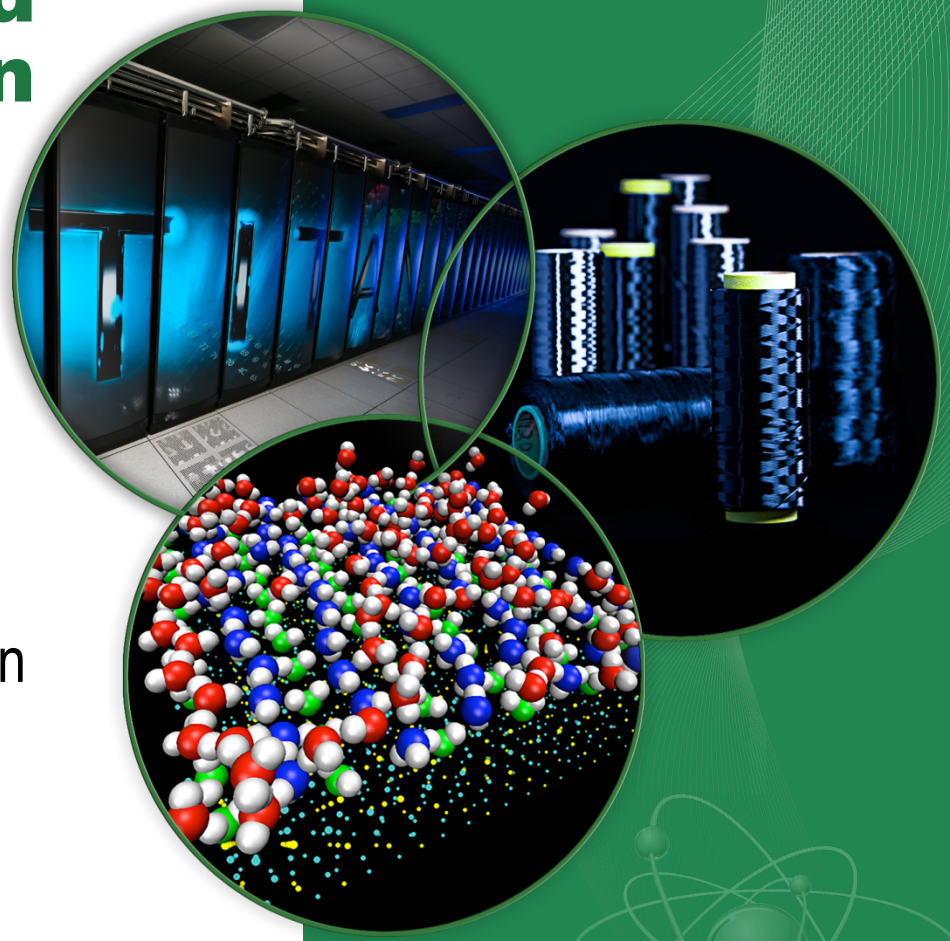
Status of SCALE and AMPX Modernization Efforts at ORNL



Brad Rearden

Manager, SCALE Code System

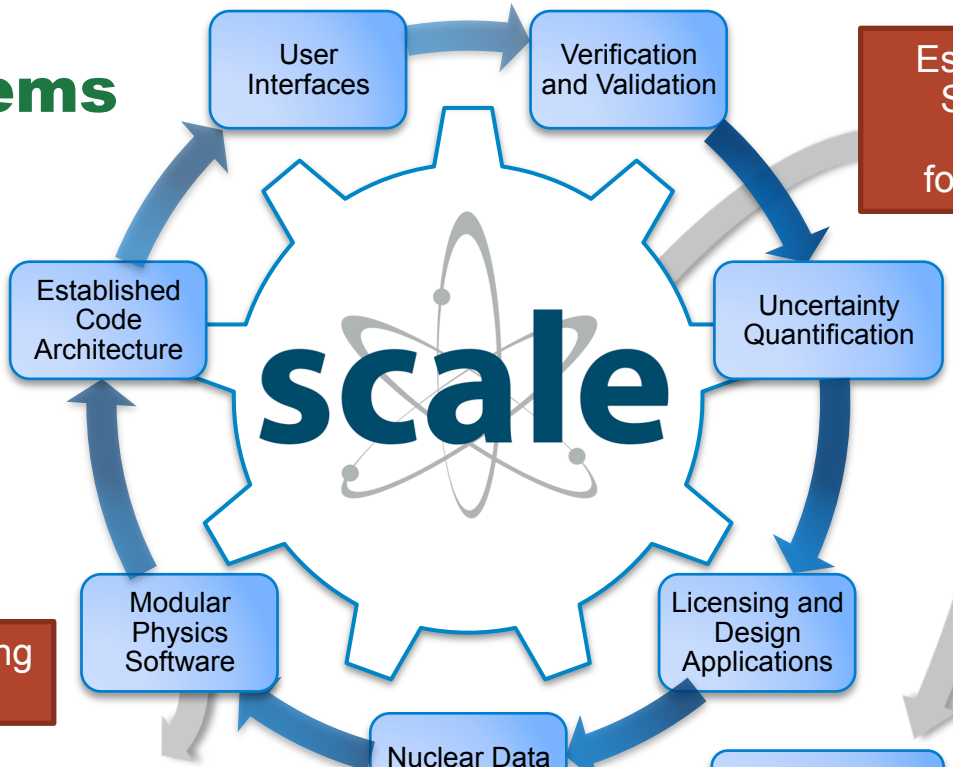
Reactor and Nuclear Systems Division

Nuclear Criticality Safety Program
Technical Program Review
Lawrence Livermore National Laboratory
March 18, 2015

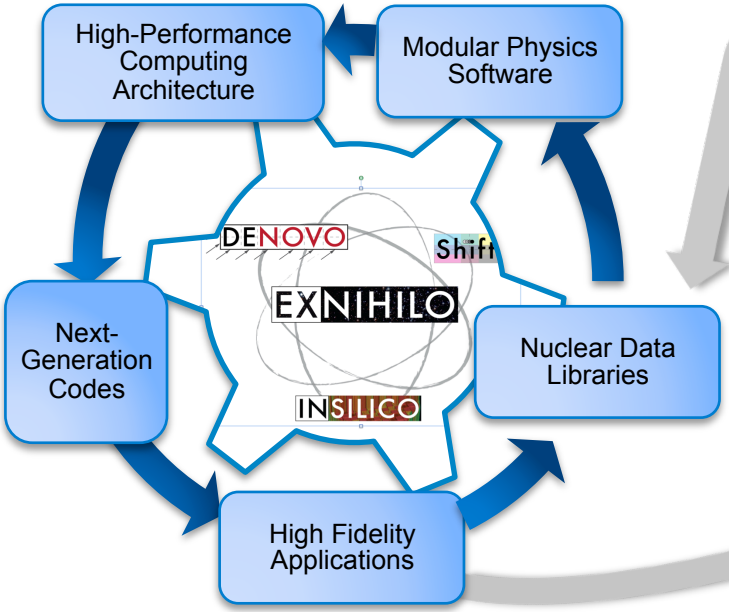
ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

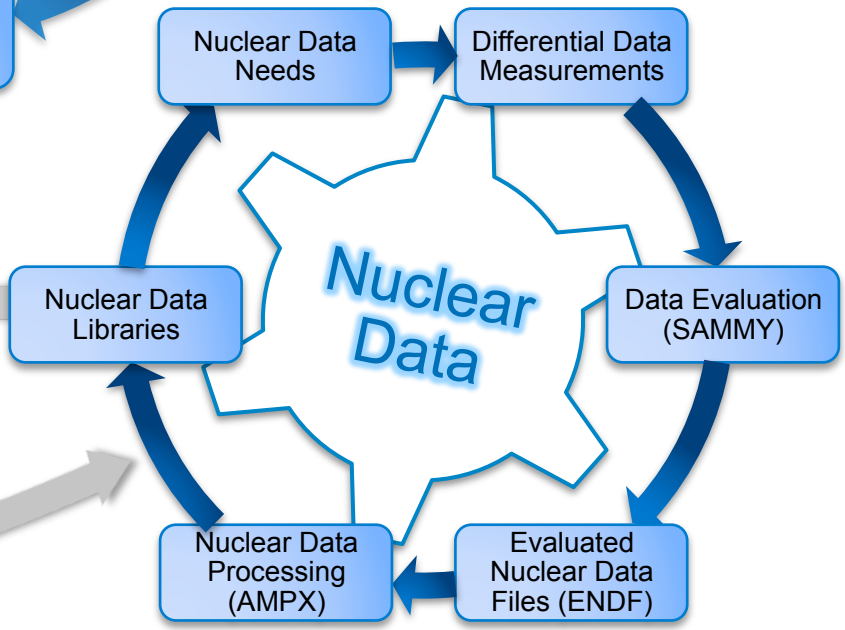
Reactor and Nuclear Systems Division's Modeling and Simulation Capabilities



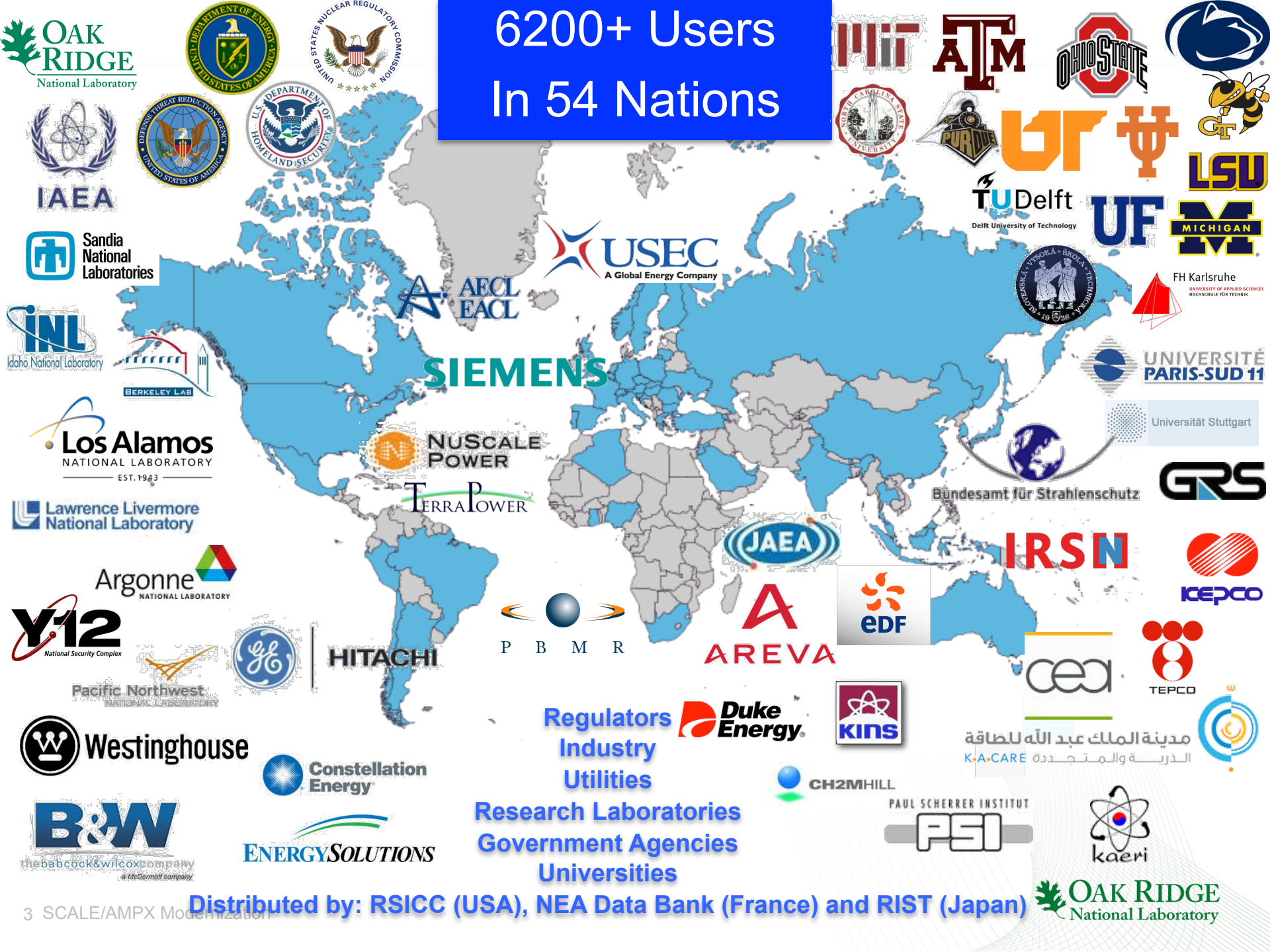
Established Modeling and Simulation Capabilities Used Worldwide for Licensing and Design



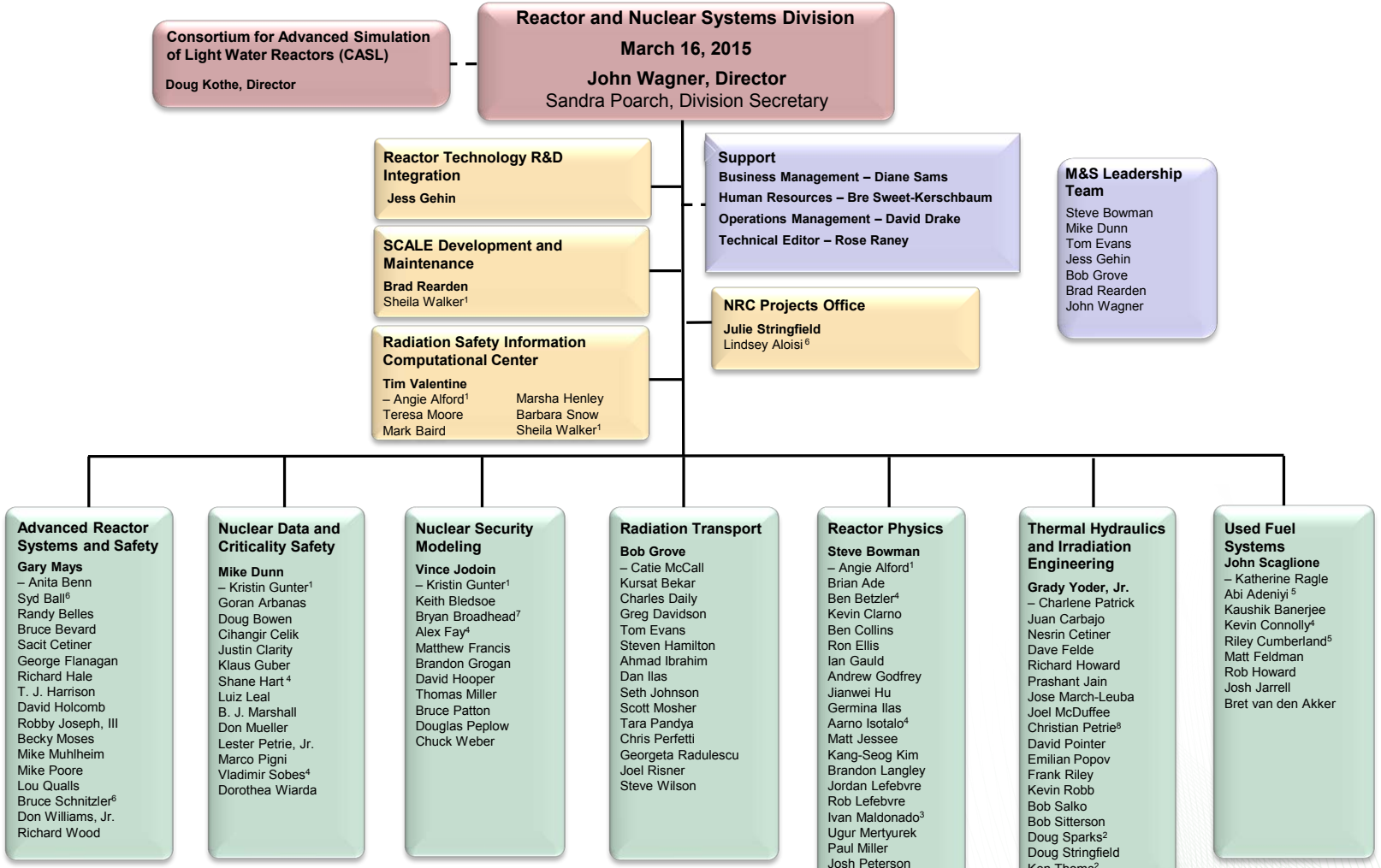
High-Performance Computing for Advanced Applications



Nuclear Data: From Fundamental Measurements to Production Libraries


6200+ Users
In 54 Nations
Regulators
Industry
Utilities
Research Laboratories
Government Agencies
Universities
Distributed by: RSICC (USA), NEA Data Bank (France) and RIST (Japan)

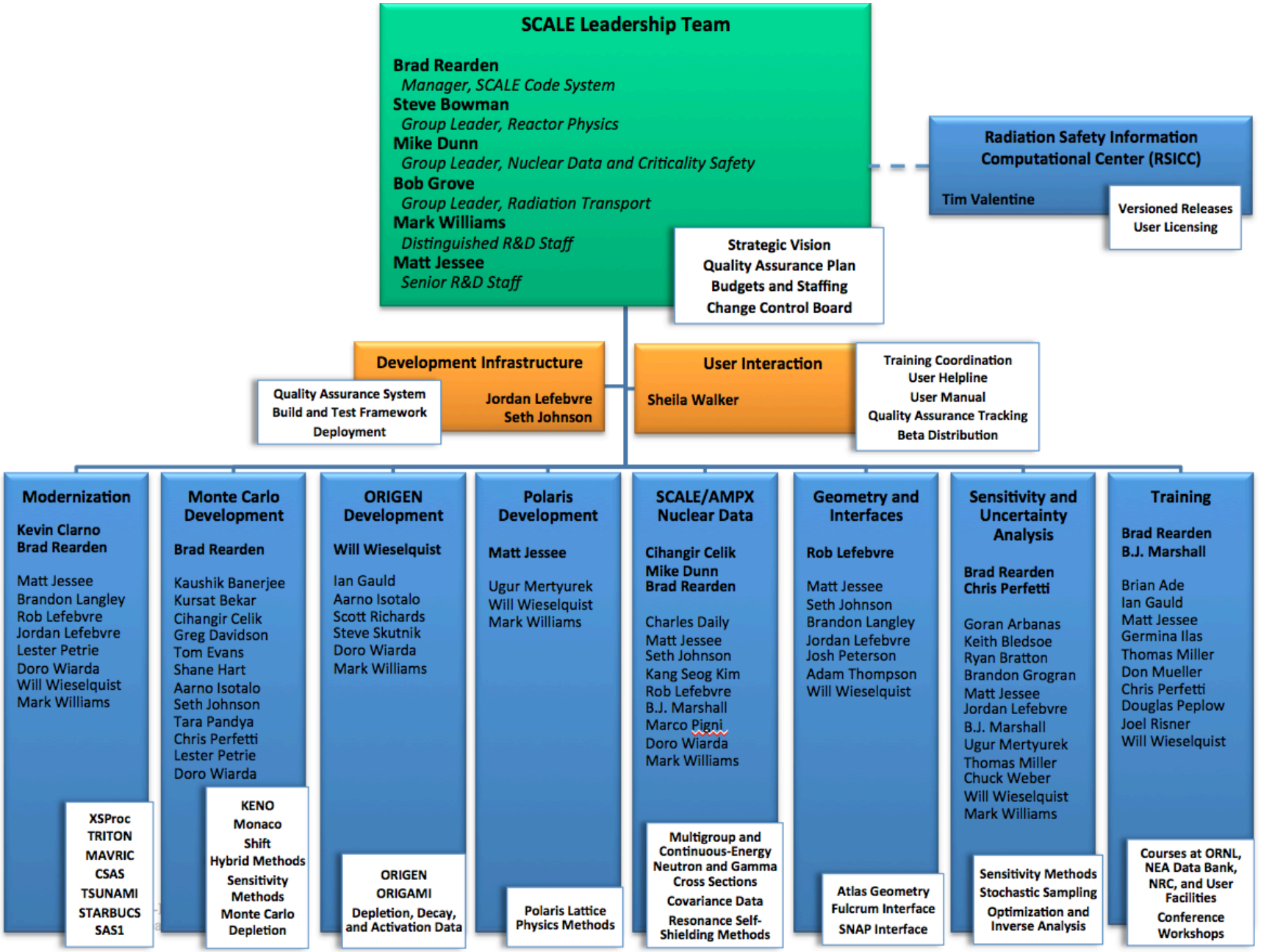
SCALE is Developed within the ORNL Reactor and Nuclear Systems Division



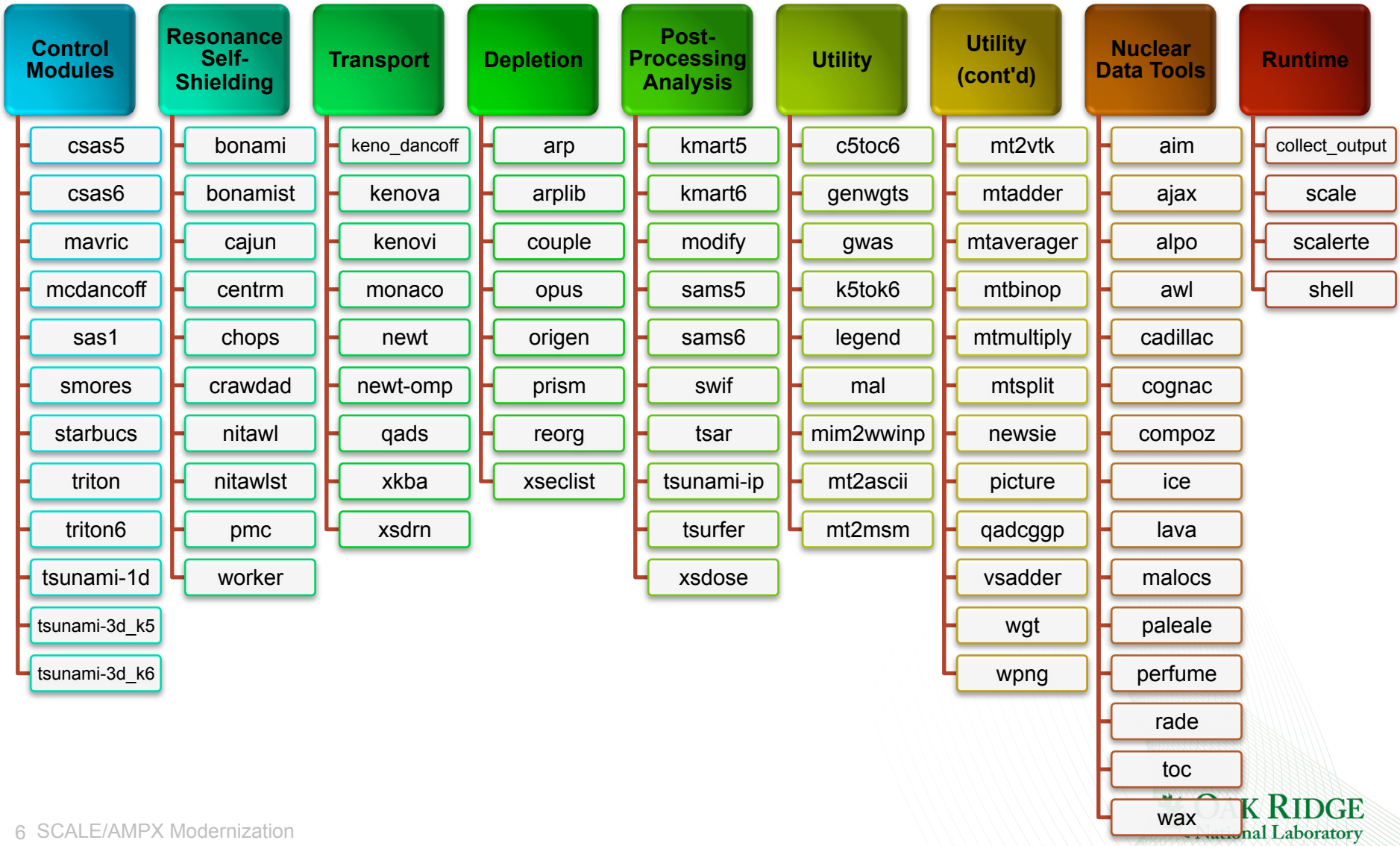
[1] Dual Capacity
[2] Subcontractor
[3] Joint Faculty
[4] Postdoc
[5] Postmaster
[6] Casual/Part-time
[7] Off-site Assignment

OAK RIDGE National Laboratory

SCALE Team Structure

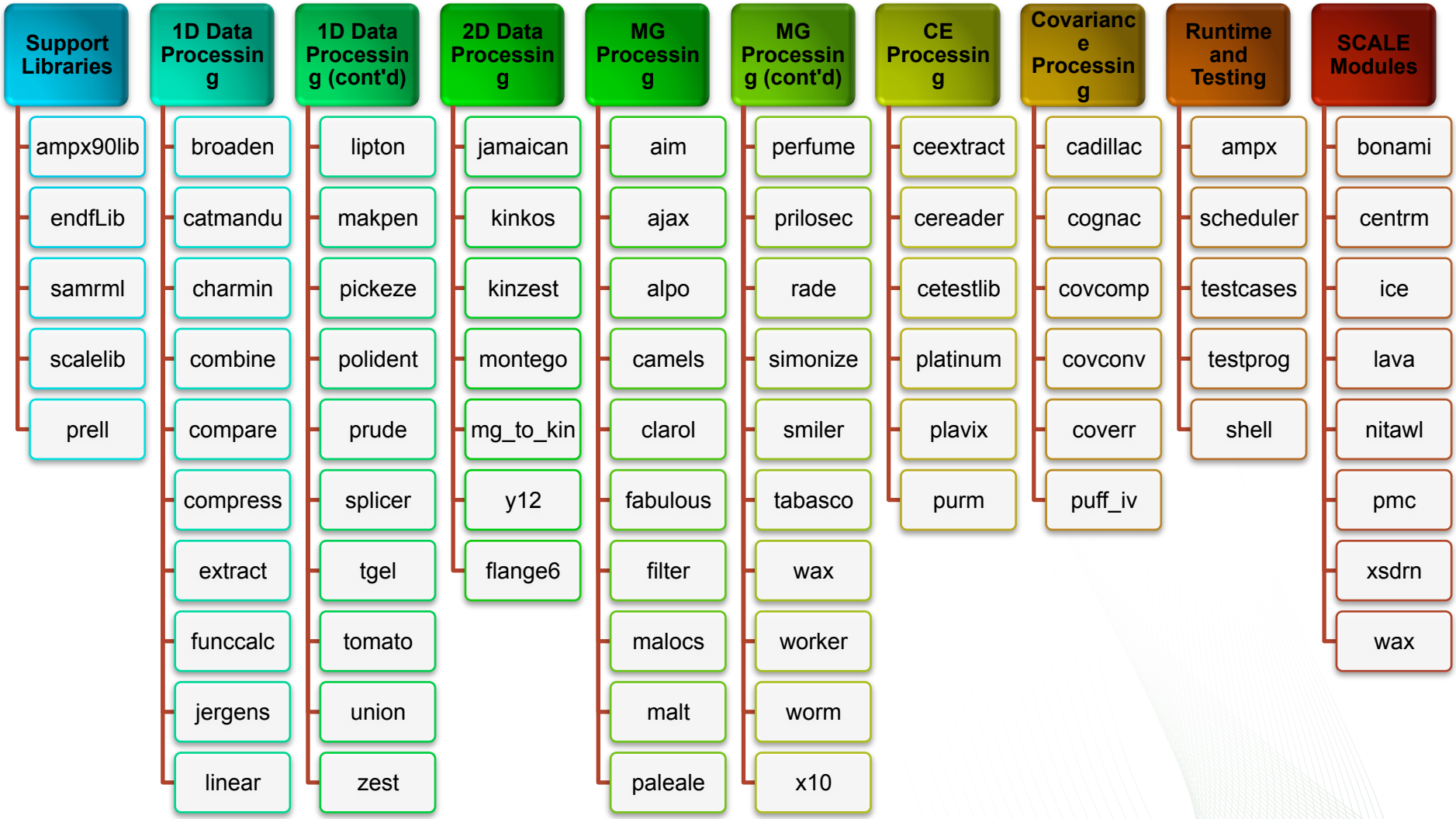


89 Independent Executable Modules in SCALE 6.1



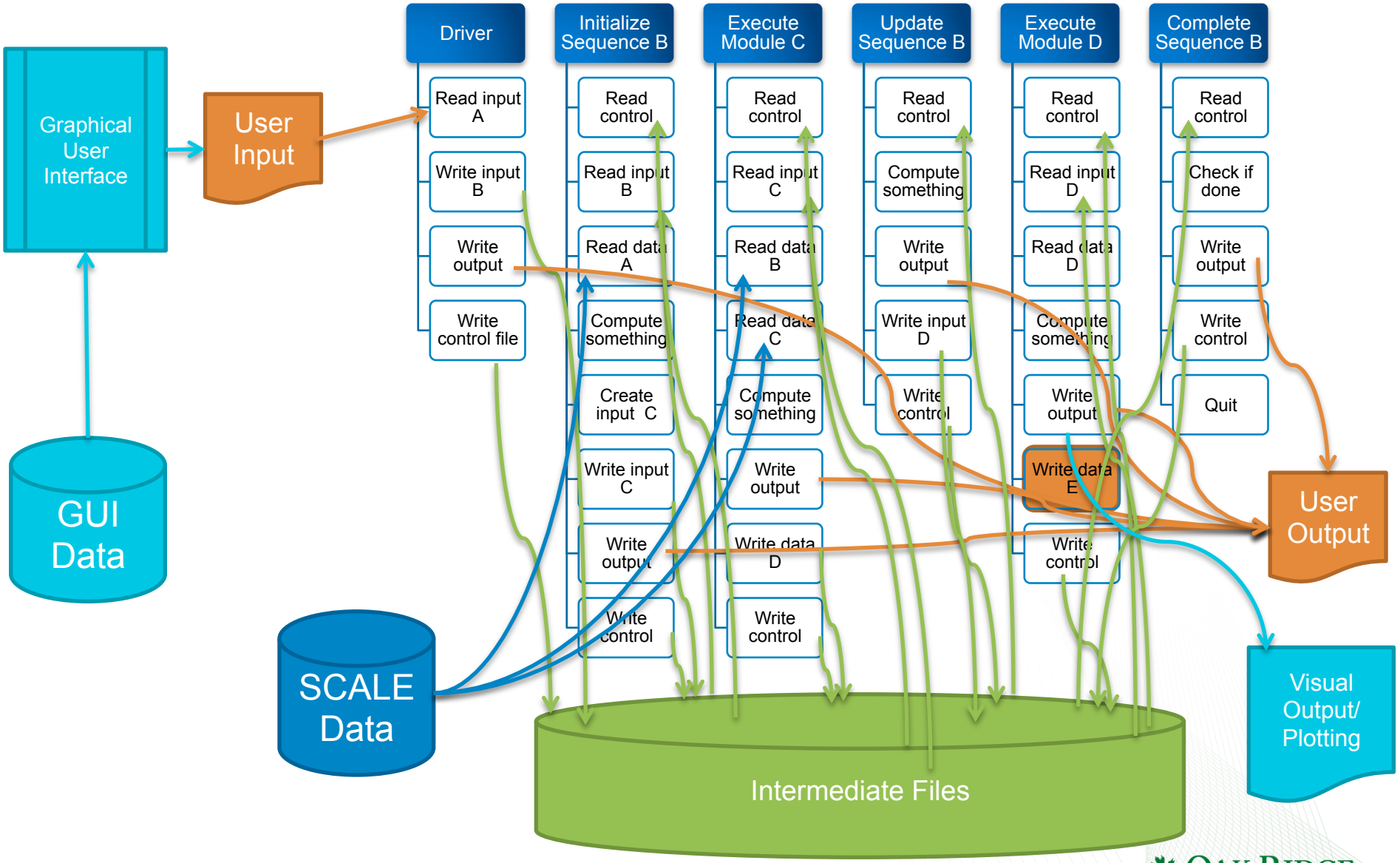
OAK RIDGE National Laboratory

AMPX Modular Code System (pre-Modernization Effort)



OAK RIDGE National Laboratory

Hypothetical SCALE 6.1 Calculation



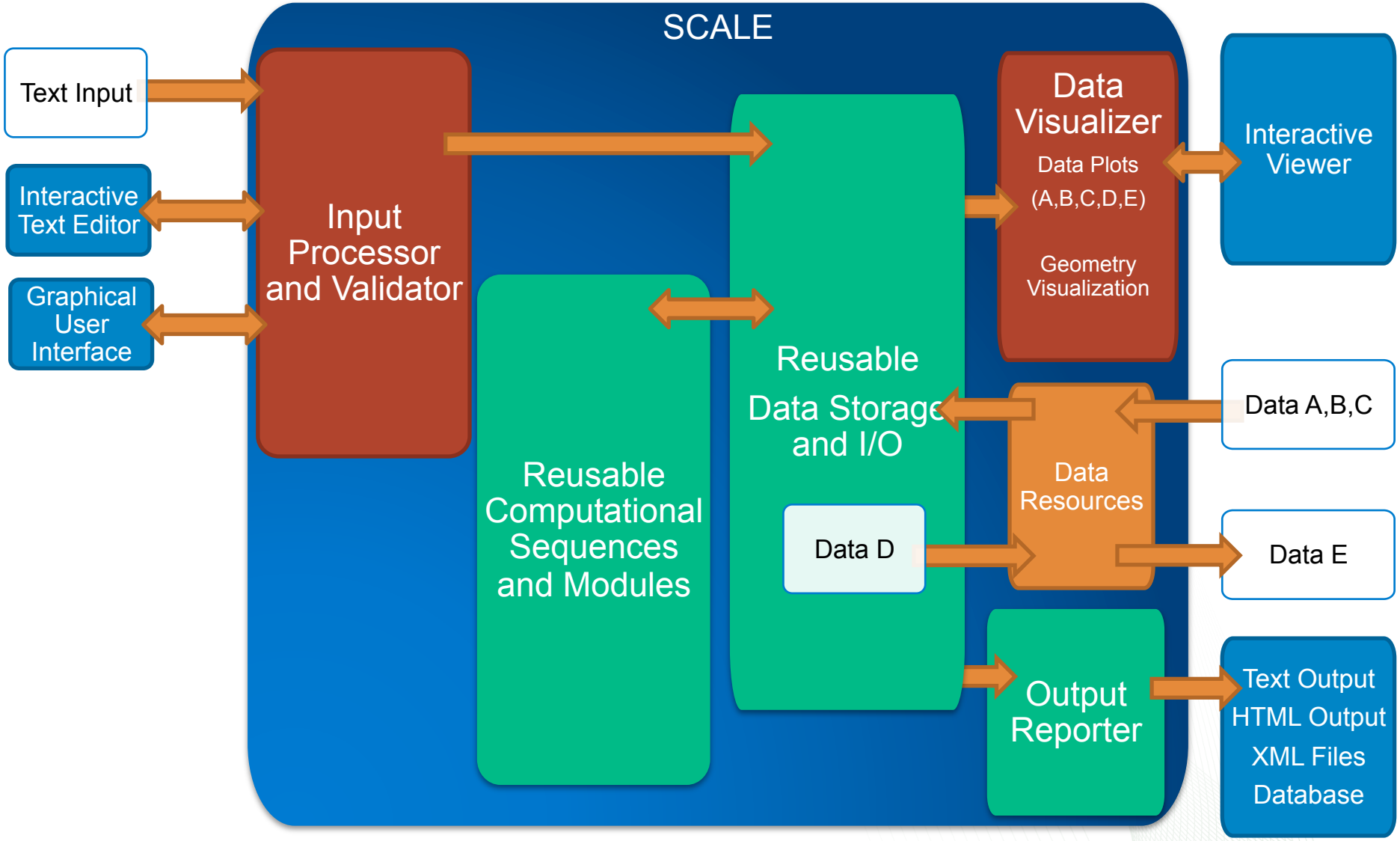
OAK RIDGE National Laboratory

Legacy AMPX Framework (pre-Modernization Effort)

- AMPX framework and operation are similar to SCALE 5
- 77 modules
- Testing not integral to system: these legacy practices leave many features untested as changes occur
  - Need improved testing suite to more readily identify ENDF data and processing issues
- Several codes that provide key functionalities are "fragile" and difficult to update
- Leverages some SCALE features, but integration is loose and features can easily get out of phase
- Legacy AMPX software not updated under formal quality assurance plan
- Objective: Modernize AMPX software to improve overall reliability and quality of nuclear data libraries for SCALE

OAK RIDGE National Laboratory

SCALE 7 Modernized Concept



OAK RIDGE National Laboratory

Progress Towards Modernization

Modular Data

- Neutron and Gamma Cross Sections
- Cross-section Covariance Libraries
- Activation, Depletion, and Decay Libraries
- Composition data

Modular Physics

- Cross-section processing
- Continuous-energy and multigroup physics for Monte Carlo analysis
- ORIGEN Depletion, Decay and Activation Methods
- Sensitivity / Uncertainty Methods
- Geometry Package for Monte Carlo and Method-of-Characteristics (MoC) Transport and Visualization

OAK RIDGE National Laboratory

Computational Benefits of Modernization

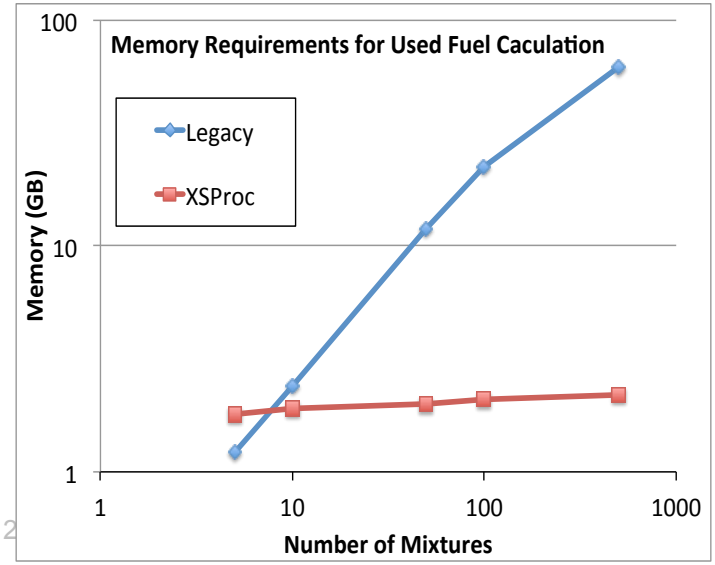
- As loaded canister with 24 fuel assemblies with 18 axial zones
- Nearly 2000x speedup for extreme case

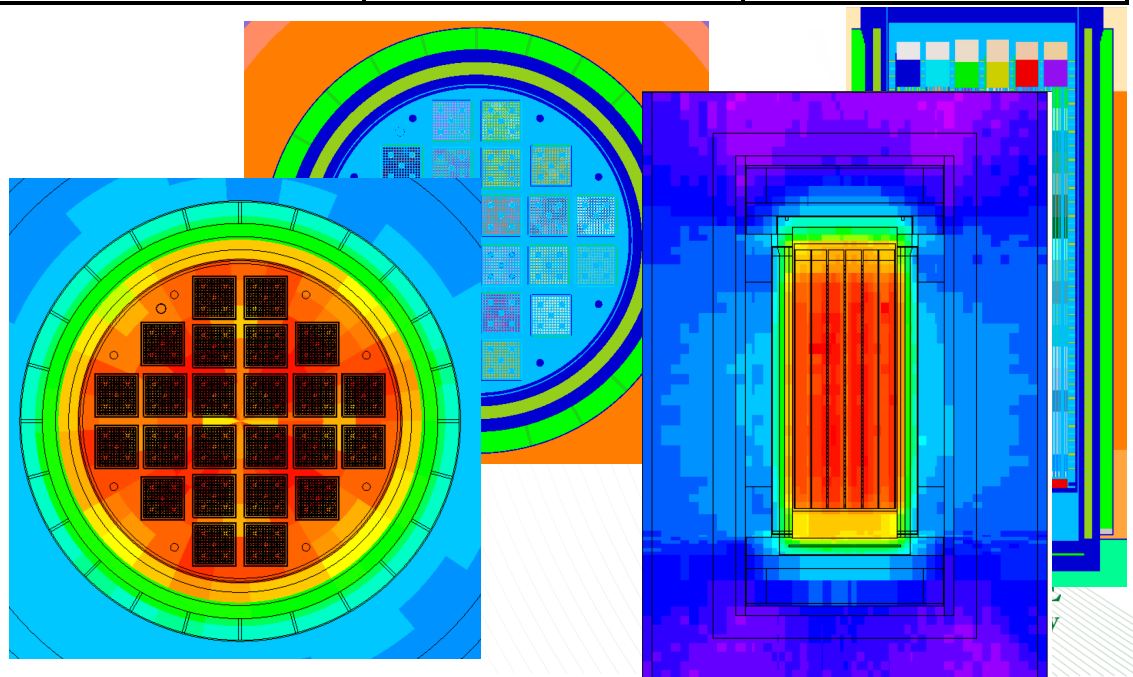
3.7 Minutes with SCALE 6.2

5 Days with SCALE 6.1

Model			Total Time (sec)	
Assemblies	Materials	Homogenized Cells	XSProc	Legacy
1	79	18	10.23	92
2	153	36	19.18	389
3	227	54	28.97	1,100
4	301	72	39.51	2,398
24	1781	432	223.66	440,000*

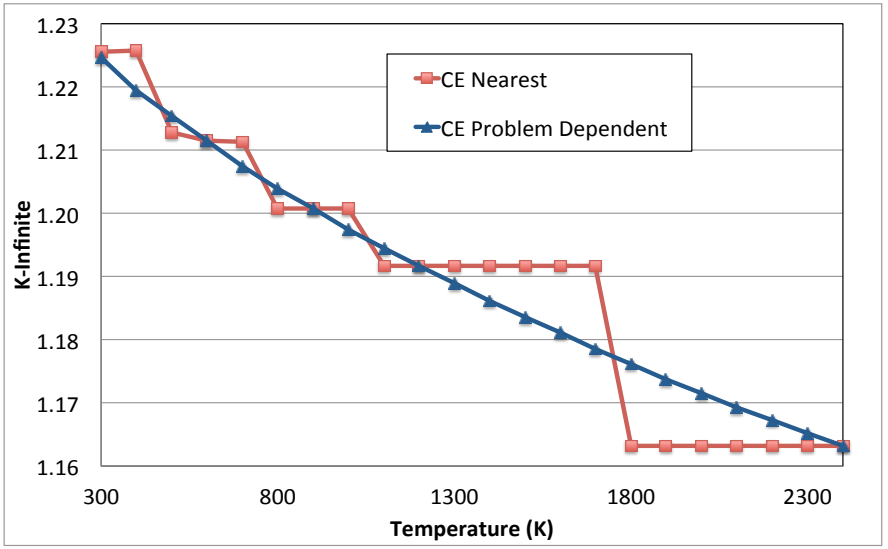
*Projected runtime.





Problem-dependent Doppler Broadening

- KENO updates CE data to user-specified temperature
  - S(α,β)
  - Resolved resonance
  - Unresolved resonance



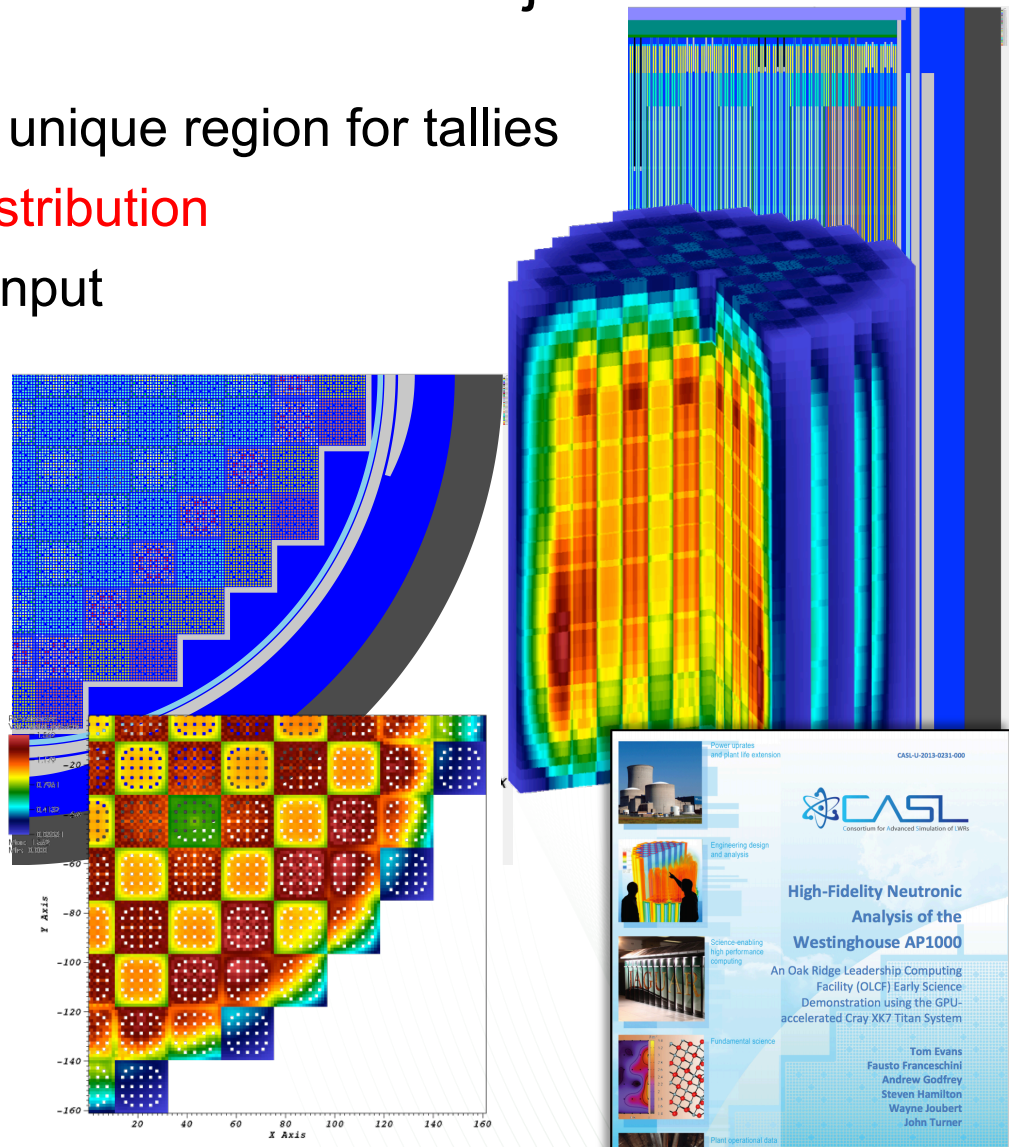
- Significant impact on thermal solutions, such as Silene benchmark

Temperature (K)	k_{eff}	Rel. Unc.
293.0	1.022831	0.000057
326.8	1.016286	0.000055
Delta k_{eff} (pcm)	-655	

OAK RIDGE National Laboratory

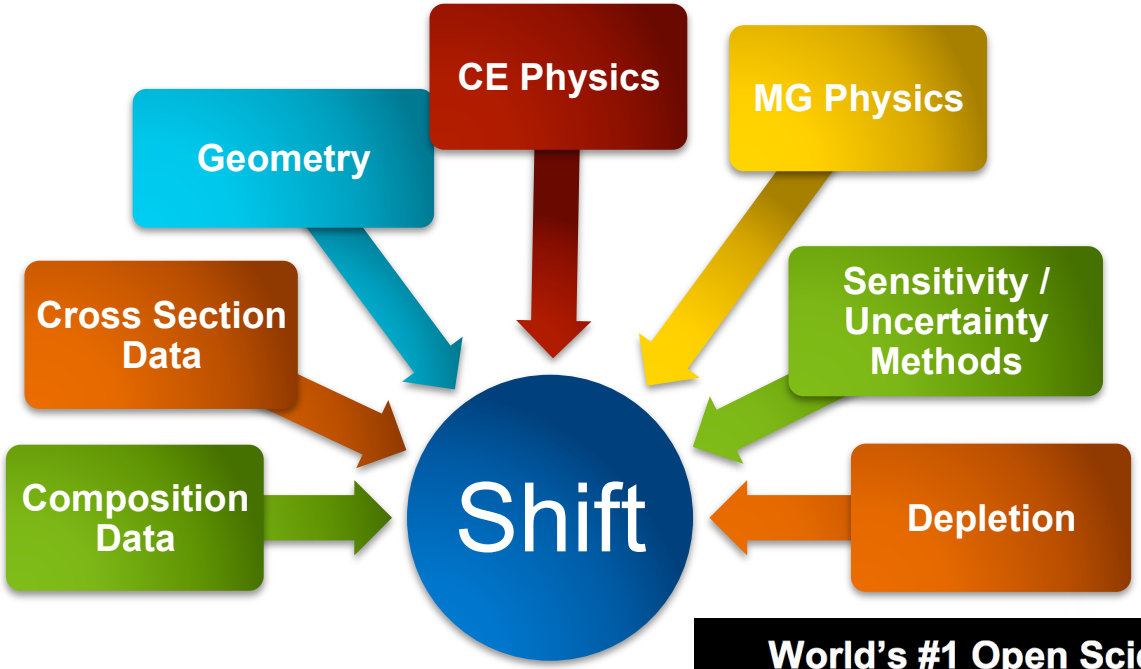
Application of Enhanced KENO

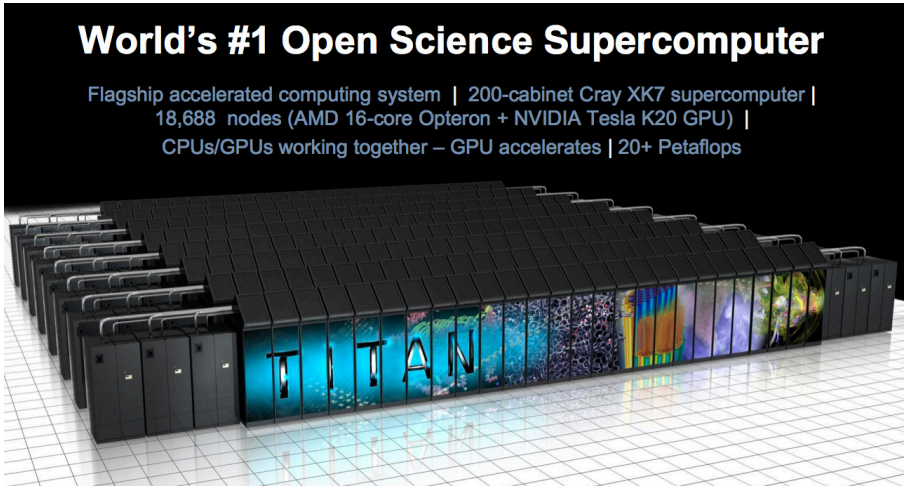
- High-fidelity AP-1000 startup calculations in conjunction with Westinghouse and CASL
  - Each axial region of each pin is unique region for tallies
  - Reference solution for power distribution
  - Auto-generated 8,000,000 line input
  - 688,000 units
  - 50 billion total particles
  - 180 processors
  - 10 days on wall clock
  - Max uncert. 3.4%
  - Credit: Andrew Godfrey



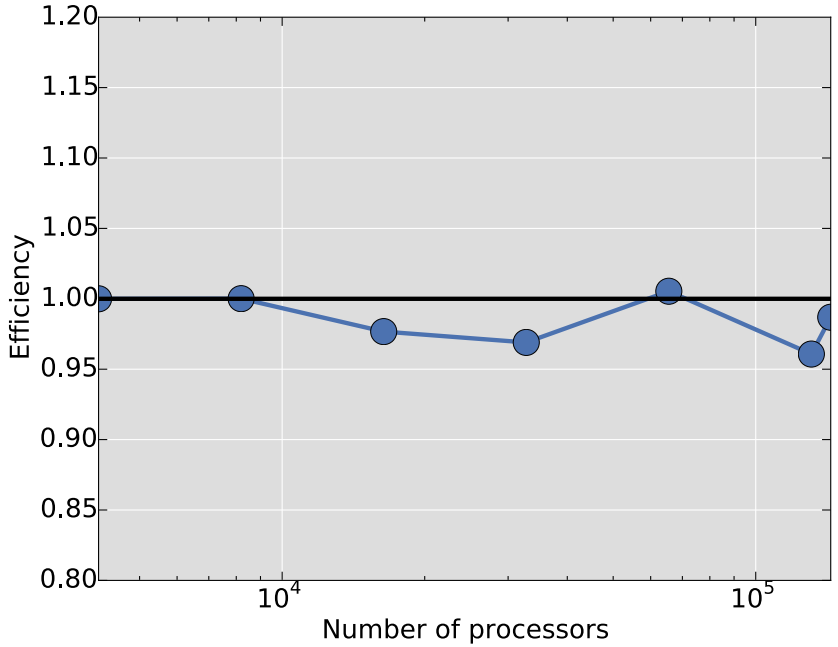
Modular Capabilities Integrated for High-Performance Computing

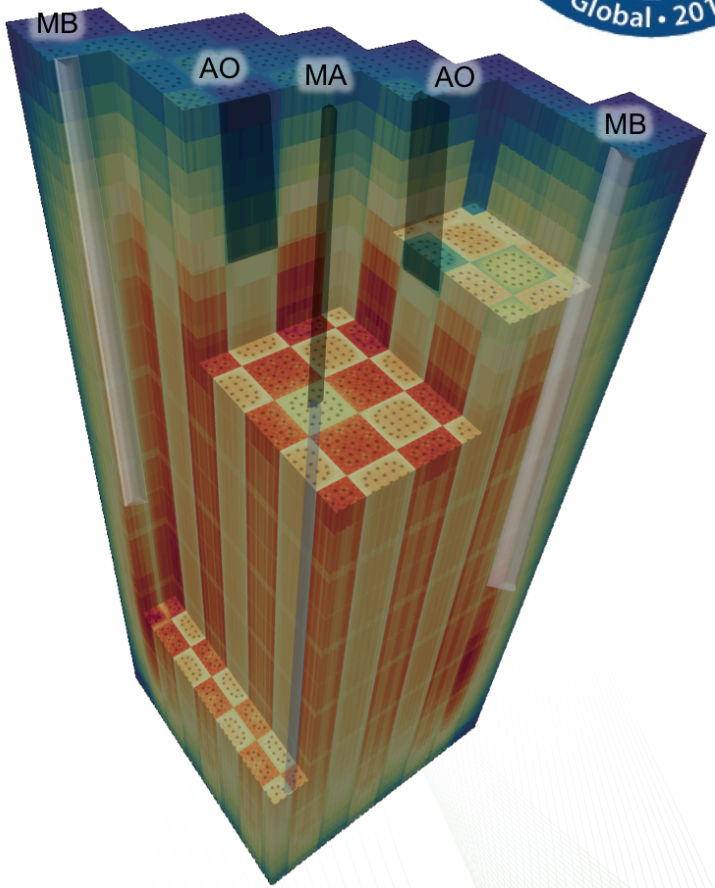
Future SCALE Monte Carlo Code - Shift





Shift Early Science – AP1000©





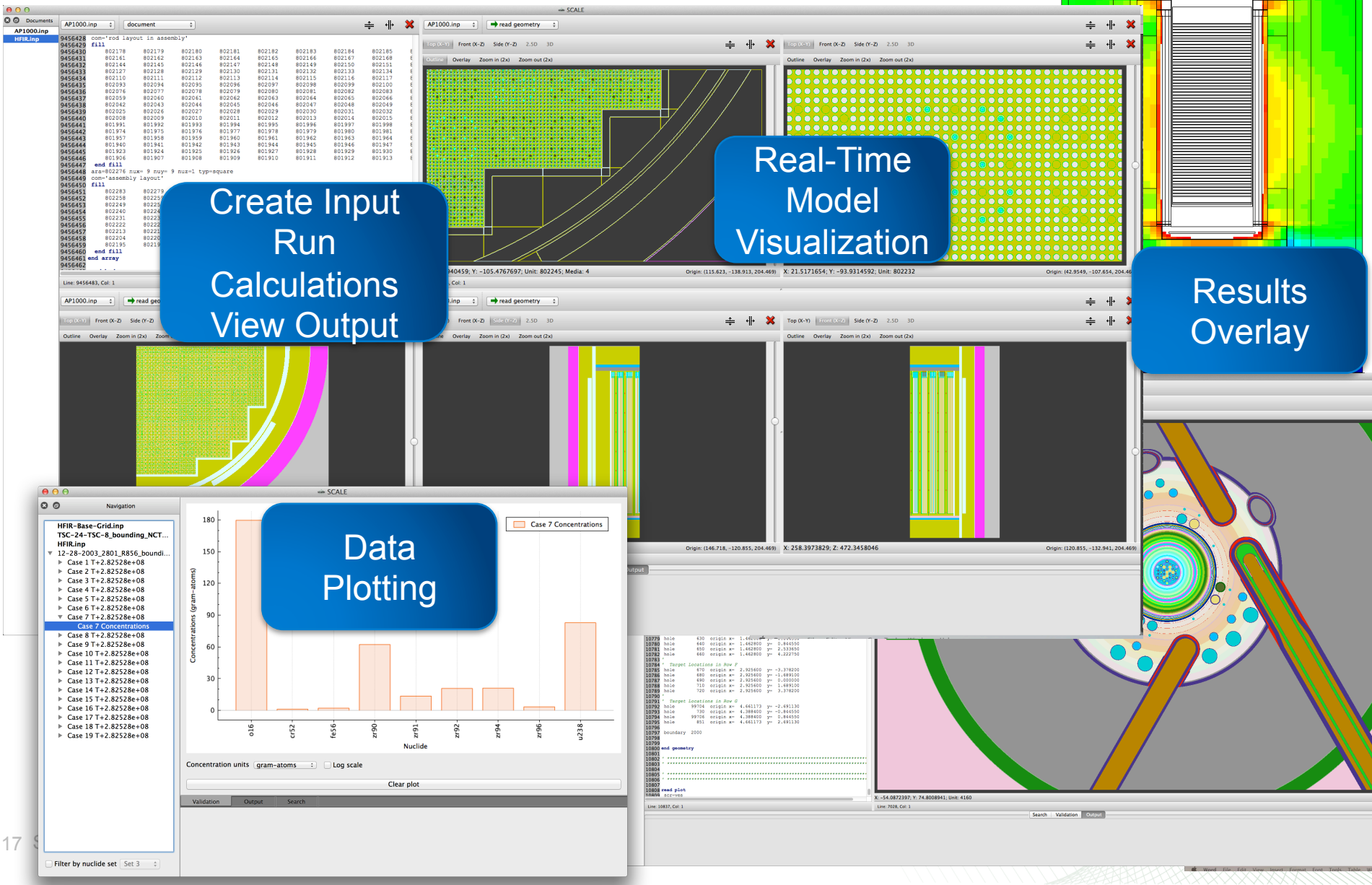
Early science modeling of AP1000©

- 10^{12} particle histories
- 232 000 cores (TITAN)
- pin-by-pin power (49 axial levels)
- ~4 hour wall-time (25 MCPU-Hours)

Shift is being integrated to run from SCA

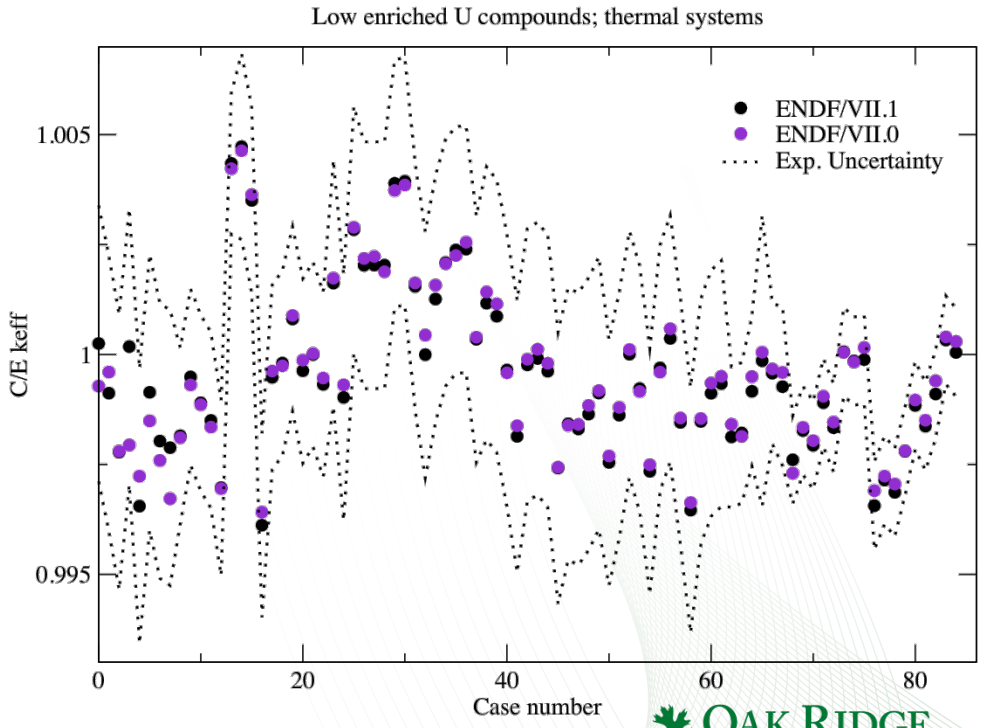
OAK RIDGE National Laboratory

Fulcrum –
Emerging Integrated Interface
"SCALE Workbench"



New Data Libraries

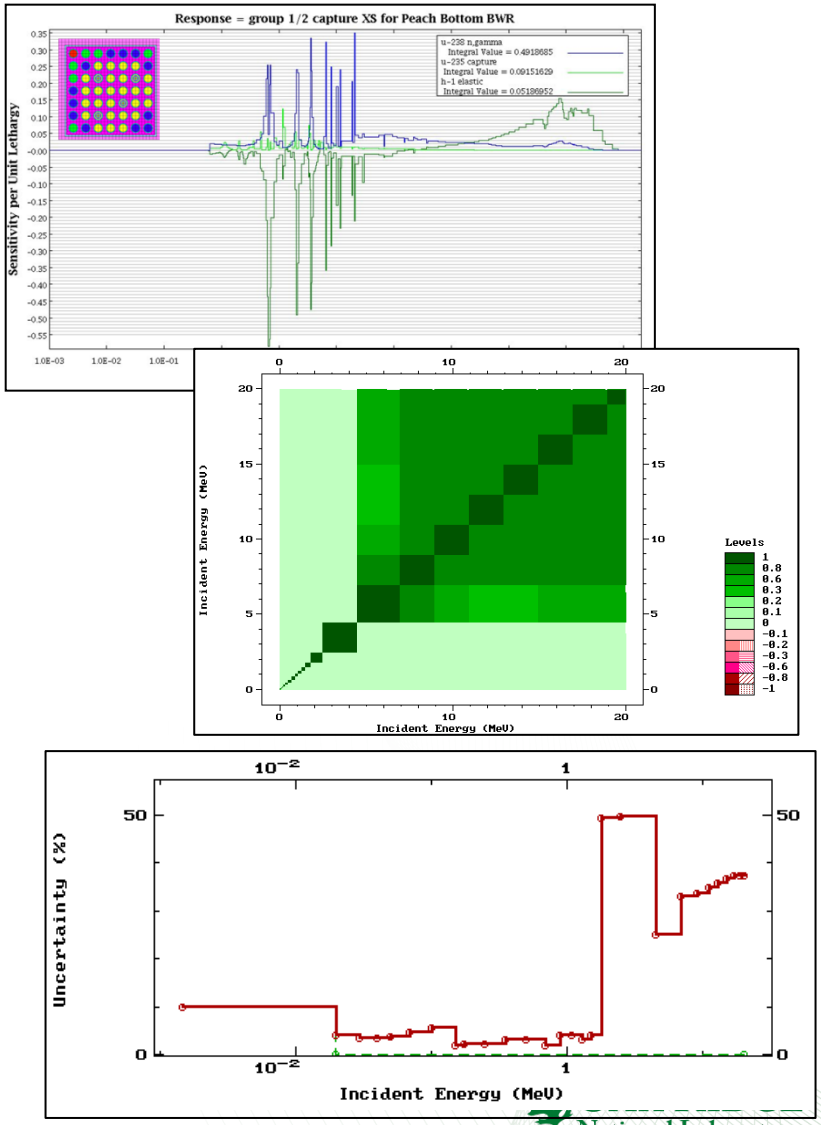
- New CE cross-section data for neutron interactions, gamma yield, and gamma interactions (sponsored by NRC)
- New MG neutron libraries
  - Provides parameters for intermediate resonance approximation for rapid resonance self-shielding techniques
  - 252-group energy structure (sponsored by NRC)
  - 56-group energy structure (sponsored by NRC and DOE NE)
- Extensive test suite
  - 381 VALID benchmarks
  - 6300 transmission tests
  - 5000 infinite medium tests
- ENDF/B-VII.0 libraries released with SCALE 6.2 Beta1-3
- ENDF/B-VII.1 libraries will also be included in Beta4



OAK RIDGE National Laboratory

Sensitivity and Uncertainty Enhancements

- New cross section covariance library based on ENDF/B-VII.1 and previous SCALE 6.1 data
- Sensitivity computations with continuous-energy Monte Carlo
- New statistical sampling code “Sampler” for general UQ of Scale MG Sequences
- New fission product yield covariances
- New decay data covariances
- New gamma interaction covariances



SCALE 6.0–6.1 Covariance Library (401 materials)

Data Source	Materials
ENDF/B-VII.0	$^{152,154\text{-}158,160}$Gd, ^{191,193}Ir, ^{7}Li, ^{99}Tc, ^{232}Th
ENDF/B-VII-p	^{197}Au, ^{209}Bi, ^{59}Co, ^{23}Na, ^{93}Nb, ^{58}Ni, ^{239}Pu, ^{48}Ti, ^{233,235,238}U*, V
ENDF/B-VI	^{27}Al, ^{241}Am, C, C-graphite, $^{50,52\text{-}54}$Cr, ^{65}Cu, ^{156}Dy, $^{54,56\text{-}58}$Fe, In, ^{55}Mn, $^{60\text{-}62,64}$Ni, $^{206\text{-}208}$Pb, ^{242}Pu, ^{185,187}Re, ^{45}Sc, Si, $^{28\text{-}30}$Si, ^{89}Y
JENDL 3.3	^{11}B, ^{240,241}Pu
JENDL 3.3+BLO	^{16}O
SG-26	^{234,236}U, ^{242,242m}Am, $^{242\text{-}245}$Cm, ^{237}Np, ^{238}Pu
BLO LANL evaluation +JENDL 3.3	^{10}B, ^{1}H, H-ZrH, H-poly, Hfreegas
BLO LANL evaluation	^{6}Li
BLO Approximate Data	$^{225\text{-}227}$Ac, ^{107,109,110m,111}Ag, ^{243,244,244m}Am, ^{36,38,40}Ar, $^{74\text{-}75}$As, $^{130,132,133,135\text{-}138,140}$Ba, ^{7,9}Be, Bebound, ^{249,250}Bk, ^{79,81}Br, Ca, $^{40,42\text{-}44,46,48}$Ca, Cd, $^{106,108,110\text{-}114,115m,116}$Cd, $^{136,138,139\text{-}144}$Ce, $^{249\text{-}254}$Cf, Cl, ^{35,37}Cl, $^{241,246\text{-}250}$Cm, ^{58,58m}Co, $^{133\text{-}137}$Cs, ^{63}Cu, $^{158,160\text{-}164}$Dy, $^{162,64,166\text{-}168,170}$Er, $^{253\text{-}255}$Es, $^{151\text{-}157}$Eu, ^{19}F, ^{255}Fm, Ga, ^{69,71}Ga, ^{153}Gd, $^{70,72\text{-}74,76}$Ge, ^{2,3}H, Dfreegas, ^{3,4}He, Hf, $^{174,176\text{-}180}$Hf, $^{196,198\text{-}202,204}$Hg, ^{165}Ho, $^{127,129\text{-}131,135}$I, ^{113,115}In, K, $^{39\text{-}41}$K, $^{78,80,82\text{-}86}$Kr, $^{138\text{-}140}$La, ^{175,176}Lu, Mg, $^{24\text{-}26}$Mg, Mo, $^{92,97\text{-}100}$Mo, ^{14,15}N, ^{94,95}Nb, $^{142\text{-}148,150}$Nd, ^{59}Ni, ^{235,236,238,239}Np, ^{17}O, ^{31}P, $^{231\text{-}233}$Pa, ^{204}Pb, $^{102,104\text{-}108,110}$Pd, ^{147,148,148m,149,151}Pm, $^{141\text{-}143}$Pr, ^{236,237,243,244,246}Pu, $^{85\text{-}87}$Rb, ^{103,105}Rh, $^{96,98\text{-}106}$Ru, S, $^{32\text{-}34,36}$S, $^{121,123\text{-}126}$Sb, $^{74,76\text{-}80,82}$Se, $^{144,147\text{-}154}$Sm, $^{112\text{-}120,122\text{-}125}$Sn, $^{84,86\text{-}90}$Sr, ^{181,182}Ta, ^{159,160}Tb, $^{120,122\text{-}126,127m,128,129m,130}$Te, $^{227\text{-}230,233,234}$Th, Ti, ^{46,47,49,50}Ti, $^{232,237,239\text{-}241}$U, W, $^{182\text{-}184,186}$W, $^{123,124,126,128\text{-}136}$Xe, ^{90,91}Y, Zr, $^{90\text{-}96}$Zr

ENDF/B-VII.0: evaluated covariance data released with ENDF/B-VII.0

ENDF/B-VII-p: recently evaluated data proposed for future release of ENDF/B-VII.1

ENDF/B-VI: evaluated covariance data released with ENDF/B-VI

JENDL-3.3: evaluated covariance data in JENDL-3.3

BLO approximate data: lo-fi covariances from BLO project (**B**rookhaven, **L**os Alamos, **O**RNL)

BLO LANL evaluation: LANL R-matrix evaluation from BLO project

* ^{235}U thermal nubar data from JENDL-3.3

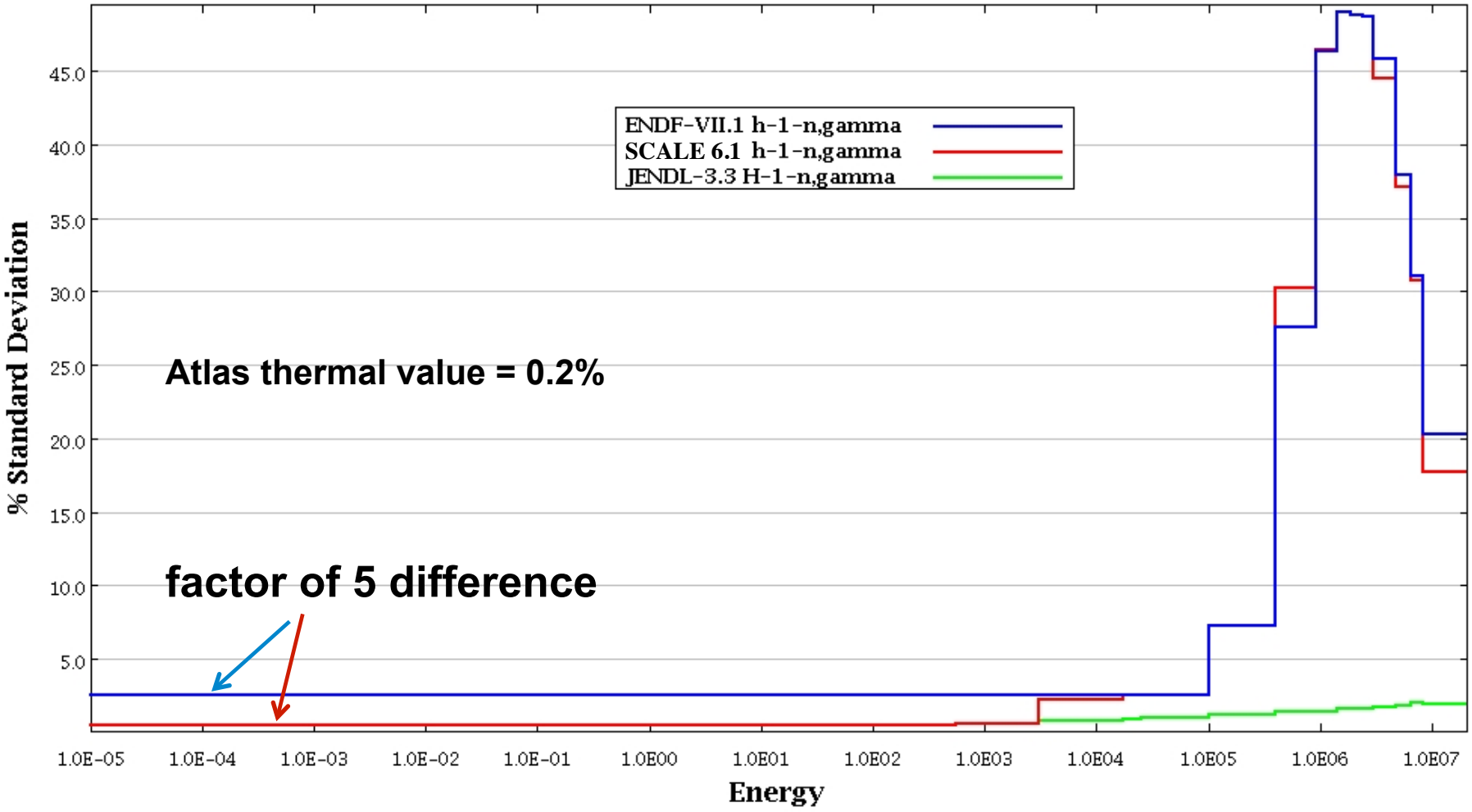
SG-26: approximate covariances from WPEC Subgroup-26

ENDF/B-VII.1 Neutron Covariance Nuclides

h1	ti50	tc99	sm151	pb204	np235	bk245	h-zr2
h2	cr50	ru101	sm152	pb206	np236	bk246	o-beo
he4	cr52	ru102	eu153	pb207	np237	bk247	o-u2o
li6	cr53	ru103	eu155	pb208	np238	bk248	si28_si2o
li7	cr54	ru104	gd152	bi209	np239	bk249	si29_si2o
be9	mn55	ru106	gd153	ac225	pu236	bk250	si30_si2o
b10	fe54	rh103	gd154	ac226	pu237	cf246	u235_u2o
b11	fe56	pd105	gd155	ac227	pu238	cf248	zr90_zr_zrh
c	fe57	pd106	gd156	th227	pu239	cf249	zr91_zr_zrh
n15	co59	pd107	gd157	th228	pu240	cf250	zr92_zr_zrh
o16	ni58	pd108	gd158	th229	pu241	cf251	zr93_zr_zrh
f19	ni60	ag109	gd160	th230	pu242	cf252	zr94_zr_zrh
na23	y89	i127	er166	th231	pu244	cf253	zr95_zr_zrh
mg24	zr90	i129	er167	th232	pu246	cf254	zr96_zr_zrh
mg25	zr91	xe131	er168	th233	am240	es251	h-benzene
mg26	zr92	xe132	er170	th234	am241	es252	benzene
al27	zr93	xe134	tm169	pa229	am242m1	es253	graphite
si28	zr94	cs133	tm170	pa230	am243	es254	h-liquid_ch4
si29	zr95	cs135	w180	pa232	cm240	es254m1	d-cryo_ortho
si30	zr96	la	w182	u230	cm241	es255	h-cryo_ortho
cl35	nb95	ce141	w183	u231	cm242	fm255	d-cryo_para
cl37	mo92	pr141	w184	u232	cm243	al_thermal	h-cryo_para
k39	mo94	nd143	w186	u233	cm244	fe_thermal	h-solid_ch4
k41	mo95	nd145	ir191	u234	cm245	bebound	
ti46	mo96	nd146	ir193	u235	cm246	be-beo	
ti47	mo97	nd148	au197	u236	cm247	h-h2o	
ti58	mo98	pm147	tl203	u238	cm249	d-d20	
ti49	mo100	sm149	tl205	np234	cm250	h-poly	

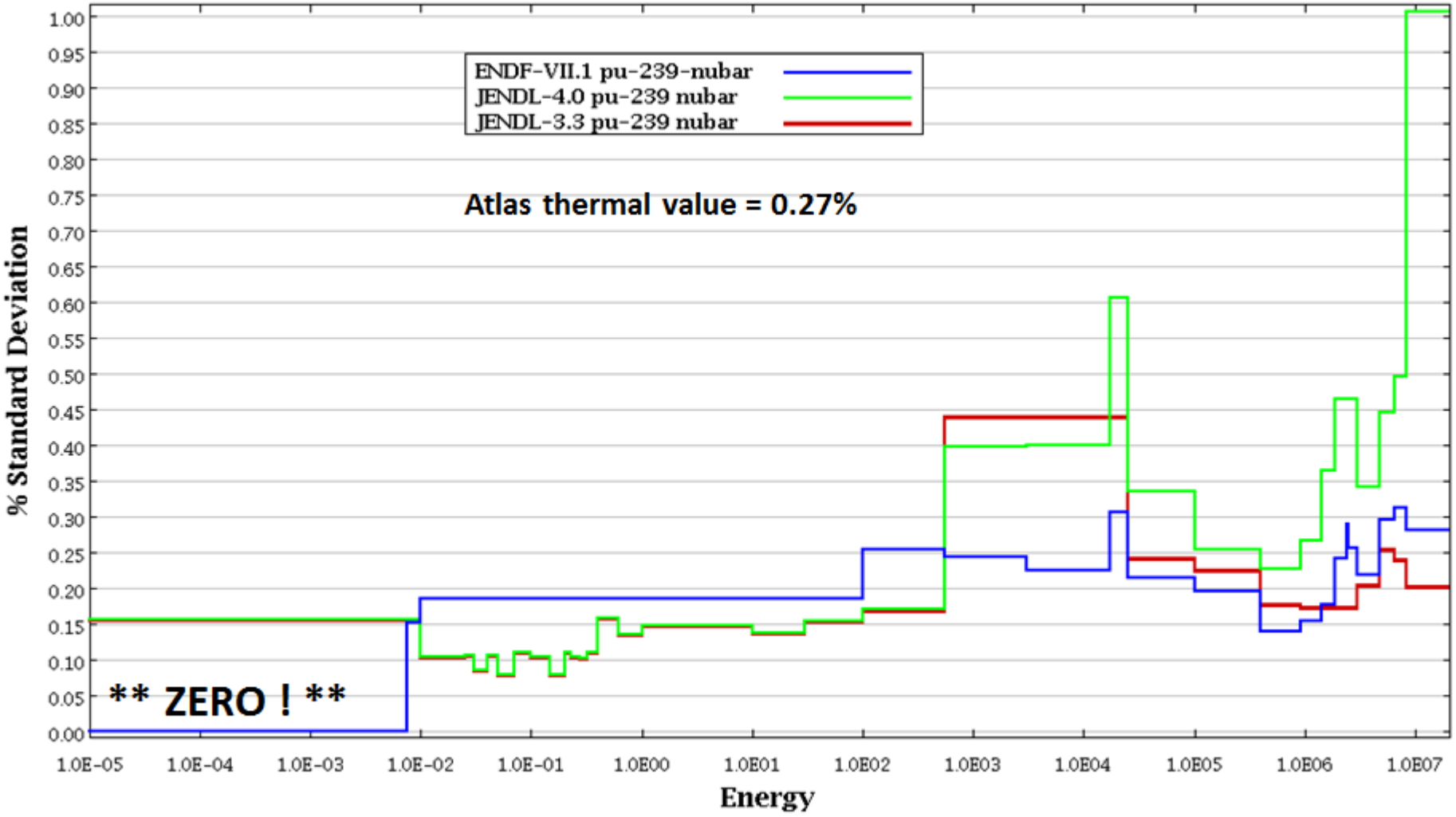
OAK RIDGE National Laboratory

H Capture Uncertainty



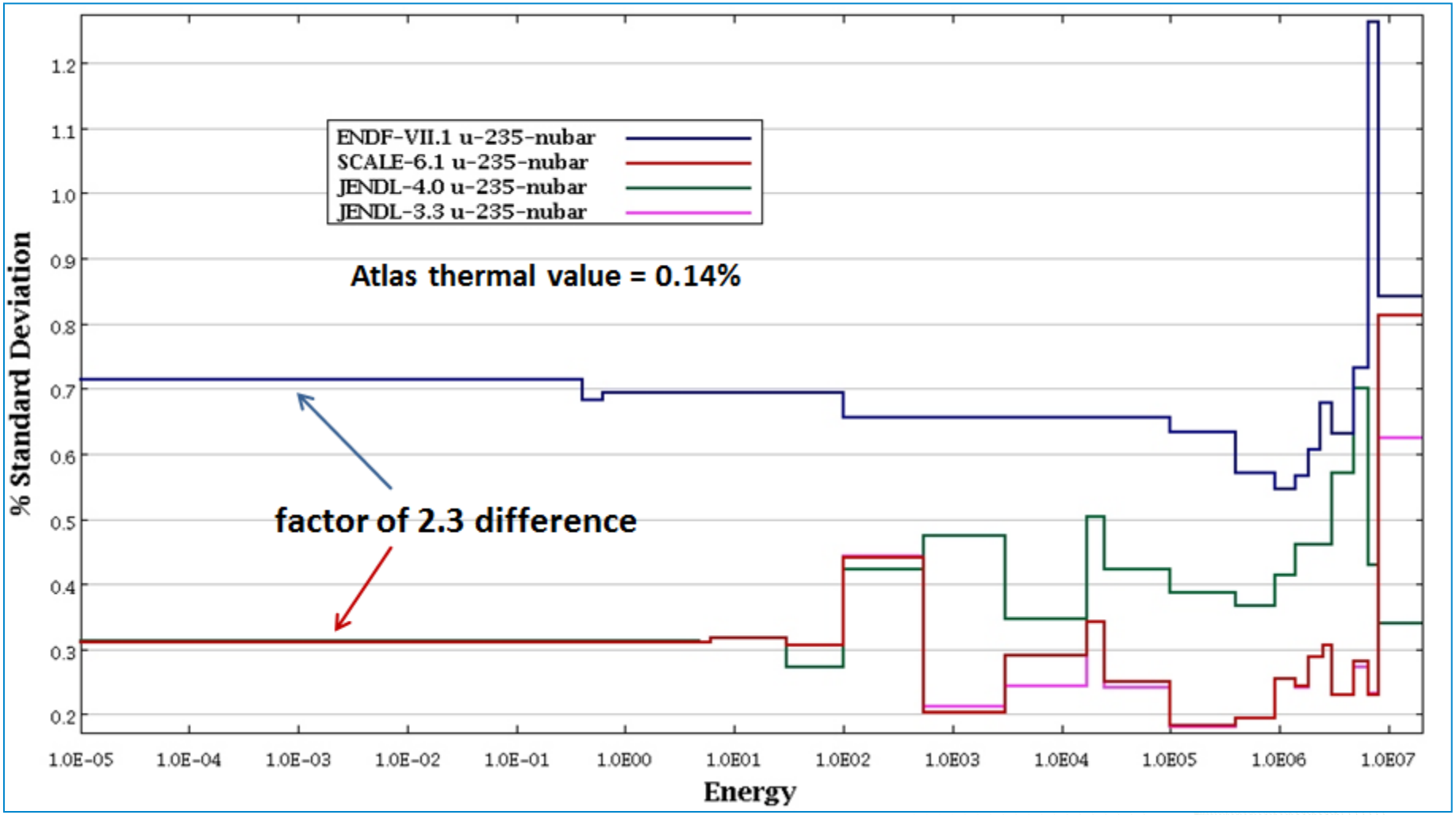
OAK RIDGE National Laboratory

Pu-239 nubar uncertainty



OAK RIDGE National Laboratory

U-235 nubar uncertainty



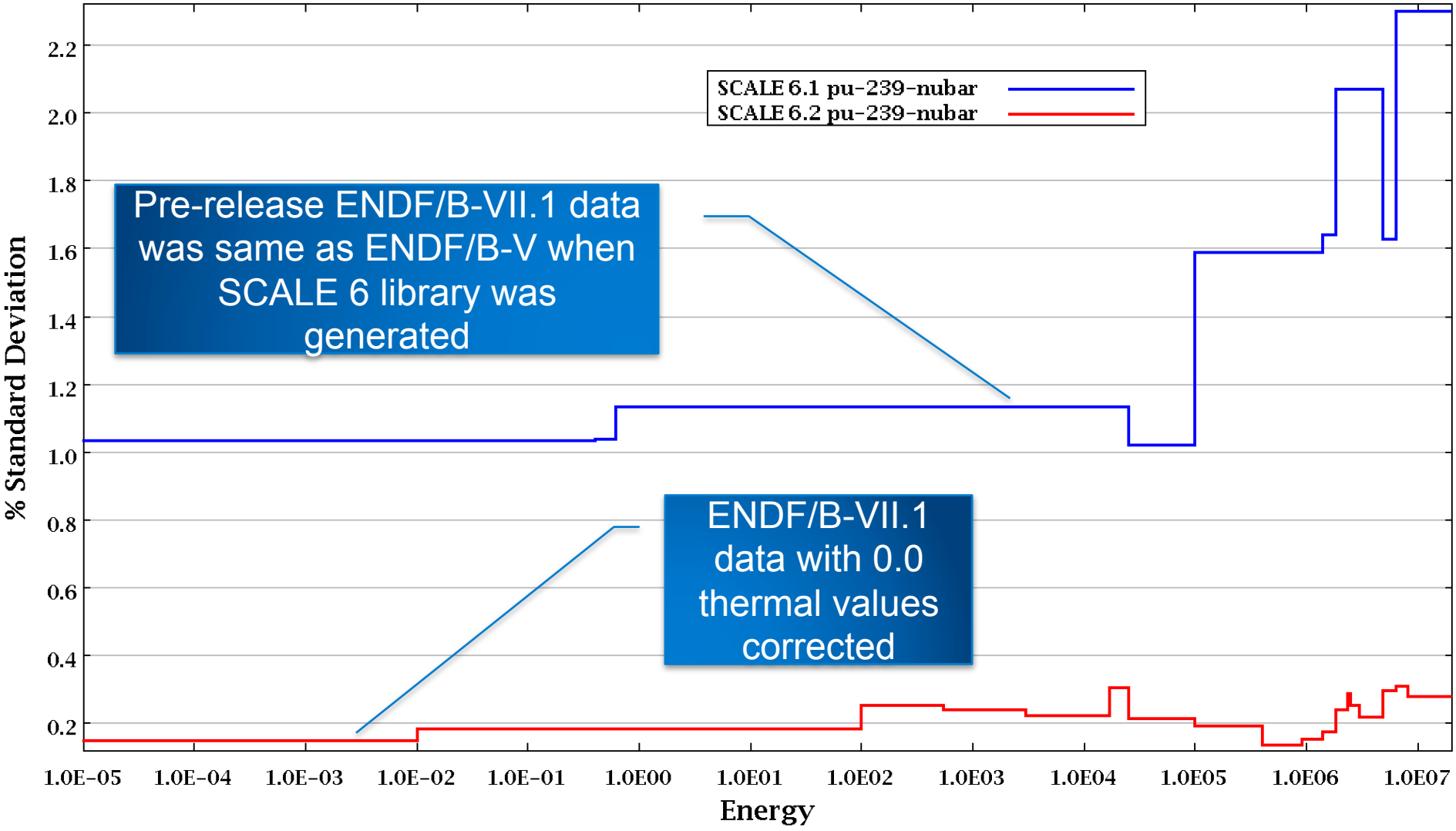
OAK RIDGE National Laboratory

SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes;
- SCALE 6.1 data retained for ~215 missing nuclides
  - SCALE 6.1 includes covariance data from ENDF/B-VII.0, pre-released ENDF/VII.1, Lo-Fi uncertainties from BNL-LANL-ORNL, and other sources
- Modified ENDF/B-VII.1 ^{239}Pu nubar and H capture uncertainties
- ENDF/B-VII.1 ^{235}U nubar covariance replaced by SCALE 6.1 covariance
- Chi uncertainties processed from new ENDF/B-VII.1 file 35
  - Previous SCALE chi uncertainties were generated from Watt spectrum data
- ****SCALE 6.2 covariances similar to SCALE 6.1 for many nuclides*

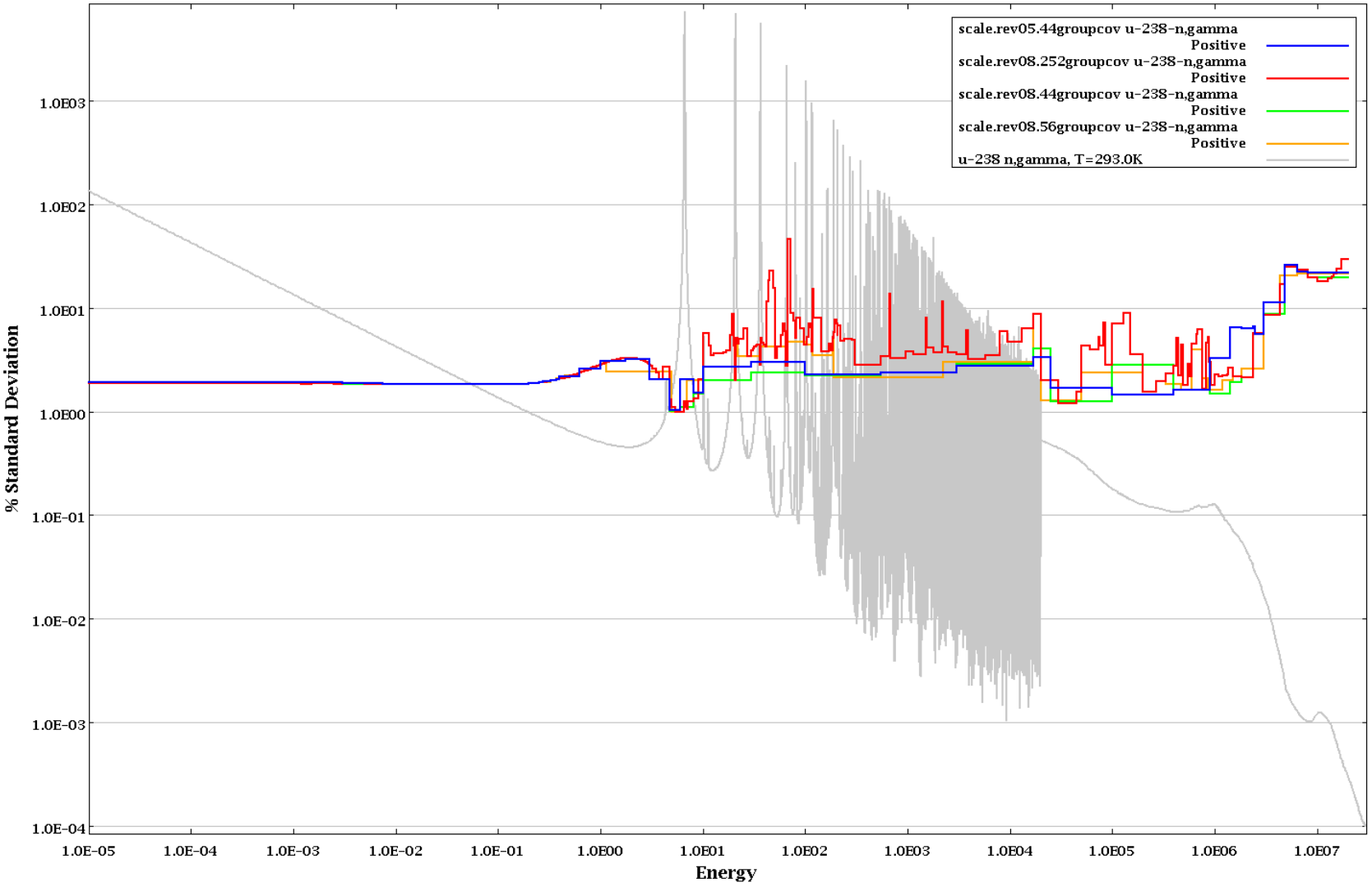
OAK RIDGE National Laboratory

Pu-239 nubar uncertainty



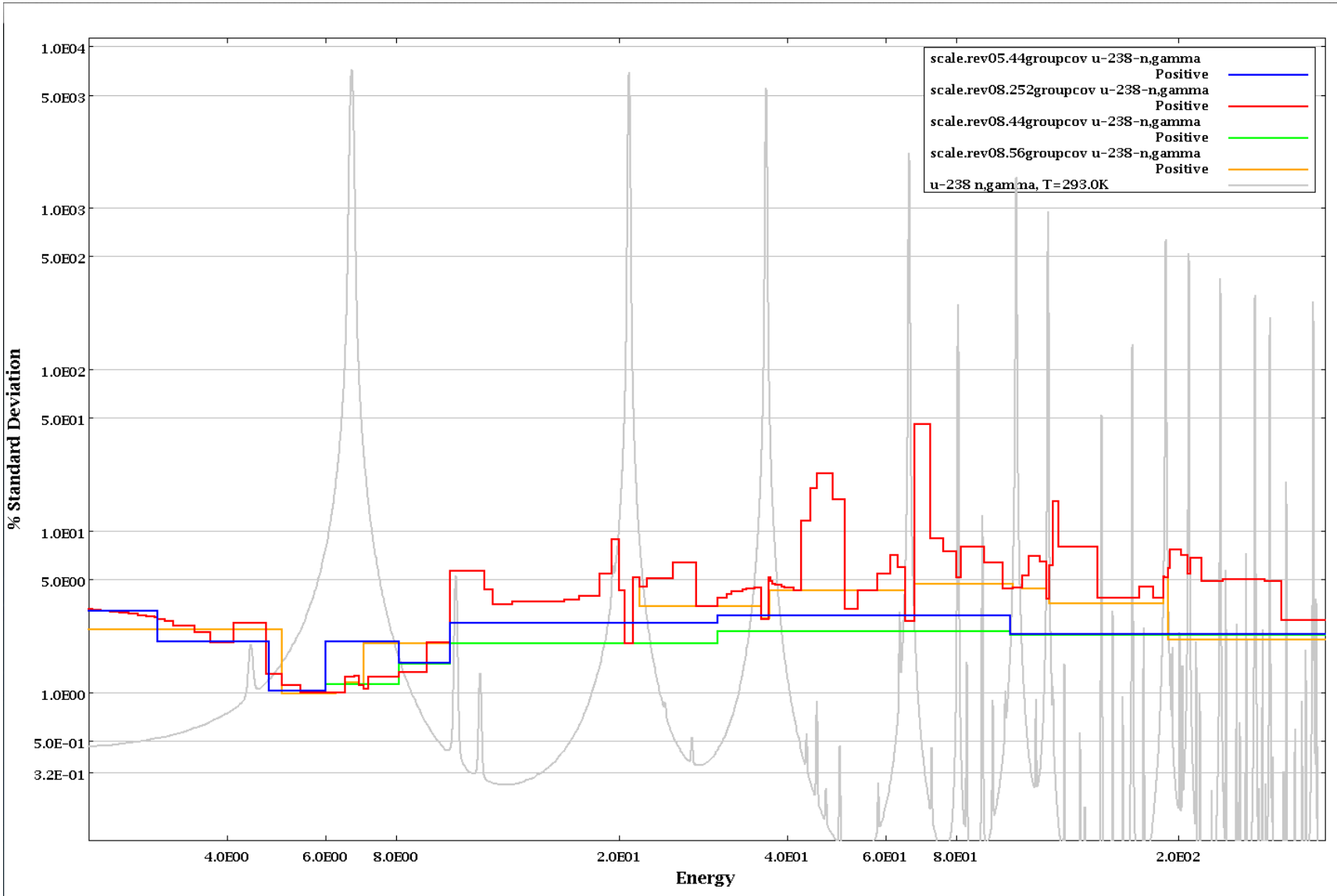
OAK RIDGE National Laboratory

Three covariance group structures investigated: 44, 56, and 252 - U-238 n,gamma shown



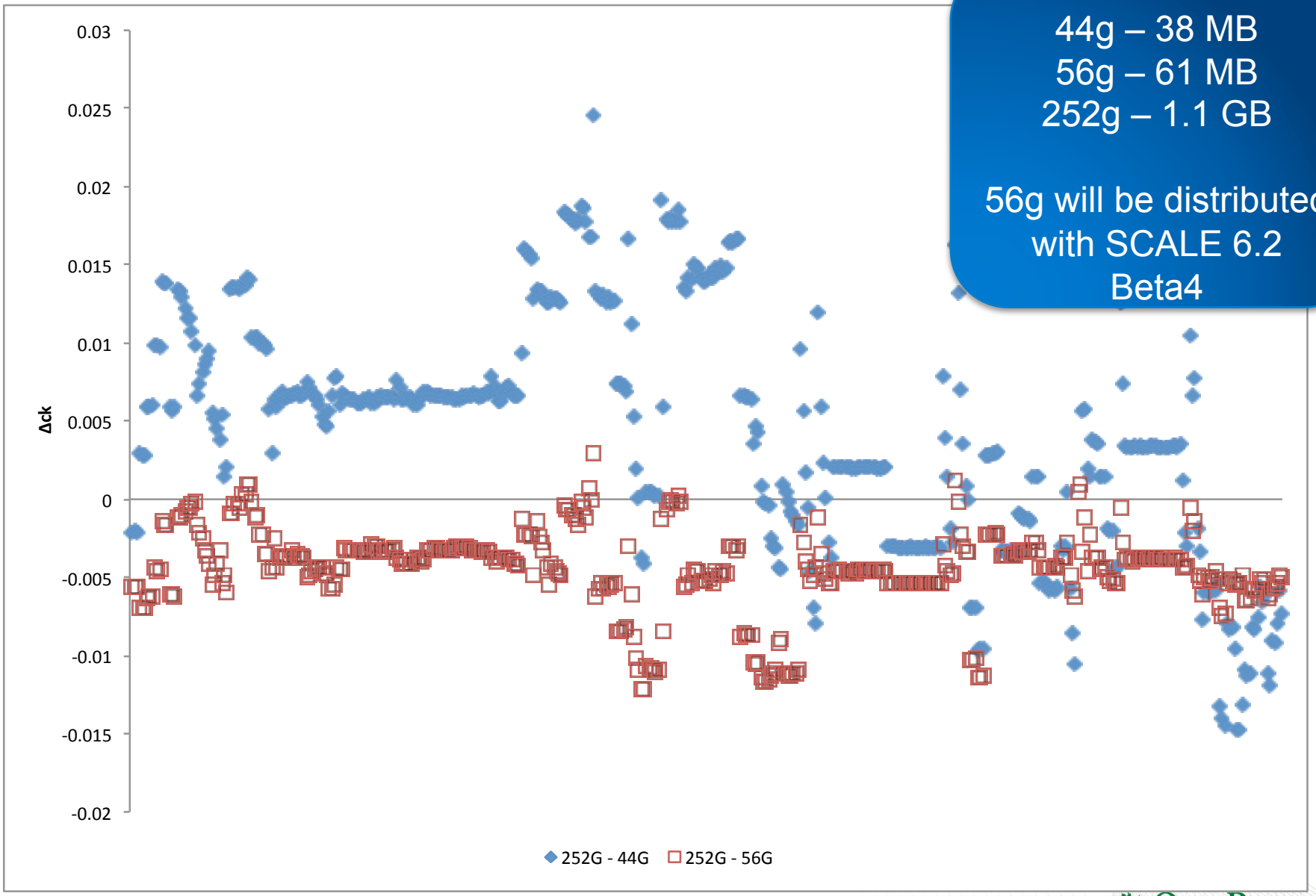
OAK RIDGE National Laboratory

44, 56, and 252 group structures U-238 n,gamma



National Laboratory

Impact of Group Structures



File sizes:
44g – 38 MB
56g – 61 MB
252g – 1.1 GB

56g will be distributed with SCALE 6.2 Beta4

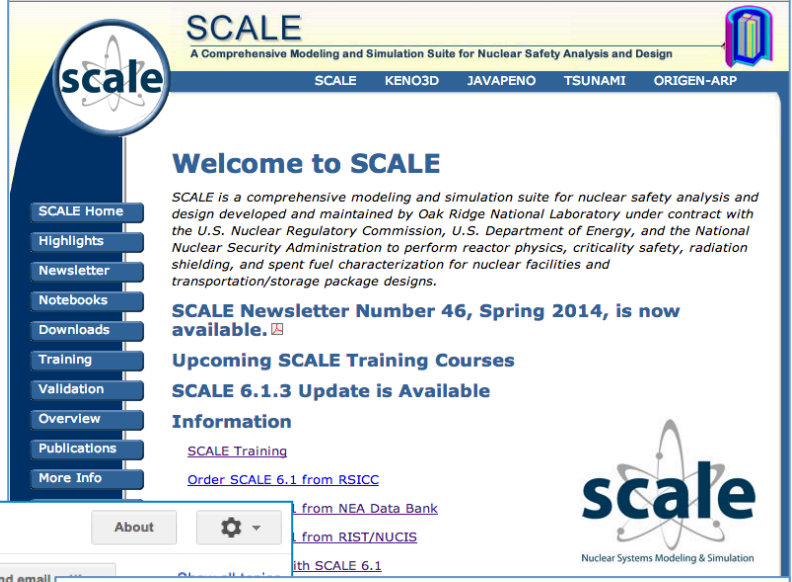
OAK RIDGE National Laboratory

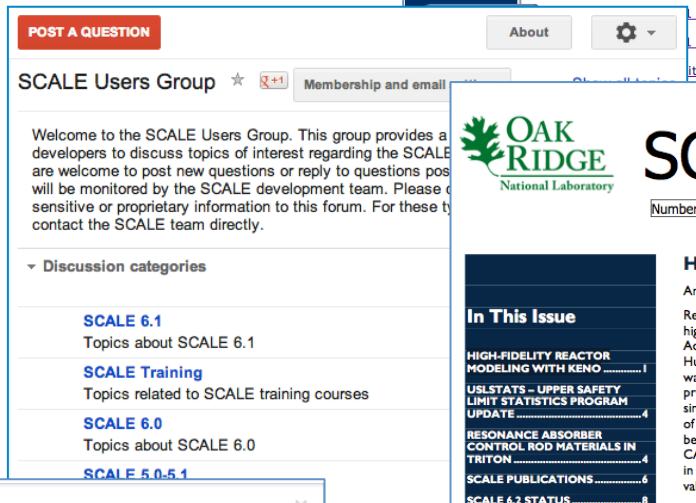
SCALE Training

- Hands-on training courses and workshops presented at
  - ORNL
  - OECD/NEA Data Bank in Paris
  - NRC Headquarters, conference venues, and user facilities
- FY14 Statistics:
  - 14 week-long courses
  - 2 conference tutorials
  - 233 participants from 24 nations

More Information

- SCALE Website (scale.ornl.gov)
  - Publications/Training
  - Validation and benchmark reports
  - Downloads
- SCALE Newsletter
- SCALE Users Group forum
- On-demand assistance
  - scalehelp@ornl.gov
- Facebook page
  - facebook.com/scale.codes



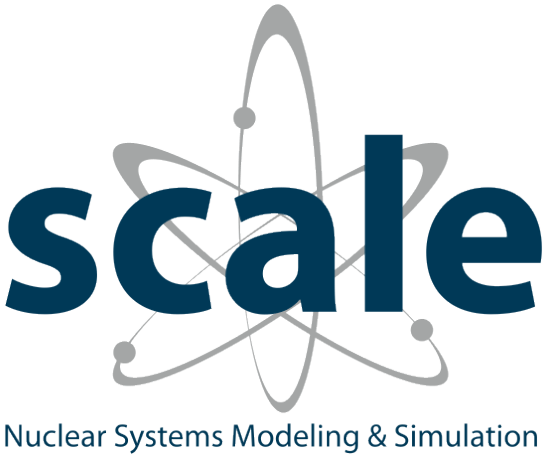


Conclusions

- SCALE has been continuously developed and deployed since 1980 and is relied on by 6200 users in 54 nations for nuclear safety analysis and design, regulation, and research
- SCALE modernization provides improved performance, accelerated integration of new features, and a solid physics foundation for advanced high-performance computing
- Consolidation of SCALE / AMPX development and deployment processes provides cross-section generation capabilities for external users and improves efficiency of development process

OAK RIDGE National Laboratory

Questions?



Brad Rearden

Manager, SCALE Code System

reardenb@ornl.gov