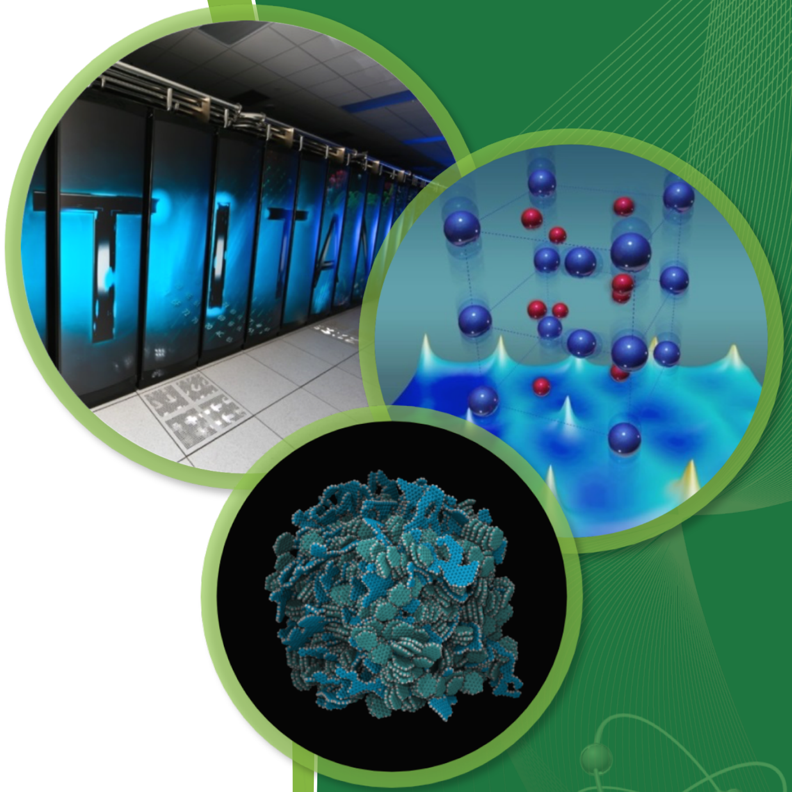
Modeling and Simulation for Advanced Reactors



Presented to:
U.S. Nuclear Regulatory Commission

Presented by:
Bradley T. Rearden, Ph.D.
Leader, Modelling and Simulation Integration
Reactor and Nuclear Systems Division
Oak Ridge National Laboratory

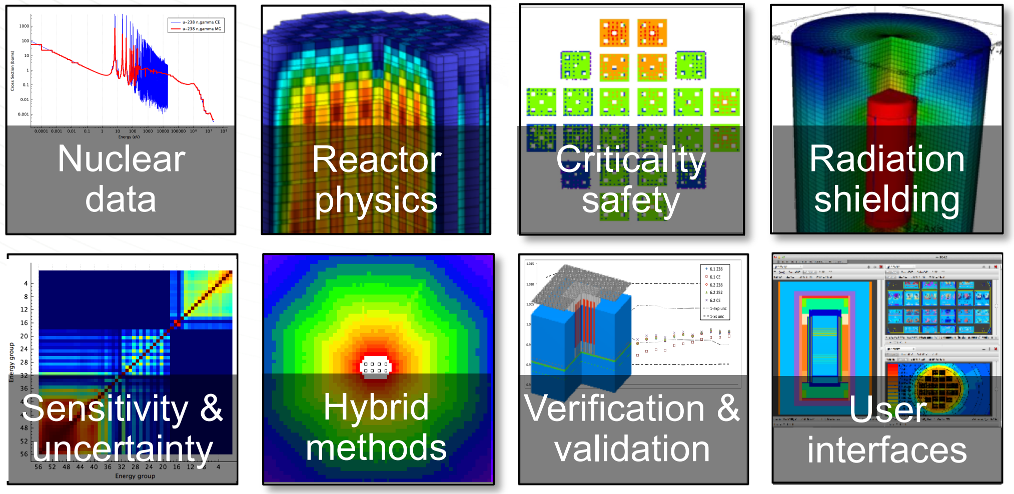
June 2018

SCALE code system

Neutronics and shielding analysis enabling nuclear technology advancements

http://scale.ornl.gov

Practical tools relied upon for design, operations, and regulation



scale

Global distribution: 8,700 users in 58 nations

Over 4,000 distributions of SCALE 6.2 since 2016!

Professional training for practicing engineers and regulators

FY17 statistics:

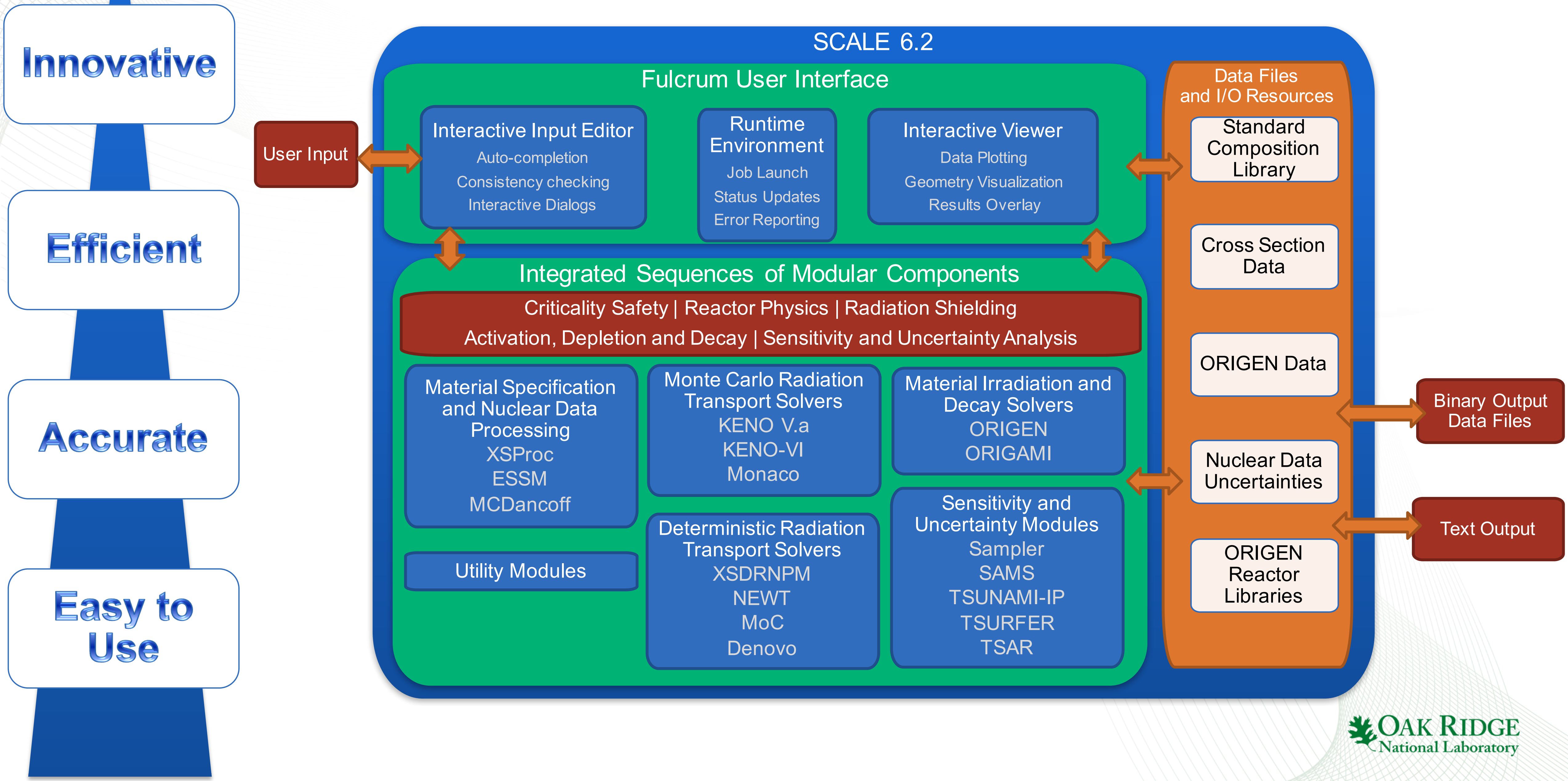
- 10 one-week courses
- 4 conference tutorials
- 150 participants from 15 nations

Primary sponsors

Robust quality assurance program based on multiple standards

OAK RIDGE National Laboratory

SCALE is an Integrated System with Many Features



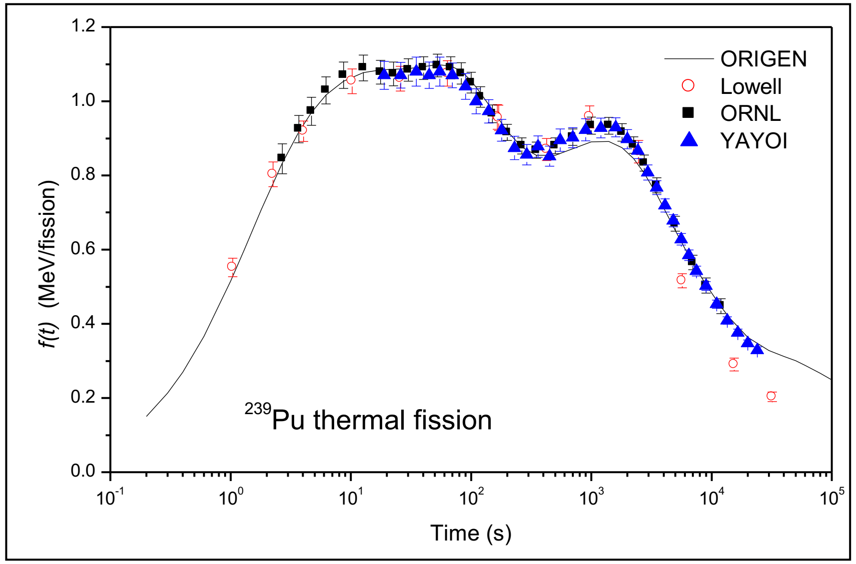
SCALE Verification and Validation

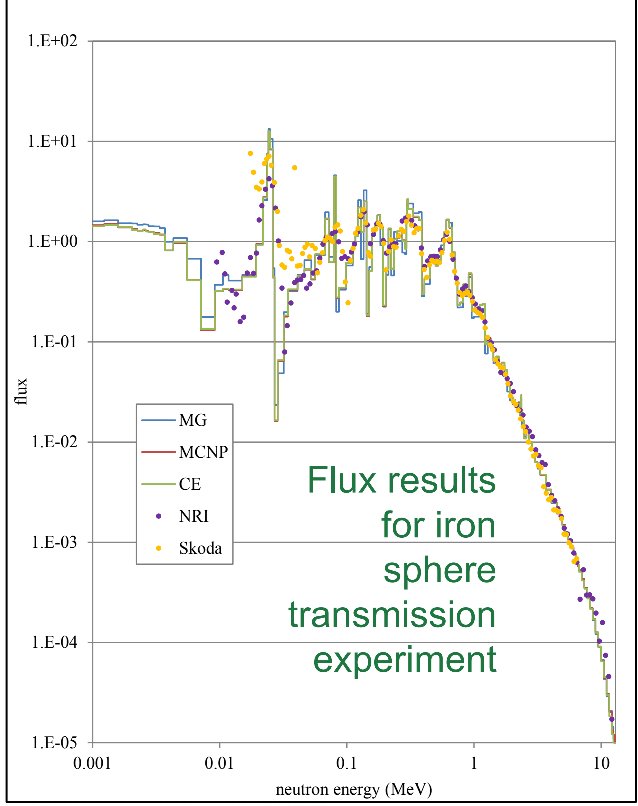
Verification

Continuous unit and regression testing
>7000 fixed-source transmission tests for neutron/gamma spectral data
Every nuclide/element at multiple energies
>5000 infinite medium k_{inf} tests

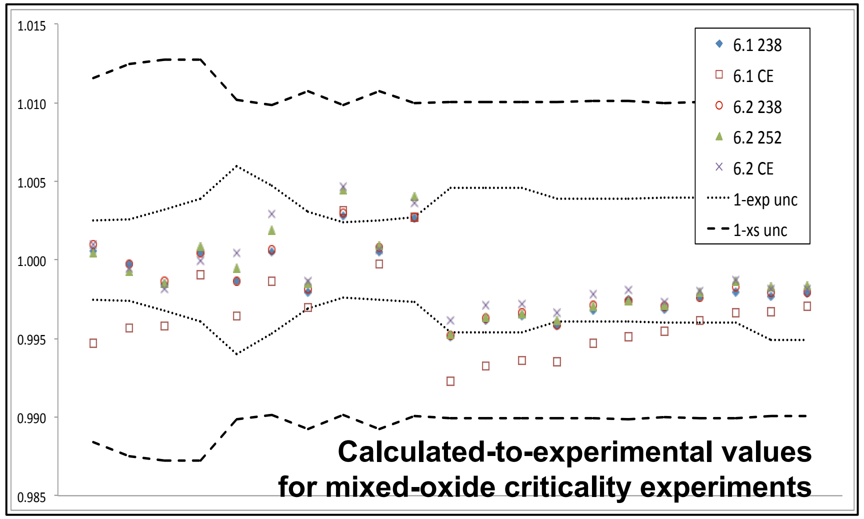
Validation

600 criticality and shielding benchmarks
120 isotopic assays samples
121 decay heat measurements
Gamma spectra - burst fission
Neutron spectra – spent fuel and (α,n) sources

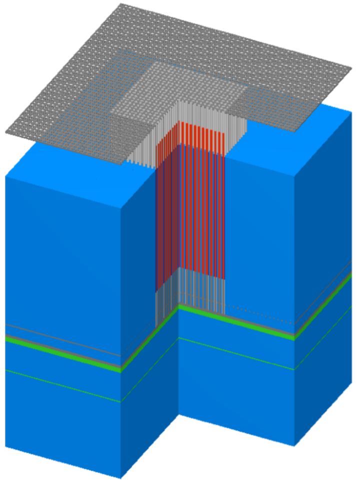




Flux results for iron sphere transmission experiment



Calculated-to-experimental values for mixed-oxide criticality experiments

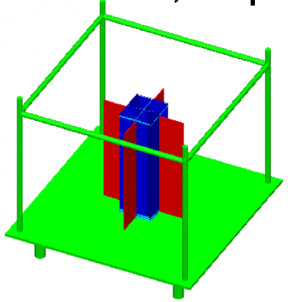


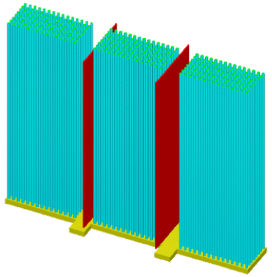
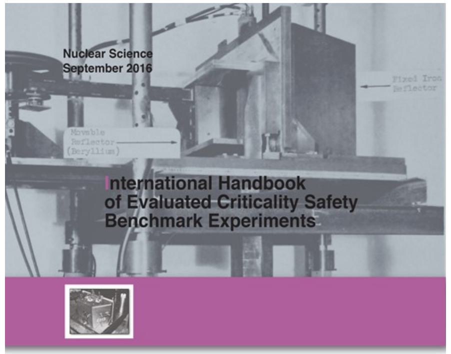
MIX-COMP-THERM-004 Critical Experiment

- **Fissile materials**
  - High-enriched uranium (HEU),
  - Intermediate-enriched uranium (IEU)
  - Low-enriched uranium (LEU)
  - Plutonium (Pu)
  - Mixed uranium/plutonium oxides (MOX)
  - Uranium-233 (U233)
- **Fuel form**
  - Metal (MET),
  - Fissile solution (SOL)
  - Multi-material composition (e.g. fuel pins – COMP)
- **Neutron spectra**
  - Fast
  - Intermediate (INTER)
  - Thermal
  - Mixed

SCALE criticality validation: Verified, Archived Library of Inputs and Data (VALID)

- 611 configurations from International Criticality Safety Benchmark Evaluation Project (ICSBEP)
- 200 additional configurations, especially for ^{233}U systems

Sequence / Geometry	Experiment class	ICSBEP case numbers	Number of configurations
CSAS5 / KENO V.a	HEU-MET-FAST	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 52, 65	19
	HEU-SOL-THERM	1, 13, 14, 16, 28, 29, 30	52
	IEU-MET-FAST	2, 3, 4, 5, 6, 7, 8, 9	8
	LEU-COMP-THERM	1, 2, 8, 10, 17, 42, 50, 78, 80	140
	LEU-SOL-THERM	2, 3, 4	19
	MIX-MET-FAST	5, 6	2
	MIX-COMP-THERM	1, 2, 4	21
	MIX-SOL-THERM	2, 7	10
	PU-MET-FAST	1, 2, 5, 6, 8, 10, 18, 22, 23, 24, 25, 26	12
	PU-SOL-THERM	1, 2, 3, 4, 5, 6, 7, 11, 20	81
	U233-COMP-THERM	1	3
	U233-MET-FAST	1, 2, 3, 4, 5, 6	10
	U233-SOL-INTER	1	29
	U233-SOL-MIXED	1, 2	8
	U233-SOL-THERM	1, 2, 3, 4, 5, 8, 9, 11, 12, 13, 15, 16, 17	140
CSAS6 / KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93, 94	27
	IEU-MET-FAST	19	2
	MIX-COMP-THERM	8	28

- **Fissile materials**
  - High-enriched uranium (HEU),
  - Intermediate-enriched uranium (IEU)
  - Low-enriched uranium (LEU)
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- **Fuel form**
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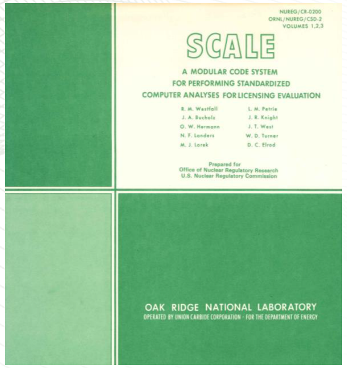
  - Multi-material composition (e.g. fuel pins – COMP)
- **Neutron spectra**
  - Fast
  - Intermediate (INTER)
  - Thermal
  - Mixed

SCALE training courses are routinely provided to the user community at ORNL and NEA, regulatory training is provided twice annually to NRC, and application-specific training provided at user facilities

Fall 2018 SCALE training classes at ORNL, October 15 – November 9	
October 15-19	Sensitivity and Uncertainty Analysis for Criticality Safety Assessment and Validation
October 22-26	SCALE/TRITON Lattice Physics and Depletion
October 29 - November 2	SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis
November 5 – 9	SCALE Criticality Safety and Radiation Shielding

Point-of-contact: Germina Ilas, ilasg@ornl.gov

SCALE Evolution



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 Class of Problems & Sponsors

Reactor physics

Shielding analysis with automated variance reduction

Sensitivity and uncertainty analysis

High-fidelity criticality safety in continuous energy

Graphical user interfaces and visualization tools

Expanded visibility

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

Initiated modern, modular software design

Expanded Use

Over 8,000 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

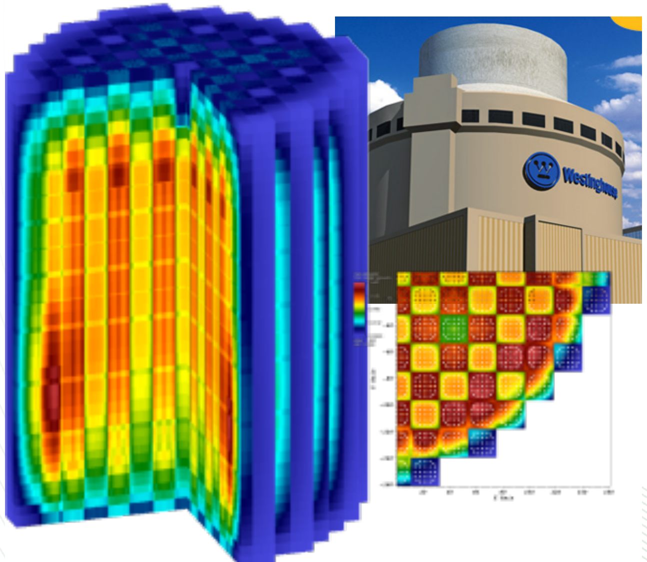
Solutions for extremely complex systems

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

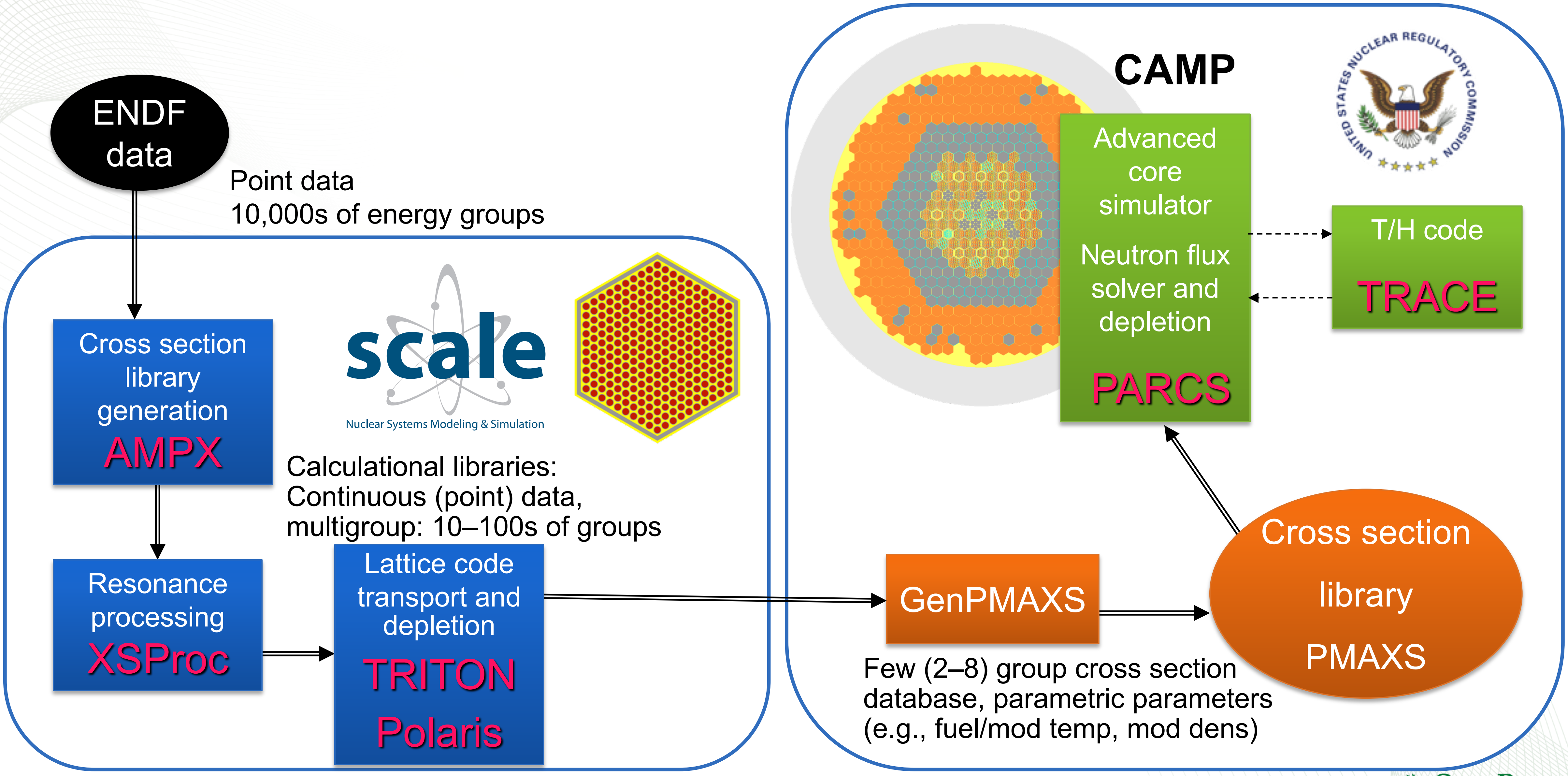
Extended modern, modular software design

Expanded Integration

Tools directly integrated with many projects

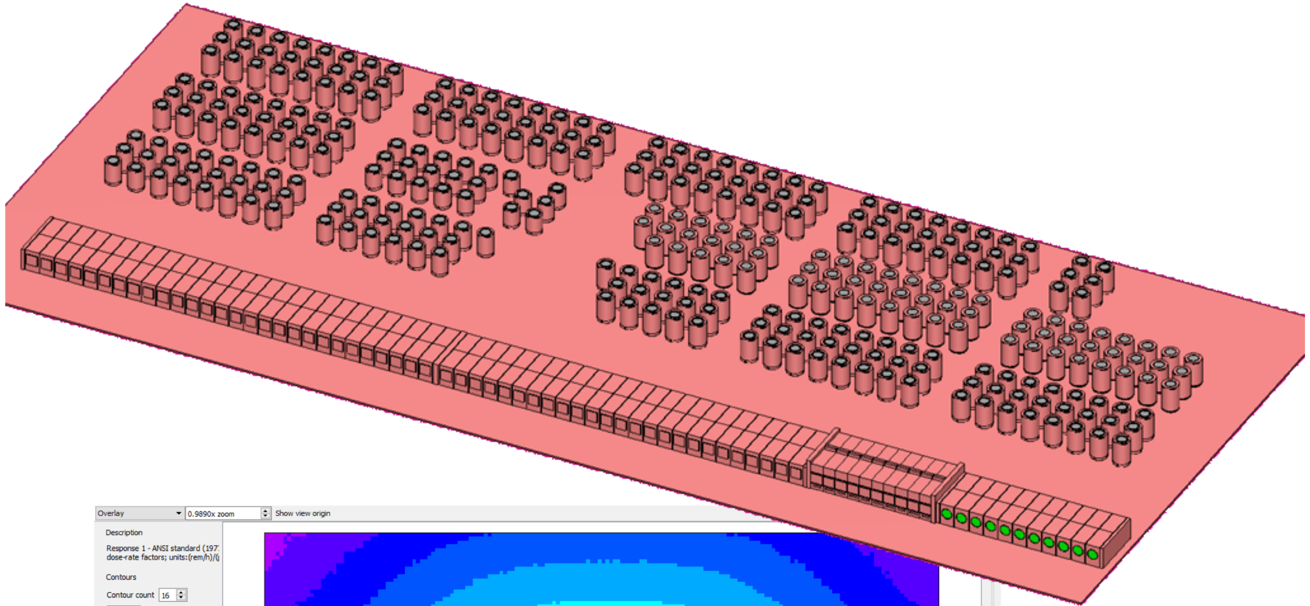


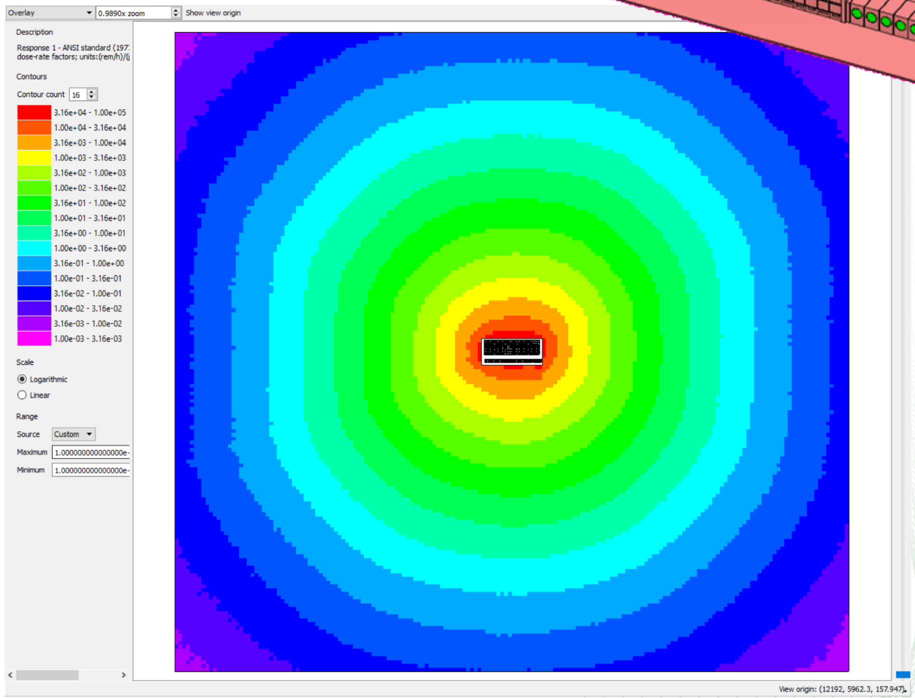
SCALE is part of the NRC's reactor licensing path



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

http://wcsstorage.com/resources/



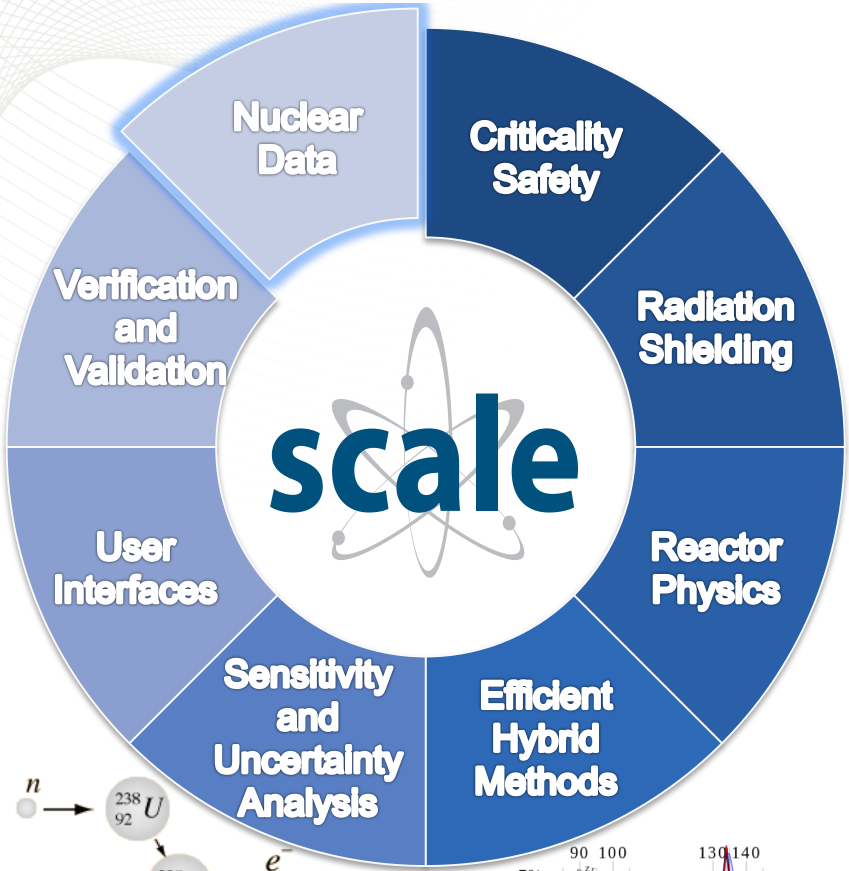


Waste Control Specialists
Consolidated Interim Storage Facility
Phase 1:

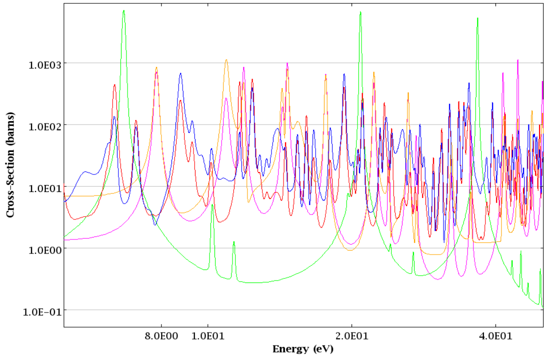
- 467 canisters
- Phase 1 concrete pad: 243.84 m × 106.68 m
- Site boundary 2713 m × 2576 m
- Air: 959.1 m for skyshine
- Soil: 1 m for ground return

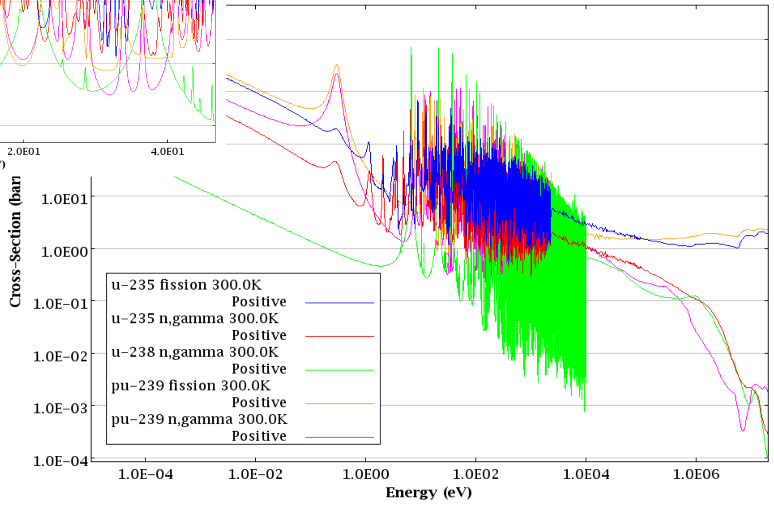
Nuclear Data from ORNL AMPX Tools

AMPX now included with SCALE distribution so users can create their own libraries!

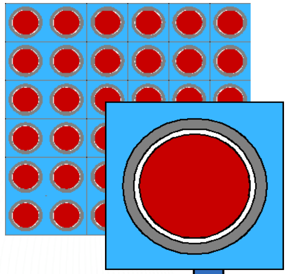


Continuous-Energy Neutron and Gamma Cross Sections

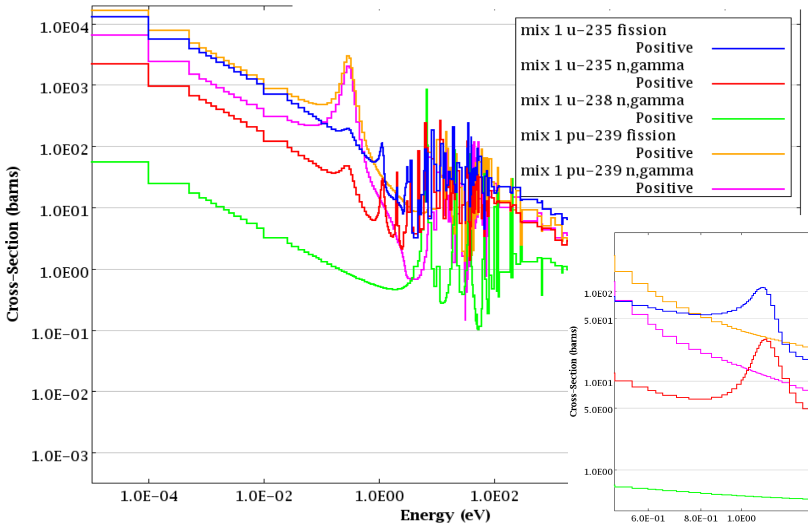


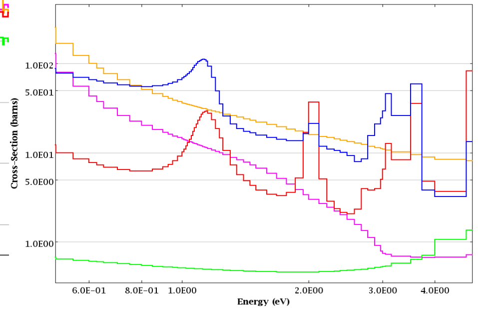


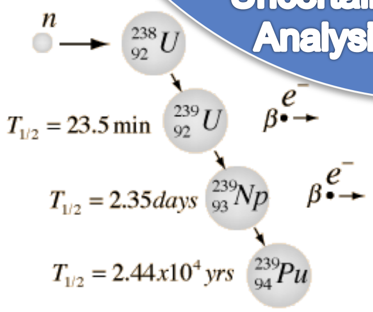
Resonance Self-Shielding

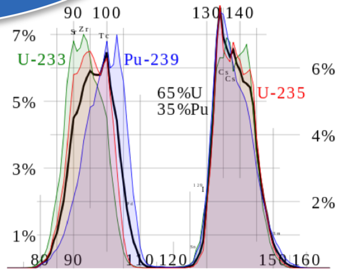


Multigroup Neutron and Gamma Cross Sections









Depletion, Decay, and Activation Data

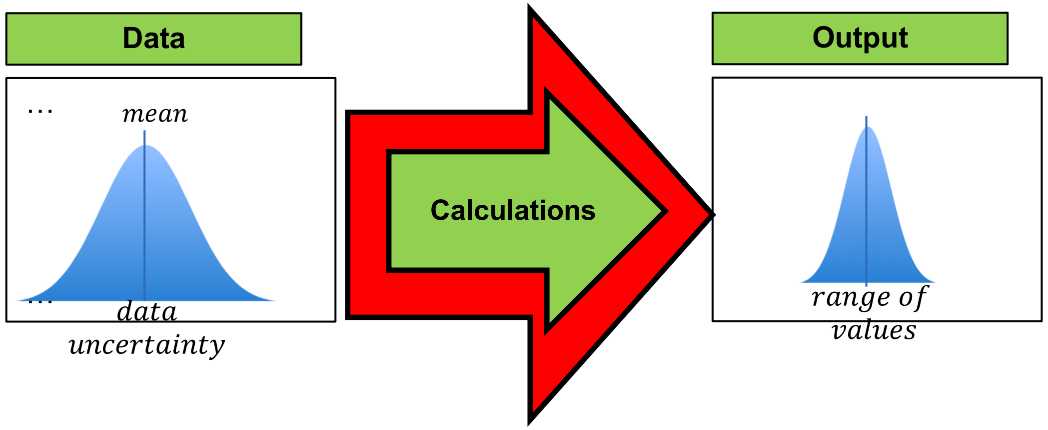
Two Approaches to Uncertainty Analysis

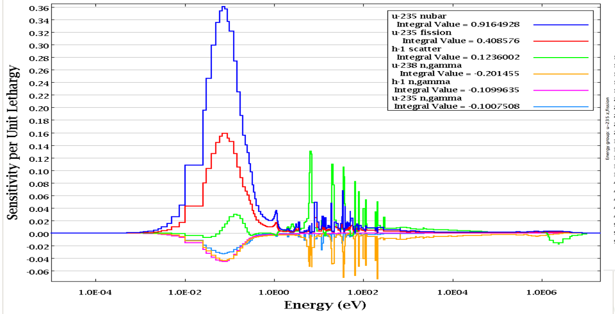
Stochastic Sampling (SCALE/Sampler)

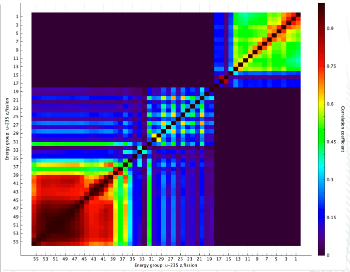
- Covariances of input data sampled; statistical analysis of output distribution gives uncertainties
- Pros
  - Typically minimally invasive to code
  - Can address complex simulations with coupled codes
- Cons
  - Quantification of separate effects (sensitivity coefficients) is challenging

Sensitivity Methods (SCALE/TSUNAMI)

- Sensitivities are computed and combined with covariances to obtain uncertainties
- Pros
  - Quantifies uncertainty contributors
  - Obtains all data sensitivities for a single response in single calculation
- Cons
  - Requires invasive implementation of adjoint solution in simulation codes
  - Limited to radiation transport applications

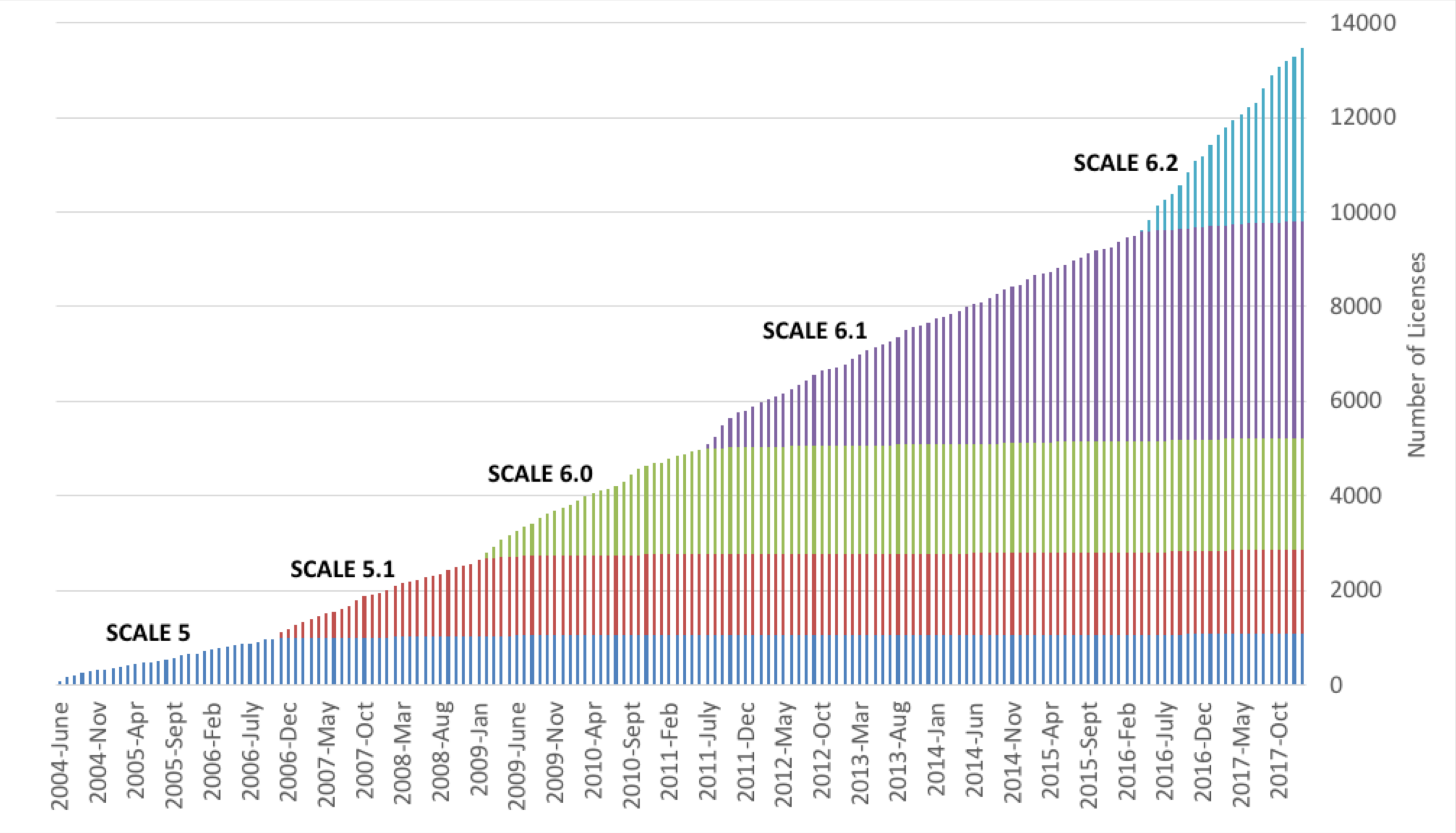






$$\mathrm{Var}(k) \equiv \underbrace{S^T}_{\text{sensitivity}} \underbrace{C_{\alpha\alpha}}_{\text{covariance}} S$$

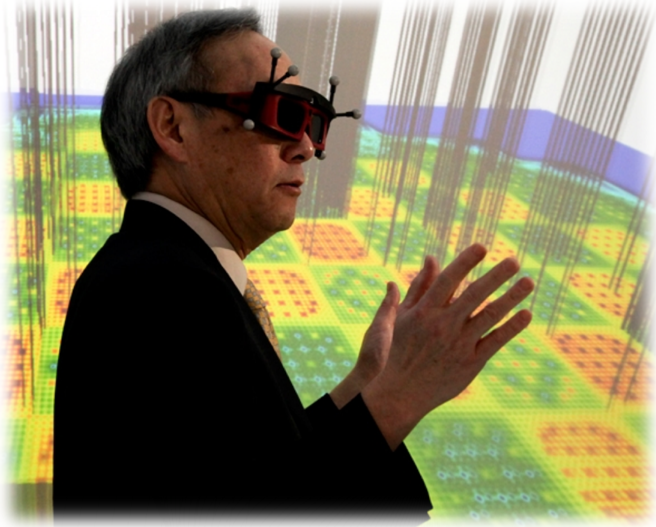
SCALE licenses by version



OAK RIDGE National Laboratory

The Consortium for the Advanced Simulation of Light Water Reactors (CASL): an Energy Innovation Hub

- Established by former DOE Energy Secretary Steven Chu
- Modeled after the scientific management characteristics of AT&T Bell Labs:
  - Addressing critical problems
  - Combines basic and applied research with engineering
  - Integrated team to take discovery to application
- 10-year focused R&D effort (2010–2019)



"Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges"

– *Steven Chu*

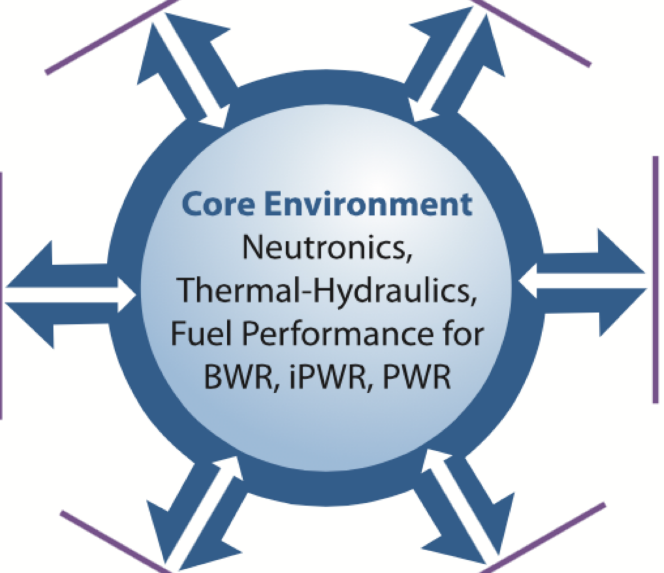
CASL MISSION
Provide leading-edge modeling and simulation (M&S) capabilities to improve the performance of currently operating and future light water reactors (LWRs)

Our challenge problems are focused on key commercial reactor performance areas

Pellet-Clad Interation (PCI)
Predict core wide PCI margin and missing pellet surface PCI for BWR, iPWR, PWR
Neutronics, Thermal-Hydraulics, Fuel/Cladding Performance

CRUD
Predict CRUD thickness, boron uptake, and impact on power and cladding corrosion for iPWR, PWR
Neutronics, Thermal-Hydraulics, Fluid Flow (CFD), Chemistry

Cladding Integrity Reactivity Insertion Accident
Predict pellet-clad mechanical interaction for BWR, iPWR, PWR
Reactor Kinetics, Transient Fuel/Cladding Performance



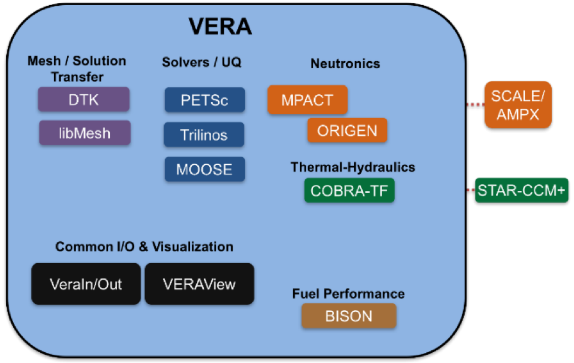
Cladding Integrity Loss of Coolant Accident
Predict peak clad temperature and oxidation margin for BWR iPWR, PWR
Fuel/Cladding Performance

Departure from Nucleate Boiling (DNB) and Flow Regimes
Predict PWR DNB margin for steam line break, predict thermal and solutal flow, BWR flow regimes
Neutronics, Thermal-Hydraulics/Fluid Flow (CFD)

Grid to Rod Fretting
Predict fluid structure excitation forces, grid-clad gap, and cladding wear for iPWR, PWR
Fluid Flow (CFD), Fuel/Clad Performance, Materials Performance

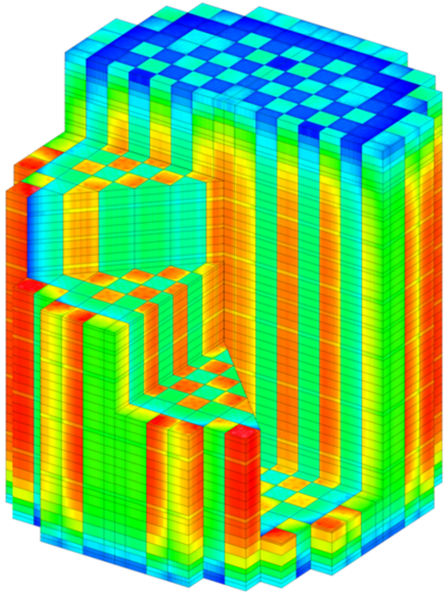
VERA core simulator

Virtual Environment for Reactor Applications

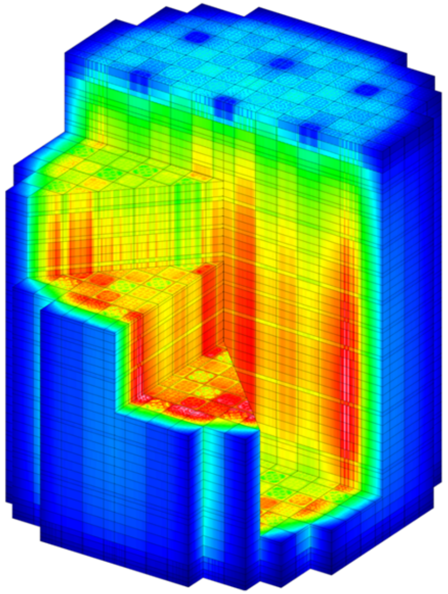


ORIGEN

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



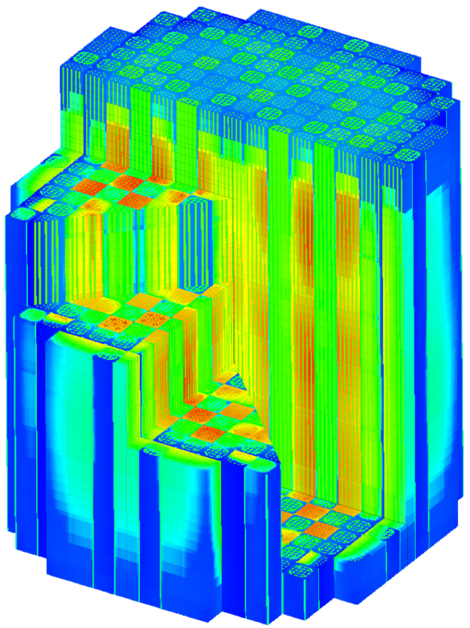
WB1C11 end-of-cycle pin exposure distribution



WB1C11 beginning-of-cycle Pin power distribution

MPACT

Advanced pin-resolved 3-D whole-core deterministic neutron transport in 51 energy groups



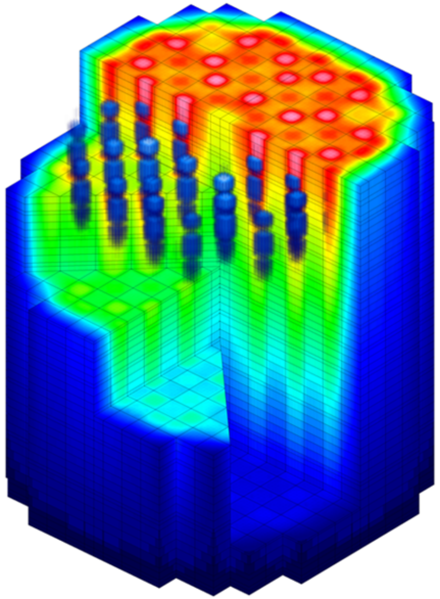
WB1C2 middle-of-cycle clad hoop stress

BISON

Fuel performance code modeling thermo-mechanics of standard and advanced fuel and cladding for every rod in the core

CTF

Subchannel thermal hydraulics with transient two-fluid, three-field (i.e., liquid film, liquid drops, and vapor) solutions in 14,000 coolant channels with crossflow

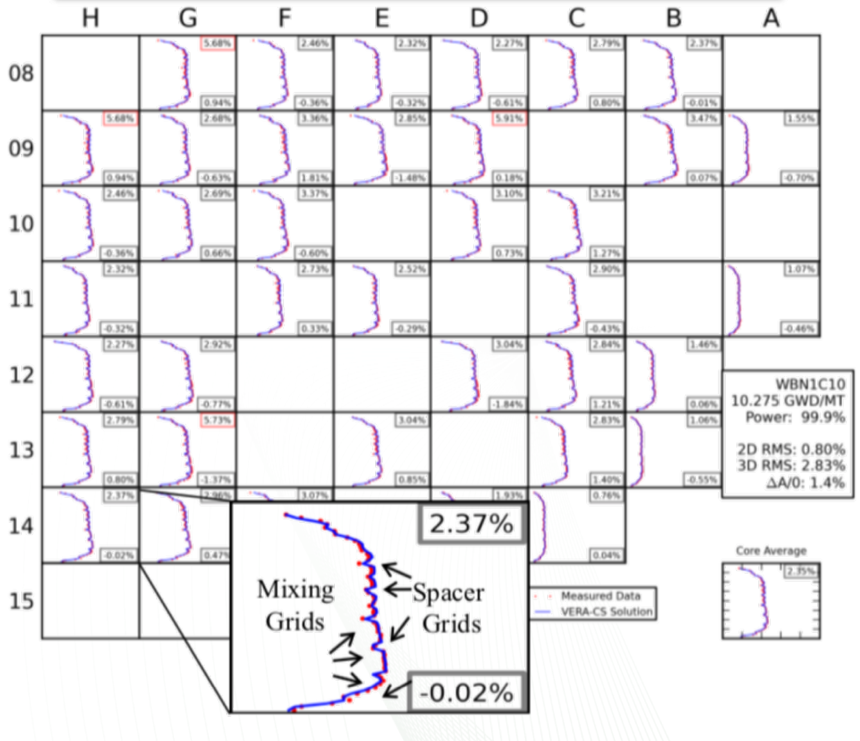


WB1C11 middle-of-cycle coolant density distribution

Watts Bar Unit 1 Benchmark

- VERA used to model Cycles 1-14 (20 years of operation)
- Good agreement with measured data (provided by TVA)
  - RCCA bank worths (-0.7 ± 3.4%)
  - Isothermal temperature coefficients (-1.6 ± 0.7 pcm/F)
  - Critical boron concentrations (*-16 ± 17 ppm*)
  - In-core power distributions (*1.7% radial, 3.3% total error, 0.2% AO*)

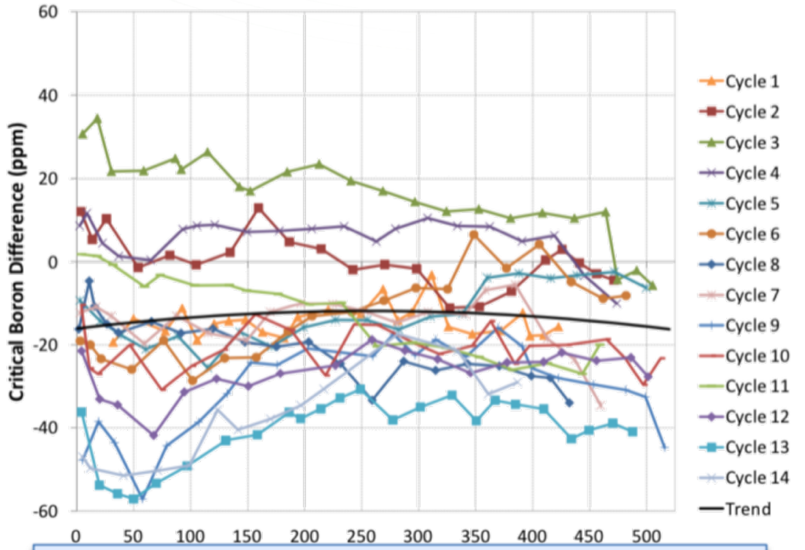
195 in-core flux maps



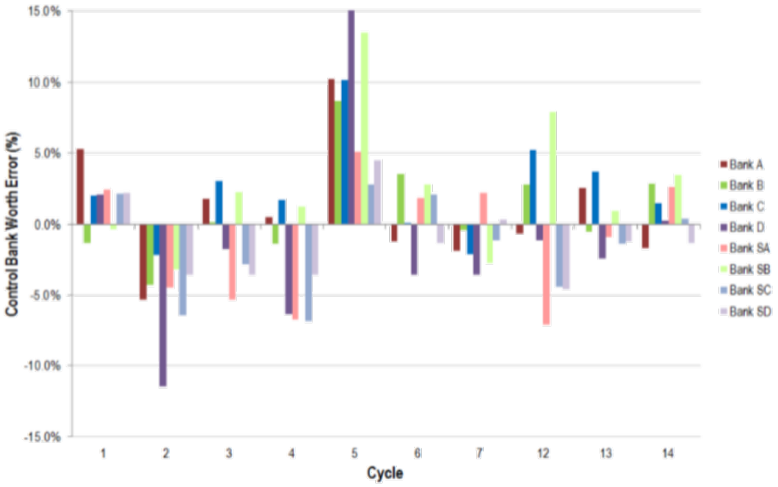
960 processors

~22 statepoints per cycle

~21 hours per cycle

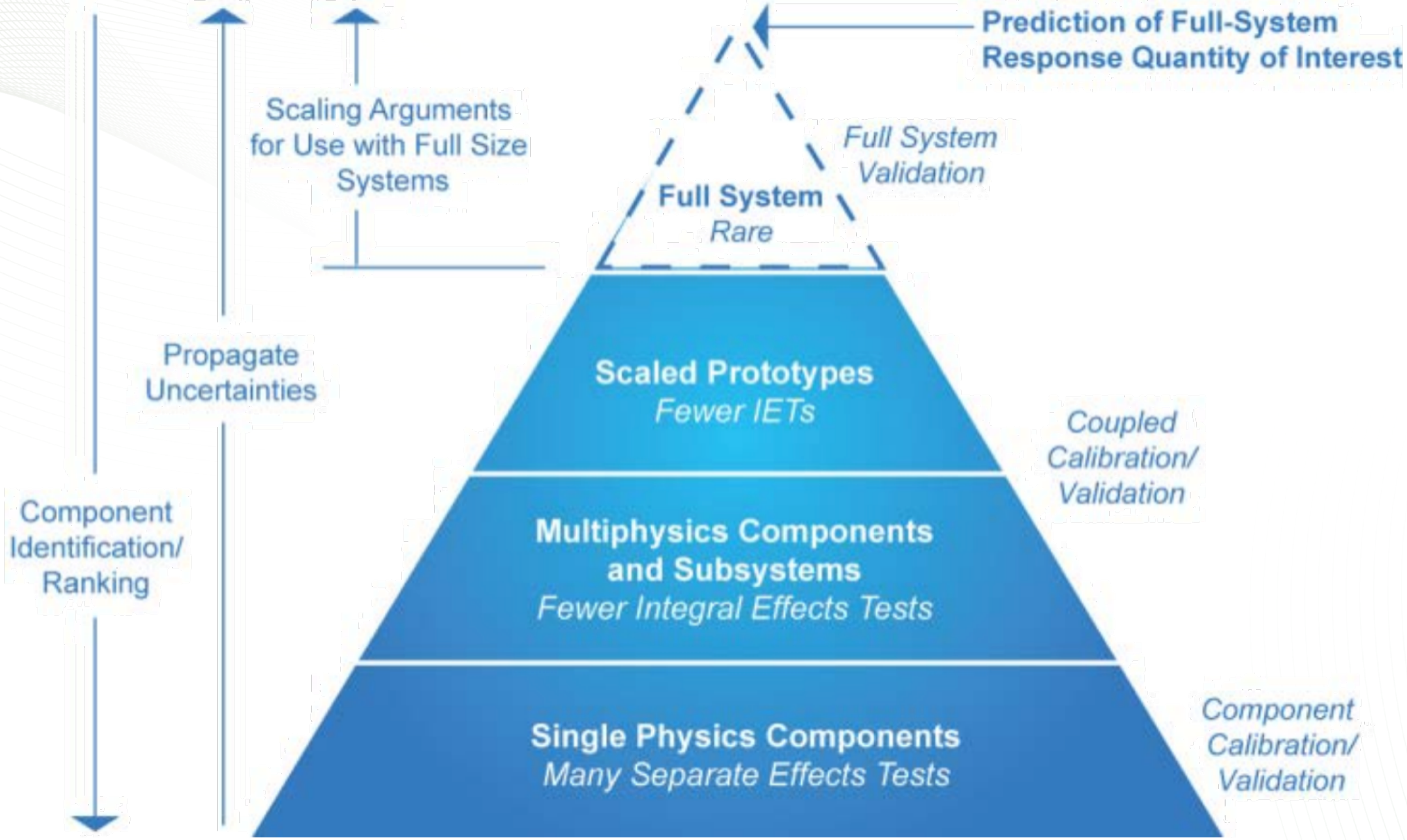


critical boron comparisons



Bank worths

An Approach to Multiphysics V&V



W. J. Rider and V. Mousseau, *Validation and Uncertainty Quantification (VUQ) Strategy, Revision 1*, CASL-U-2014-0042-001 (2014)

Advanced Reactors

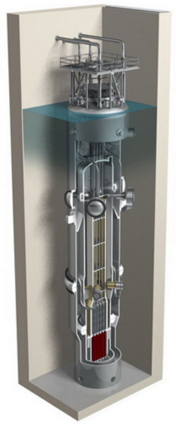
Over two dozen companies are entering the advanced reactor market today

Develop intrinsically safe designs with lower costs, high burnup, and minimal waste

Retain or increase electricity baseload in lieu of retiring LWR fleet

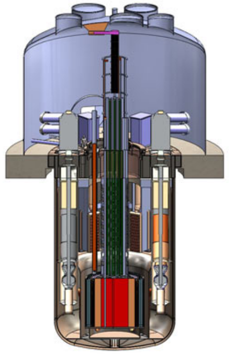
Achieve greenhouse gas reductions and clean air goals

NuScale Power



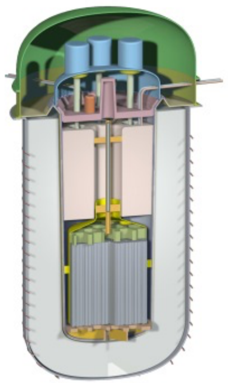
Small modular reactor (PWR)

TerraPower



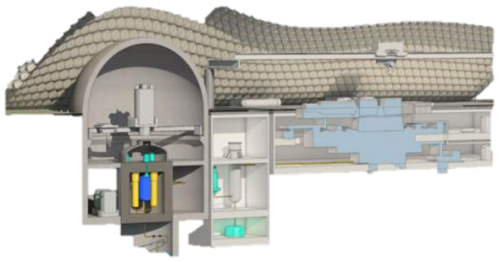
Sodium and salt-cooled fast reactors

Terrestrial Energy



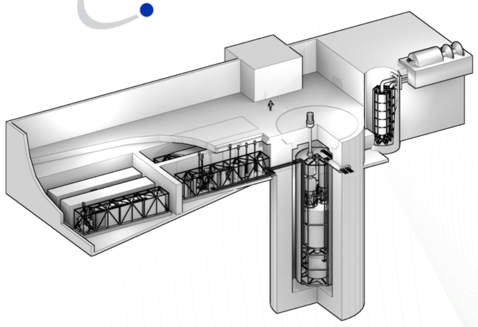
Integral molten salt thermal reactor (IMSR)

Transatomic



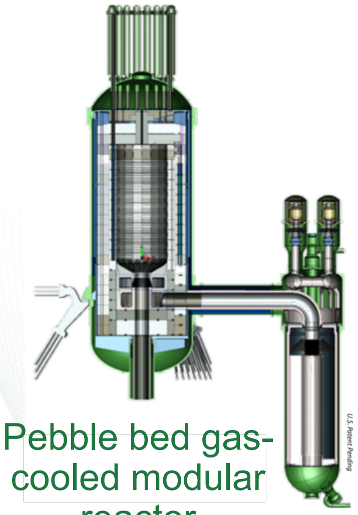
Molten salt thermal reactor, LEU fuel

Flibe Energy



Liquid fluoride thorium thermal reactor (LFTR)

X-energy



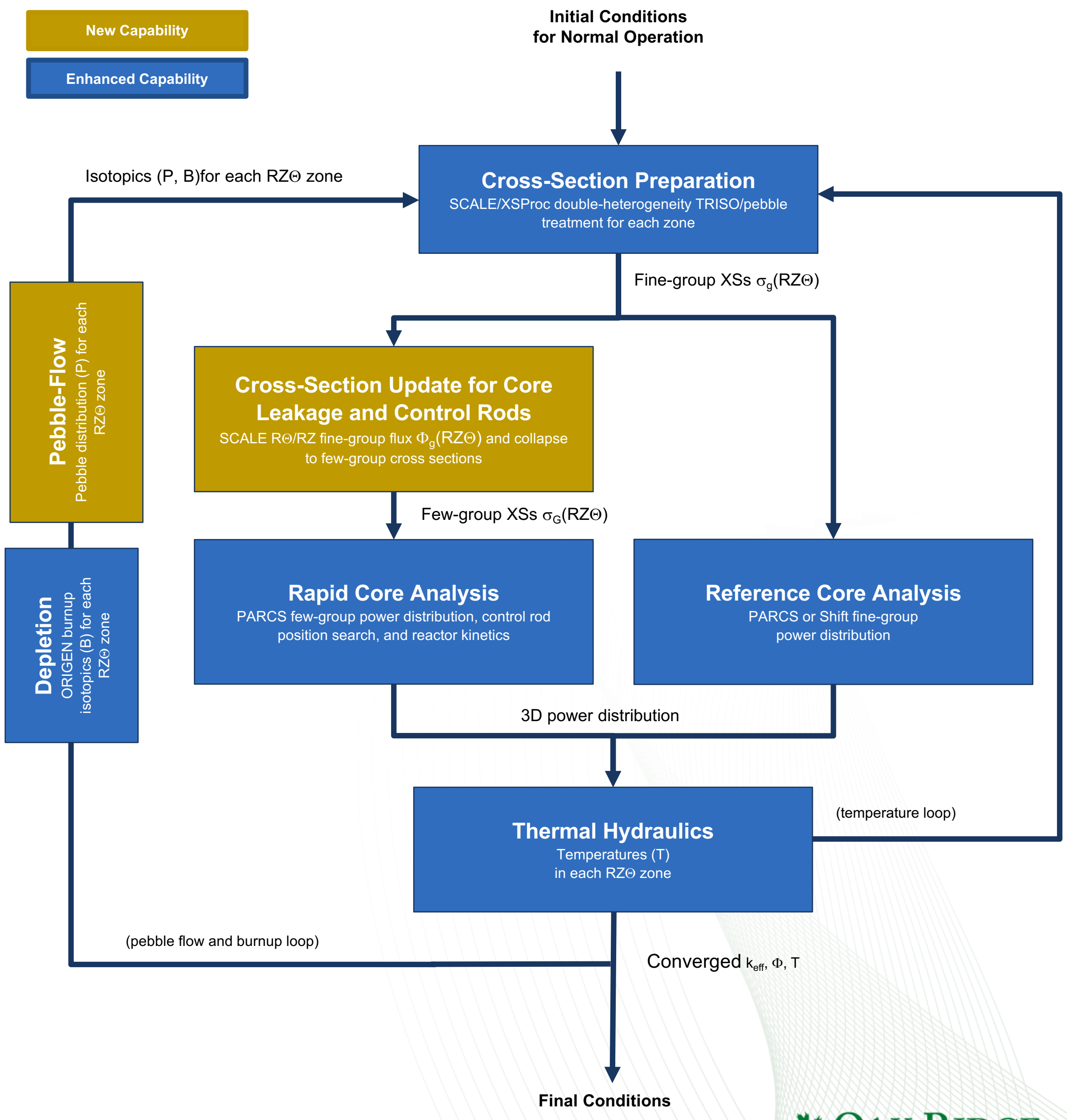
Pebble bed gas-cooled modular reactor

Abbreviated advanced reactor technology matrix

Reactor Type	Companies	Licensing action expected	Fuel / Enrichment	Thermal spectrum	Fast Spectrum	Coolant	Radial core expansion	Flowing Fuel	External control elements	TRISO Fuel	Metallic Fuel
SFR	Oklo	2019	~20%		✓	Sodium heat pipes	✓		✓		✓
	TerraPower (TWR)		~20%		✓	Sodium	✓				✓
	GE PRISM				✓	Sodium	✓				✓
HTGR	X-energy (Xe100)	2020s	15.5%	✓		Helium		✓	✓	✓	
	Areva (SC-HTGR)		~20%	✓		Helium				✓	
FHR	Kairos	2020s	~17%	✓		FLiBe		✓	✓	✓	
MSR	Terrestrial Energy (IMSR)	2019	~5%	✓		Proprietary		✓			
	Transatomic	2020s		✓		FLiBe		✓			
	TerraPower (MCFR)	2020s	~20%		✓	Chloride salt		✓			
	Elysium		~20%		✓	Chloride salt		✓			
	FLiBe Energy		Thorium	✓		FLiBe		✓			

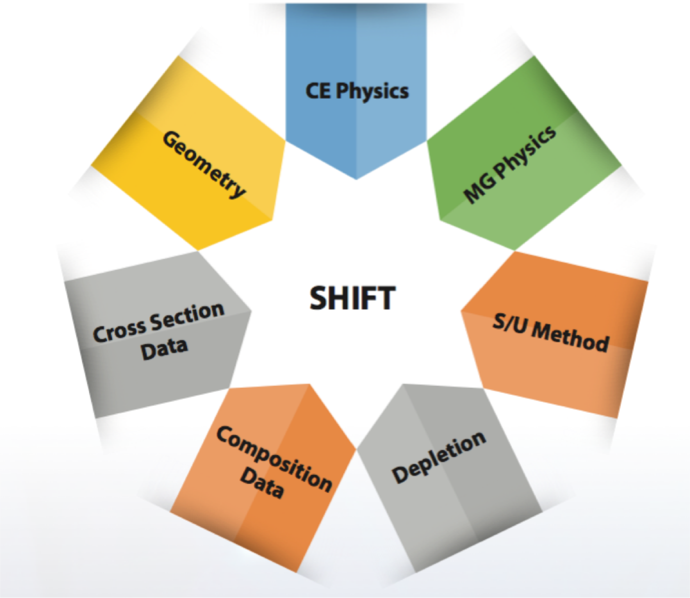
Needs for advanced reactors

- New materials / geometry / nuclear data needs
- Most use high-assay LEU fuel
- Flowing fuel
  - Slow flow for pebble bed
  - Rapid flow with reactivity effects for MSR
- New spectra
- Core leakage effects
- Control systems external to the core
- Chemistry effects
- Material expansion/deformation with temperature as a control mechanism
- Need for tight coupling with PARCS, T/H, material flow, chemistry



Shift Monte Carlo Code

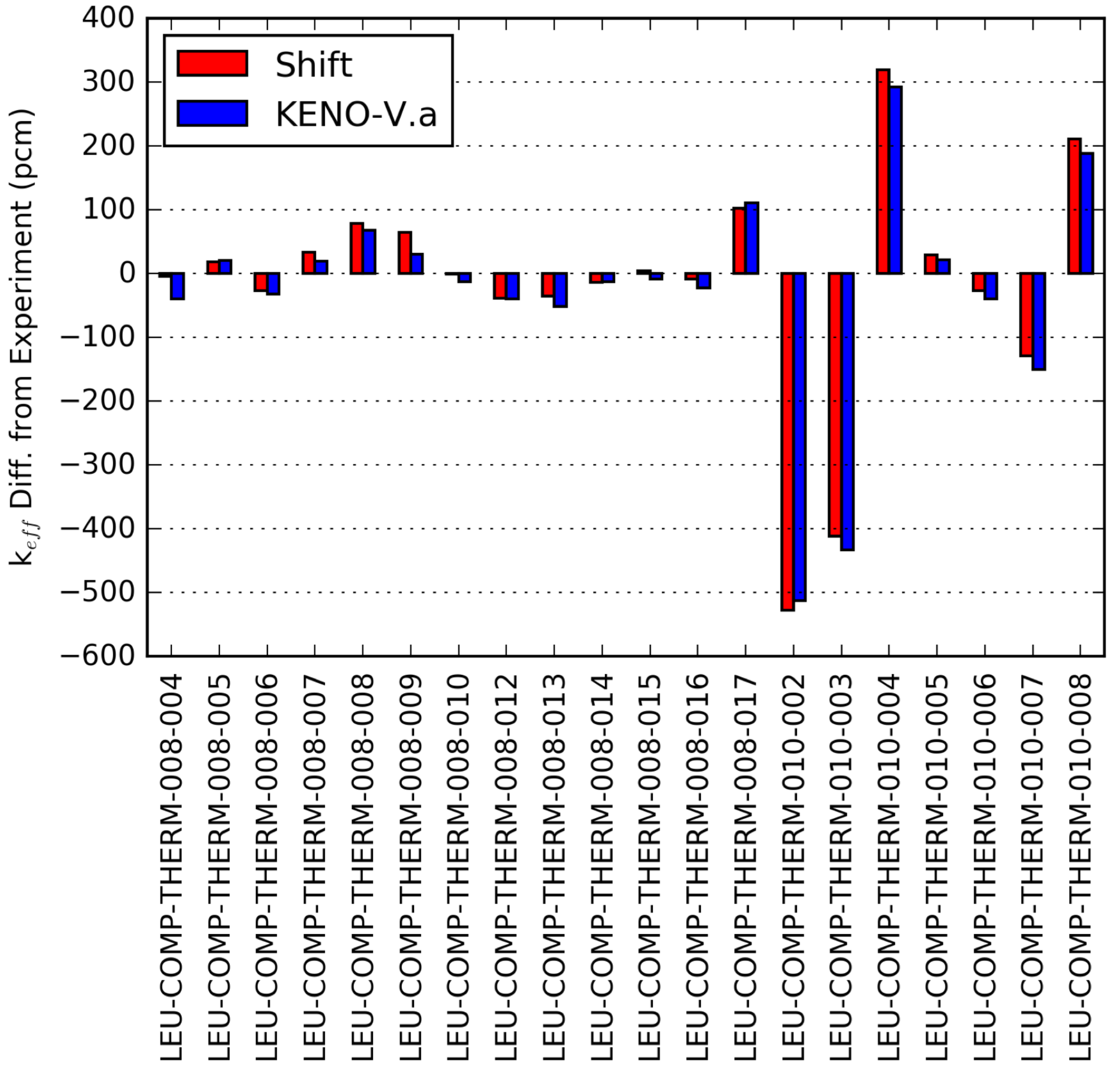
Shift Monte Carlo code system



- 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

Validation of CSAS5-Shift

- VALID results for Shift correspond well with KENO V.a and KENO-VI results
- VALID calculations were run on a single processor, to compare computational time between KENO and Shift



Experiment type	Number of cases	Difference from KENO[a] (pcm)	Standard deviation[b] (pcm)
LEU-COMP-THERM	128	21	31
IEU-MET-FAST	11	16	160
PU-MET-FAST	10	-23	27
MIX-SOL-THERM	3	23	21
MIX-COMP-FAST	2	506	19
MIX-COMP-THERM	20	18	17
HEU-MET-FAST	22	-14	18
PU-SOL-THERM	81	6	20

[a] Computed as the average over all KENO and Shift simulations for an experiment set.
[b] Computed as the standard deviation of the difference in k_{eff} between Shift and KENO.

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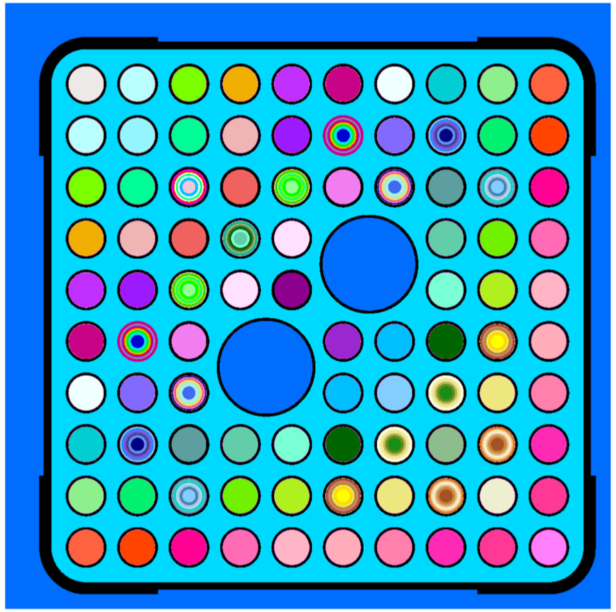
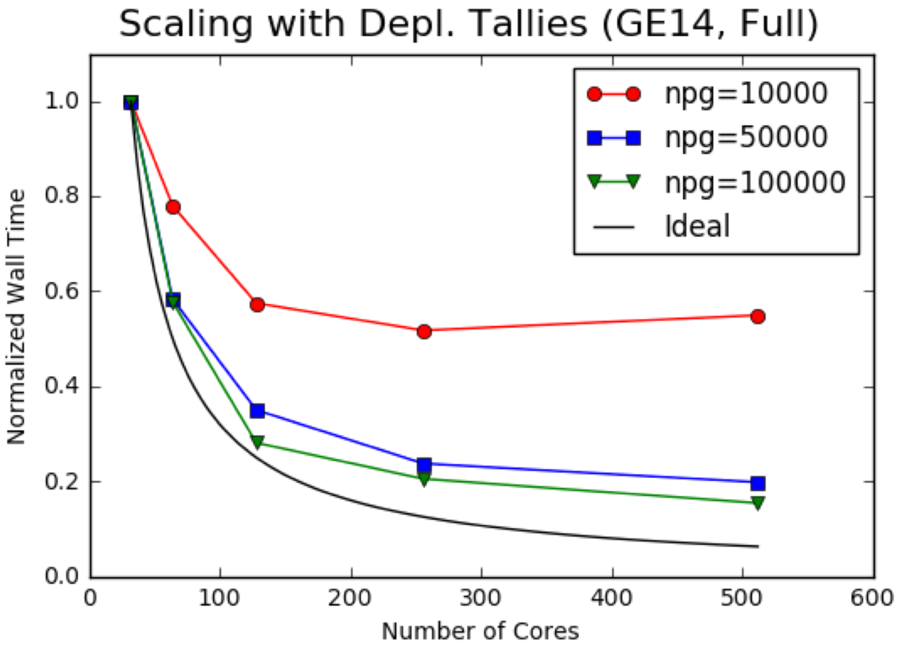
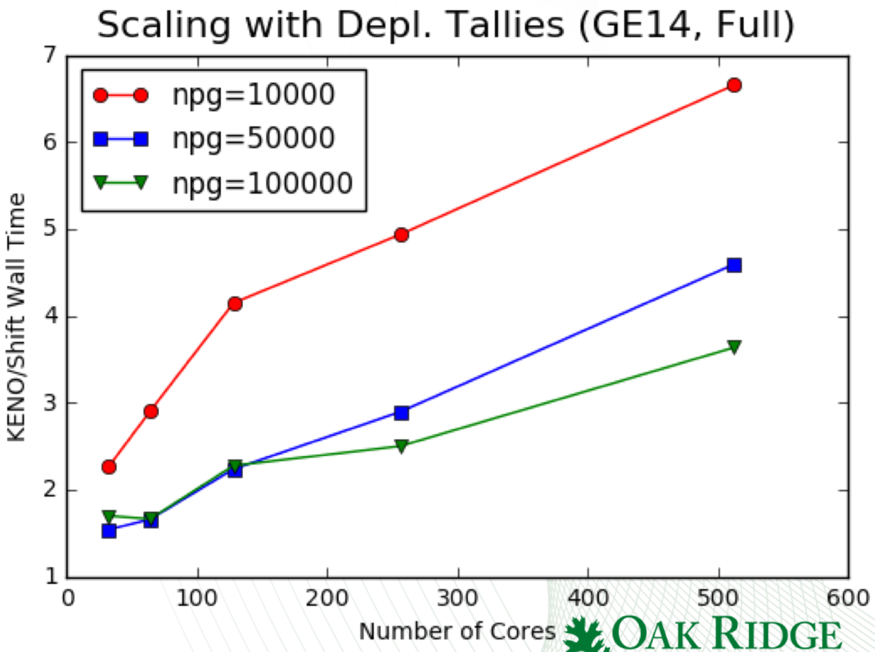
Shift parallel scaling compared to KENO

- **Test Case:** GE14 fuel assembly with depletion tallies
  - A number of identical simulations were run and the average time over the set simulations was used to estimate CPU time
- Shift is only slightly faster than KENO on a single node (1.5x – 2x), but much faster on many nodes (3x - 7x)
- Shift scales close to ideally up to hundreds of processors when using O(50k) particles per generation



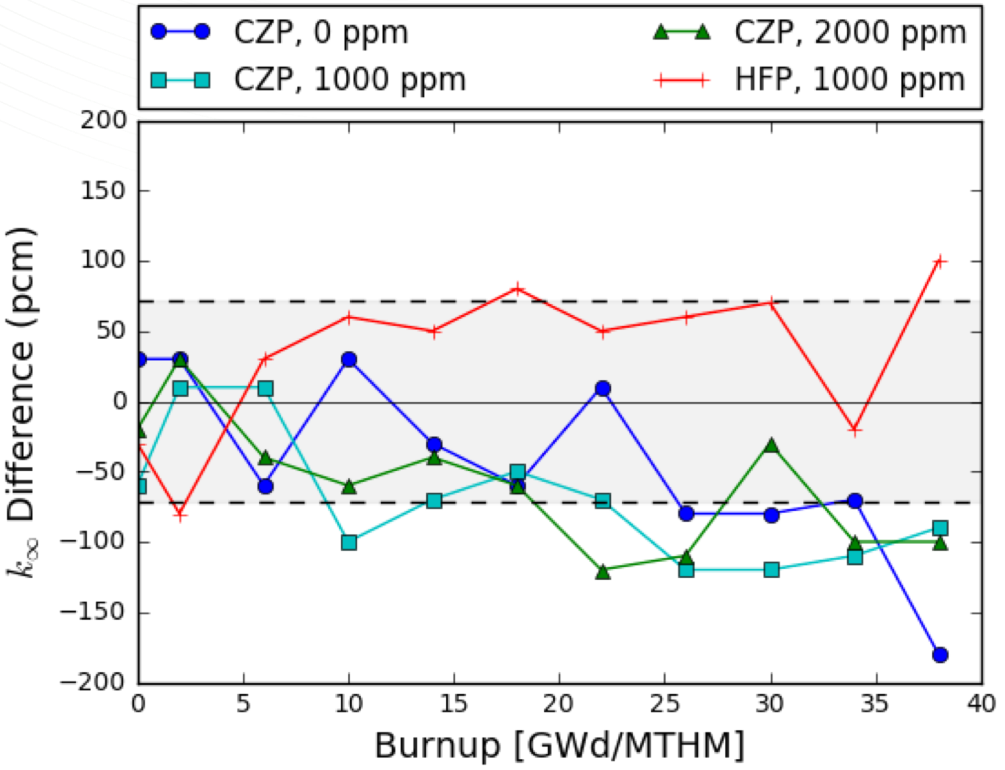




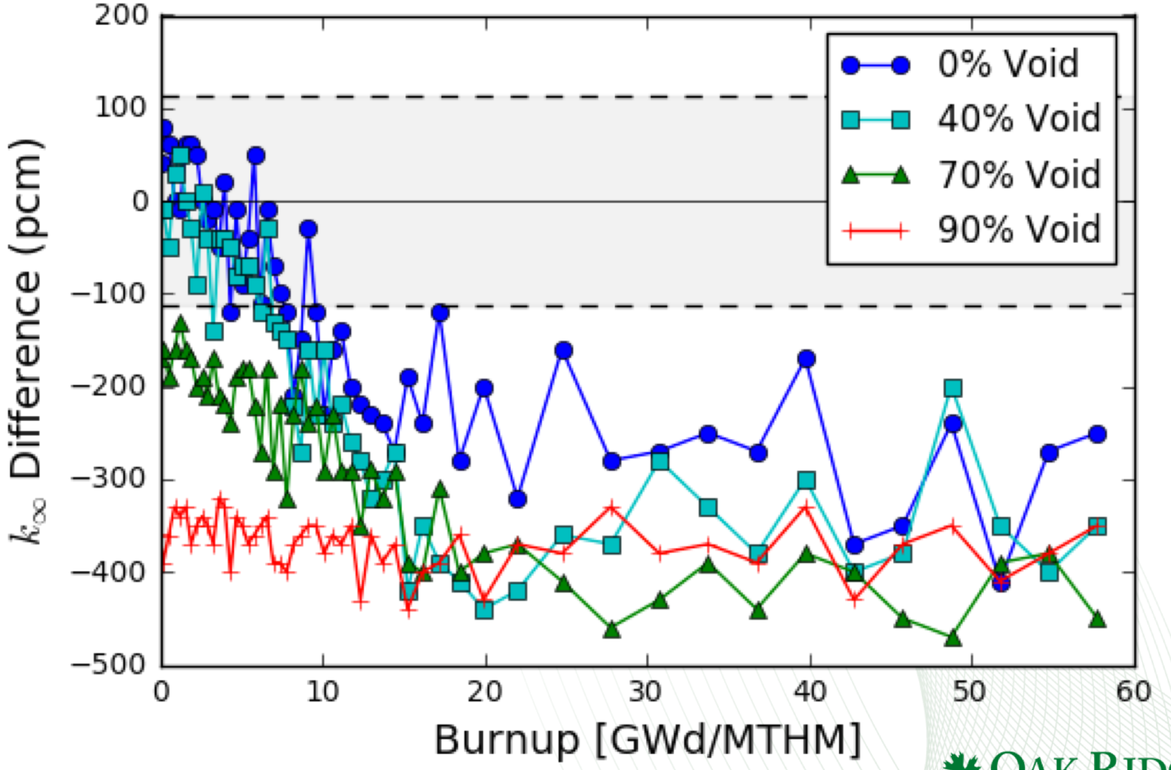
TRITON/Shift Depletion Testing

- Simple LWR test cases were run in all of SCALE's depletion methods
  - Long history of validation for LWR's provides confidence in SCALE's multigroup methods
  - Results show consistency between TRITON/Shift depletion and SCALE's multigroup depletion methods

PWR KENO-CE and Shift Comparison



BWR KENO-MG and Shift Comparison



Generating Few-Group XS Data using SCALE/Shift

- Tally capability has been added to Shift and a new input definition has been implemented to allow generation of few-group cross sections using Shift
- Highlights:
  - Arbitrary energy group structure
  - Multiple tally regions in a single model
  - Supports typical XS data, ADFs, scatting matrix, etc.
  - Based on a rectangular mesh
  - Can be used in Shift-based TRITON or CSAS sequences

Input Format

```
read fgxs
      shape cuboid id=NUM Xmax Xmin Ymax Ymin Zmax Zmin
      energy       id=NUM  E0 E1 E2 ... EN end
      tallytype    id=NUM [options]
end fgxs
```

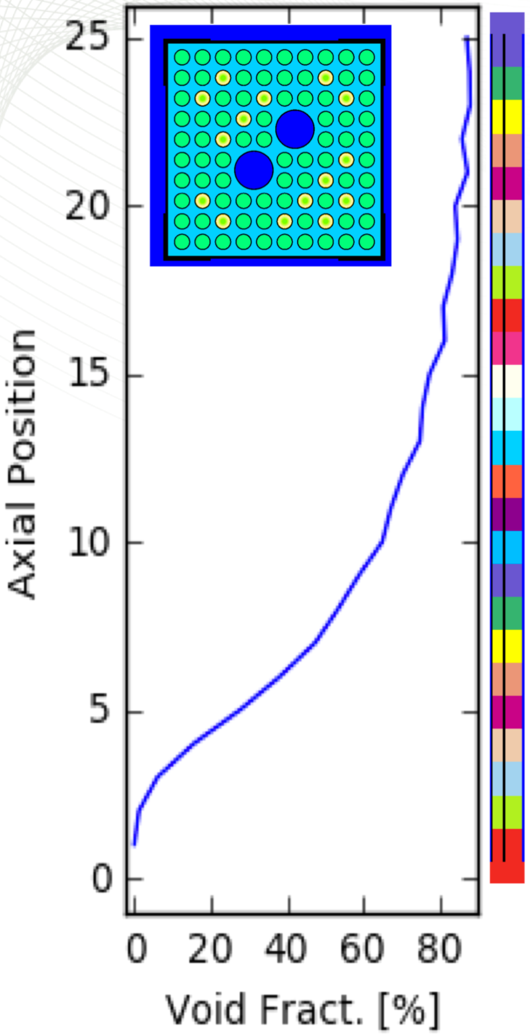
3 Tally Region Example:

```
read fgxs
     shape cuboid id=10  5.0 -5.0  5.0 -5.0   40.0  0.0
     energy       id=10  0 0.625 20E6 end
     tallyset t16 id=10

     shape cuboid id=20  5.0 -5.0  5.0 -5.0   70.0 40.0
     energy       id=20  0 0.625 20E6 end
     tallyset t16 id=20

     shape cuboid id=30  5.0 -5.0  5.0 -5.0  100.0 70.0
     energy       id=30  0 0.625 20E6 end
     tallyset t16 id=30
end fgxs
```

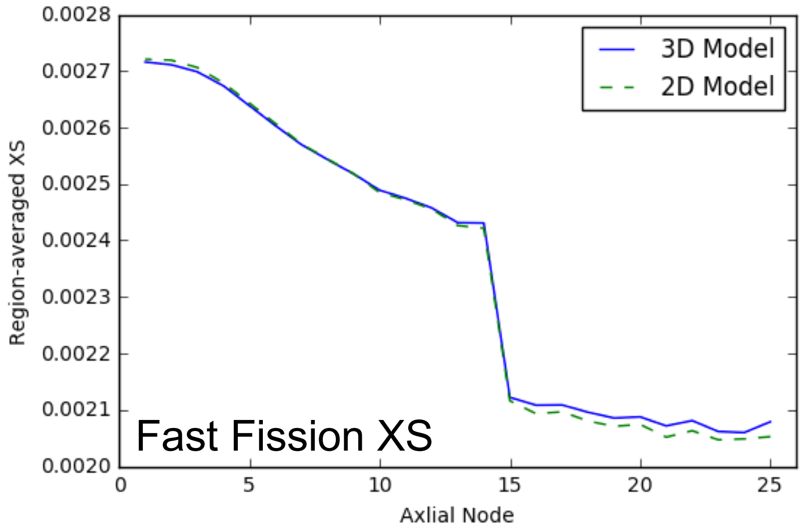
Tally ID=0 Example:

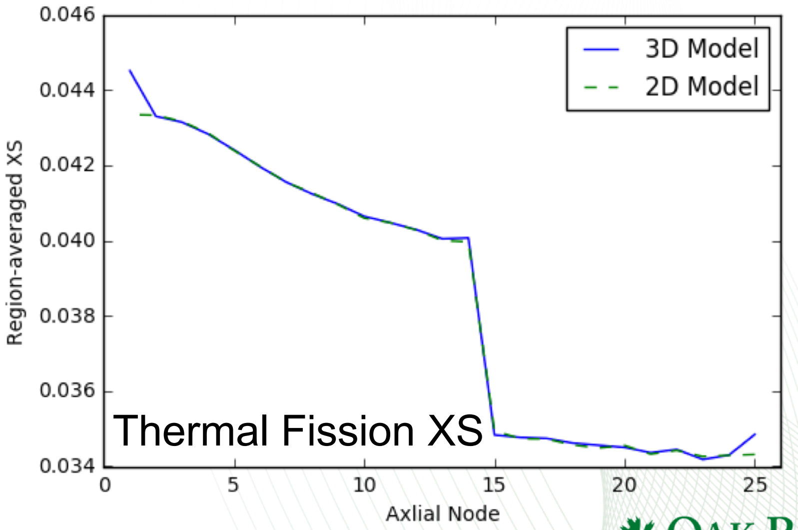
```
read fgxs
     energy       id=0  0 0.625 20E6 end
     tallyset t16 id=0
     shape cuboid id=10  5.0 -5.0  5.0 -5.0   40.0  0.0
     shape cuboid id=20  5.0 -5.0  5.0 -5.0   70.0 40.0
     shape cuboid id=30  5.0 -5.0  5.0 -5.0  100.0 70.0
end fgxs
```

Shift Nodal Data for 3D Assemblies



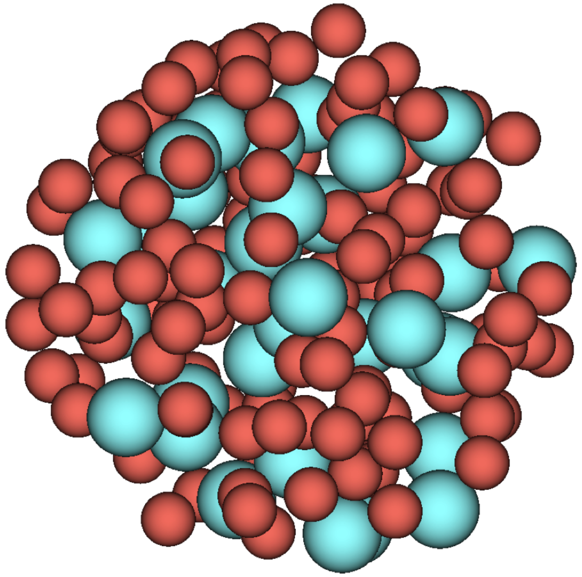
- GE14 fuel assembly modeled with full and vanished regions at BOL.
- Realistic axial void fraction distribution taken from previous BWR BUC work
- Full 3D fuel assembly model compared to typical axial slice models, both modeled in Shift.
  - Designed to test the assumption of using 2D slices to generate XS data for a 3D core simulator
- Results indicate relatively minor differences between cross sections generated with true 3D model versus 2D slice model





Stochastic Geometry in SCALE

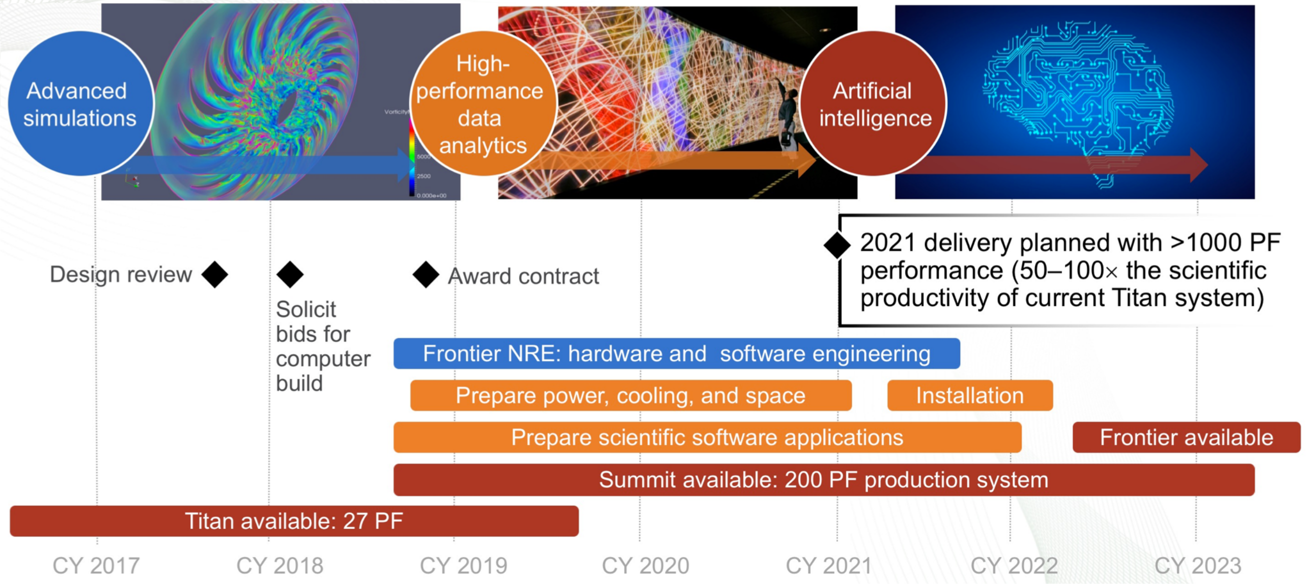
- **Goal:** Enable more straightforward generation of reference solutions for stochastic geometry (TRISO, pebble bed, FCM, etc.)
- Current capabilities
  - Multiple particle types and sizes (spherical only)
  - Sphere, cylinder, and cuboid boundaries
  - Random or regular array placement
  - Visualization of geometry enabled in Fulcrum
- Implemented only in Shift-based sequences



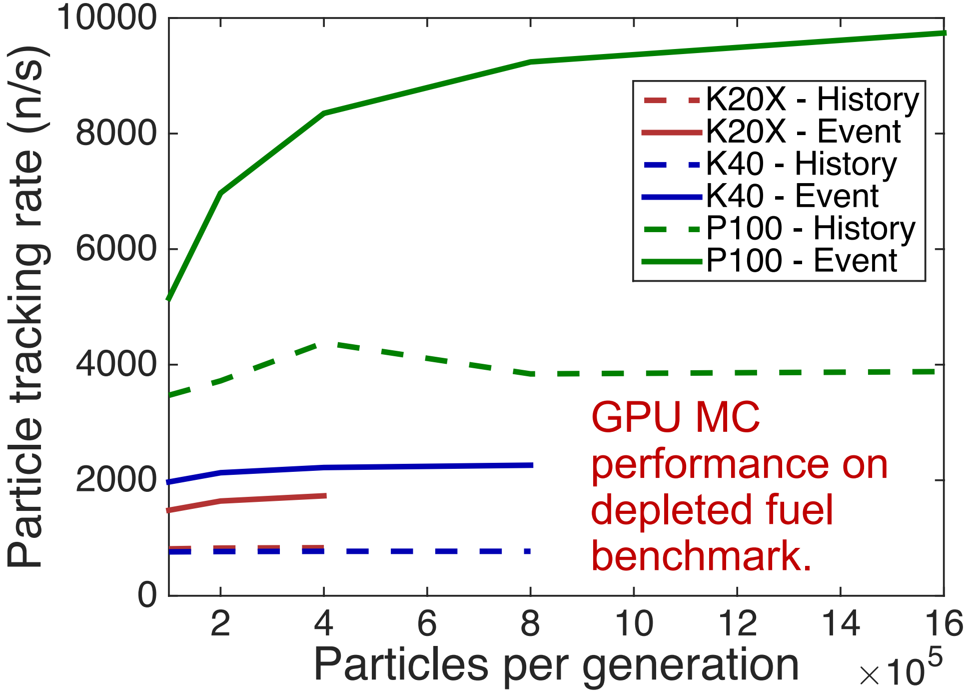
Pebble Input Example

```
=csas-shift
...
unit 1
    sphere 1    2.500000e-02
    sphere 2    3.400000e-02
    sphere 3    3.800000e-02
    sphere 4    4.150000e-02
    sphere 5    4.550000e-02
    media  100 1    1
    media  101 1    2  -1
    media  102 1    3  -2
    media  103 1    4  -3
    media  104 1    5  -4
    boundary 5
unit 10
    com='pebble'
    sphere 1    2.500000e+00
    sphere 2    3.000000e+00
    media  101 1    1  randommix='trisos'
    media  106 1    2  -1
    boundary 2
...
end geometry
...
read randomg eom
  randommix = 'trisos'
    type=    random
    units=    1  end
    pfs=    0.10 end
    clip=    no
    seed=    1000
  end randommix
end randomgeom
...
end
```

Shift is being extended for operation on GPUs as part of the Exascale Computing Project



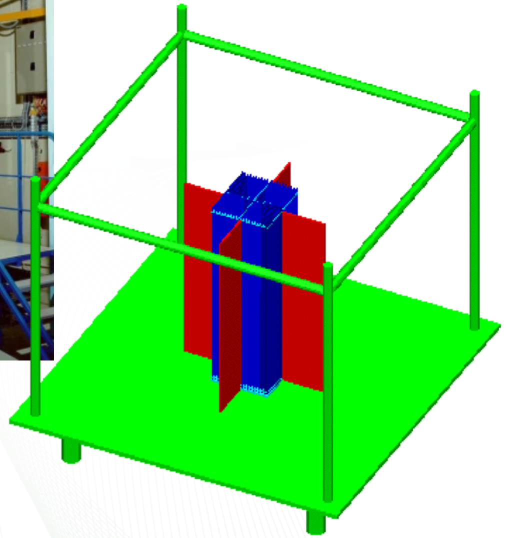
- Improved Monte Carlo particle tracking rate allows reduction in statistical errors
- Cost of tallies and data access is implicit in this measure
- Improved device performance yields better results – Algorithms are tracking hardware improvements



http://www.nvidia.com/object/what-is-gpu-computing.html

Shift/SCALE integration

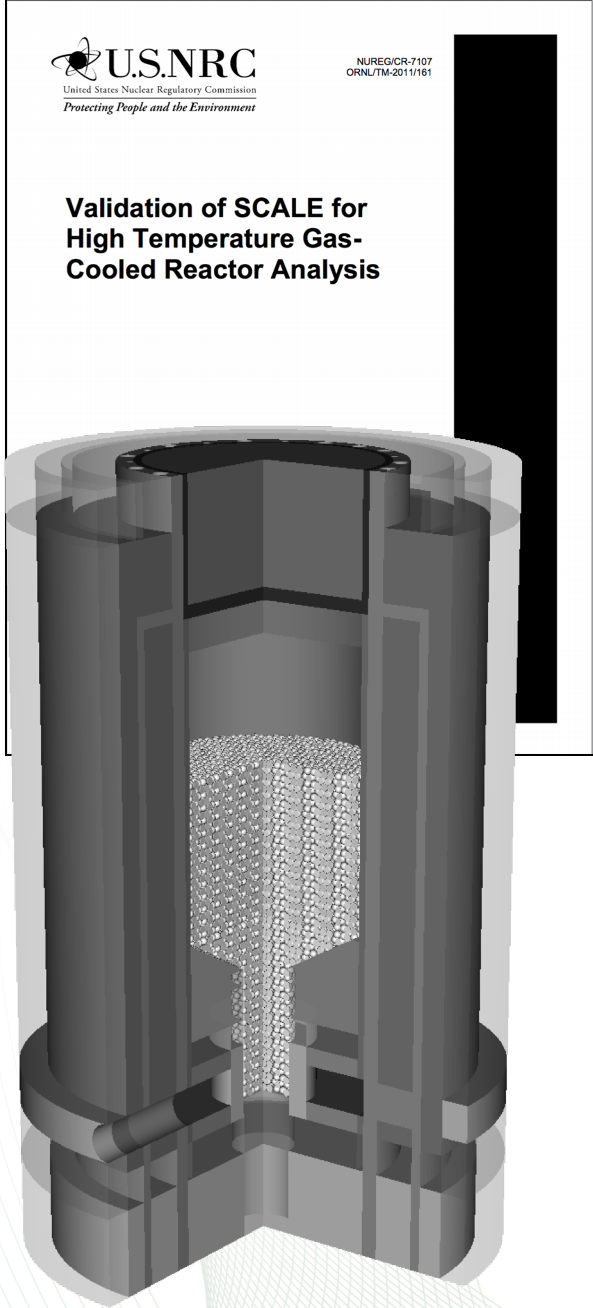
- **Integrated in CSAS criticality sequence**
  - Eigenvalue mode for criticality safety
  - KENO V.a and KENO-VI geometry
  - Uses standard SCALE geometry, material, and control specifications
  - Validated with over 400 benchmark experiments
- **Integration in TRITON depletion sequence**
  - Currently in development
  - Flux-solver
  - Depletion
  - Multigroup cross section generation for nodal codes
  - Randomized geometry for TRISO and pebble bed
- **Integration in TSUNAMI sensitivity/uncertainty sequences**
  - Capability demonstrated
  - 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
  - Currently in development



HTR Modeling Capabilities

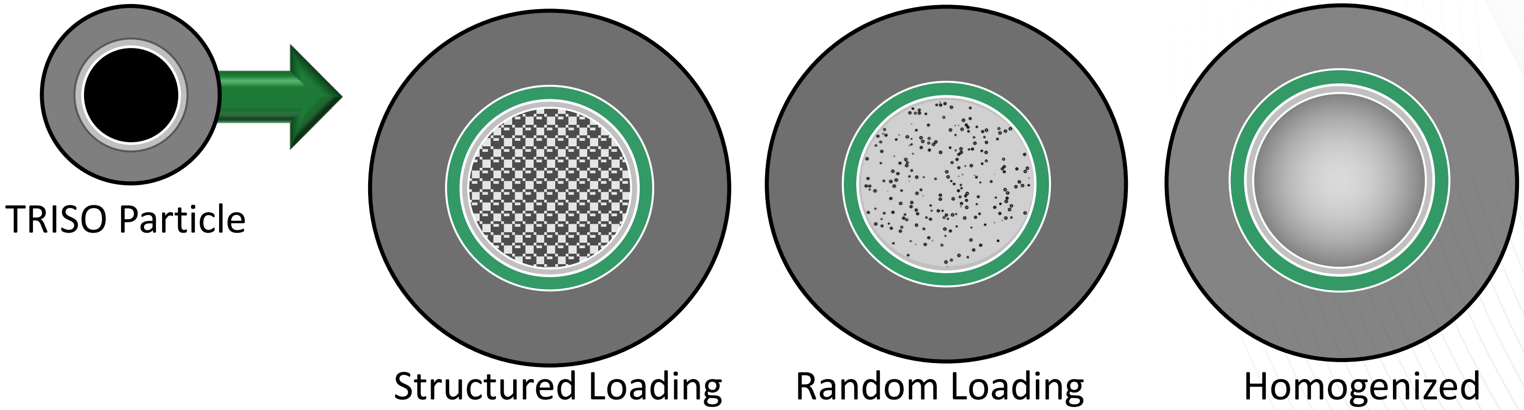
Previous efforts for HTRs

- SCALE provides unique capabilities for the neutronics and source terms analysis of high-temperature reactors (HTRs), including gas-cooled HTGRs, as well as fluoride-salt cooled FHRs.
- Through the US Department of Energy's Next Generation Nuclear Plant (NGNP) program, the NRC supported enhancements to SCALE for tristructural isotropic (TRISO) fuel modeling, especially for interoperability with the PARCS core simulator for HTGR license reviews.
- These capabilities were further enhanced under a cooperative research and development agreement with the Chinese Academy of Sciences and the Shanghai Institute of Applied Physics (SINAP) to integrate and extend TRISO features within the modernized SCALE framework and to develop enhanced features for additional fuel forms and molten salt coolants.
- Sensitivity and uncertainty analysis features of SCALE have been applied extensively with IAEA Coordinated Research Project on HTRs.



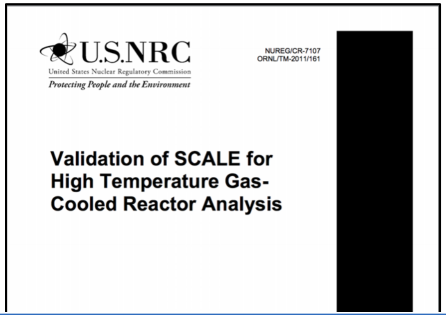
Ongoing efforts for HTR

- Current development activities involve advanced 3D capabilities with the Shift Monte Carlo code, including generation of nodal cross sections for core simulator calculations and modeling random TRISO particle loading.
- Planned developments include improved core simulator coupling for thermal feedback, pebble flow and depletion, reflector and control rod effects, and transient analysis.



Some applications of SCALE to HTGRs

G. Ilas, D. Ilas R. P. Kelly, and E. E. Sunny, *Validation of SCALE for High Temperature Gas Cooled Reactor Analysis*, NUREG/CR-7107, ORNL/TM-2011/161, Oak Ridge National Laboratory (2011). https://www.nrc.gov/docs/ML1220/ML12201A080.pdf

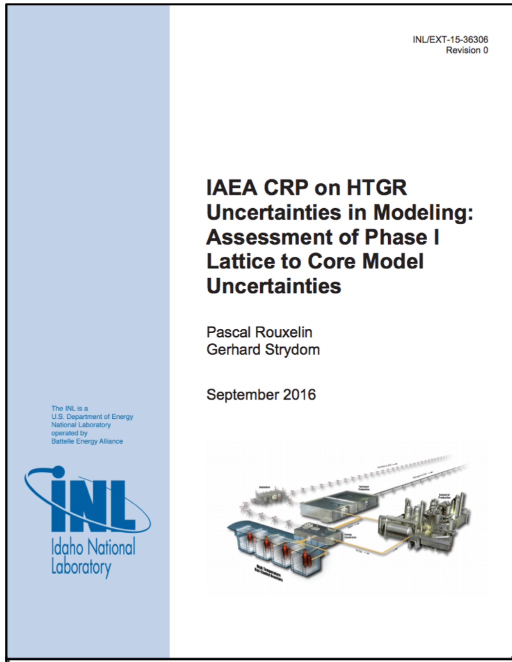

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment
NUREG/CR-7107
ORNL/TM-2011/161
Validation of SCALE for High Temperature Gas-Cooled Reactor Analysis

IAEA
International Atomic Energy Agency
Atoms for Peace

#	Reference of publications - Provided by Frederik Reitsma - Project Manager for Gas Cooled Reactor Technology at IAEA (HTGRs and Molten Salt Reactors)	Year	Reference to SCALE
1	V F Boyarinov, A V Grol, P A Fomichenko and M Yu Ternovykh, "Improvement of Modeling HTGR Neutron Physics by Uncertainty Analysis with the Use of Cross-Section Covariance Information", 2017 J. Phys.: Conf. Ser. 781 012032	2017	Yes
2	Friederike Bostelmann, Hans R. Hammer, Javier Ortensi, Gerhard Strydom, Kiril Velkov, Winfried Zwermann, "Criticality calculations of the Very High Temperature Reactor Critical Assembly benchmark with Serpent and SCALE/KENO-VI" Annals of Nuclear Energy 90 (2016) 343–352	2016	Yes
3	Lidong Wang, Jiong Guo, Fu Li, Jason Hou, Kostadin N. Ivanov "Effect of Double Heterogeneity Treatment on Neutronics Modeling of HTGR Unit Cell", International Topical Meeting on High Temperature reactor technology (HTR2016), November 6-10, Las Vegas, NV, USA	2016	Yes
4	V.F. Boyarinov, P.A. Fomichenko, A.V. Grol, "Use of Cross-Section Covariance Information in Uncertainty Analysis at Modeling HTHR Neutron Physics", International Topical Meeting on High Temperature reactor technology (HTR2016), November 6-10, Las Vegas, NV, USA	2016	Yes
5	Pascal Rouxelin, Gerhard Strydom, Andrea Alfonsi, Kostadin Ivanov, "IAEA CRP on HTGR Uncertainties: Sensitivity Study of PHISICS/RELAP5-3D MHTGR-350 Core Calculations using Various SCALE/NEWT Cross-Section Sets for Ex. II-1a" International Topical Meeting on High Temperature reactor technology (HTR2016), November 6-10, Las Vegas, NV, USA	2016	Yes
6	Frederik Reitsma, "The Activities at the IAEA in Support of High Temperature Reactors Technology Development", International Topical Meeting on High Temperature reactor technology (HTR2016), November 6-10, Las Vegas, NV, USA	2016	Yes
7	Frederik Reitsma and Wonkyeong Kim, "The contribution of cross-section uncertainties to pebble bed reactor eigenvalues results: IAEA cooperative research project Phase I standalone neutronics", Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
8	Wonkyeong Kim, Frederik Reitsma and Deokjung Lee, "IAEA Coordinated Research Program on HTGR Uncertainty Analysis: Results of Exercise I-1 Model and the Application of the RPT Method", Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
9	V.V. Naicker, D.A. Maretele, F. Reitsma, F. Bostelmann, G Strydom, "Quantification of the SCALE 6.1 Eigenvalue Uncertainty due to Cross-Section Uncertainties for Exercise I-1 of the IAEA CRP on HTGR Uncertainties." Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
10	Lidong Wang, Jiong Guo, Fu Li, Chen Hao, Kostadin Ivanov, Pascal Rouxelin "Direct Evaluation of Nuclear Data Uncertainty Propagation in Pebble-Bed HTR Core", Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
11	Friederike Bostelmann, Kiril Velkov, Winfried Zwermann (GRS), Hans Hammer (Texas A&M), Gerhard Strydom (INL), "Impact of Nuclear Data Uncertainties on Criticality Calculations of the Very High Temperature Reactor Critical Assembly Benchmark", Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
12	P. Rouxelin (NCSU), G. Strydom (INL), K. Ivanov (NCSU), "IAEA CRP on HTGR Uncertainties: Comparison of Ex. I-2c Nominal Results and Coupling with the PHISICS/RELAP5-3D Core Model for Ex. II-1", Reviewed paper presented at the PHYSOR2016 conference, Sun Valley, Idaho, May 1-5, 2016.	2016	Yes
13	Friederike Bostelmann, Gerhard Strydom, Frederik Reitsma, Kostadin Ivanov "The IAEA coordinated research programme on HTGR uncertainty analysis: Phase I status and Ex. I-1 prismatic reference results" Nucl. Eng. Des. (2015). http://dx.doi.org/10.1016/j.nucengdes.2015.12.009	2015	Yes
14	G. Strydom, F. Bostelmann, "IAEA Coordinated Research Project on HTGR Reactor Physics, Thermal Hydraulics and Depletion Uncertainty Analysis: Prismatic HTGR Benchmark Definition: Phase 1" INL/EXT-15-34868, Revision 1, August 2015	2015	No
15	Tae Young Han, Hyun Chul Lee, Jae Man Noh, "Development of a sensitivity and uncertainty analysis code for high temperature gas-cooled reactor physics based on the generalized perturbation theory", Annals of Nuclear Energy 85 (2015) 501–511	2015	Yes
16	Frederik Reitsma "The IAEA Activities in Support of the Near Term Deployment of High temperature Gas Cooled Reactors" 2014 ANS Winter Meeting and Nuclear Technology Expo; Transactions of the American Nuclear Society Volume 111, TRANSAO 111, p 1082-1084 (2014); ISSN: 0003-018X	2014	No
17	F. Reitsma, G. Strydom, F. Bostelmann K. Ivanov, "The IAEA Coordinated Research Program on HTGR Uncertainty Analysis: Phase I Status and Initial Results", Paper HTR2014-51106, Proceedings of HTR 2014, Weihai, China, October 27 – 31, 2014	2014	Yes

Additional References for Applications of SCALE to HTRs

- R. Rouxelin and G. Strydom, *IAEA CRP on HTGR Uncertainties in Modeling: Assessment of Phase I Lattice to Core Model Uncertainties,* INL/EXT-15-36303 (2016).
- F. Bostelmann, G. Strydom, F. Reitsma, and K. Ivanov, *The IAEA coordinated research programme on HTGR uncertainty analysis: Phase I status and Ex. I-1 prismatic reference results*, INL/JOU-15-34866 (2016).
- F. Bostelmann and G. Strydom, "Nuclear data uncertainty and sensitivity analysis of the VHTRC benchmark using SCALE," *Ann. Nucl. Eng.*, 110, p. 317-329 (2017).
- P. Avigni, *On-line refueling for the Advance High Temperature Reactor,* Georgia Institute of Technology 2017.


INL/EXT-15-36306
Revision 0

IAEA CRP on HTGR Uncertainties in Modeling: Assessment of Phase I Lattice to Core Model Uncertainties

Pascal Rouxelin
Gerhard Strydom

September 2016

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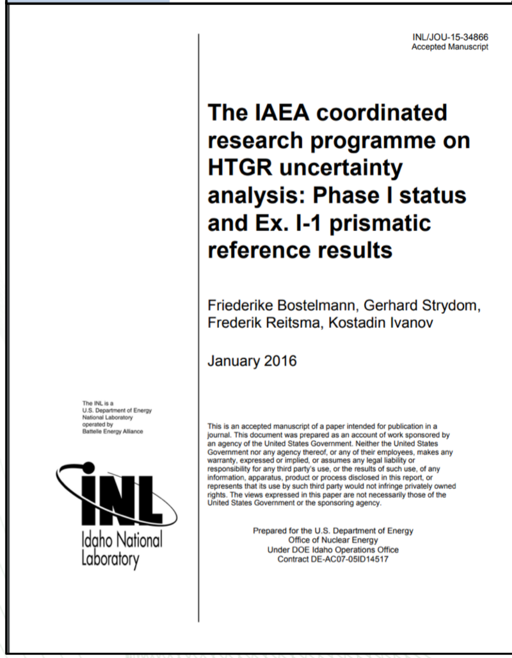
INL/JOU-15-34866
Accepted Manuscript

The IAEA coordinated research programme on HTGR uncertainty analysis: Phase I status and Ex. I-1 prismatic reference results

Friederike Bostelmann, Gerhard Strydom, Frederik Reitsma, Kostadin Ivanov

January 2016

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Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

X-energy Neutronics Roadmap

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- Feasibility study published by Idaho National Laboratory in August 2017

Table 2. High-level requirements and functionalities matrix.

Code	Basic Code Suitability to Development and Verification and Validation					Basic Functional Capabilities					
	Pedigree (Doc. and V&V)	*Level of Support*		*Availability*		*Core Neutron Transport in Cylindrical (2D or 3D) Geometry*		*Burnup (Micro Depletion)*	*Fuel Management (Shuffling)*	*Cross-section (XS) Generation*	
		Code	*User*	*Source*	*Exe.*	*Transient*	*SS*			*Double Het.*	*Leakage Feedback*
VSOP-A	L	H	H	✓	✓	✗	✓	✓	✓	✓	✓
VSOP-99	L	L	M	✗	✓	✗	✓	✓	✓	✓	✓
MGT	L	L	M	✗	✓	✓	✓	VSOP99 can support this.			
HCP	L	L	L	✗	✗	✓	✓	✓	✓	✓	✓
PARCS-SCALE	H	M	M	✓	✓	✓	✓	✓	✗	✓	✗
PEBBED	L	M	M	✓	✓	✗	✓	✓	Equilibrium. Core	✓	✓
CYNOD	L	L	L	✓	✓	✓	✓	Third-party codes can support this.			
DYN3D	L	L	L	✓	✓	✗	✗	✓	✗	Unknown	Unknown
NEM	L	M	M	✓	✓	✓	✓	✗	✗	MICROX-2	
DORT/TORT	L	M	M	✓	✓	✓	✓	✗	✗	MICROX-2	
DALTON	L	L	L	Unknown	Unknown	✓	✓	✗	✗	SCALE, but might need more work.	
RZ-KIND	L	L	L	Unknown	Unknown	✓	✓	✗	✗	Unknown	Unknown
PANTHER	M	M	M	Unknown	✓	✗	✗	unknown	unknown	WIMMS.	
PHISICS	L	M	M	✓	✓	✗	✗	✓	✓ (tested on LWRs only)	Third-party codes only.	
MAMMOTH/ RATTLESNAKE	L	M	M	✓	✓	✓	✓	✓	✗	Third-party codes only.	
CAPP	L	L	L	Unknown	Unknown	✓	✓	✓	✓	HELIOS w. RPT, ECF, method.	
Hexpedite	L	L	L	✗	✗	✗	✗	✗	✗	Unknown	Unknown

H = High, M = Medium, L = Low

4

X-ENERGY BUSINESS SENSITIVE

INL/LTD-17-42500
Revision 0

X-energy Core Neutronics Simulation Code Technical Feasibility Study

Work For Others Agreement No.14803 between Battelle Energy Alliance, LLC, and X-energy, LLC., Modification No. 5

Sonat Sen
Gerhard Strydom
Hans Gougar

August 2017

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Idaho National Laboratory

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X-ENERGY BUSINESS SENSITIVE

OAK RIDGE National Laboratory

X-energy Neutronics Roadmap

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- X-Energy, LLC (X-energy) requires a fully functional high-temperature reactor core design and analysis code to support Xe-100 reactor design, licensing, and commercial operation. The code suite should be able to simulate all neutronic and thermal-fluid core scenarios and phenomena needed to show that the Xe-100 reactor plant design can meet technical requirements, and enable understanding of potential licensing and economic impacts. This report documents the process used by Idaho National Laboratory (INL) engineering staff to evaluate candidate neutronic simulation codes and recommend a viable option for meeting X-energy's needs.
- A two-step selection process was employed. In the first step, neutronics codes that were applied to previous pebble bed reactor core neutronics simulations (as indicated through publication or participation in international benchmark projects) were measured against high-level code accessibility and functionality criteria. Those that met a large number of these criteria were deemed suitable for a more detailed evaluation of capabilities and gaps. The challenges to acquisition and development posed by the remaining codes were deemed too great such that overcoming them would not be an effective use of X-energy's resources.
- The code systems that passed the first filter were then assessed against a set of detailed Technical and Functional Requirements (TFRs). Individual requirements were categorized as either Essential (E), Recommended (R), or just Desirable (D) in terms of the capability to simulate pebble bed reactor neutronics and fuel management. The maturity level of the selected codes was assessed against these TFRs using the Predictive Capability Maturity Model (PCMM) methodology developed at Sandia National Laboratory (SNL).
- This process led to the SCALE/PARCS/Flownex code set as being the recommended option for calculations beyond the scoping phase, based on the combined package's verification and validation (V&V) pedigree, choice of high-fidelity solvers, and flexibility. It will, however, require improvements in the coupling with Flownex or another thermal-fluid code, the addition of a fuel management (shuffling) capability, and a leakage feedback correction methodology.

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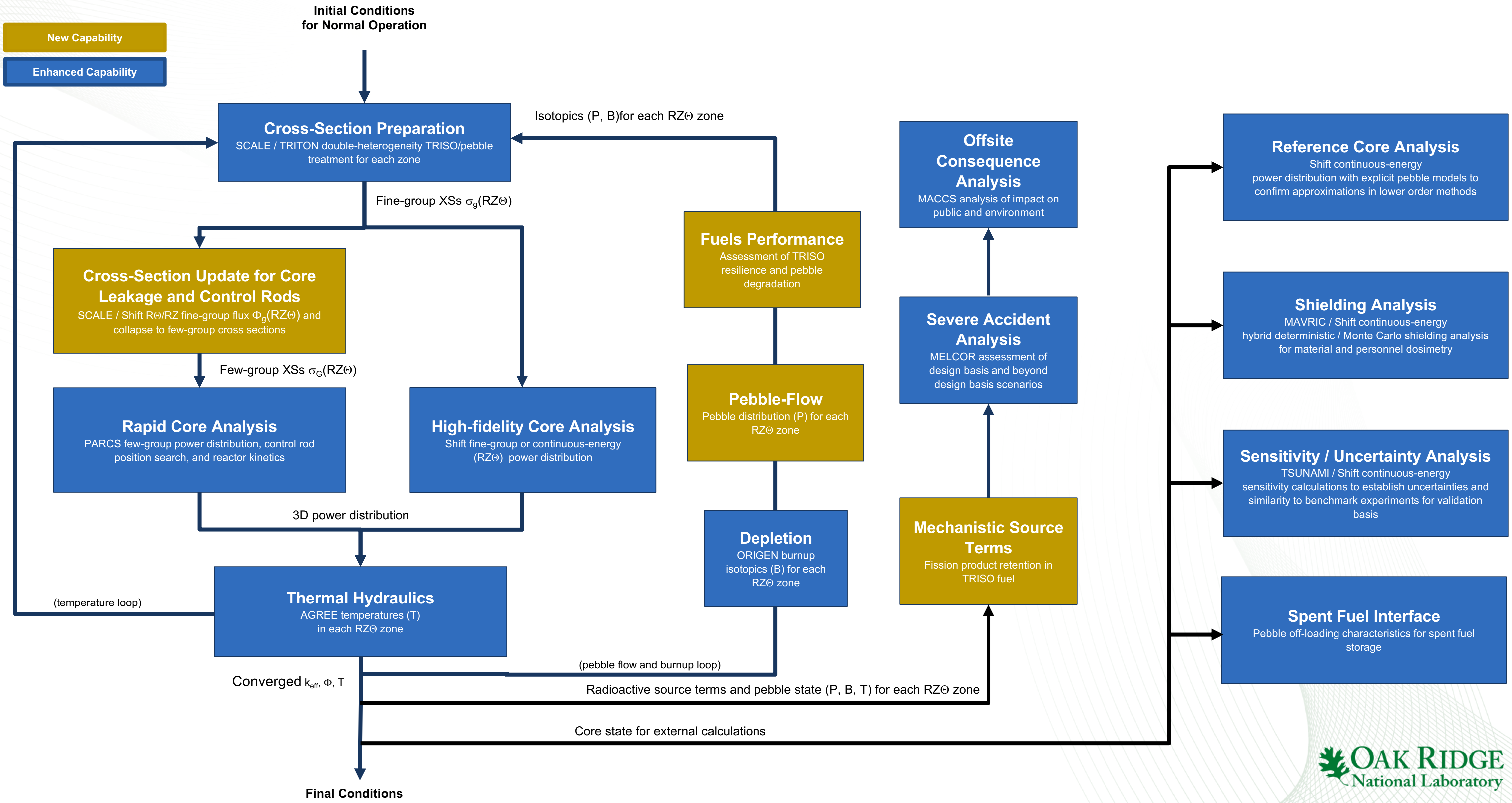
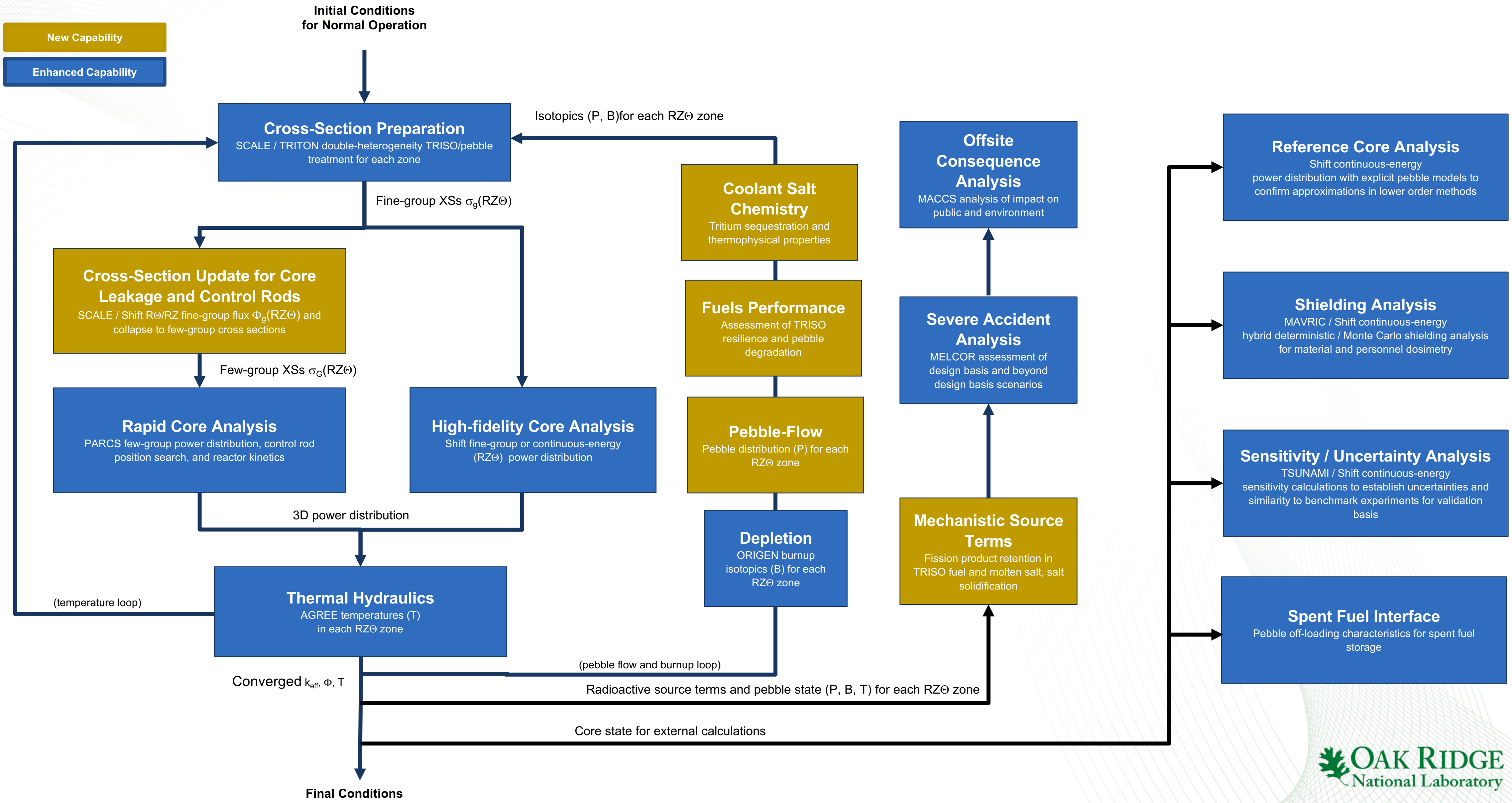
SCALE-HTGR Integrated Modeling and Simulation



Modeling and Simulation Gaps - HTGR

- Pebbles flowing through core and reloaded
- >5% enrichment
- Nuclear data libraries optimized for graphite spectrum
- Leakage effect in cross section treatment
- Treatment of control rods in reflector
- Steaming paths through core
- 3D effects of non-uniform burnup distribution and history effects
- Mechanistic source terms
- Fuels performance

SCALE-FHR Integrated Modeling and Simulation

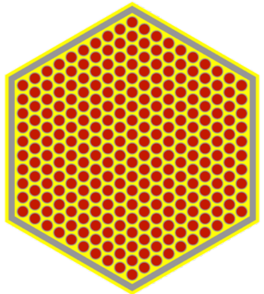


Modeling and Simulation Gaps - FHR

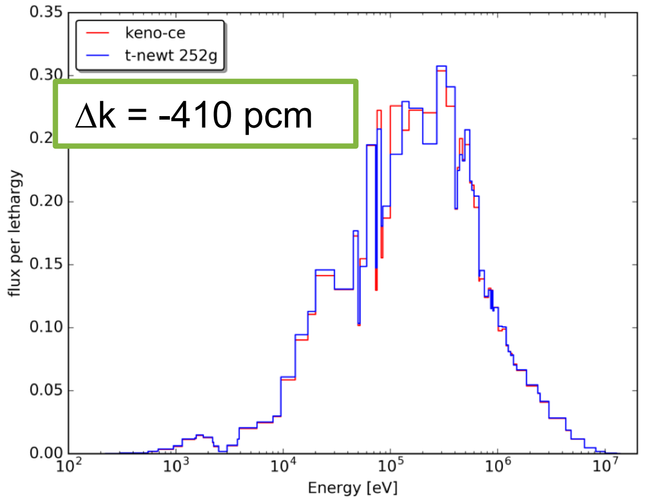
- Pebbles flowing through core and reloaded
- >5% enrichment
- Nuclear data libraries optimized for graphite spectrum with molten salt
- Tritium production in FLiBe
- Leakage effect in cross section treatment
- Treatment of control rods in reflector
- 3D effects of non-uniform burnup distribution and history effects
- Mechanistic source terms
- Fuels performance

SFR Modeling Capabilities

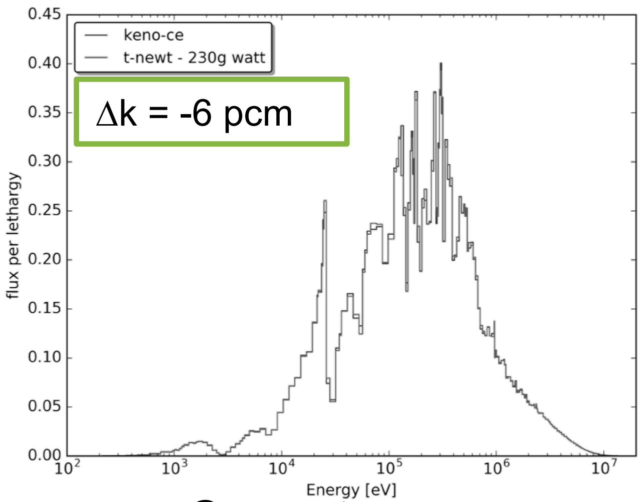
Nuclear Data Libraries from AMPX



- Continuous-energy data serve as reference solution to confirm multigroup approximations
- Multigroup cross sections can be generated for any type of system
  - LWR, HTGR, MSR, FHR, SFR, etc. with appropriate energy group structure and weighting spectrum
- Uncertainties in cross sections (covariance data) quantify confidence in deployed data libraries
- AMPX developed and deployed with SCALE



Incorrect group structure/weighting



Correct group structure/weighting

Uncertainty in k_{eff} Due to Nuclear Data Uncertainties: 1,435 pcm!

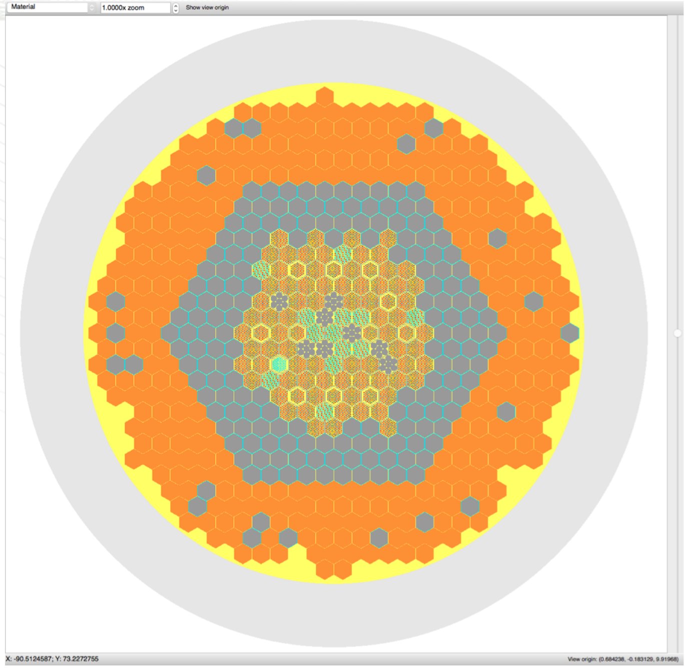
covariance matrix nuclide-reaction		with	nuclide-reaction		% Δk/k due to this matrix
u-238	n,n'		u-238	n,n'	1.2053(9)
na-23	elastic		na-23	elastic	0.3242(2)
fe-56	elastic		fe-56	elastic	0.2590(3)
u-238	n,gamma		u-238	n,gamma	0.2435(1)
fe-56	n,n'		fe-56	n,n'	0.2388(1)

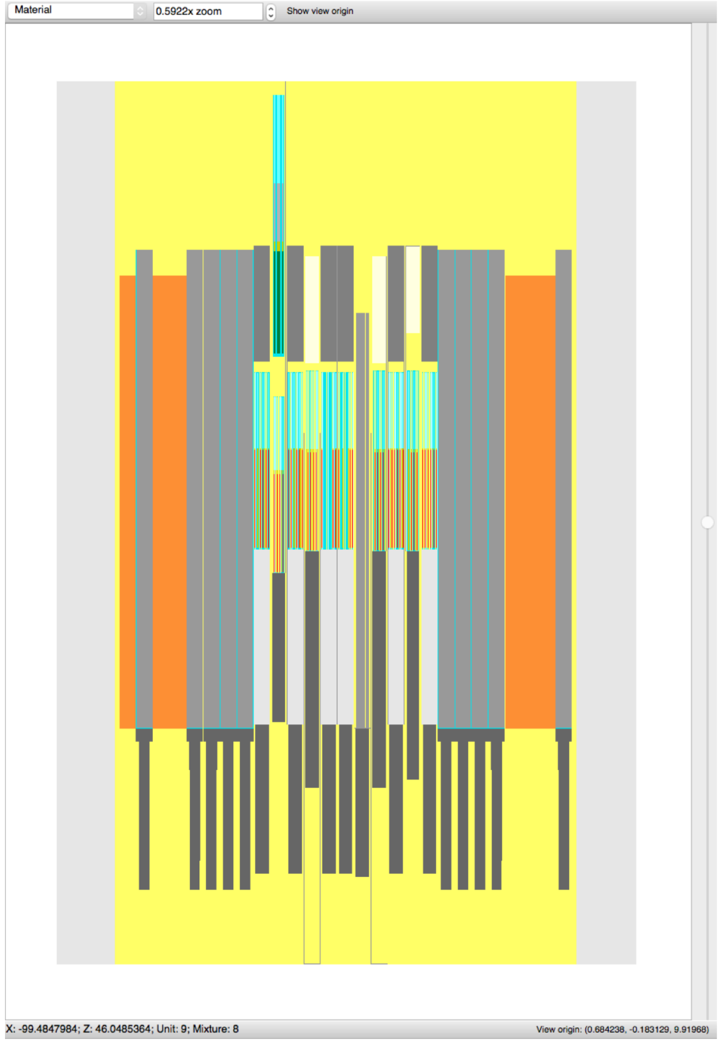
Oak Ridge National Laboratory

Some applications of SCALE to SFRs

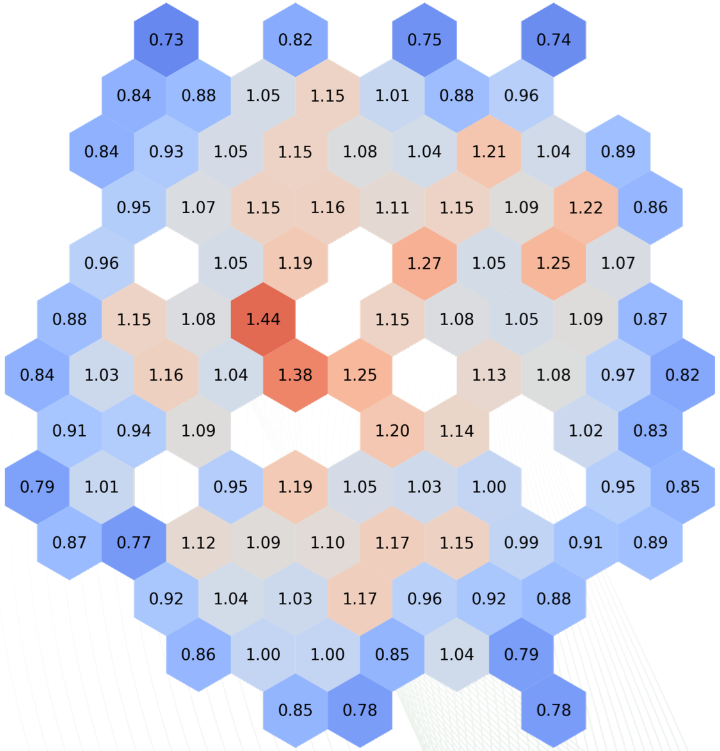
- F. Bostelmann, W. Zwermann, A. Pautz, "SCALE Covariance Libraries For Sodium-Cooled Fast Reactor Systems," Proc. PHYSOR 2018, Cancun, Mexico, April 22-26, 2018
- F. Bostelmann, N. R. Brown, A. Pautz, B. T. Rearden, K. Velkov, and W. Zwermann, "SCALE Multi-Group Libraries for Sodium-cooled Fast Reactor Systems," *M&C 2017 – International Conference on Mathematics & Computational Methods Applied to Nuclear Science and Engineering*, Jeju, Korea, April 16–20, 2017.
- F. Bostelmann, B. T. Rearden, W. Zwermann, A. Pautz, "Preliminary SCALE/TSUNAMI Results for the Sub-exercises of the OECD/NEA Benchmark for Uncertainty Analysis in Modeling of Sodium-Cooled Fast Reactors," *Trans. Am. Nucl. Soc.* (2018) (submitted)
- F. Bostelmann, N. Brown, B. Rearden, K. Velkov, W. Zwermann, "Assessing and Enhancing SCALE Capabilities to Model Fast Neutron Spectrum Systems," FR-UAM-2 meeting: Paul Scherrer Institut, Villigen, Switzerland, June 2-3, 2016
- J. Bousquet, F. Bostelmann, K. Velkov, W. Zwermann, "Macroscopic Cross Section Generation with SCALE 6.2 for the MYRRHA Minimal Critical Core," *M&C 2017 – International Conference on Mathematics & Computational Methods Applied to Nuclear Science and Engineering*, Jeju, Korea, April 16–20, 2017.
- P. Romojaro, et al, "Nuclear data sensitivity and uncertainty analysis of effective neutron multiplication factor in various MYRRHA core configurations," *Ann. Nucl. Eng.,* 101, p. 330-338 (2017).
- R. Stewart, *Sensitivity and Uncertainty Analysis in the Homogenization of the EBR-II Core*, Idaho State University 2017.
- N. E. Stauff, et al, "Evaluation of the OECD/NEA/SFR-UAM Neutronics Reactivity Feedback and Uncertainty Benchmarks," IAEA-CN245-149 2017.

EBR-II Model with TRITON / Shift



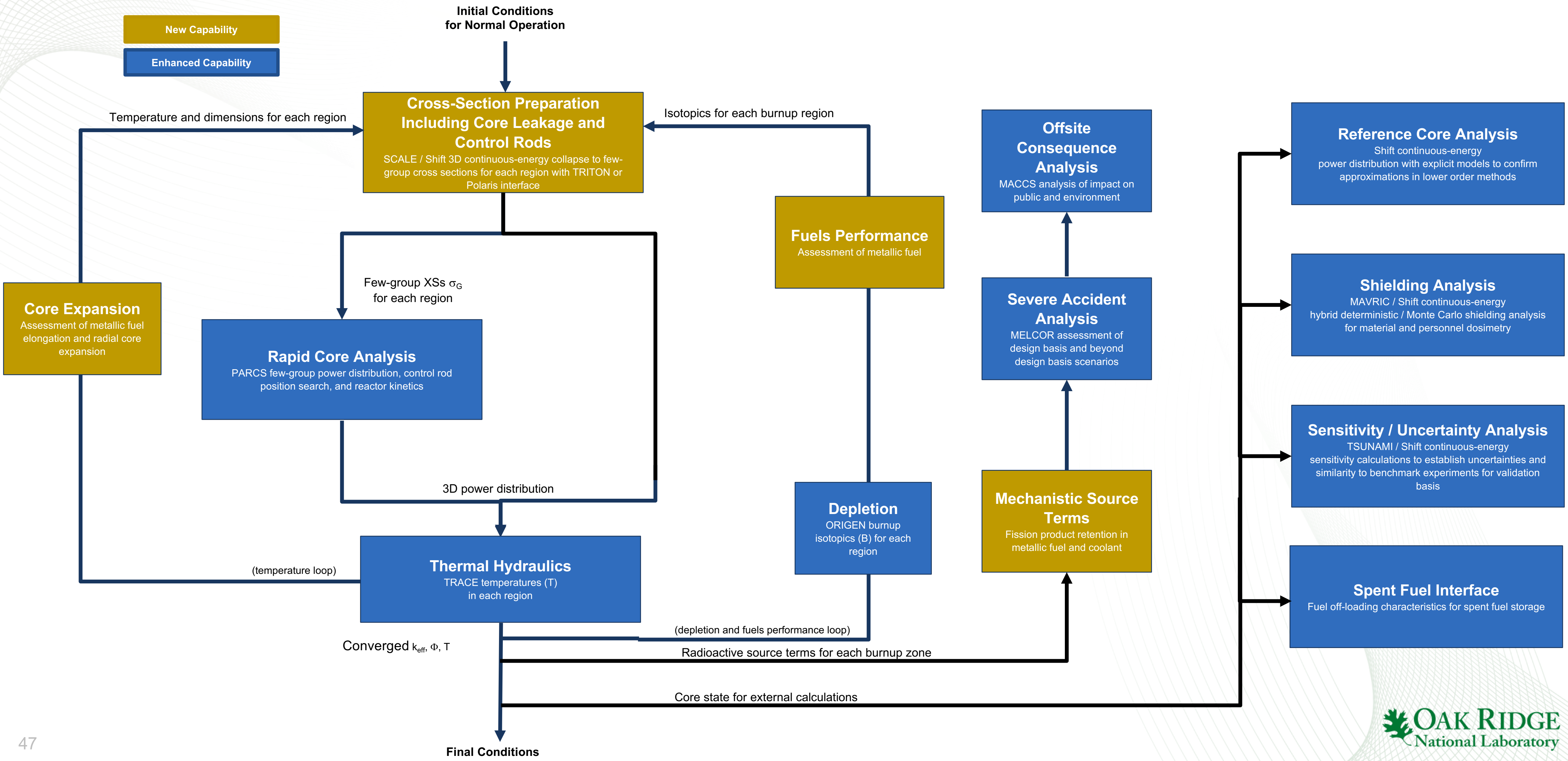


- Radial power distribution



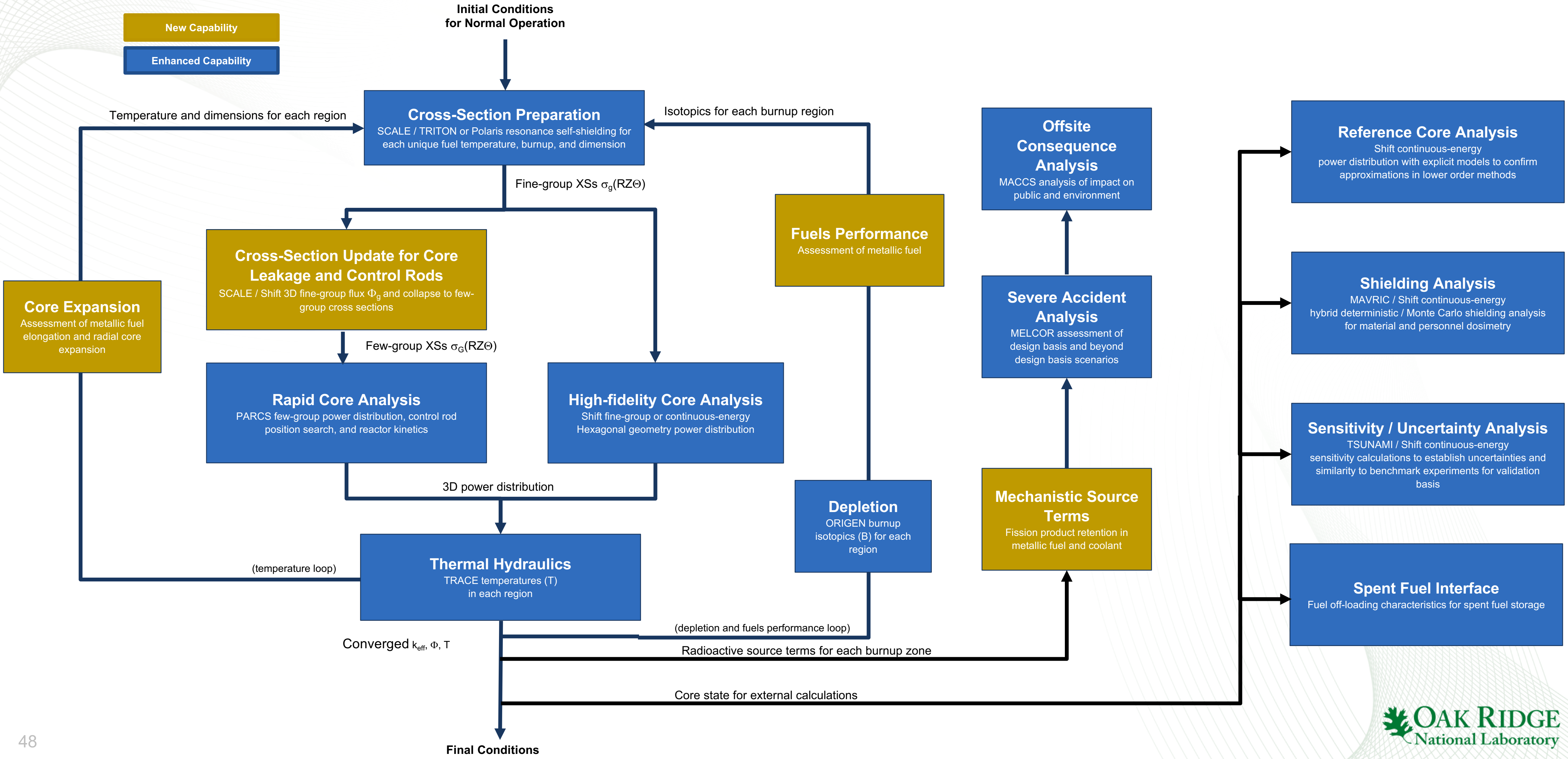
SCALE-SFR Integrated Modeling and Simulation

Continuous-energy Shift/PARCS Path



SCALE-SFR Integrated Modeling and Simulation

Multigroup TRITON (or Polaris) / PARCS Path



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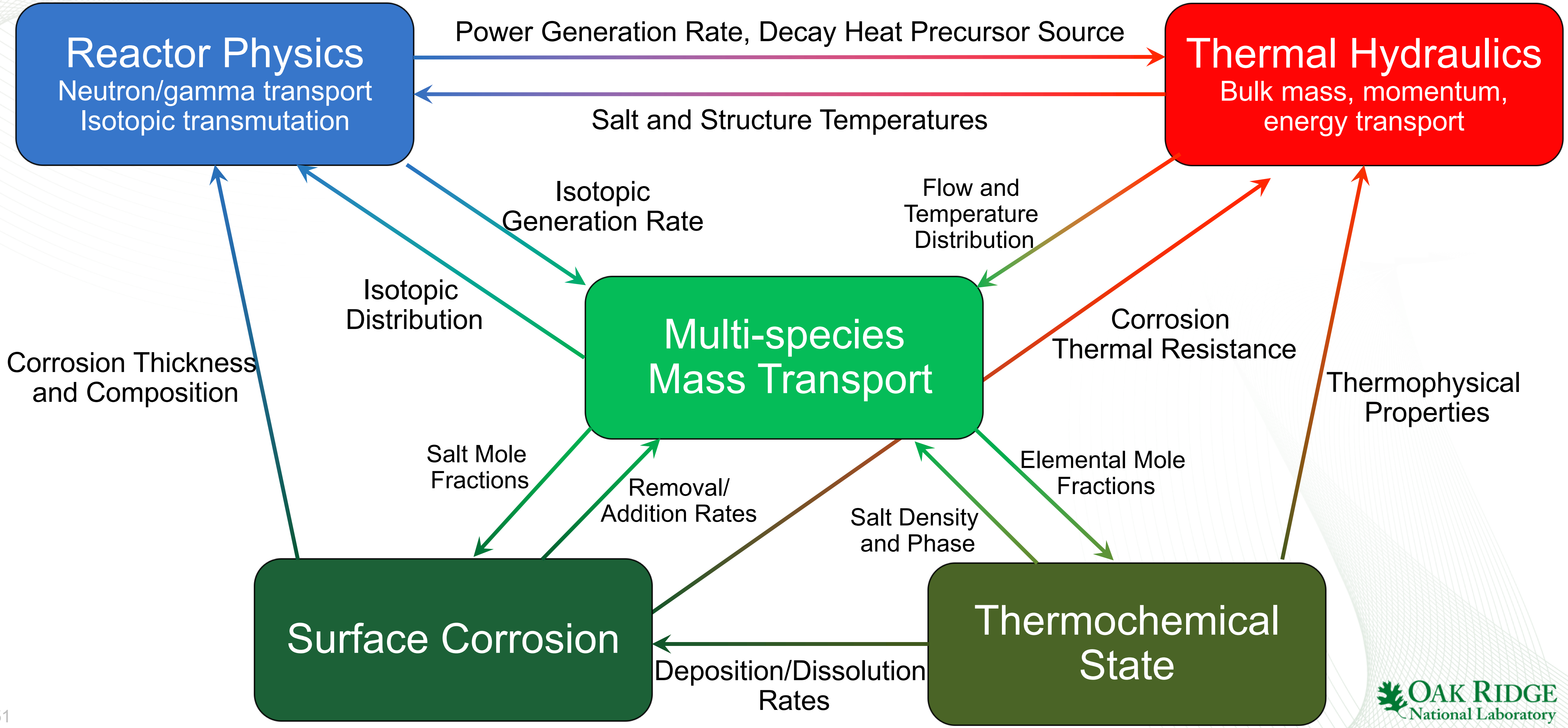
Modeling and Simulation Gaps - SFR

- >5% enrichment
- Nuclear data libraries optimized for fast spectrum
- Core expansion as safety feature
- Leakage effect in cross section treatment
- Treatment of control rods in reflector
- Steaming paths through core
- Mechanistic source terms
- Fuels performance

Discussion on MSRs

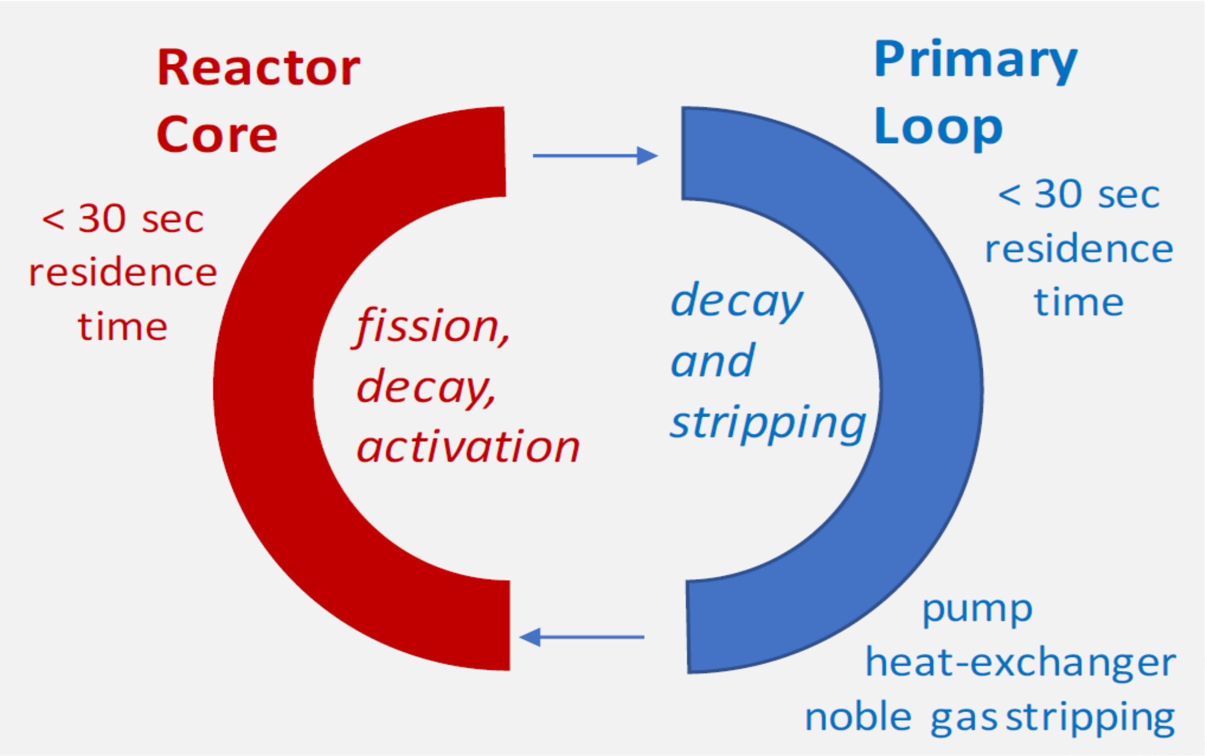
Multiphysics simulations are required for MSRs



Mass Transport with Nuclear Decay

$^{137}\mathrm{I} \xrightarrow{\text{25 sec.}} {}^{137}\mathrm{Xe} \xrightarrow{\text{4 min.}} {}^{137}\mathrm{Cs}$

$^{99}\mathrm{Zr} \xrightarrow{\text{2.1 sec.}} {}^{99}\mathrm{Nb} \xrightarrow{\text{15 sec.}} {}^{99}\mathrm{Mo} \xrightarrow{\text{2.75 days}} {}^{99}\mathrm{Tc}$



soluble
sometimes soluble
insoluble
gaseous

$^{131,132}\mathrm{Cd} \xrightarrow{\text{<1 sec}} {}^{131}\mathrm{In} \xrightarrow{\text{<1 sec}} {}^{131}\mathrm{Sn} \xrightarrow{\text{1 min.}} {}^{131}\mathrm{Sb} \xrightarrow{\text{23 min.}} {}^{131}\mathrm{Te} \xrightarrow{\text{25 min.}} {}^{131}\mathrm{I} \xrightarrow{\text{8 days}} {}^{131}\mathrm{Xe}$

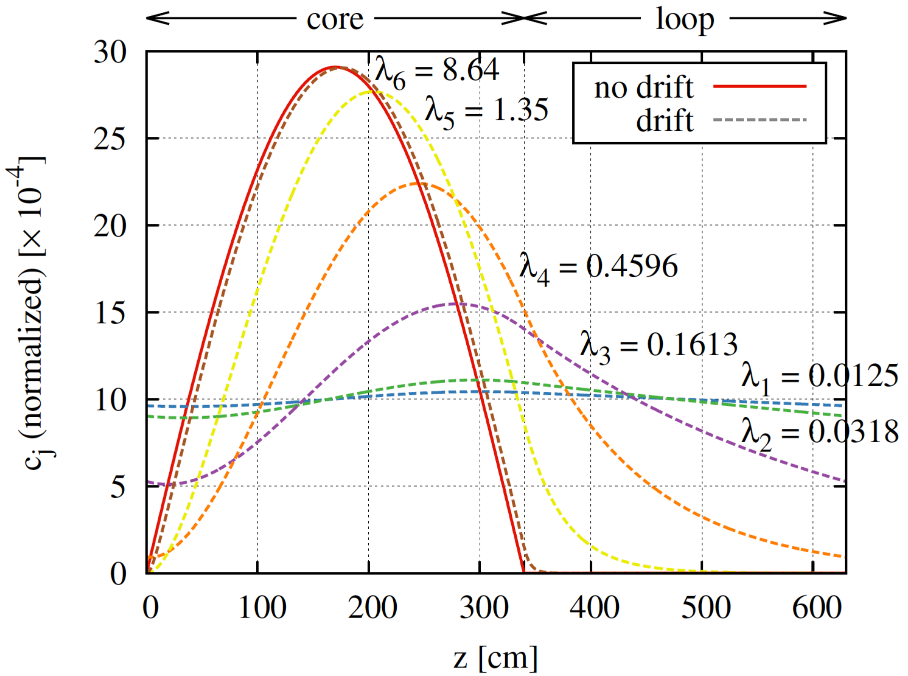
TRITON for MSR neutronics

Analytical solutions for precursor drift, material removal and feed

- To provide solutions for testing precursor drift modules
- 0D model is unable to account for effects from power shapes

Analytic Correction Factors (F) Using Different Models

j	0-D	Core-averaged 1-D $p(z) = C$	Core-averaged 1-D $p(z) \sim \sin(z)$
1	0.5493	0.5403	0.5403
2	0.5635	0.5417	0.5421
3	0.6480	0.5788	0.5885
4	0.7772	0.7236	0.7660
5	0.9059	0.8961	0.9518
6	0.9840	0.9838	0.9987
total	0.7405	0.6994	0.7287

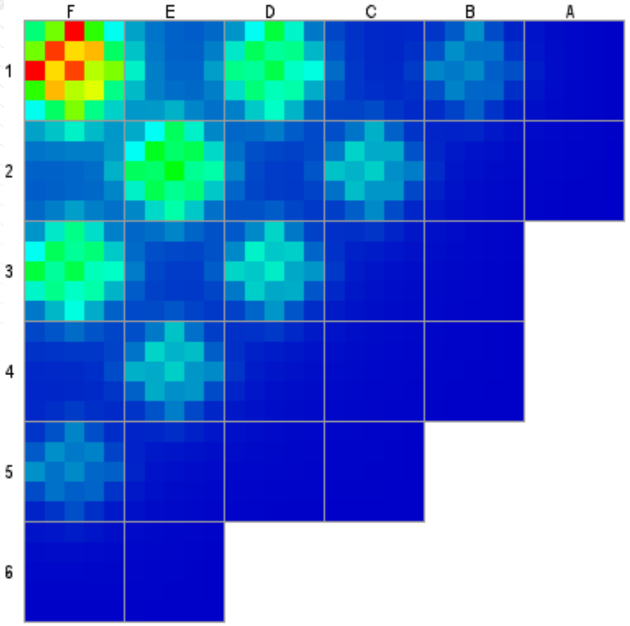


Delayed neutron precursor concentrations in the primary loop of a liquid-fueled MSR.

Initial Assessment CASL VERA-MSR for 3D Multiphysics Analysis with delayed neutron precursor drift and thermal feedback

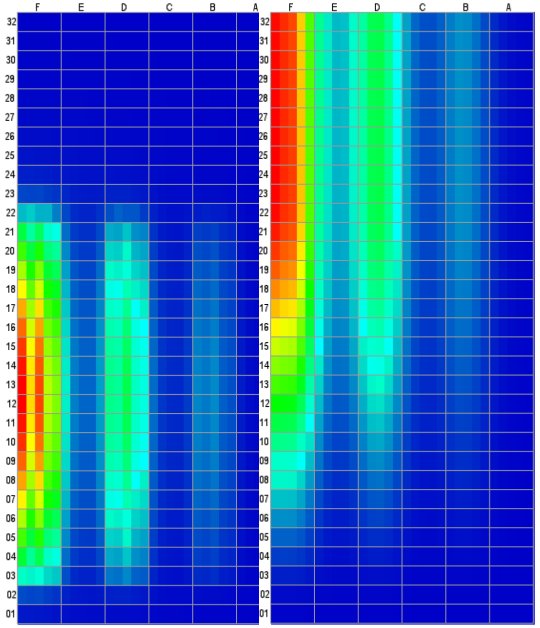
First moderator bank inserted to 66%

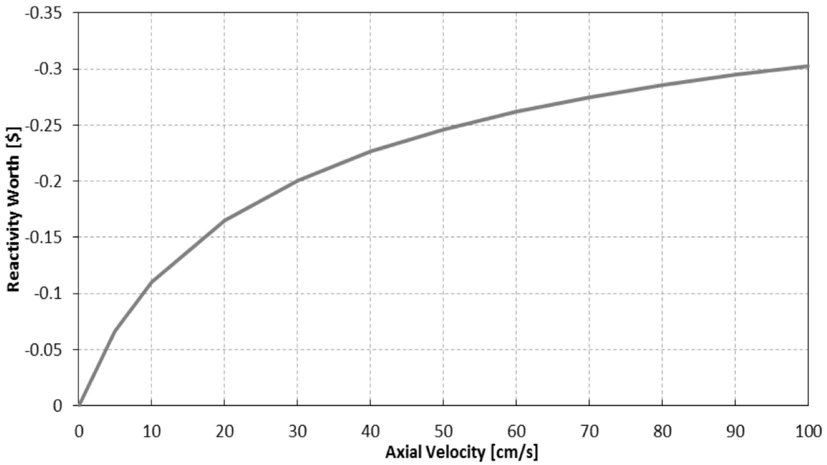
Radial Power Distribution



Axial Power Distribution

Axial Temp Distribution

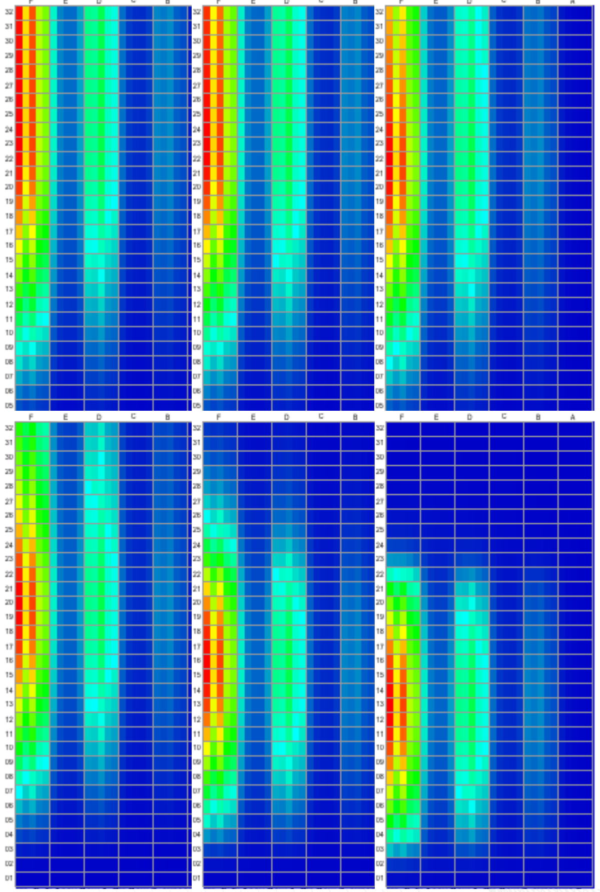




Group 1
T=55.45 s

Group 2
T=21.80 s

Group 3
T=6.36 s



Group 4
T=2.19 s

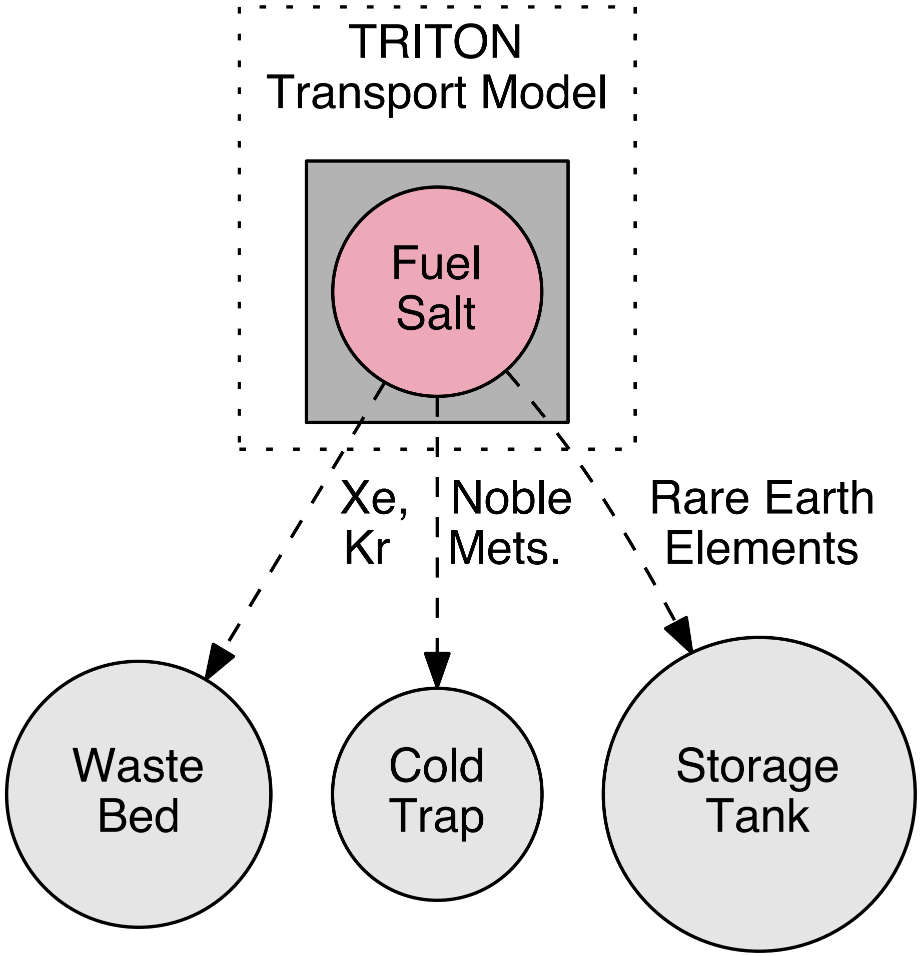
Group 5
T=0.51 s

Group 6
T=0.08 s

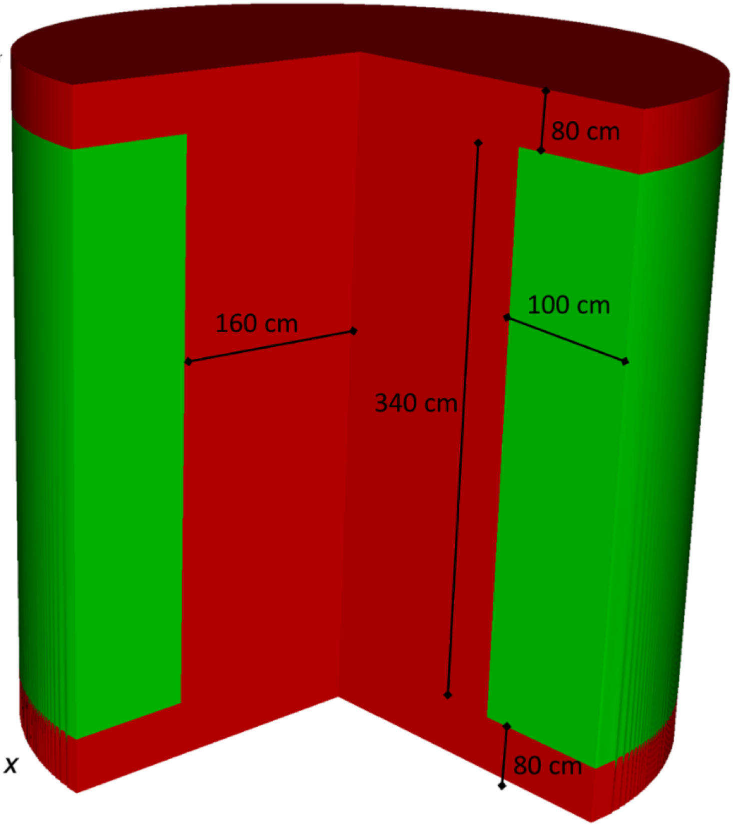
Delayed Neutron Precursor Concentrations

Ongoing Efforts
Molten Salt Reactor Tools

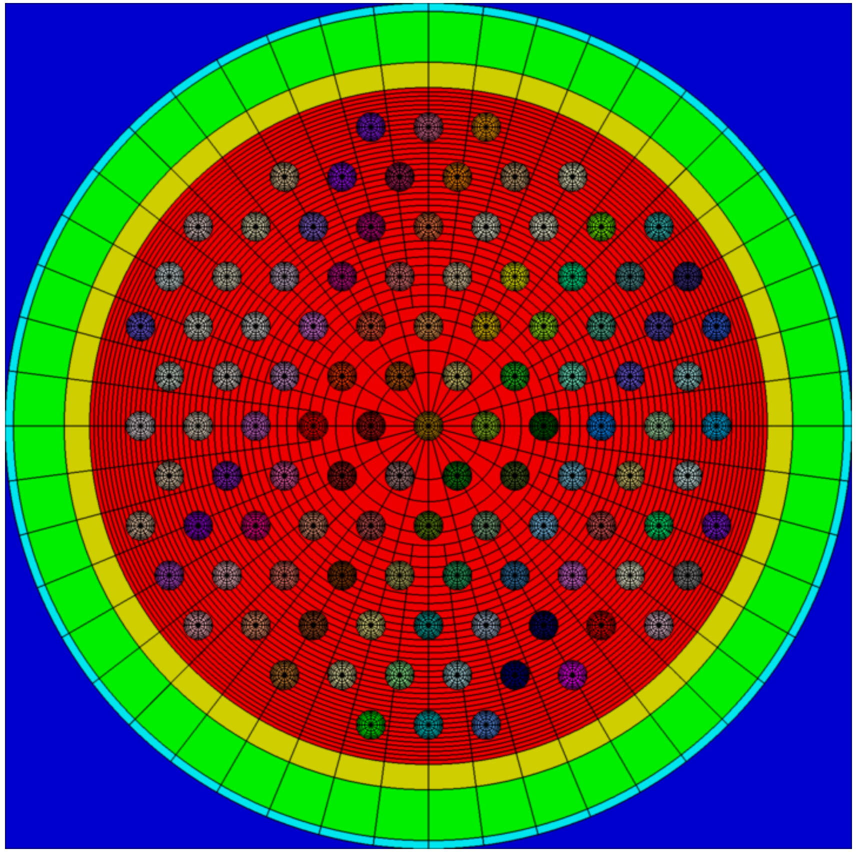
- Finalize integration into SCALE/TRITON
- Finalize generic implementation inputs
- Demonstrate applicability with examples (feeds potential training materials)
- Finalize TM on these tools
  - Recommendations for parameterizing chemical processes



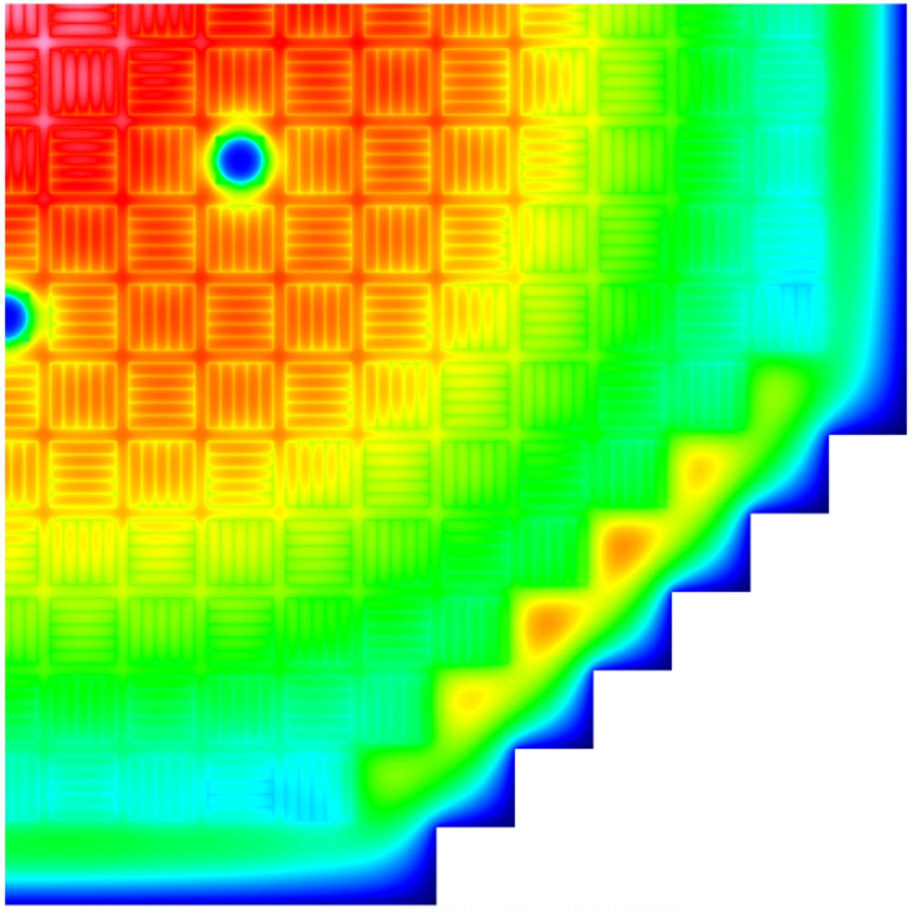
Extending capability to support more reactors



Molten Chloride Reactor



Hexagonal Pitch Graphite Moderated

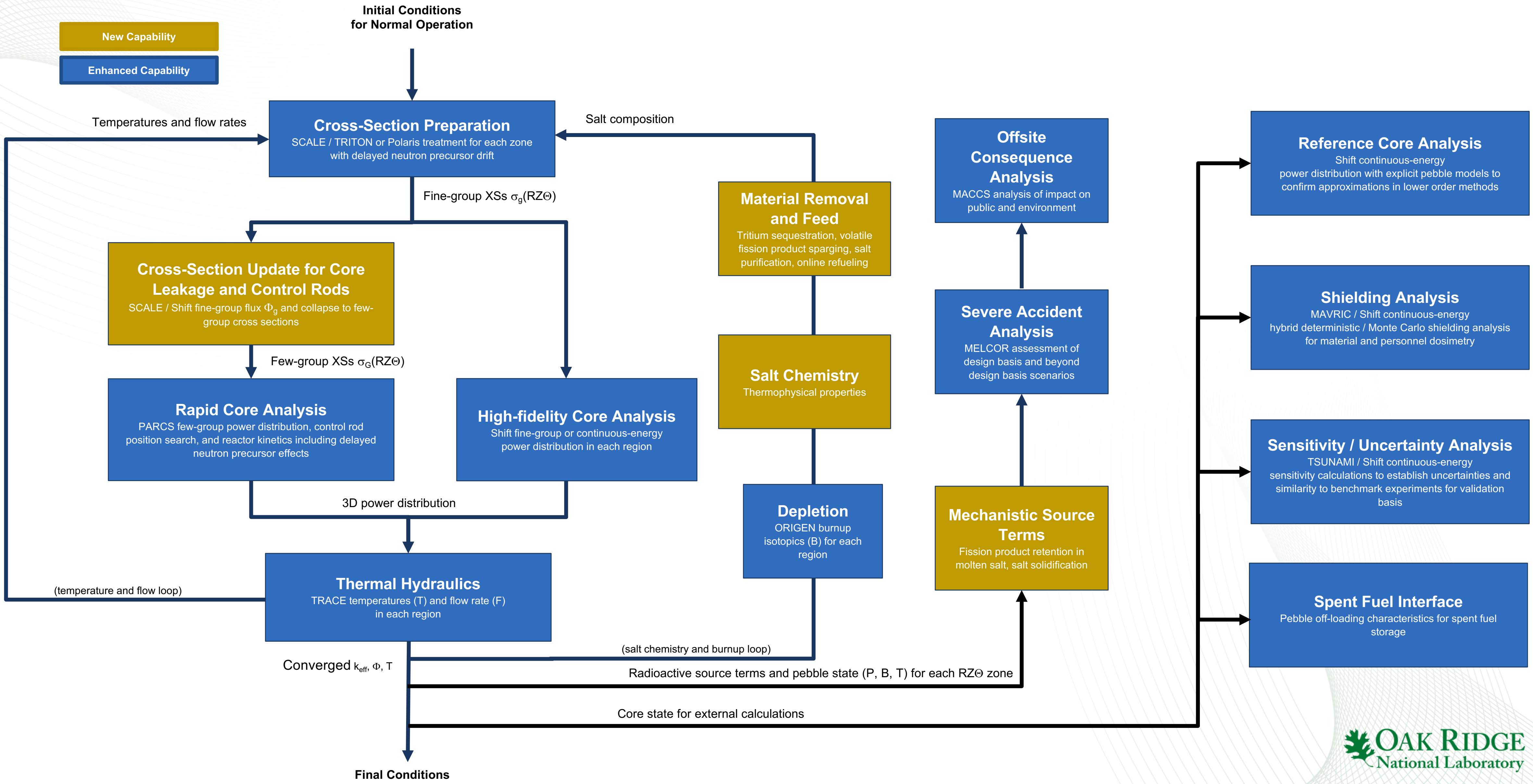


Molten Salt Demonstration Reactor

Some applications to MSRs

- B. R. Betzler, **S. Robertson**, E. E. Davidson, J. J. Powers, A. Worrall, **L. Dewan**, **M. Massie**, *Assessment of the Neutronic and Fuel Cycle Performance of the Transatomic Power Molten Salt Reactor Design,* ORNL/TM-2017/475 (2017).
- B. R. Betzler,S. Robertson, E. E. Davidson, J. J. Powers, A. Worrall, L. Dewan, M. Massie, "Fuel cycle and neutronic performance of a spectral shift molten salt reactor design," *Ann. Nucl. Eng.*, 119 p. 396-410 (2018).
- B. R. Betzler, el al, *Two-Dimensional Neutronic and Fuel Cycle Analysis of the Transatomic Power Molten Salt Reactor*, ORNL/TM-2016/742 (2017).
- N. R. Brown, et al, *Complete Sensitivity/Uncertainty Analysis of LR-0 Reactor Experiments with MSRE FLiBe Salt and Perform Comparison with Molten Salt Cooled and Molten Salt Fueled Reactor Models*, ORNL/TM-2016/729 (2016).
- B. R. Betzler, J. J. Powers, and A. Worrell, "Molten salt reactor neutronics and fuel cycle modeling and simulation with SCALE," *Ann. Nucl. Eng.,* 101, p. 489-503 (2017).
- E. Losa, et al, "Neutronic experiments with fluorine rich compounds at LR-0 reactor," *Ann. Nucl. Eng.*, 120, p. 286-295 (2018).
- B. Collins, C. Gentry, and S. Stimpson, "Molten Salt Reactor Simulation Capability Using MPACT," *M&C 2017 – International Conference on Mathematics & Computational Methods Applied to Nuclear Science and Engineering*, Jeju, Korea, April 16–20, 2017.

SCALE-MSR Integrated Modeling and Simulation



Modeling and Simulation Gaps - MSR

- Flowing fuel creates integrated multiphysics effects
- >5% enrichment
- Nuclear data libraries optimized for thermal and fast spectrum molten salts, also with graphite stringers and zirconium moderator rods
- Delayed neutron “precursor drift”
- Continuous fuel feed and fission product removal
- Tritium production in FLiBe
- Leakage effect in cross section treatment
- Treatment of control rods in reflector
- 3D effects of non-uniform burnup distribution and history effects
- Mechanistic source terms

Summary

- For four decades, ORNL and the SCALE team have responded to a wide range of regulatory needs with innovative, useable, production level capabilities integrated under a robust quality assurance program, with an experienced team to provide user support and training
- Projects have been underway for some time to make the next update to SCALE to support non-LWRs licensing activities
- As features are implemented, early beta releases will be made to NRC staff with hands-on training provided
- Analyst feedback from training will be used as input to guide enhancements

SCALE Users' Group Workshop

- The first ever SCALE Users' Group Workshop was held at ORNL, September 26-28, 2017
  - attended by 117 participants from academia, industry, research institutions, and government agencies
  - provided an interactive forum for discussions between SCALE end users and developers

Save the date: August 27–29, 2018
Application-specific technical tracks
Latest capabilities in SCALE 6.3
SCALE Help *Live!*

Backup Slides on SCALE Modernization

SCALE Modernization Plan:

89 Independent Executable Modules in SCALE 6.1

Control Modules
- csas5
- csas6
- mavric
- mcdancoff
- sas1
- smores
- starbucs
- triton
- triton6
- tsunami-1d
- tsunami-3d_k5
- tsunami-3d_k6

Resonance Self-Shielding
- bonami
- bonamist
- cajun
- centrm
- chops
- crawdad
- nitawl
- nitawlst
- pmc
- worker

Transport
- keno_dancoff
- kenova
- kenovi
- monaco
- newt
- newt-omp
- qads
- xkba
- xsdrn

Depletion
- arp
- arplib
- couple
- opus
- origen
- prism
- reorg
- xseclist

Post-Processing Analysis
- kmart5
- kmart6
- modify
- sams5
- sams6
- swif
- tsar
- tsunami-ip
- tsurfer
- xsdose

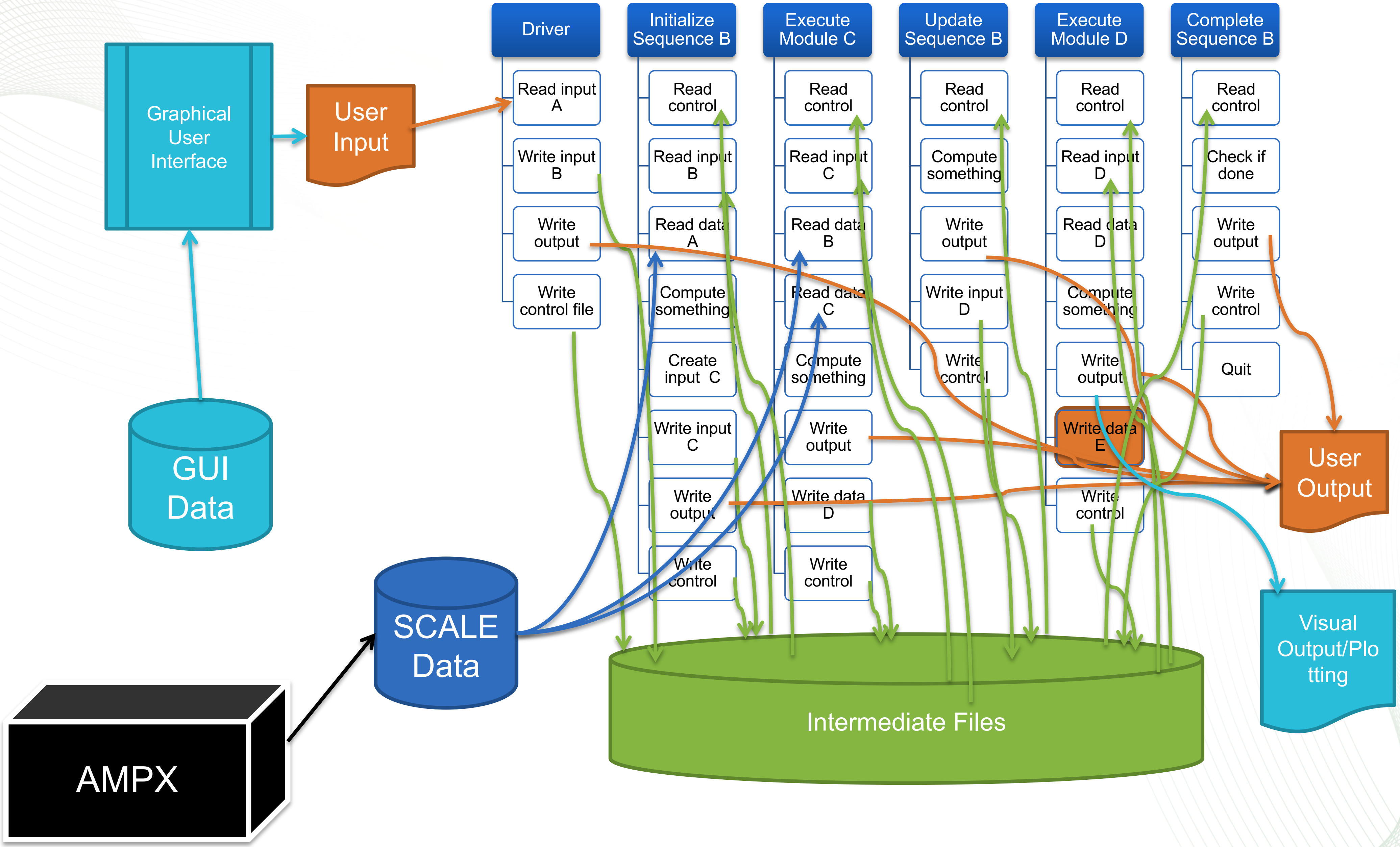
Utility
- c5toc6
- genwgts
- gwas
- k5tok6
- legend
- mal
- mim2wwinp
- mt2ascii
- mt2msm

Utility (cont'd)
- mt2vtk
- mtadder
- mtaverager
- mtbinop
- mtmultiply
- mtsplit
- newsie
- picture
- qadcggp
- vsadder
- wgt
- wpng

Nuclear Data Tools
- aim
- ajax
- alpo
- awl
- cadillac
- cognac
- compoz
- ice
- lava
- malocs
- paleale
- perfume
- rade
- toc
- wax

Runtime
- collect_output
- scale
- scalerte
- shell

Hypothetical SCALE 6.1 Calculation



SCALE 7 Modernized Concept