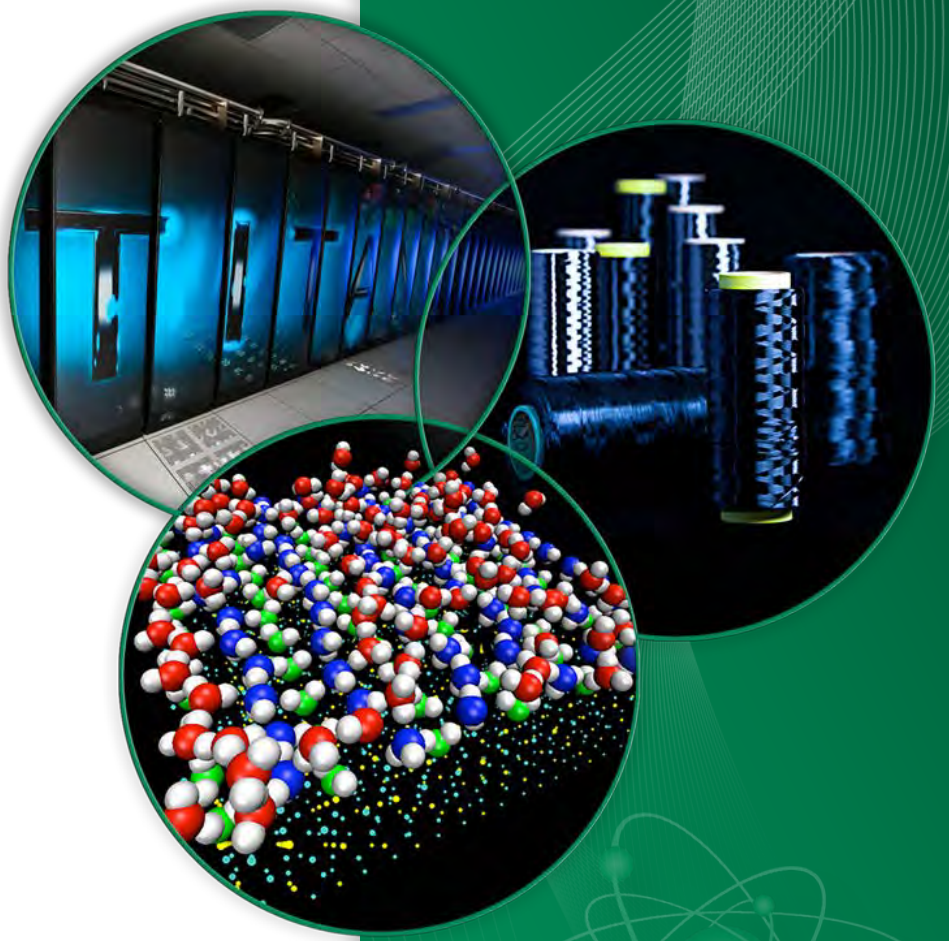
FY13 Accomplishments for SCALE

B. T. Rearden, M. E. Dunn, D. Wiarda,
C. Celik, K. Bekar, M. L. Williams,
D. E. Peplow, C. M. Perfetti,
J. P. Lefebvre, and R. A. Lefebvre

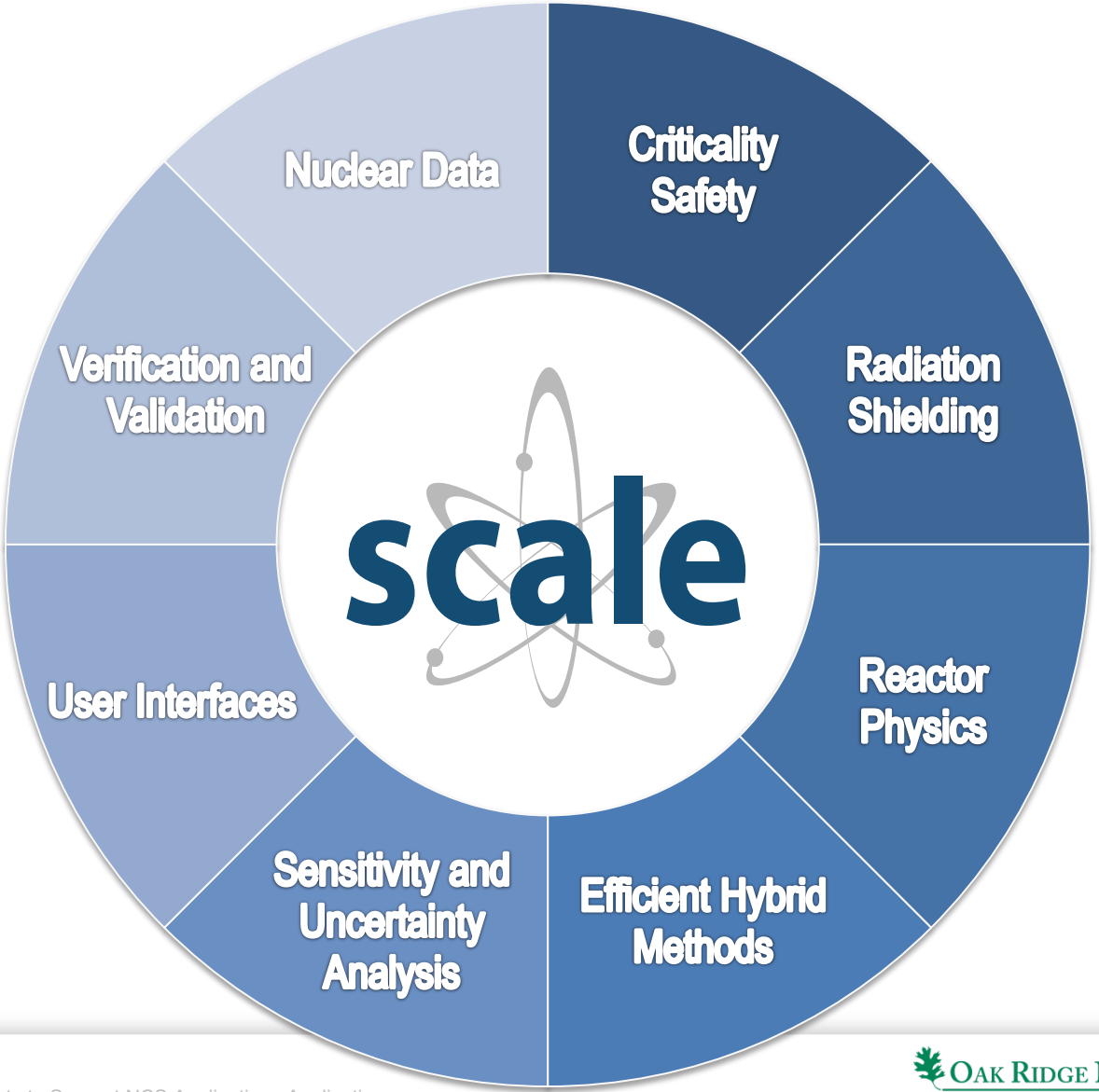
Oak Ridge National Laboratory



Nuclear Criticality Safety Program
Technical Program Review
Los Alamos, NM, March 26, 2014

The SCALE Code System

Neutronics and Shielding Analysis For Enabling Nuclear Technology Advancements



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The SCALE Code System

Neutronics and Shielding Analysis For Enabling Nuclear Technology Advancements

scale

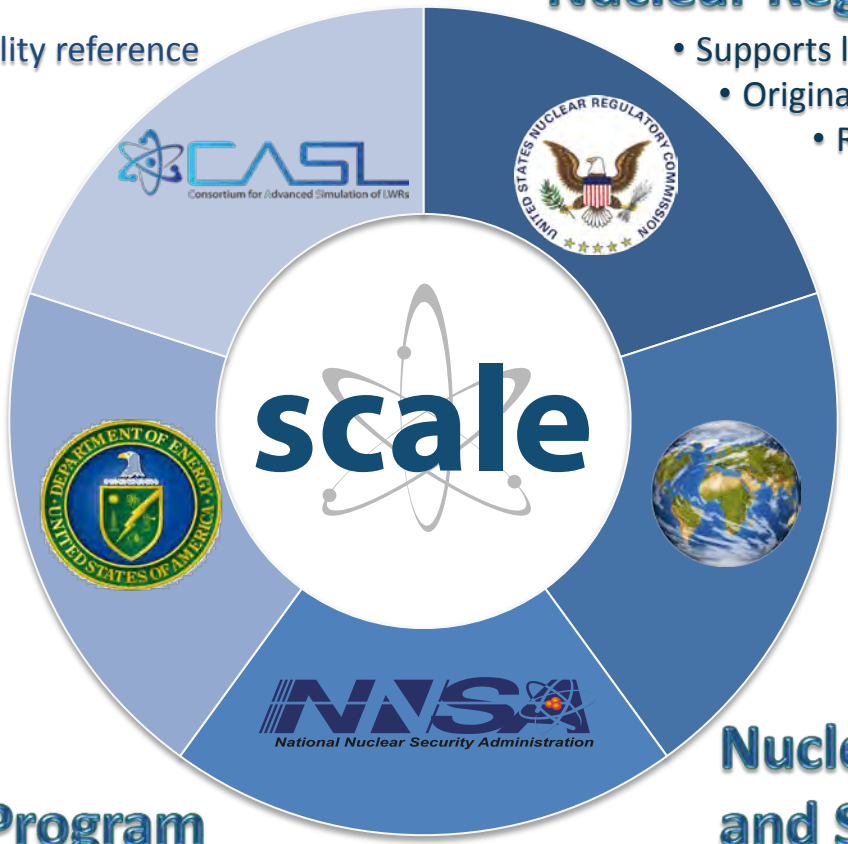
OAK RIDGE National Laboratory

CASL

- Continuous-energy, high-fidelity reference solutions for reactor physics
- Cross-section data libraries
- Reactor fuel depletion
- Uncertainty quantification

Nuclear Regulatory Commission

- Supports licensing and regulatory research
- Original sponsors of SCALE – since 1976
- Reactor physics and source terms
- Criticality safety and shielding
- Cross section data libraries



DOE Used Fuel Disposition

- Radiation shielding
- Nuclear fuel depletion
- Used fuel source terms
- Criticality safety analysis
- Uncertainty quantification

Global Distribution

- 5600 users in 51 nations
- Regulators
- Industry
- Research and Development

DOE Nuclear Criticality Safety Program

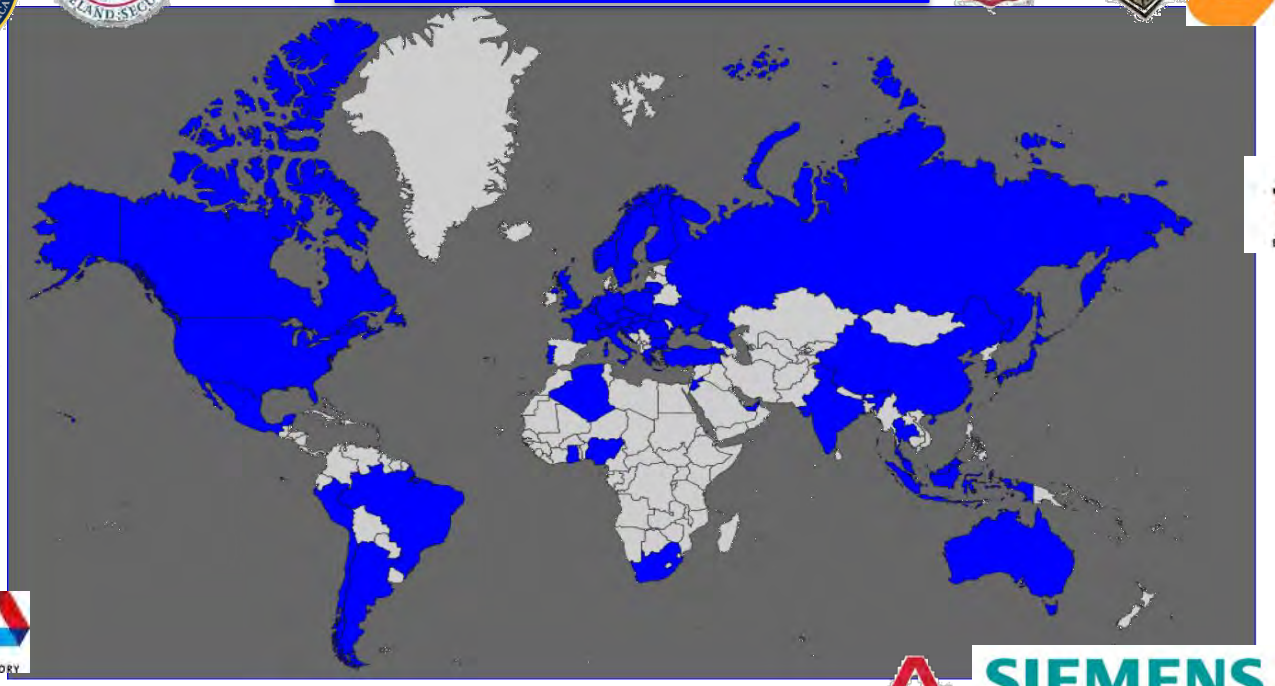
- Criticality safety assessments
- Sensitivity and uncertainty analysis
- Advanced validation methods
- Experiment design
- Criticality accident alarm system analysis and design

Nuclear Nonproliferation and Safeguards

- Used fuel and radionuclide source terms
- Reactor depletion analysis
- Radiation transport
- Nuclear forensics

5600+ Users

51 Nations



Regulators
Industry
Utilities
Research Laboratories
Government Agencies
Universities

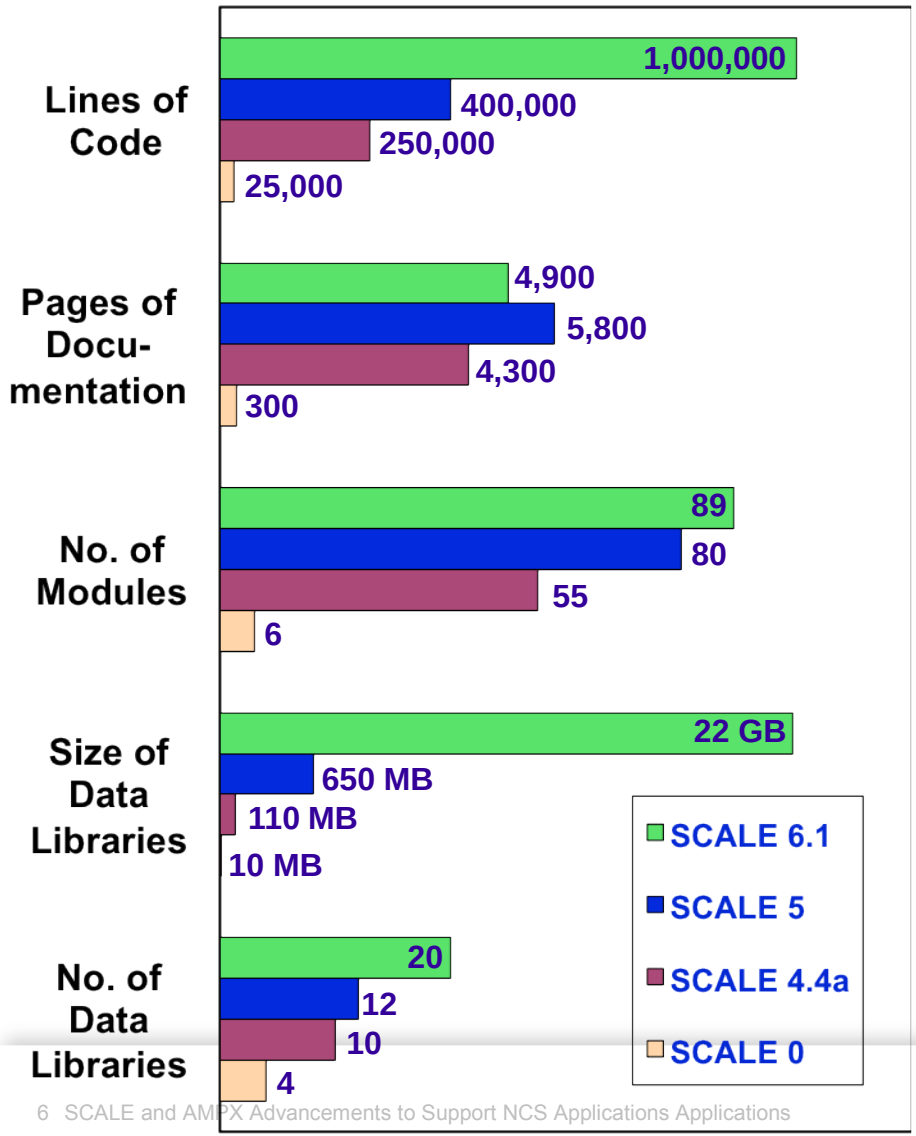
Distributed by RSICC (USA), NEA Data Bank (France) and RIST (Japan)

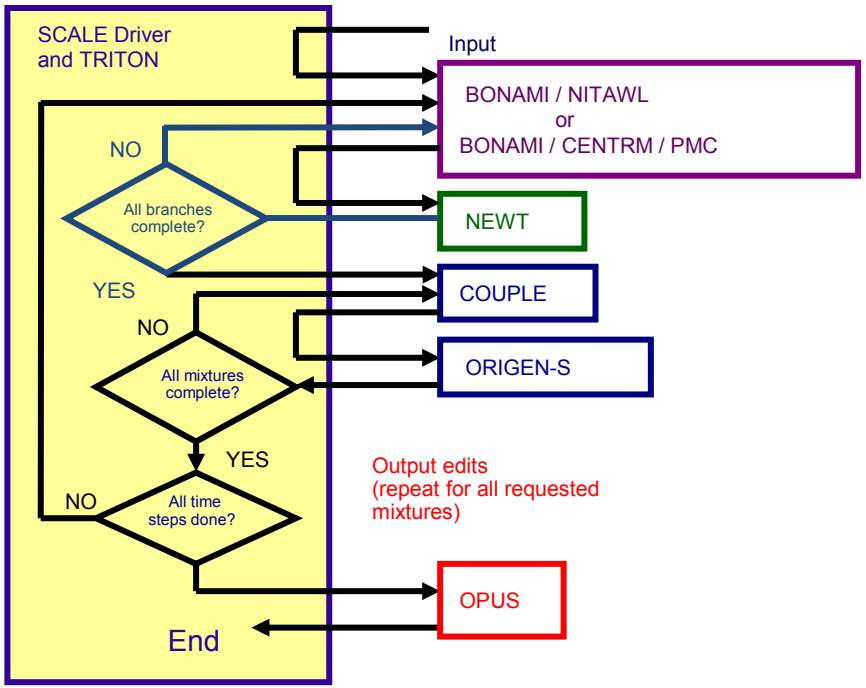
Outline

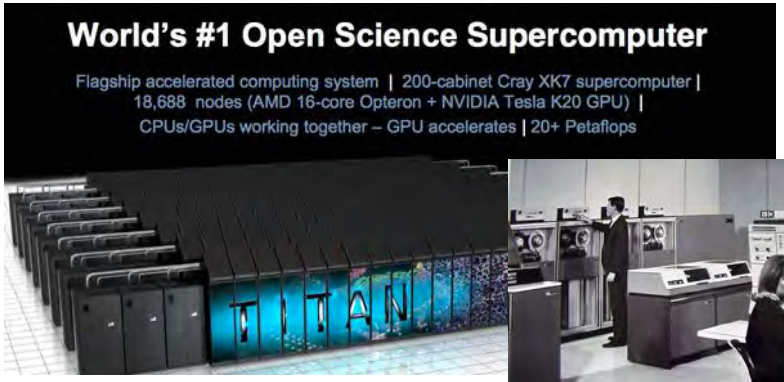
- Quality Assurance
- Advanced Features
- Modernization

Evolution of SCALE – 1980–2011

Each era with differing tools and developers, same design and management strategy







2000 – Quality Assurance Document

SCALE MODULE REVISION REPORT

Part I - Change Request — Report No. MRR 00-001

Module/Library Name	Version	Code Design Requirements attached ___ Report No. ___ / Discrepancy Report attached ___ Report No. ___
KENOVA	4.2	

Description: Changing PULL in MRR 00-003 requires minor changes to KENO v.a. The changes made in generating angles & probabilities in perfume in MRR99034 should also be incorporated in KENO v.a

Prepared by (Requestor): L M Petrie — Date: 1/4/00

Part II - Approval / Disapproval — Approved ✓ / Not approved ___ by (Project Leader): S. M. Bowman — Date: 1/4/2000

Explanation (if not approved):

Part III - Documentation of Changes — Code Manager: L. M. Petrie

Attached are the following:
Description of changes X (required) — Verification report X (required) — Validation report ___
Description of testing X (required) — Test case inputs X (required)

Fix Makefile. (add new subroutine) Do after MRR 00-003

Do changes impact documentation? Yes ___ No X (if yes, attached updated / new pages)
Were sample inputs revised? Yes ___ No X (if yes, attach updated / new input decks)

Modified source modules and their locations: X4S.WORKING, MASTER — K5FIND, K5GETMIX, K5GUIDE, K5MAKANG, K5MIXER, K5PRANG, K5REPORT → REPORTIT.F (new)

Locations of test problem inputs As tested by Code Manager	Prepared for Software Coordinator
/home/lmp/MRR/mrr00001/ smp17b.inp smp17d.inp	← x4s case1.input x4s case2.input

Other SCALE Executable Modules affected: csas, modify, o0o009

Effect of change on previous calculations: Should be none, although possibly the random sequence could change

Prepared by (Code Manager): L M Petrie — Date: 1/5/00

Part IV - Technical Review — Technical Reviewer: S. M. Bowman

The following are acceptable: (If "No," Technical Review Form No. _____ is attached)
Code design requirements satisfied Yes ✓ No ___ — Code Documentation Yes ✓ No ___
Verification and / or validation Yes ✓ No ___ — Current sample problems Yes ___ No ___

Reviewed by (Technical Reviewer): S M Bowman — Date: 1/13/2000

Part V - Approval for Revision — Approved by (Configuration Coordinator): MB (Peggy Dimmett) — Date: 1/13/2000

Test cases to be performed with the production executable code: Run test cases from Part III

Part VI - Implementation

NY12N : Production Implementation Dates			
Name/Version	Source	Object	Executable
KENOVA/N/A	1/14/00	N/A	N/A

DEC Alpha Production Implementation Dates			
Name/Version	Source	Object	Executable
kenova/4.3	1/14/00	1/14/00	1/14/00
o0o009/4.3	N/A	N/A	1/14/00
csas/4.6	N/A	N/A	1/14/00
modify/4.7	N/A	N/A	1/14/00

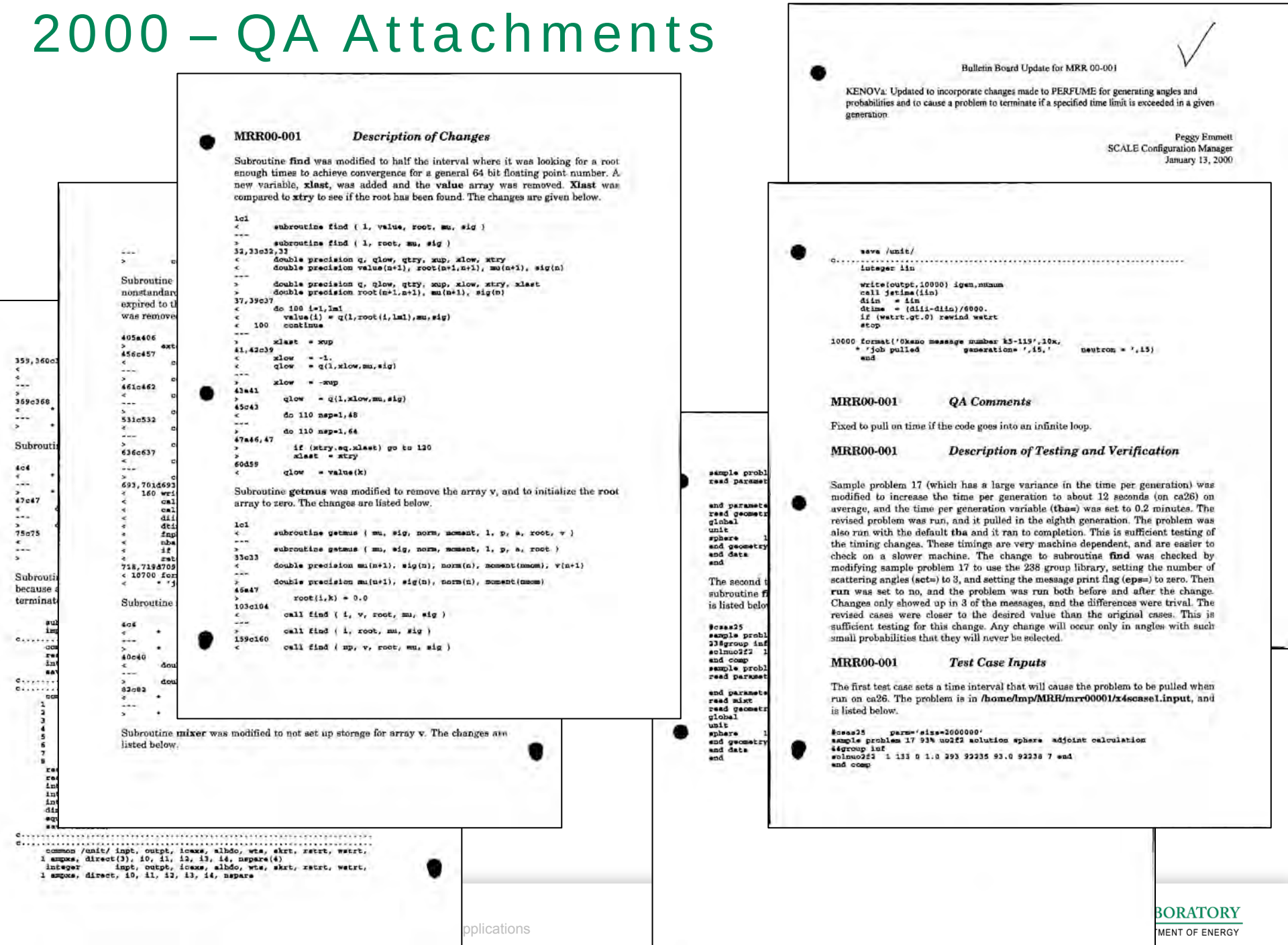
Performed by (Software Coordinator): Kay Rittenwalter

Describe results of testing production executables
Machine: NY12N
TESTING NOT REQUIRED.

Machine: DEC Alpha
Results of testing were as expected and verified by L.M. Petrie.

Tested by (Software Coordinator): Kay Rittenwalter — Date: 01/14/00 — Bulletin board updated: ok

2000 – QA Attachments



Bulletin Board Update for MRR 00-001

KENOVa: Updated to incorporate changes made to PERFUME for generating angles and probabilities and to cause a problem to terminate if a specified time limit is exceeded in a given generation

Peggy Emmett
SCALE Configuration Manager
January 13, 2000

MRR00-001 ***Description of Changes***

Subroutine **find** was modified to half the interval where it was looking for a root enough times to achieve convergence for a general 64 bit floating point number. A new variable, **xlast**, was added and the **value** array was removed. **Xlast** was compared to **xtry** to see if the root has been found. The changes are given below.

```
1c1
<       subroutine find ( i, value, root, mu, sig )
---
>       subroutine find ( i, root, mu, sig )
32,33c32,33
<       double precision q, qlow, qtry, xup, xlow, xtry
<       double precision value(n+1), root(n+1,n+1), mu(n+1), sig(n)
---
>       double precision q, qlow, qtry, xup, xlow, xtry, xlast
>       double precision root(n+1,n+1), mu(n+1), sig(n)
37,39c37
<       do 100 i=1,lm1
<         value(i) = q(1,root(i,lm1),mu,sig)
<   100   continue
---
>       xlast  = xup
41,42c39
<       xlow   = -1.
<       qlow   = q(1,xlow,mu,sig)
---
>       xlow   = -xup
43a41
>         qlow   = q(1,xlow,mu,sig)
45c43
<         do 110 nsp=1,48
---
>         do 110 nsp=1,64
47a46,47
>           if (xtry.eq.xlast) go to 120
>           xlast  = xtry
60d59
<         qlow   = value(k)
```

Subroutine **getmus** was modified to remove the array v, and to initialize the root array to zero. The changes are listed below.

```
1c1
<       subroutine getmus ( mu, sig, norm, moment, l, p, a, root, v )
---
>       subroutine getmus ( mu, sig, norm, moment, l, p, a, root )
33c33
<       double precision mu(n+1), sig(n), norm(n), moment(nmom), v(n+1)
---
>       double precision mu(n+1), sig(n), norm(n), moment(nmom)
45a47
>           root(i,k) = 0.0
103c104
<           call find ( i, v, root, mu, sig )
---
>           call find ( i, root, mu, sig )
159c160
<           call find ( np, v, root, mu, sig )
```

Subroutine **mixer** was modified to not set up storage for array v. The changes are listed below.

```
      save /unit/
C-----------------------------------------------------------------------
      integer iin

      write(outpt,10000) igen,nthnum
      call jstime(iin)
      diin   = iin
      dtime  = (diin-diin)/6000.
      if (watrt.gt.0) rewind watrt
      stop

10000 format('0keno message number k5-119',10x,
     * 'job pulled          generations ',i5,'      neutron = ',i5)
      end
```

MRR00-001 ***QA Comments***

Fixed to pull on time if the code goes into an infinite loop.

MRR00-001 ***Description of Testing and Verification***

Sample problem 17 (which has a large variance in the time per generation) was modified to increase the time per generation to about 12 seconds (on ca26) on average, and the time per generation variable (**tba=**) was set to 0.2 minutes. The revised problem was run, and it pulled in the eighth generation. The problem was also run with the default **tba** and it ran to completion. This is sufficient testing of the timing changes. These timings are very machine dependent, and are easier to check on a slower machine. The change to subroutine **find** was checked by modifying sample problem 17 to use the 238 group library, setting the number of scattering angles (**sct=**) to 3, and setting the message print flag (**eps=**) to zero. Then **run** was set to no, and the problem was run both before and after the change. Changes only showed up in 3 of the messages, and the differences were trival. The revised cases were closer to the desired value than the original cases. This is sufficient testing for this change. Any change will occur only in angles with such small probabilities that they will never be selected.

MRR00-001 ***Test Case Inputs***

The first test case sets a time interval that will cause the problem to be pulled when run on ca26. The problem is in **/home/lmp/MRR/mrr00001/x4scase1.input**, and is listed below.

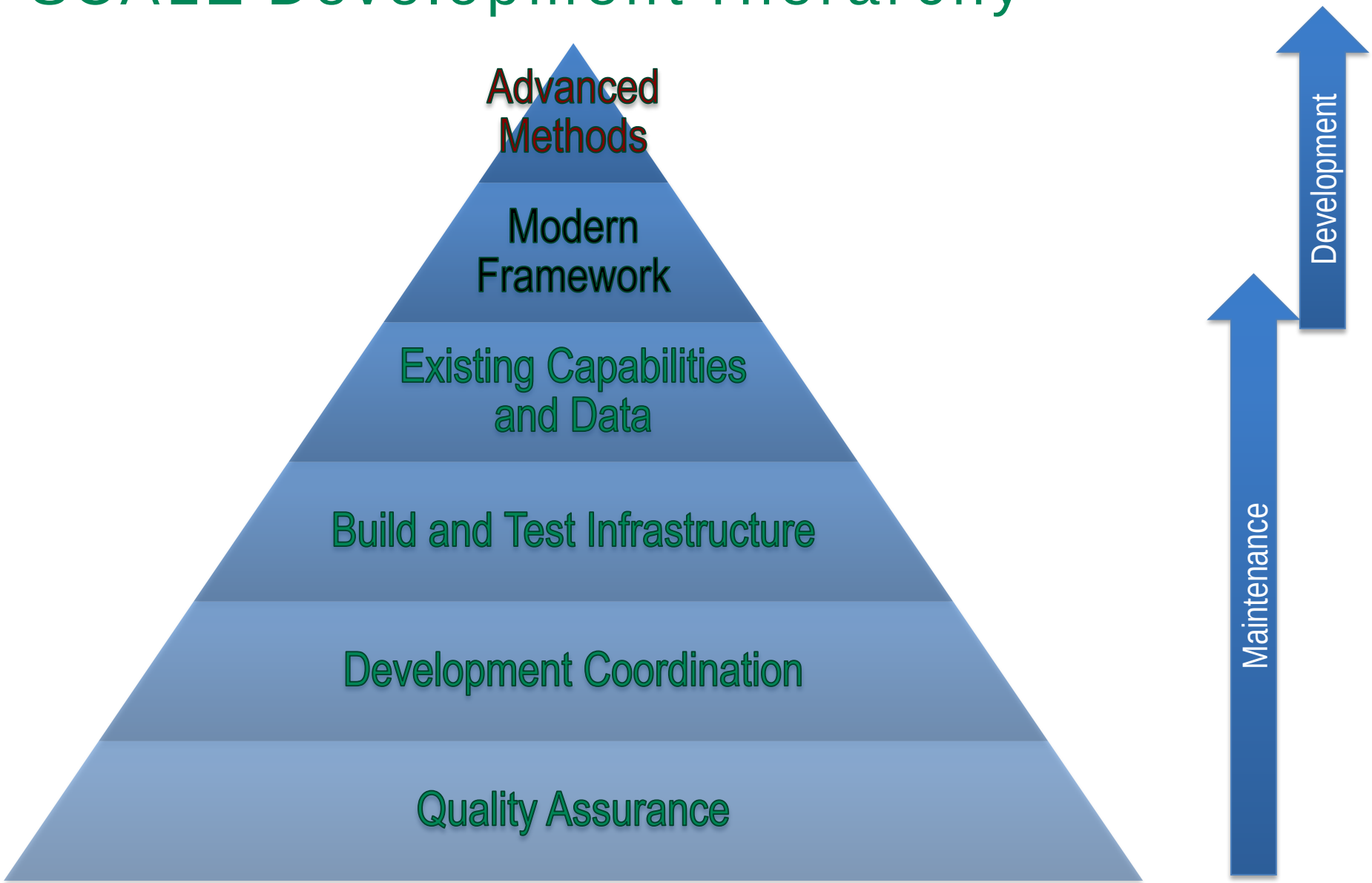
```
=csas25      parm='size=2000000'
sample problem 17 93% uo2f2 solution sphere  adjoint calculation
44group luf
solnuo2f2  1 133 0 1.0 293 92235 93.0 92238 7 end
end comp
```

```
      common /unit/ inpt, outpt, icsxs, albdo, wts, skrt, rstrt, wstrt,
     1 smpxs, direct(3), i0, i1, i2, i3, i4, nspare(4)
      integer       inpt, outpt, icsxs, albdo, wts, skrt, rstrt, wstrt,
     1 smpxs, direct, i0, i1, i2, i3, i4, nspare
```

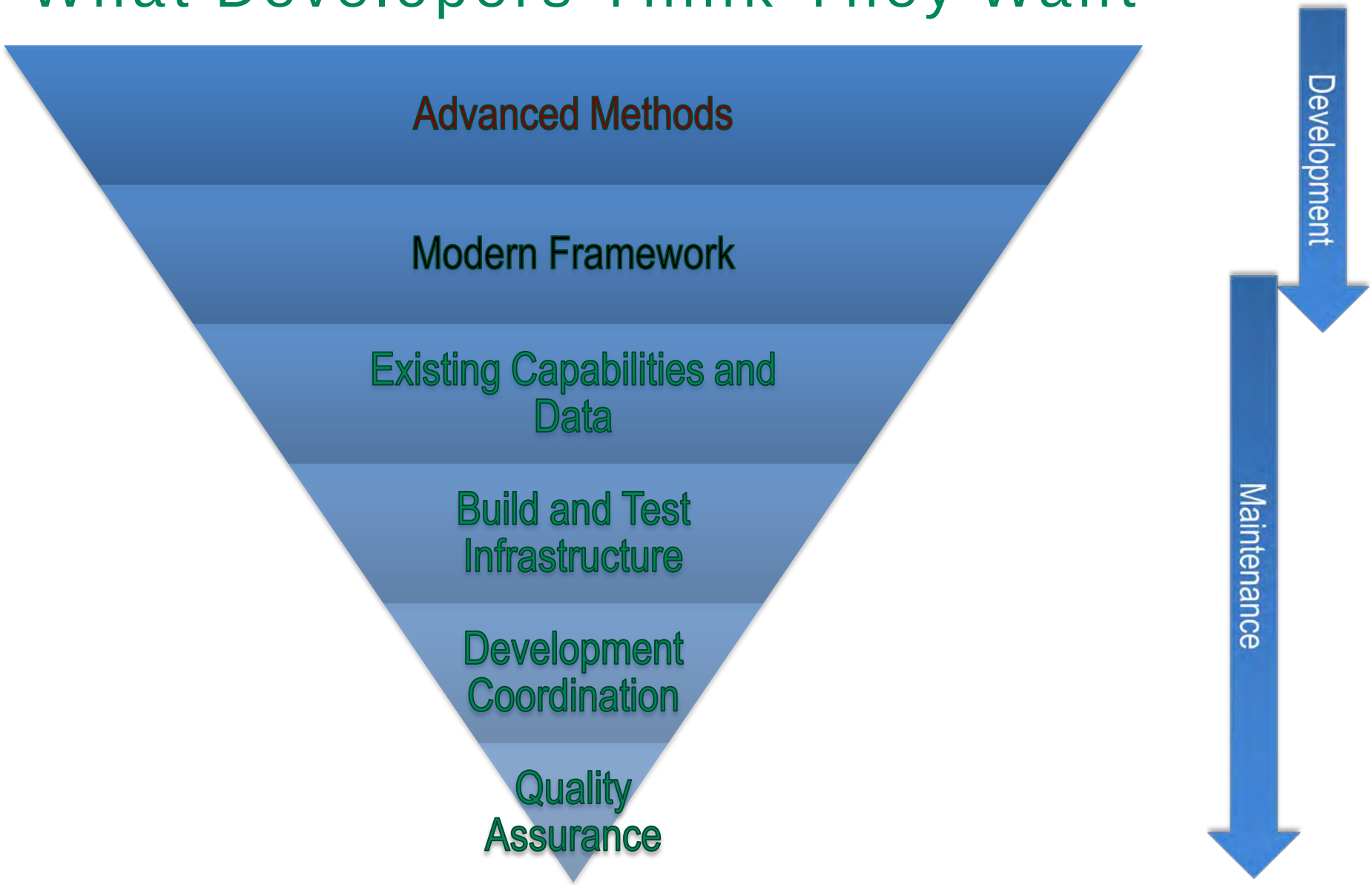
Historical SCALE Testing and Defects

- During development SCALE was tested by running ~250 sample problems every six months to assess overall performance of all features and data
- Preparation of final distribution generally required 6-9 months to synchronize all features and hand modify a specific version for Windows
- Frustrated developers spent large percentage of time fixing bugs and helping frustrated users
- Corrective Actions Taken After Release
  - 2004 - SCALE 5.0
    - 7 patches
  - 2006 - SCALE 5.1
    - 8 patches
  - 2009 - SCALE 6.0
    - 10 patches

SCALE Development Hierarchy



What Developers Think They Want



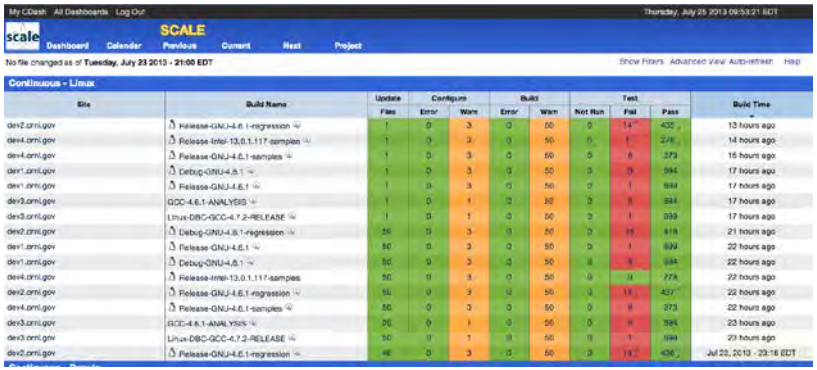
Communication and Coordination

- **SCALE Leadership Team**
  - **SCALE manager, line managers, senior staff**
  - **Coordinates overall vision for SCALE**
  - **Sets priorities and reviews progress**
  - **Meets regularly to maintain close coordination**
- **SCALE Development & Applications Teams**
  - **Multiple teams meet frequently to discuss different technical areas**
  - **Promotes collaboration**
    - **Within and across technical areas**
    - **Between developers and users**
    - **Across organizational boundaries**
- **Friday Forum**
  - **Open discussions 2 hours each Friday**

New Push for Quality

- Instilled culture of quality
- Migrated to electronic QA system
- Hired team of young computer scientists
- SCALE Testing Team
  - Five students tested SCALE 6.0 and SCALE 6.1-beta during summer of 2010
  - Worked directly with developers as mentors
  - Hundreds of previously unknown defects were identified spanning nearly every module
- Automated daily testing initiated using hundreds of student test cases
- All test results posted to internal website where anyone on the team can monitor outcomes

2010 SCALE Testing Team and Mentors. First row: Oscar Lastres, Heather Connaway; Second row: David Harmangruber, Chris Perfetti; Third row: Brad Rearden, Paul Stauduhar; Forth row: Douglas Peplow, Matt Jessee



Infrastructure Investments

- 384 core, 4 Teraflop Linux cluster for SCALE development and testing
- Additional 30 Teraflop for capacity computing

SCALE 6.1 – July 2011

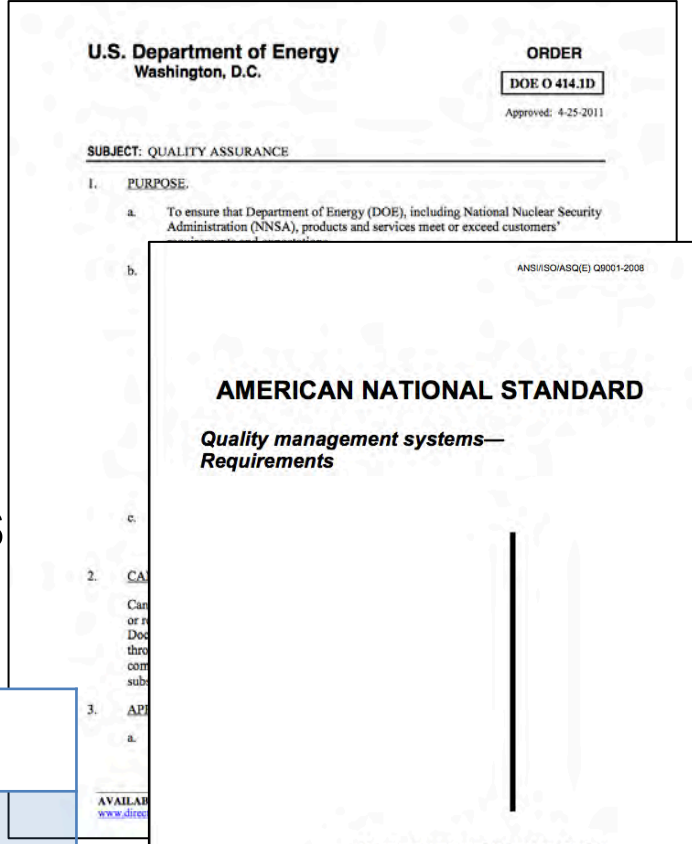
- New quality philosophy communicated through conference presentations and newsletter
- 2700 licenses issued through February 2014
- >1700 new users that had never used any previous version of SCALE (2500 total SCALE users in 2009)
- Record training attendance
- Many publications and license applications from other teams using SCALE for innovative analyses
- Only two patches issued
- Enhanced opportunities with cross-project collaboration, Ph.D. projects, etc.
- Rest and enjoy fruits of labor?

scale
Nuclear Systems Modeling & Simulation

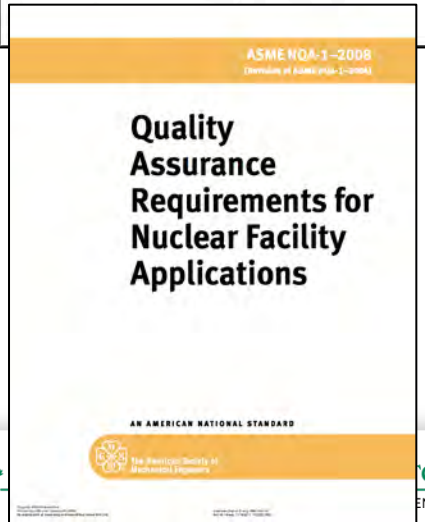
FY13 Updated QA Program

- Designed for Compliance with:
  - ISO 9001-2008
  - DOE 414.1D
  - ORNL SBMS
  - Consistent with ASME NQA-1
- Capabilities are tracked with the *Kanban* process through the *FogBugz* electronic *collaborative development environment*

Kanban Category	Meaning
Proposed	Task has been proposed for management approval
Approved	Task has been approved by management and assigned to a developer for implementation
In Progress	Developer is actively working to implement the feature
Ready for Testing	Developer has completed the implementation and the feature is ready for comprehensive testing
Ready to Ship	Item has passed all tests and is a candidate feature for quality assurance implementation
Shipped	Feature is implemented in quality-assured version

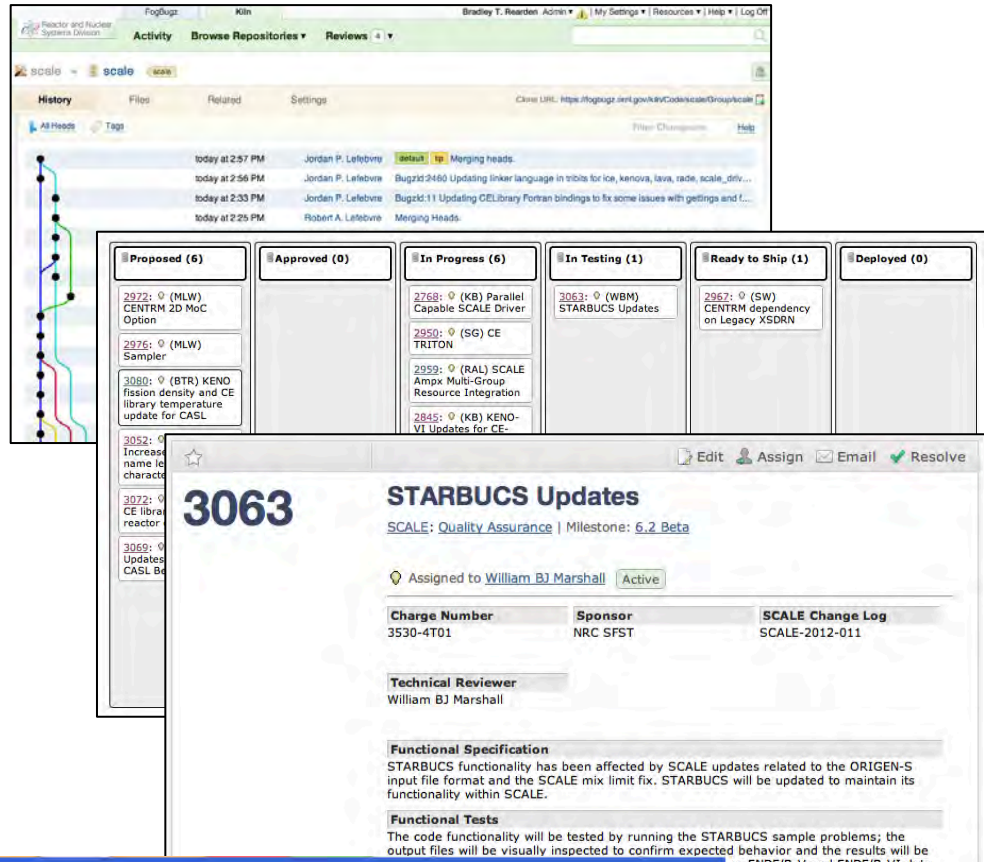

U.S. Department of Energy
Washington, D.C.
ORDER
DOE O 414.1D
Approved: 4-25-2011
SUBJECT: QUALITY ASSURANCE
1. PURPOSE.
a. To ensure that Department of Energy (DOE), including National Nuclear Security Administration (NNSA), products and services meet or exceed customers'

ANSI/ISO/ASQ(E) Q9001-2008
AMERICAN NATIONAL STANDARD
Quality management systems—Requirements
AMERICAN SOCIETY FOR QUALITY
P.O. BOX 3005
MILWAUKEE, WI 53201-3005


ASME NQA-1–2008
Quality Assurance Requirements for Nuclear Facility Applications
AN AMERICAN NATIONAL STANDARD

Build and Test Infrastructure

- **Electronic feature tracking system**
  - All developers can see all development all the time
  - Holistically review all features in development in 1 hour meeting
- **Testing fully automated and extended to ~70,000 tests/day**
- "Release candidate" prepared for distribution in 24 hours



Linux Regression

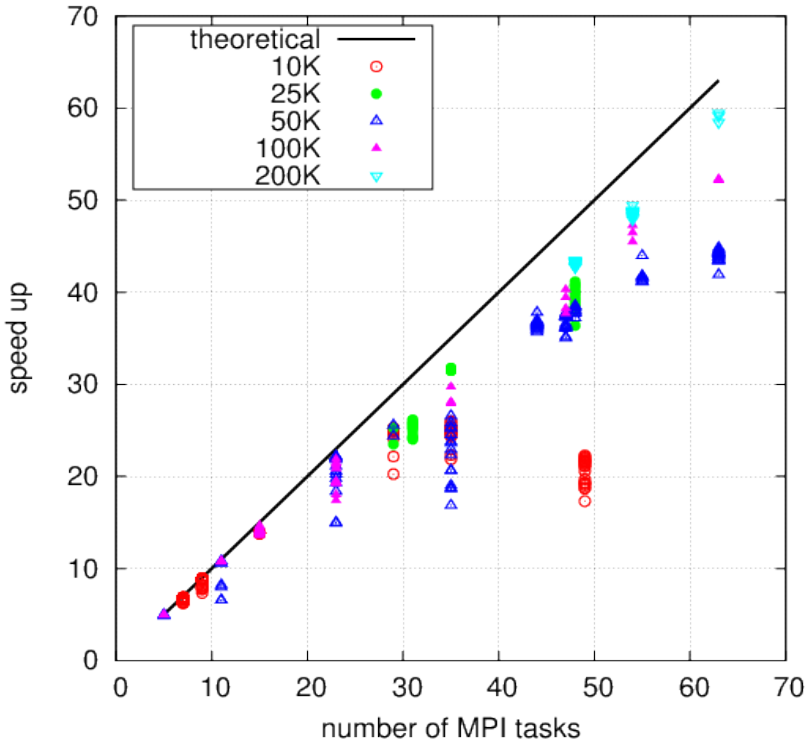
Site	Build Name	Update		Configure			Build			Test				Build Time	Labels
		Files	Min	Error	Warn	Min	Error	Warn	Min	NotRun	Fail	Pass	Min		
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	13	0.2	0	0	1.3	0	0	5.6	0	4	477	221.6	2012-03-07T11:50:42 EST	(none)
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	11	0.4	0	0	3.4	0	16	14.1	0	4	477	223.8	2012-03-07T07:48:54 EST	(none)

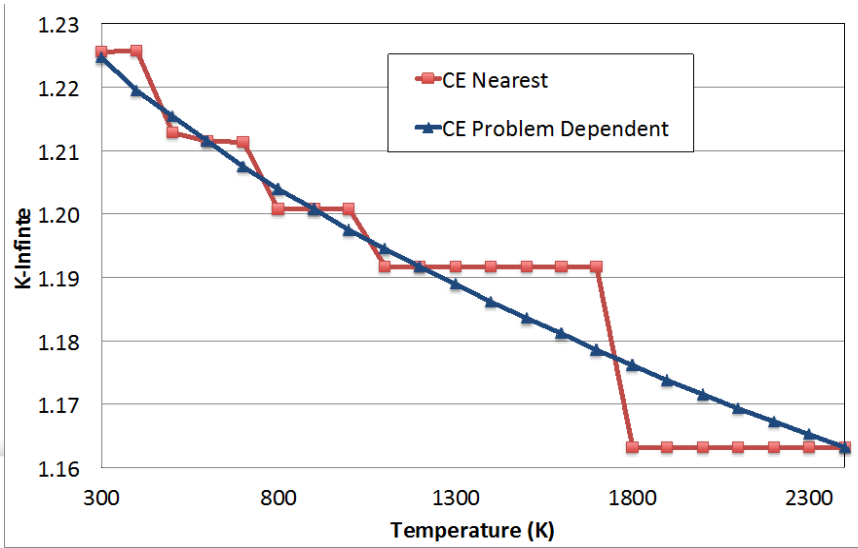
Outline

- Quality Assurance
- Advanced Features
- Modernization

Monte Carlo Improvements for Criticality

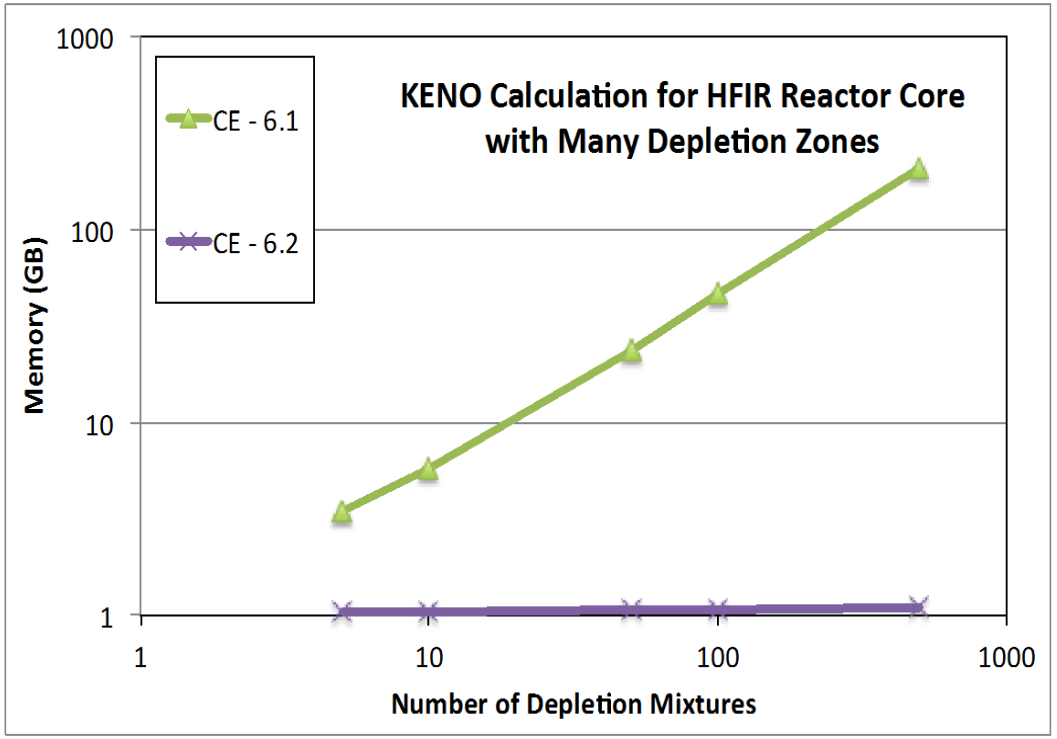
- Parallel KENO Significant speedups with MPI on Linux clusters
- Problem-Dependent Doppler broadening for CE calculations for resolved and unresolved (probability table) energy ranges (PhD)
- Doppler Broadened Rejection Correction (PhD)
  - Significant improvement in elevated temperature CE Monte Carlo





Memory Footprint

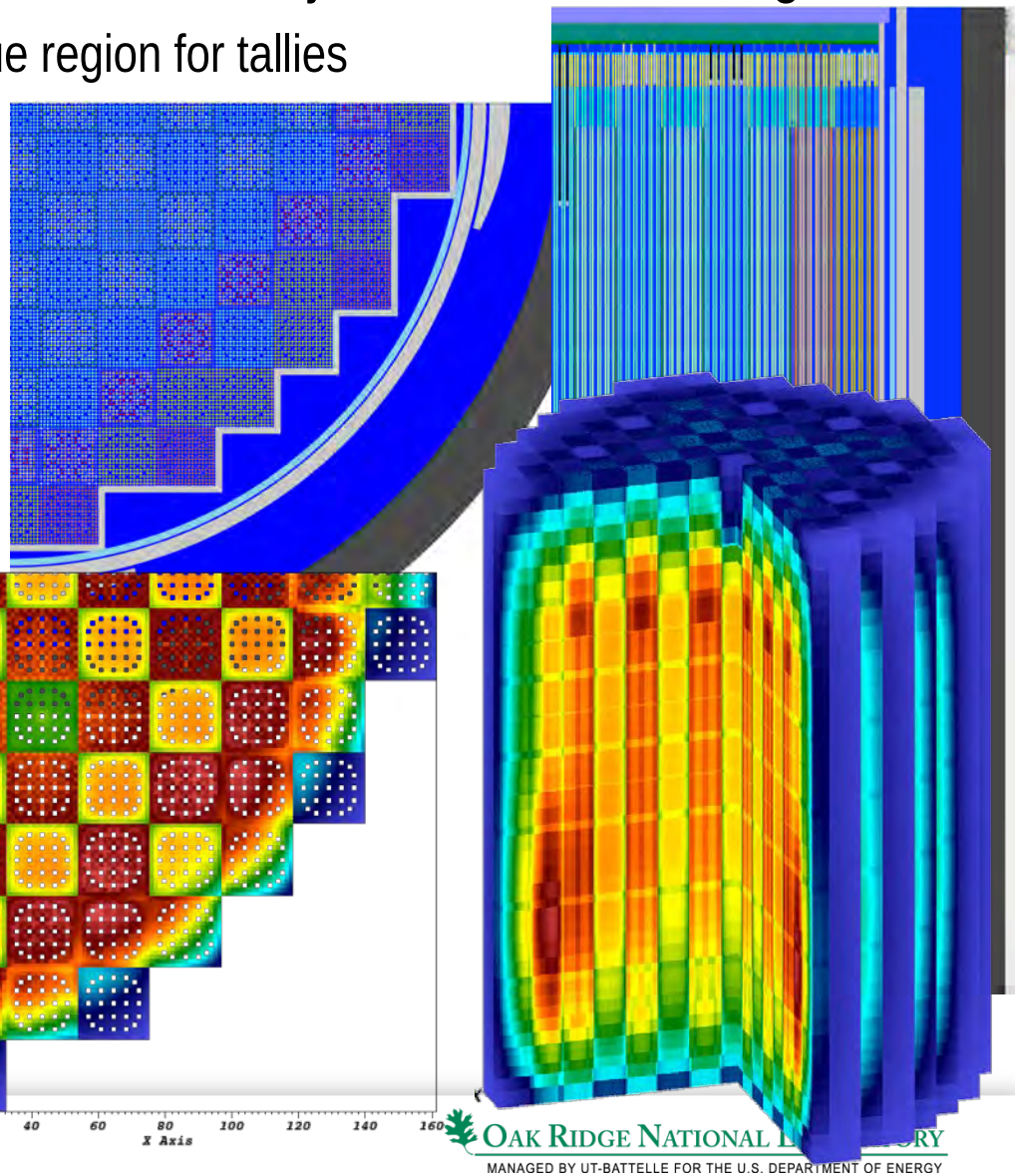
- Extensive rework of everything CE in SCALE and AMPX
- Introduction of efficient, XSProc module for MG calculations



CE Memory Improvements for Each Material	% Reduction in Memory
Conversion of internal data storage from double- to single-precision	15–45
Redesign of 2D collision kinematics data	5–30
Optimize nuclide object (in memory access to data)	3–15
Optional within-nuclide unionized reaction energy grid	10–20
TOTAL	40–95

CASL Application of Enhanced KENO-VI

- High-fidelity AP-1000 startup calculations in conjunction with Westinghouse
  - Each axial region of each pin is unique region for tallies
  - Reference solution for power dist.
  - Auto-generated 8,000,000 line input
  - 688,000 units
  - 5,000,000 particles/gen
  - 10,000 generations
  - 50 billion total particles
  - 180 cores on INL's Fission
  - 10.3 days of wall time
  - 44,500 CPU-hours
  - 11 GB/core (2 TB total)
  - Max uncert. 3.4%
  - Credit: Andrew Godfrey



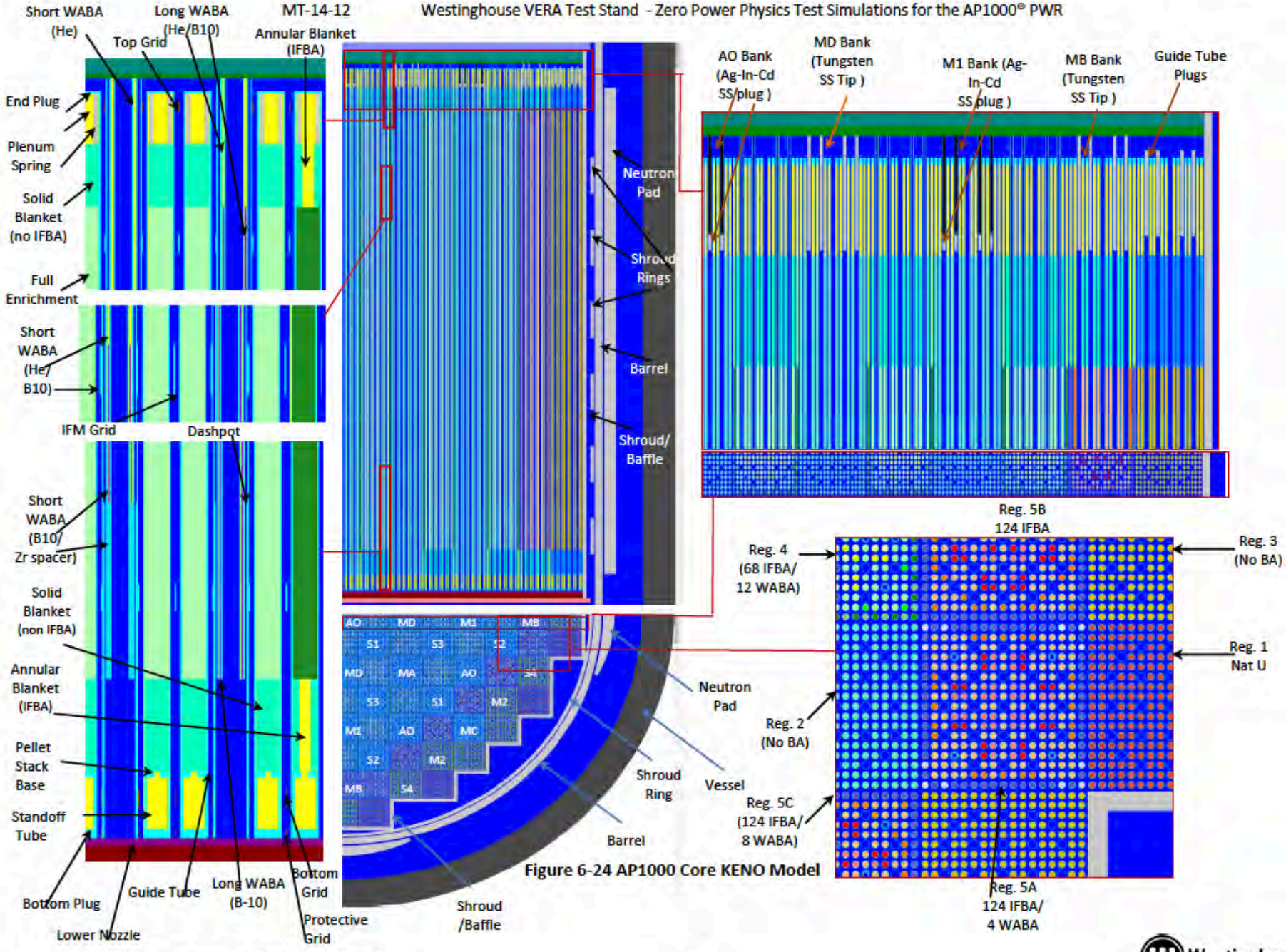
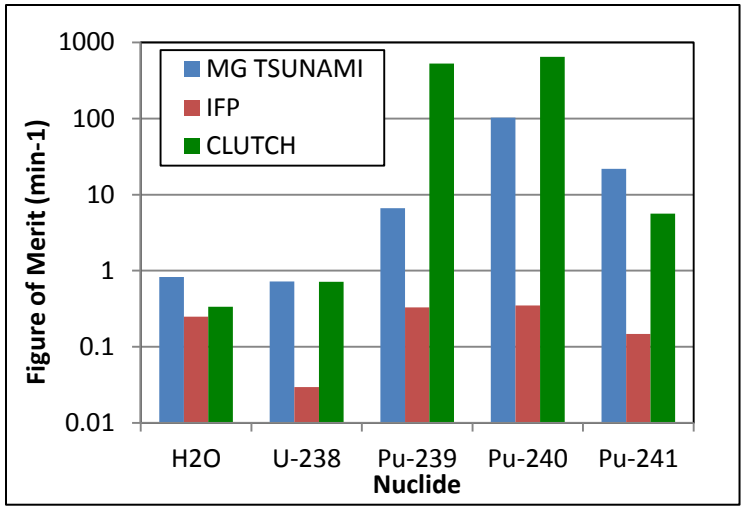


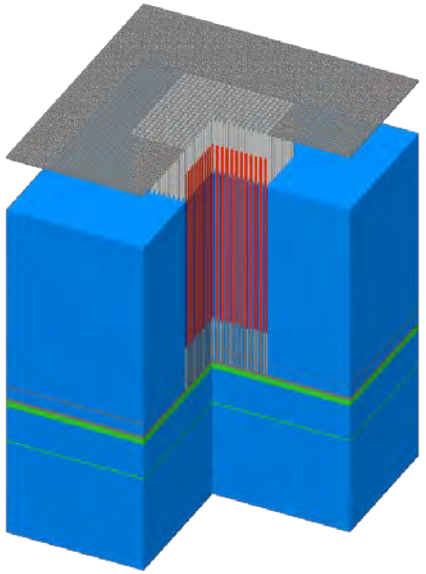
Figure 6-24 AP1000 Core KENO Model

Continuous-Energy Sensitivity Analysis

- Two new methods integrated into TSUNAMI / KENO for CE Calculations
  - Iterated Fission Probability (similar to MCNP)
  - CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization) – PhD topic



	13 GB	11 GB	0.06 GB

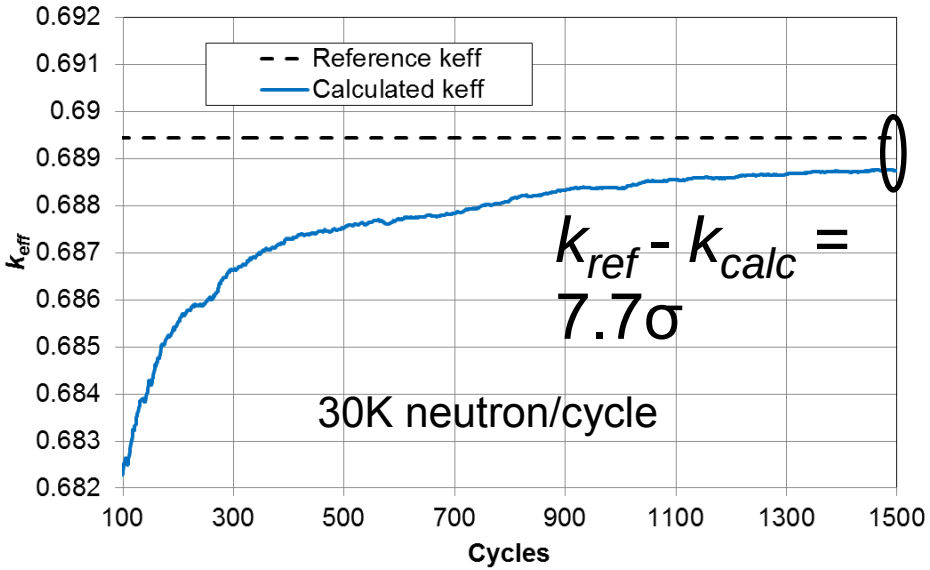


MIX-COMP-THERM-004
Critical Experiment

Convergence problems of NAC-UMS-TSC-24

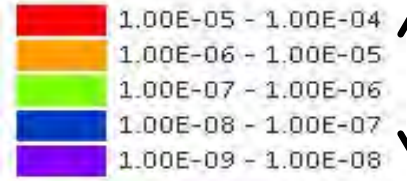
- Difficult to capture most reactive regions
- Decoupling due to water and flux traps

k_{eff} with uniform starting source

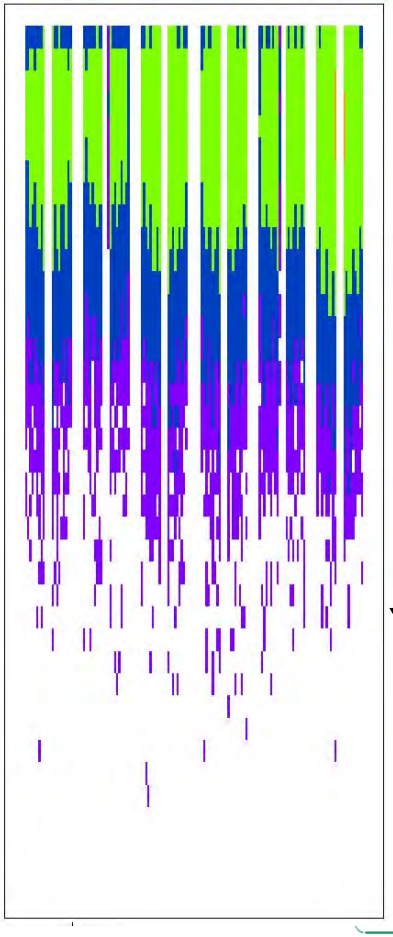


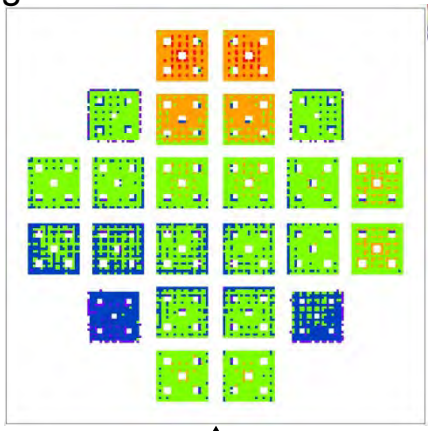
Unaffordable computer and human resources required to ensure reliability of canister-specific calculations

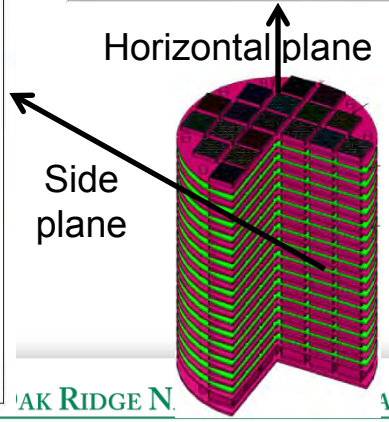
Reference fission source distribution



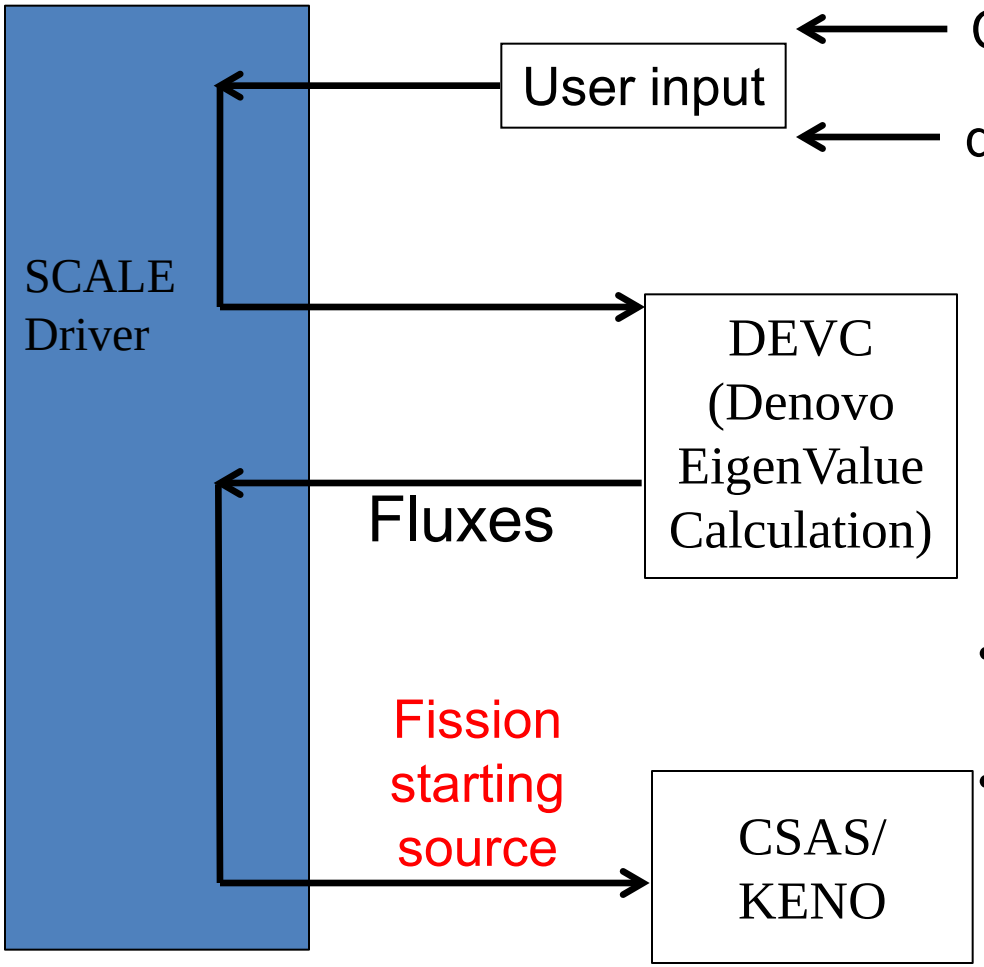
Difficulties in adequately sampling most reactive regions







Sourcerer



detSource block

- Denovo library
- Denovo mesh
- Denovo parameters

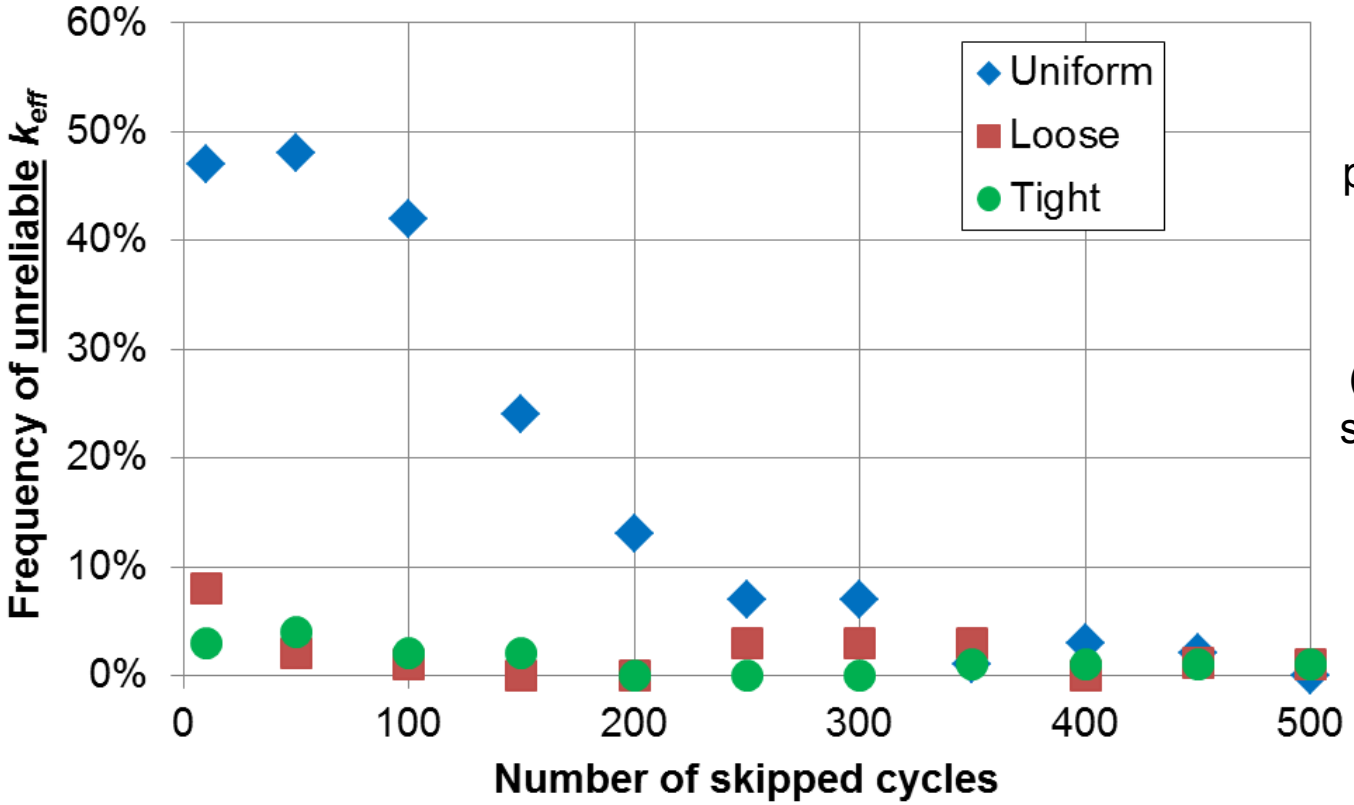
- Automatic mapping of KENO geometry on user-defined grid
- Materials mixing (macromaterials) using a volume weighted average of the materials in the MC model

Ibrahim et. al, "Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources," PHYSOR 2012

Reliability

Frequency of **not** calculating k_{eff} inside confidence interval

$k_{ref} - 3\sigma < k_{calc} < k_{ref} + 3\sigma$

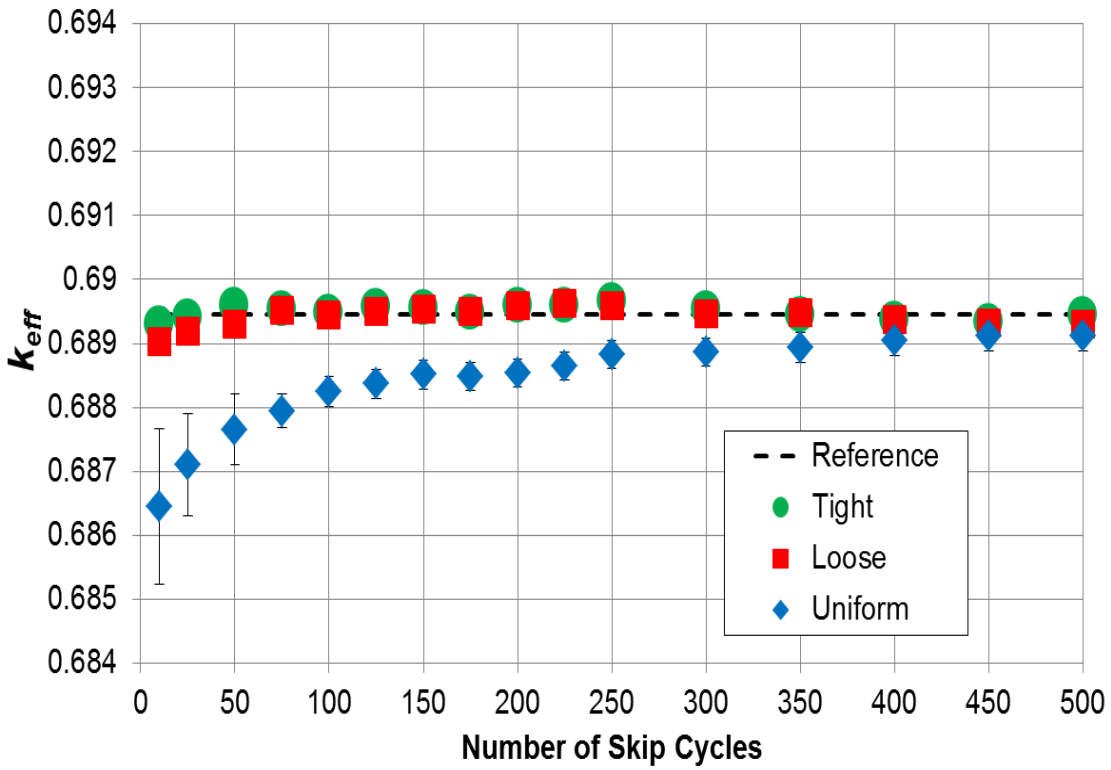


30,000 Neutrons per cycle and 500 active cycles

100 independent (different random seed) calculations for each point

Reliability of uniform source is comparable with the reliability of deterministic source after skipping 350 cycles

Efficiency
k_{eff} with 500 active generations

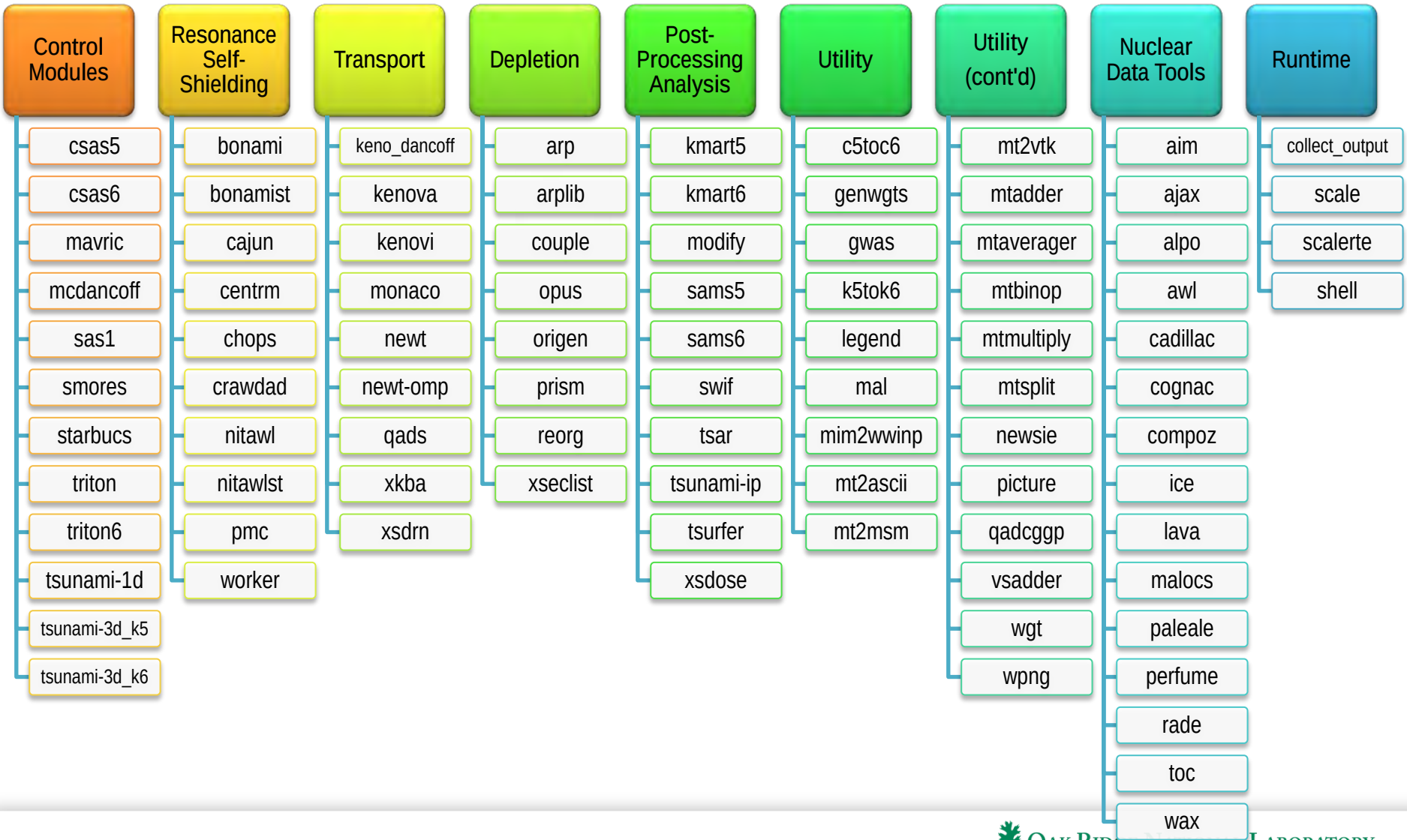


Starting source	k_{eff}	Speedup
Uniform	0.68977 ± 0.00025	1.00
Loose	0.68944 ± 0.00024	1.71
Tight	0.68900 ± 0.00024	1.36

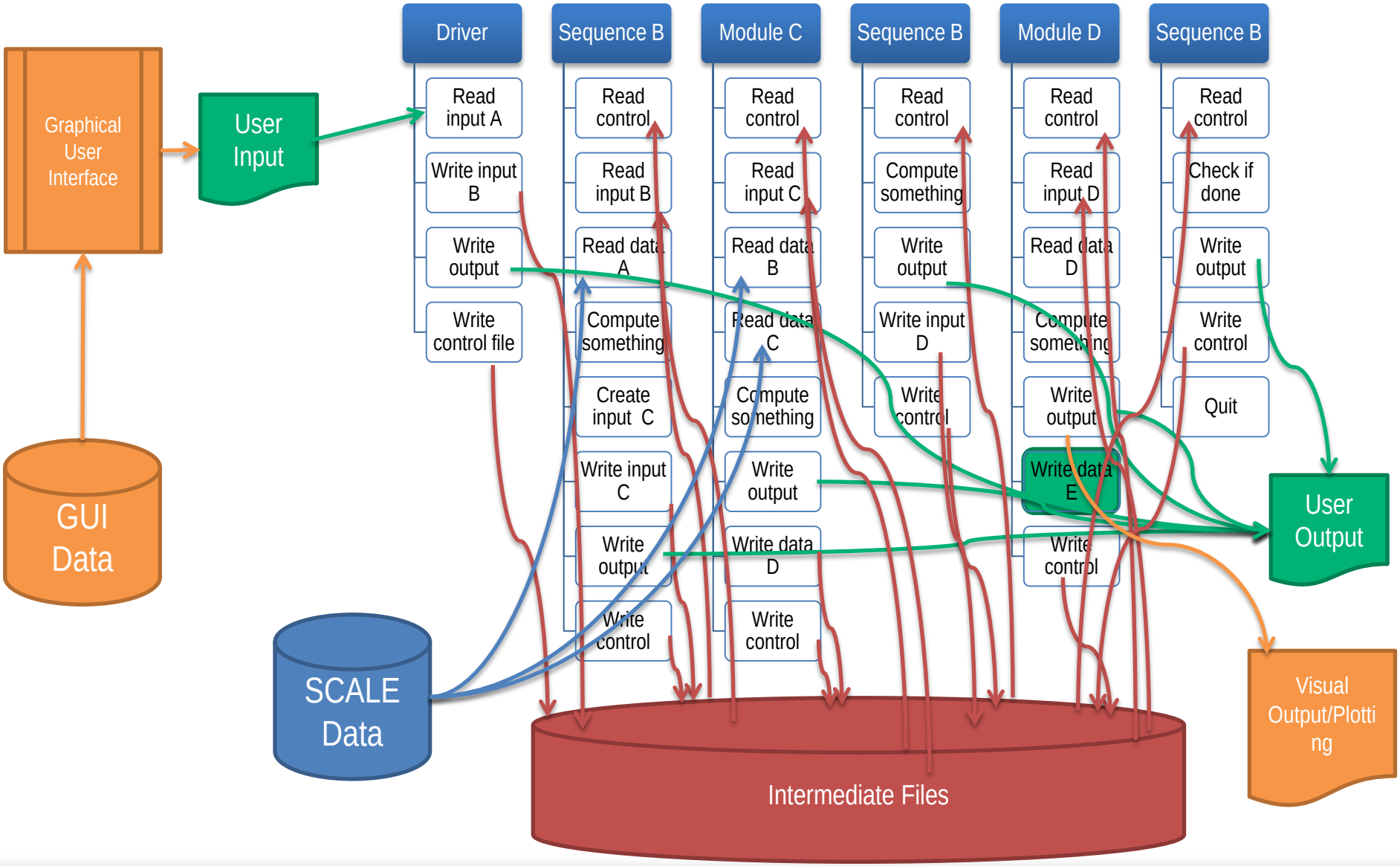
Outline

- Quality Assurance
- Advanced Features
- Modernization

89 Independent Executable Modules in SCALE 6.1

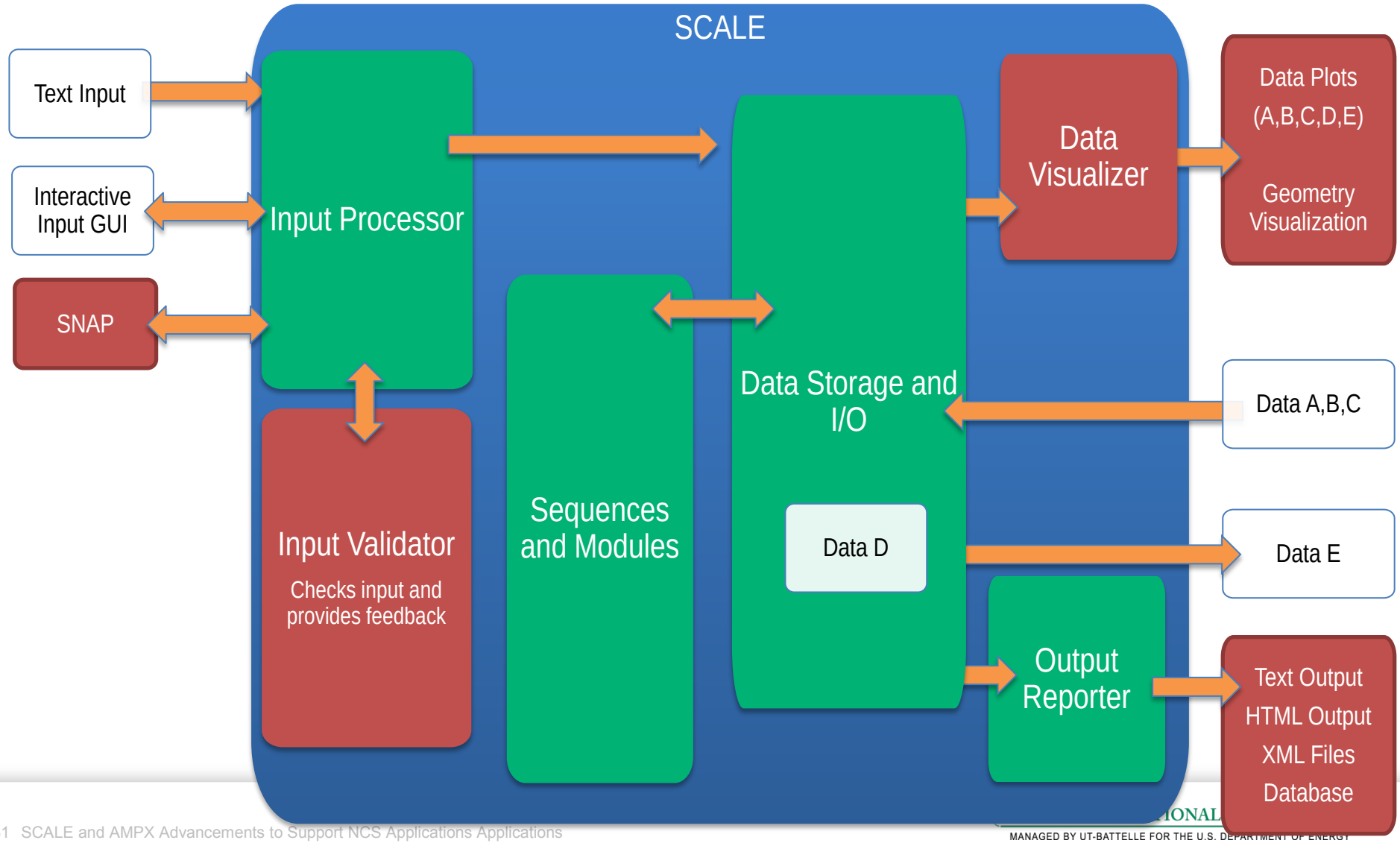


Hypothetical SCALE 6.1 Calculation



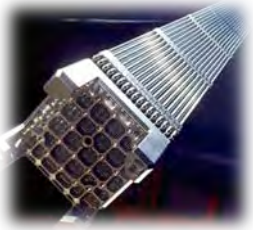
SCALE Modernization

New Framework, New Potential, New Motivation

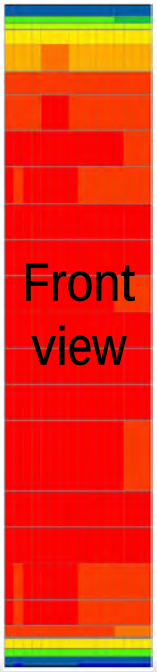


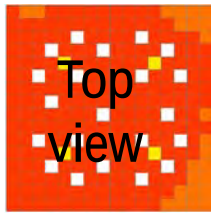
Modular Interfaces

- SCALE Continuous-Energy Modular Physics Package (SCEMPP)
  - Coupled neutron/gamma physics
  - Application Programmer Interface (API) for CE physics for next-generation Monte Carlo codes
  - Implemented for shielding in Monaco
  - HPC Monte Carlo with Shift (125K processors)
- 6300 fixed-source transmission tests used in V&V
- ORIGEN restructured to provide API and parallel capabilities
- New ORIGAMI tool developed to rapidly characterize spent fuel.
- MPI with (near)-linear speedup

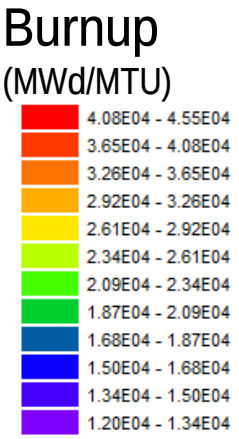


235 pins
26 axial zones



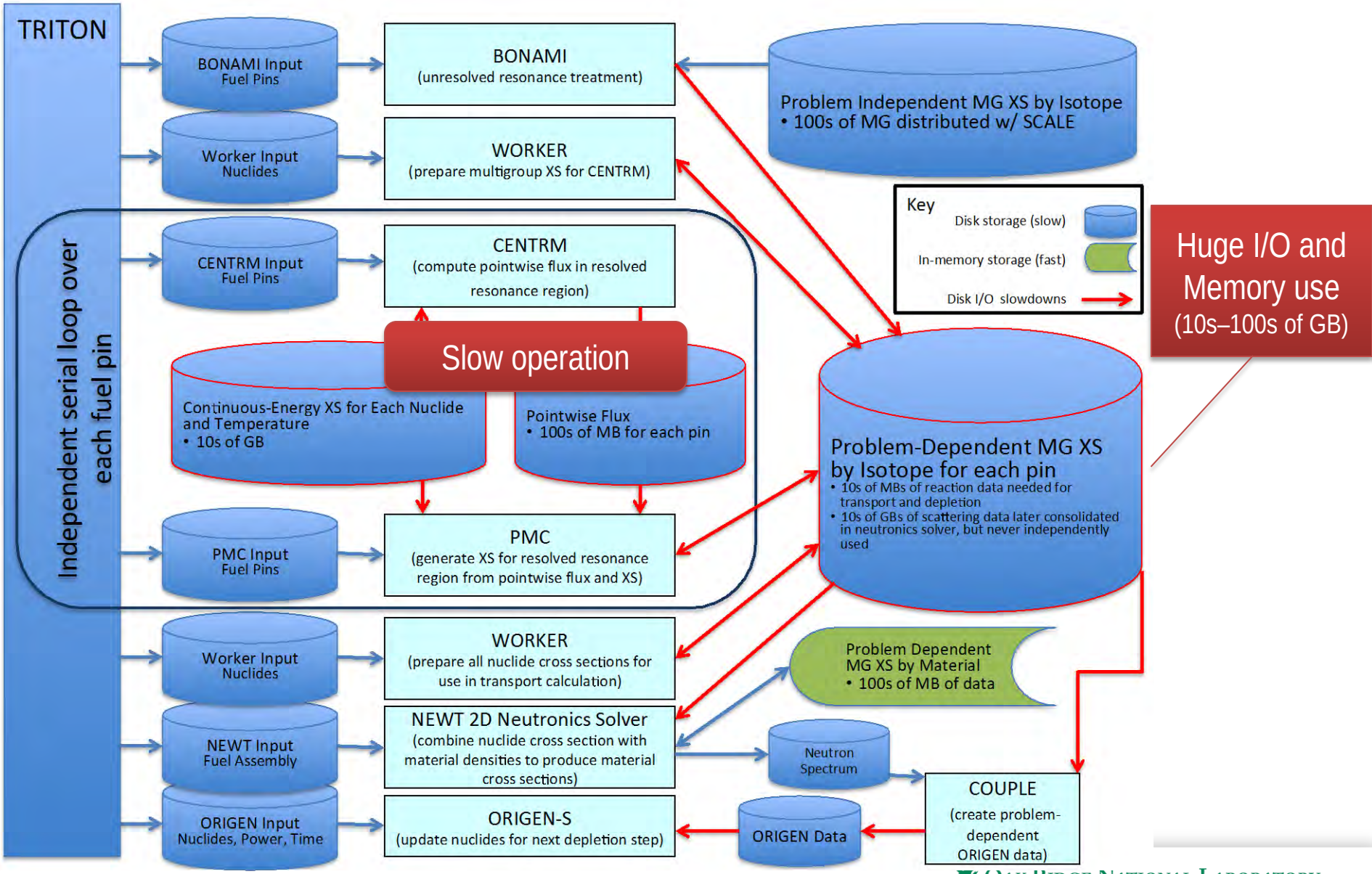


6,110 Depletion nodes

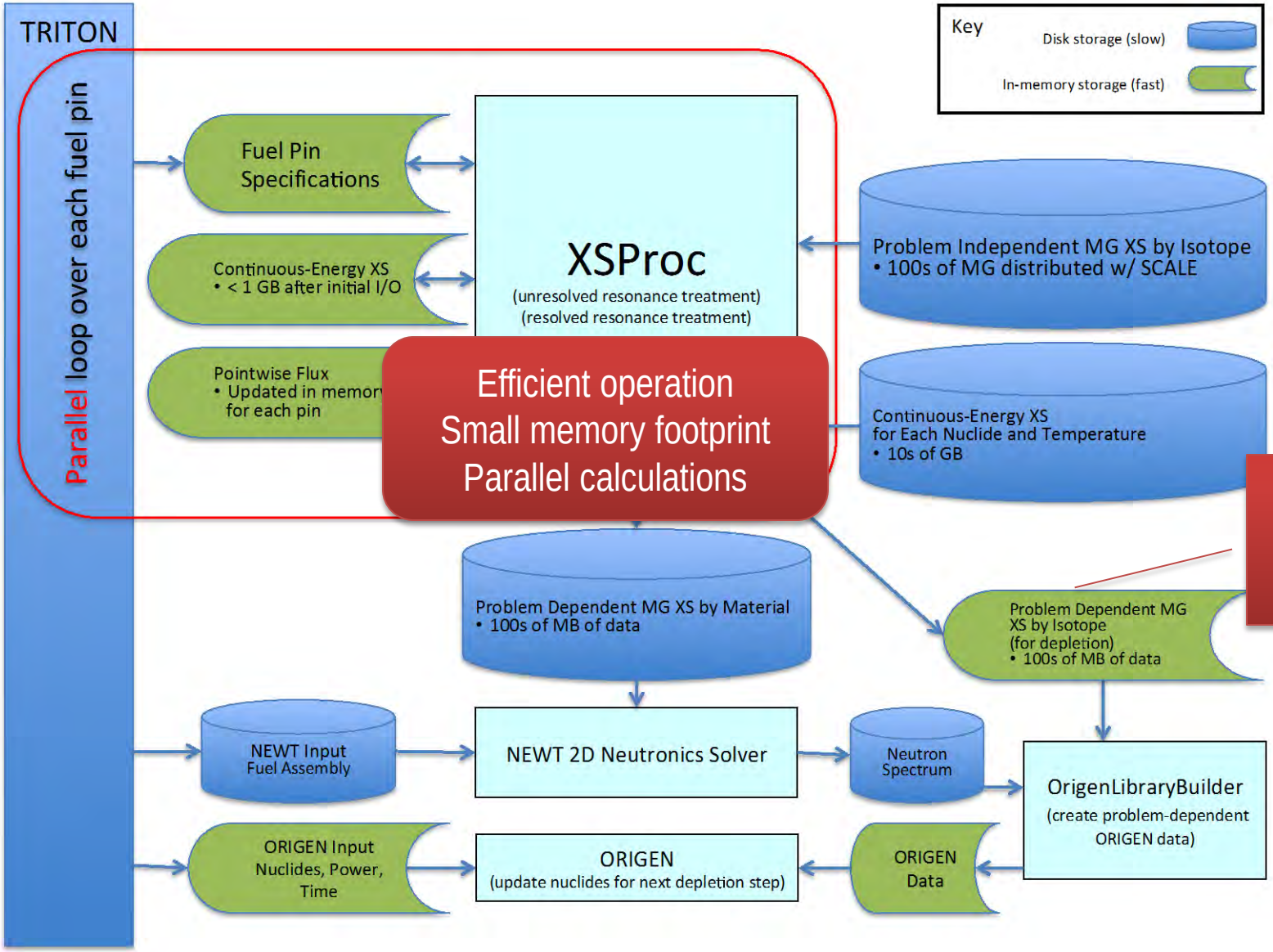


SCALE 5.0–6.1 Resonance Self-Shielding

(somewhat simplified view)

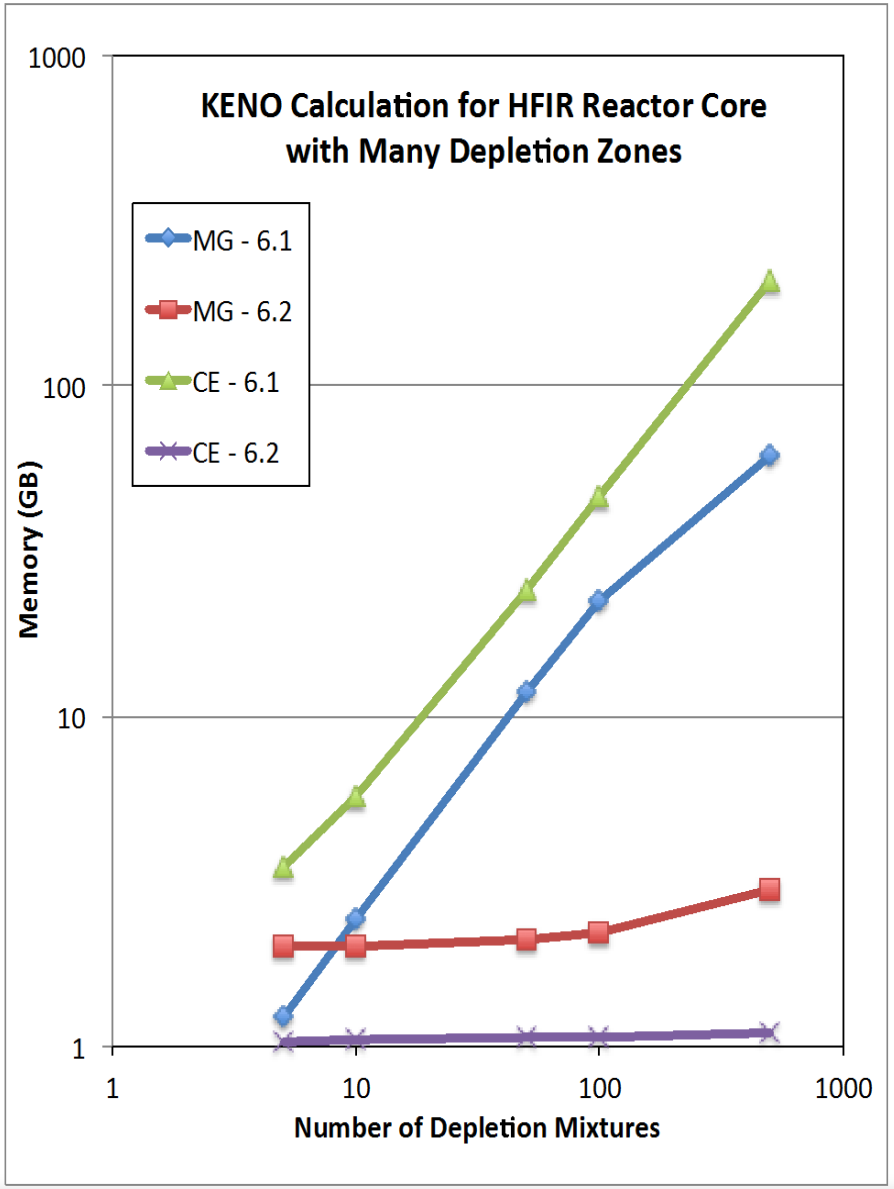


SCALE 6.2 Resonance Self-Shielding



Modernization Successes in SCALE 6.2beta

- Many calculations with 95% reduction in memory footprint
- Many calculations 3x faster, some calculations run 1800x faster
- Interfaces to physics capabilities provided to other high-profile projects and university R&D



The SCALE Code System

Neutronics and Shielding Analysis For Enabling Nuclear Technology Advancements

scale

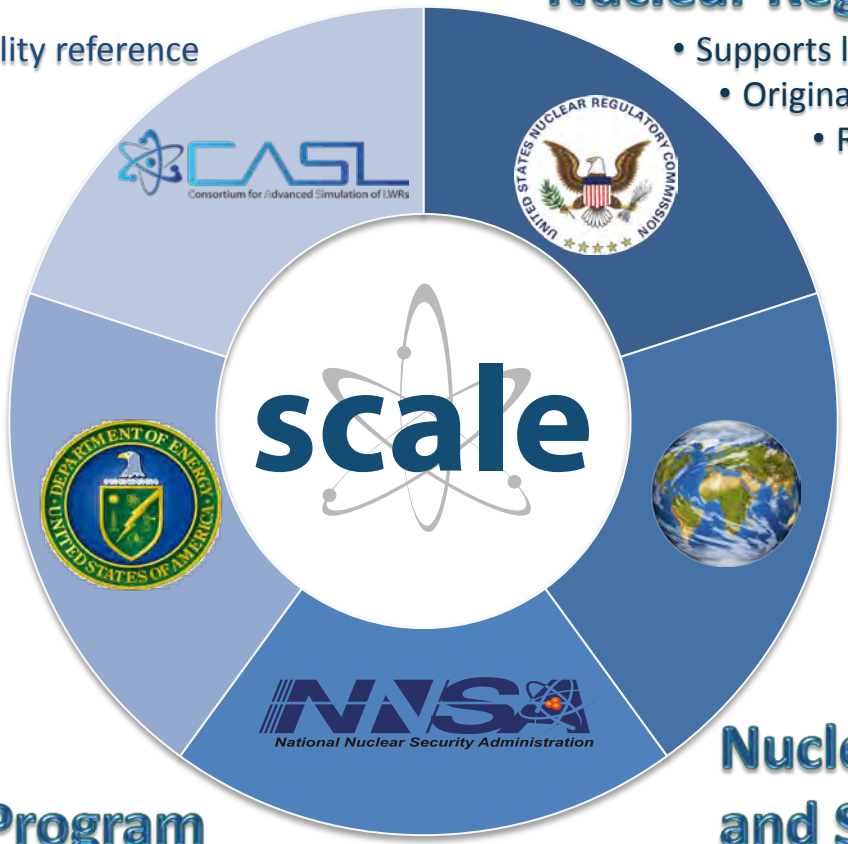
OAK RIDGE National Laboratory

CASL

- Continuous-energy, high-fidelity reference solutions for reactor physics
- Cross-section data libraries
- Reactor fuel depletion
- Uncertainty quantification

Nuclear Regulatory Commission

- Supports licensing and regulatory research
- Original sponsors of SCALE – since 1976
- Reactor physics and source terms
- Criticality safety and shielding
- Cross section data libraries



DOE Used Fuel Disposition

- Radiation shielding
- Nuclear fuel depletion
- Used fuel source terms
- Criticality safety analysis
- Uncertainty quantification

Global Distribution

- 5600 users in 51 nations
- Regulators
- Industry
- Research and Development

DOE Nuclear Criticality Safety Program

- Criticality safety assessments
- Sensitivity and uncertainty analysis
- Advanced validation methods
- Experiment design
- Criticality accident alarm system analysis and design

Nuclear Nonproliferation and Safeguards

- Used fuel and radionuclide source terms
- Reactor depletion analysis
- Radiation transport
- Nuclear forensics

SCALE 6.2 Tentative Schedule

- Beta1 – August 2013
- Beta2 – broader release January 2014
- Beta3 – expected in Spring 2014
- Production release – expected in later in 2014

Questions?

http://scale.ornl.gov

scalehelp@ornl.gov