) Transient.



SCALE is being extended for advanced fuel concepts

- ATF concepts must meet existing needs for plants <u>and</u> improve performance during accident scenarios
- High-burnup fuel will require additional validation and performance assessments
- Goals:
 - Extend tools for normal operation (NO), anticipated operational occurrences (AOOs), design basis accidents (DBAs)
 - Maintain compatibility with existing infrastructure
- Polaris has been benchmarked for AFT concepts















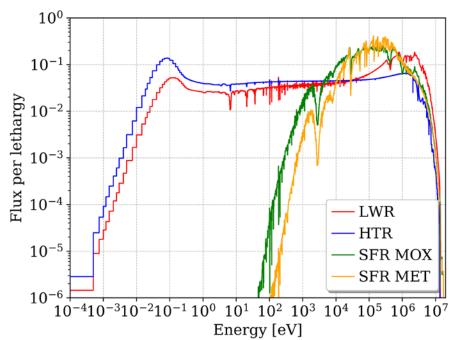
SCALE 6.3

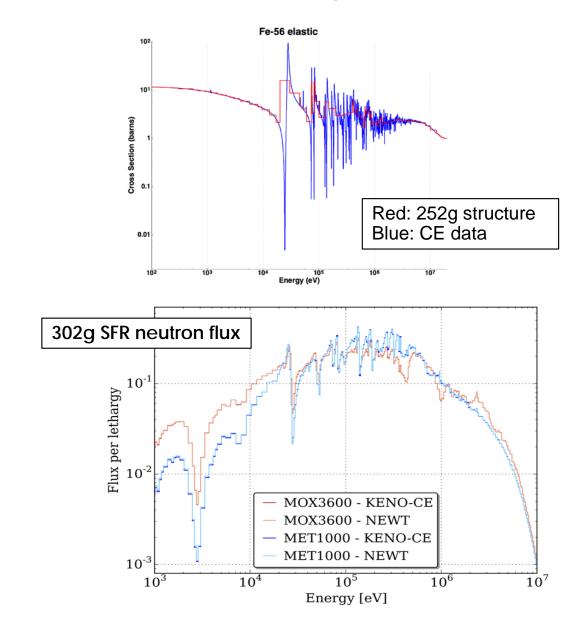
- Motivation Advanced Systems
- Nuclear data libraries
- Shift Monte Carlo Code
- Beta release



Updated nuclear data libraries for advanced systems

- With SCALE 6.2 MG libraries optimized for thermal systems are available
- Group structures and weighting spectrum are being optimized for advanced systems









SCALE 6.3

- Motivation Advanced Systems
- Nuclear data libraries
- Shift Monte Carlo Code
- Beta release



Shift/SCALE integration

Integrated in CSAS criticality sequence

- KENO V.a and KENO-VI geometry
- SCALE physics, material, and control specifications
- Validated with over 600 benchmark experiments

Integration in TRITON depletion sequence

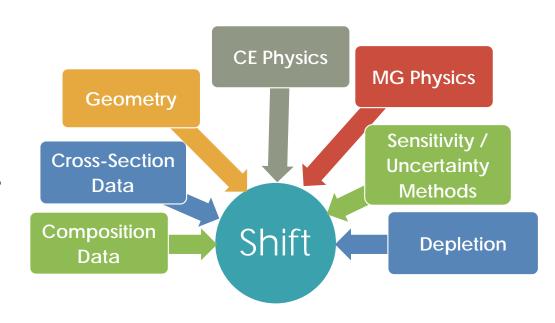
- ORIGEN depletion
- Multigroup cross section generation for nodal codes
- Randomized geometry for TRISO and pebble bed
- Validated with SFCOMPO data and full core code assessments

Integration in TSUNAMI sensitivity/uncertainty sequences

Eigenvalue and generalized perturbation theory sensitivity coefficients with CE physics

Integration in MAVRIC shielding sequence

 Fixed-source shielding problems using hybrid methods, especially for large facility and site modeling





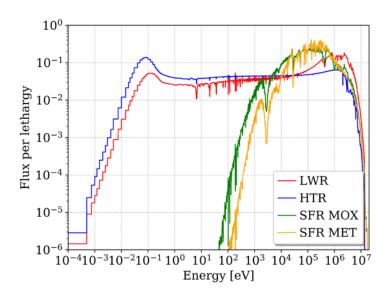
SCALE 6.3

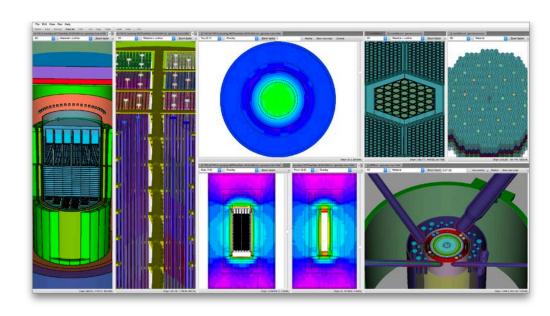
- Motivation Advanced Systems
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SCALE 6.3 Beta1 (fall 2018)

- ENDF/B-VIII.0 nuclear data libraries
 - Continuous-energy
 - LWR and nonLWR
- Shift Monte Carlo Code integration and feature extension
- Polaris enhancements for ATF and nonLWR
- TRITON MSR capability
- Fulcrum user interface enhancements, including 3D visualization
- Enhanced interoperability with MELCOR and FAST for LWR, ATF and nonLWR









Your SCALE Team



SCALE 6.2 Team Photo – May 2016



Left to right: Ahmed Ibrahim, Germina Ilas, Brandon Langley, Andrew Holcomb, Shane Hart, Cihangir Celik, Seth Johnson, Matt Jessee, Kevin Clarno, Adam Thompson, Bob Grove, Rob Lefebvre, Greg Davidson, Charles Daily, Alan Icenhour, Barbara Snow, Brian Ade, Brad Rearden, Ben Betzler, B. J. Marshall, Kursat Bekar, Will Wieselquist, Mark Baird, Mark Williams, Georgeta Radulescu, Ron Ellis, Thomas Miller, Dan Ilas, Elizabeth Jones, Cecil Parks, Sheila Walker, Teresa Moore, Marsha Henley, Sandra Poarch, Lester Petrie

SCALE Leadership Team

Brad Rearden

Manager, SCALE Code System

Will Wieselauist

Deputy Manager, SCALE Code System

Doug Bowen

Group Leader, Nuclear Data and Criticality Safety

Kevin Clarno

Group Leader, Reactor Physics

Bob Grove

Group Leader, Radiation Transport

Rob Lefebvre

Software Development Coordinator

Matt Jessee

Decay, Depletion,

and Activation

Methods

Senior R&D Staff

Radiation Safety Information Computational Center (RSICC)

Tim Valentine

Versioned Releases User Licensina

Infrastructure and Support

Tony Walsh Seth Johnson Brandon Langley Jordan Lefebvre Rob Lefebvre Paul Miller

Monte Carlo Development

Brad Rearden Brian Ade Kursat Bekar

Kaushik Banerjee Cihangir Celik Greg Davidson Tom Evans Shane Hart Seth Johnson Tara Pandya Doro Wiarda

Quality Assurance KENO/CSAS System MAVRIC/Monaco **Build and Test** Shift Framework Sourcerer Deployment

Will Wieselquist Ian Gauld Shane Hart Germina Ilas Thomas Miller Steve Skutnik (UT) Doro Wiarda

ORIGEN ORIGAMI Depletion, Decay, and Activation Data

Reactor Physics Methods

Matt Jessee Brian Ade

Kursat Bekar Ben Betzler Greg Davidson Tom Evans Cole Gentry Steven Hamilton Rob Lefebvre Ugur Mertyurek Doro Wiarda Will Wieselquist

TRITON Polaris Advanced Reactor R&D

Nuclear Data and Methods

Strategic Vision

Quality Assurance Plan

Budgets and Staffing Change Control Board

Cihangir Celik Rike Bostelmann Charles Daily Andrew Holcomb Seth Johnson Kang Seog Kim Rob Lefebyre B.J. Marshall Marco Pigni Doro Wiarda

XSProc Neutron and Gamma **Cross Section Data** (MG&CE) Covariance Data

User Interfaces

Rob Lefebvre

Brandon Langley BJ Marshall Josh Peterson Will Wieselquist

Fulcrum Geometry and Data Visualization

Sensitivity and **Uncertainty Analysis**

Vladimir Sobes Goran Arbanas Keith Bledsoe Rike Bostelmann Matt Jessee Rob Lefebvre B.J. Marshall Ugur Mertyurek Will Wieselquist

TSUNAMI TSURFER SAMPLER Optimization and **Inverse Analysis**

User Interaction and Training

Germina Ilas Brian Ade Ben Betzler Cihangir Celik Justin Clarity Ian Gauld Shane Hart Marsha Henley Matt Jessee B.J. Marshall **Thomas Miller** Douglas Peplow Will Wieselquist

Courses at ORNL, NEA Data Bank, NRC, and User **Facilities** Conference Workshops Helpline, User Groups Documentation



Reactor and Nuclear Systems Division

Kenneth Tobin, Director

Sandra Poarch, Division Secretary July 1, 2018

Consortium for Advanced Simulation of Light Water Reactors

Kevin Clamo¹, Interim Director

Support

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Operations Management Support, Angel Kennedy

Recruiter, Bre Sweet-Kerschbaum Technical Editor, Rose Raney

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Radiation Safety Information Computational Center

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Syd Ball⁶ Elvis Dominguez-Ontiveros David Holcomb Jordan Massengale Jeff Powers Kevin Robb Michael Smith⁵

Data Analytics, Instrumentation and Control Team

Sacit Cefiner, Lead Scott Greenwood Mike Muhlheim Jordan Rader

Reactor Safety and Licensing Team

T. Jay Harrison, Lead Randy Belles George Flanagan Richard Hale Mike Poore, III Askin Guler Yigitoglu

Thermal Hydraulics Team

Prashant Jain, Lead Marc-Olivier Delchini **Emilian Popoy** Bob Salko, Jr. Aaron Wysocki

Nuclear Data and Criticality Safety

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Joel McDuffee Andrea Beatty¹

David Bryant Nesrin Cetiner Ryan Gallagher Richard Howard Padhraic Mulligan Christian Petrie Kurt Smith Bob Sitterson² Ken Thoms?

Radiation Transport

Bob Grove Elaine Davis

Kursat Bekar Charles Daily Scott Mosher Georgeta Radulescu Joel Risner Katherine Royston Steve Wilson Jinan Yang

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Reactor Physics

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Kevin Clarno¹ Angle Alford¹

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Rob Lefebyre, Lead Mark Baird Brandon Langley Paul Miller Adam Thompson Tony Walsh

Neutronics Team

Germina Ilas, Lead Brian Ade Mehdi Asgari Ben Betzler Ron Ellis Ian Gauld⁶ Andrew Godfrey Jianwei Hu Kang-Seog Kim Travis Lange⁶ Ivan Maldonado³ Josh Peterson-Droogh

Reactor Multiphysics Team

Will Wieselguist1, Lead Ben Collins Eva Davidson Kevin Dugan⁴ Cole Gentry Aaron Graham⁴ Shane Henderson Matt Jessee Ugur Mertyurek Shane Stimpson

Used Fuel Systems

John Scaglione Andrea Beatty¹

Abi Adeniyis Kaushik Banerjee Bruce Beyard¹ Stylianos Chatzidakis Kevin Connolly Riley Cumberland Matt Feldman Rob Howard Robby Joseph, III Oscar Martinez Rose Montgomery Bill Reich

- Dual Capacity
- 2 Subcontractor
- 3 Joint Faculty
- 4 Postdoctoral 5 ORISE Post Master's
- ⁶Part-time
- 7 CASL ORISE Post BS



ORNL Nuclear Modeling and Simulation Portfolio



Updated SCALE Leadership

Will Wieselquist

Director, SCALE Code System

Doug Bowen

Group Leader, Nuclear Data and Criticality Safety

Kevin Clarno

Group Leader, Reactor Physics

Bob Grove

Group Leader, Radiation Transport

Rob Lefebvre

Software Development Coordinator

Matt Jessee

Senior R&D Staff

Brad Rearden (ex officio)

Leader, Modeling and Simulation Integration

