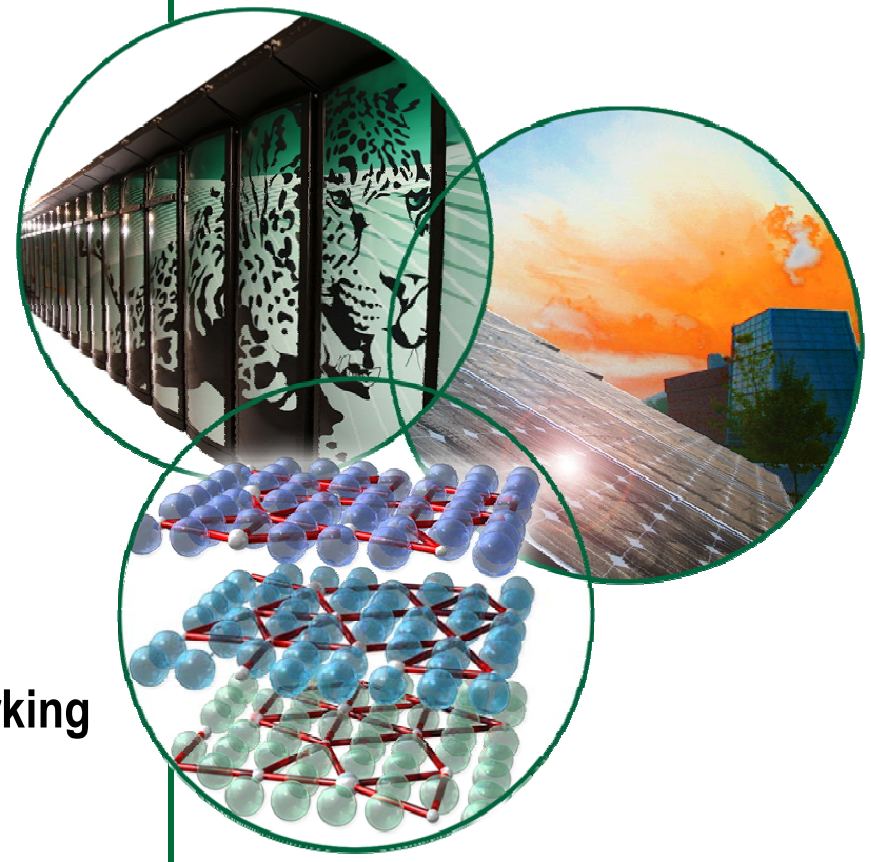
Use of Cross-Section Uncertainty Data in Scale 6.1 Validation Studies



Presenter: Michael Dunn

Contributors: W.J. Marshall, B.T. Rearden

Oak Ridge National Laboratory

DOE/NE Fuel Cycle R&D Nuclear Physics Working Group Meeting
Nuclear Data Week
November 14-18, 2011
Brookhaven, NY

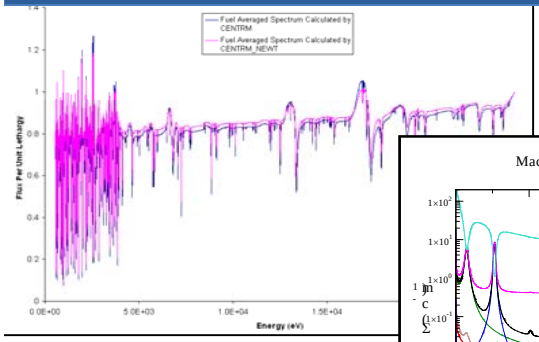
U.S. DEPARTMENT OF ENERGY

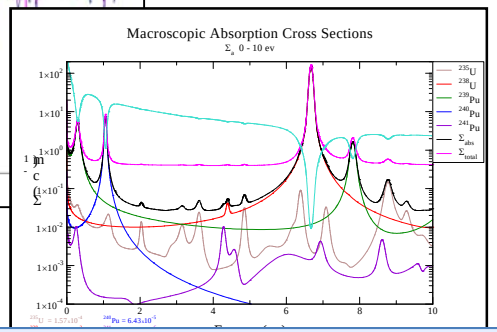
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

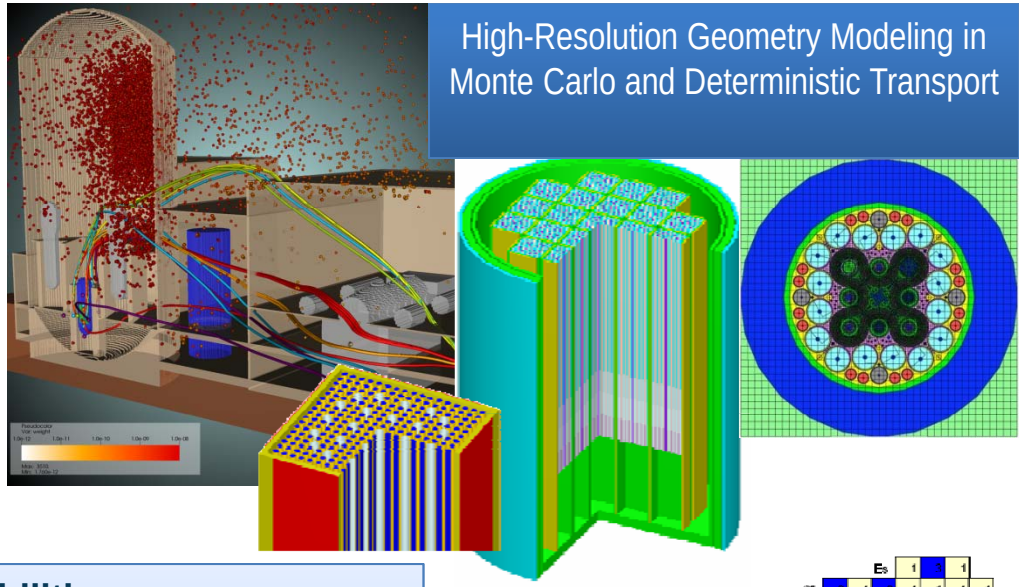
- Overview of Scale 6.1 sensitivity/uncertainty (S/U) analysis tools for validation studies
- Criticality Validation of KENO codes for Scale 6.1
- Cross section uncertainty compared to C/E values
  - Pu Metal Systems
  - Pu Solution Systems
  - MOX Lattice Systems
  - LEU Systems
  - HEU Systems
- Summary

Convenient Material Input and Current Nuclear Data with Continuous-Energy Resonance Processing





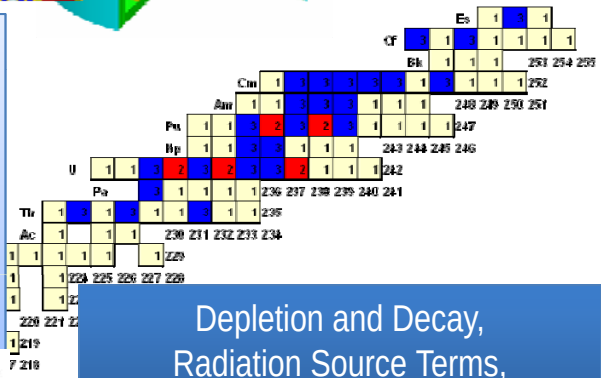
High-Resolution Geometry Modeling in Monte Carlo and Deterministic Transport



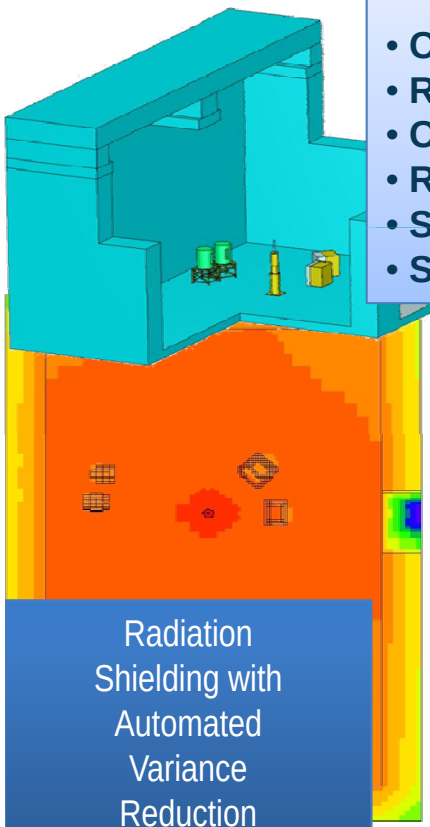
SCALE Capabilities

- Criticality safety
- Radiation shielding
- Cross-section processing
- Reactor physics
- Sensitivity and uncertainty analysis
- Spent fuel and HLW characterization

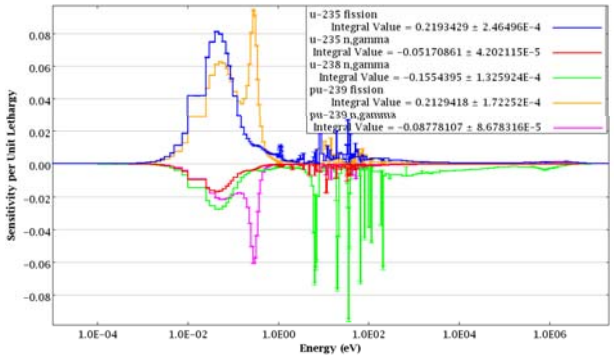
scale



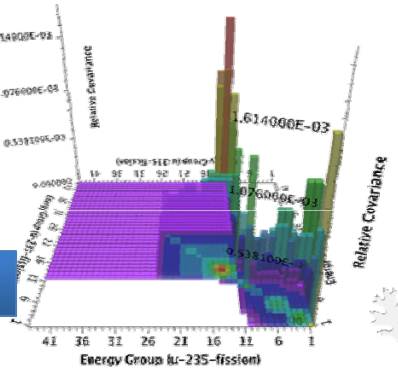
Depletion and Decay, Radiation Source Terms, and Decay Heat



Radiation Shielding with Automated Variance Reduction



Sensitivity and Uncertainty Analysis



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Computational Biases and Their Bounds

- Premise of TSUNAMI validation concept:
  - Computational biases are primarily caused by errors in the cross-section data
  - Errors are bounded by cross-section uncertainties represented in covariance data
- Uncertainties in cross sections are propagated to uncertainty in response (e.g. k_{eff}) through sensitivity coefficients
- Bias in the response should be bounded by uncertainty due to cross-section-covariance data

TSUNAMI

Tools for Sensitivity and Uncertainty Analysis Methodology Implementation

- **Produces sensitivity of responses to cross-section data.**

Scale 6.1

  - **neutron multiplication: k_{eff}**
    - **1D (XSDRNPM), 2D (NEWT), 3D (KENO)**
  - **reactivity: ρ**
    - **TSAR post-processing from 2 eigenvalue calculations (1D, 2D, or 3D)**
  - **generalized responses: fluxes, reaction rates, few group cross sections, ...**
    - **1D (XSDRNPM), 2D (NEWT)**
  - **coming soon: fixed-source responses and sources**
    - **1D (XSDRNPM), 3D (Monaco, Denovo)**
  - **coming soon: 3D GPT**
    - **Denovo**
  - **continuous-energy treatment**
    - **contributon approach**

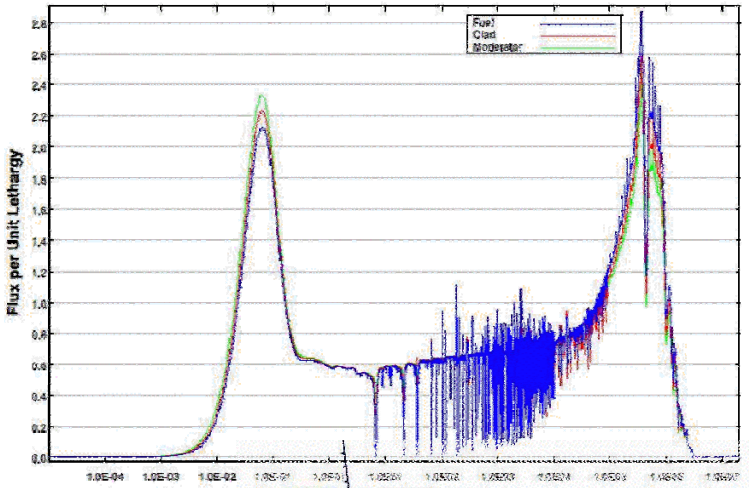
TSUNAMI Methods

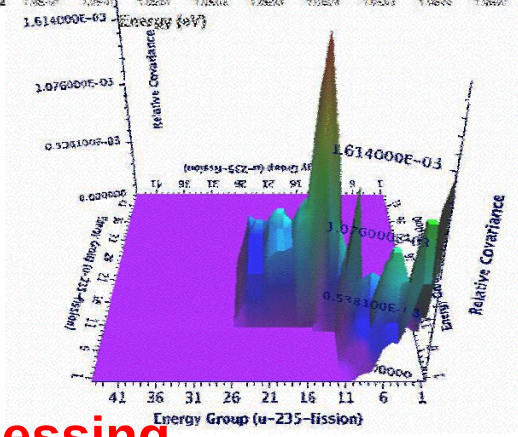
- Uses both adjoint techniques and automatic differentiation with code coupling capability to accurately compute sensitivity coefficients.
- Monte Carlo and deterministic transport sensitivity analysis tool for accurately modeling complex geometries.
- Computes uncertainty in responses due to uncertainties tabulated in cross-section-covariance data.
- Uses S/U data in code validation for system-to-system similarity quantification, bias assessment, and gap analysis.
- Customized data visualization capabilities and user-friendly GUI driven input and output.

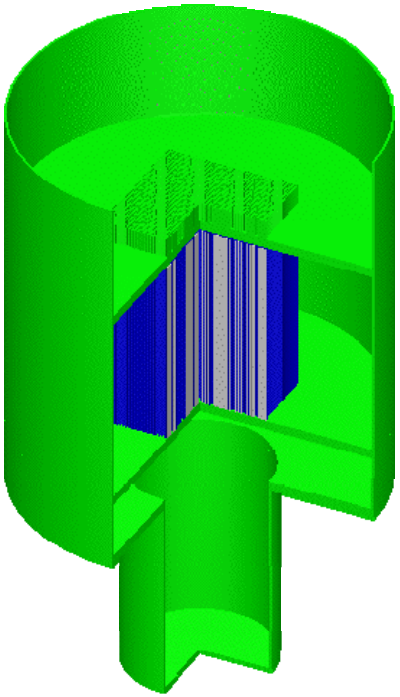
TSUNAMI-3D

Resonance Self-Shielding

Continuous energy transport and Bondarenko Factor treatment for multigroup cross-section preparation with "implicit effect", up to 40% contribution for thermal/intermediate systems

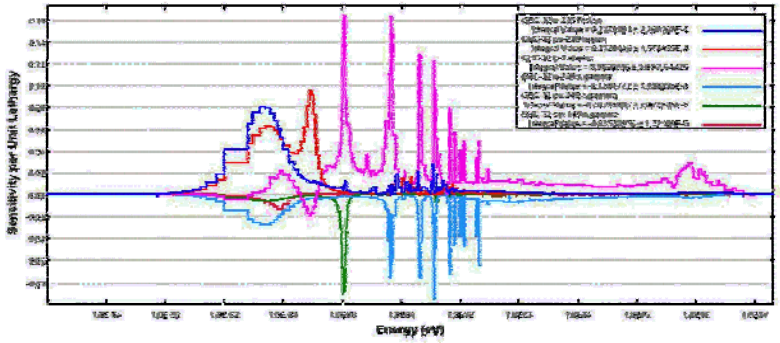






KENO V.a or KENO-VI

Forward/Adjoint multigroup Monte Carlo flux calculation with angular moments

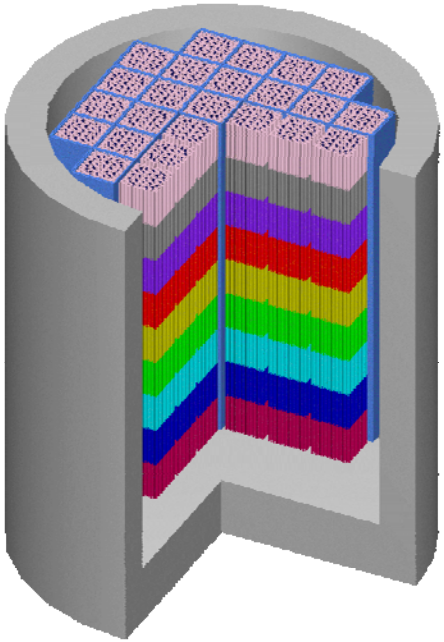


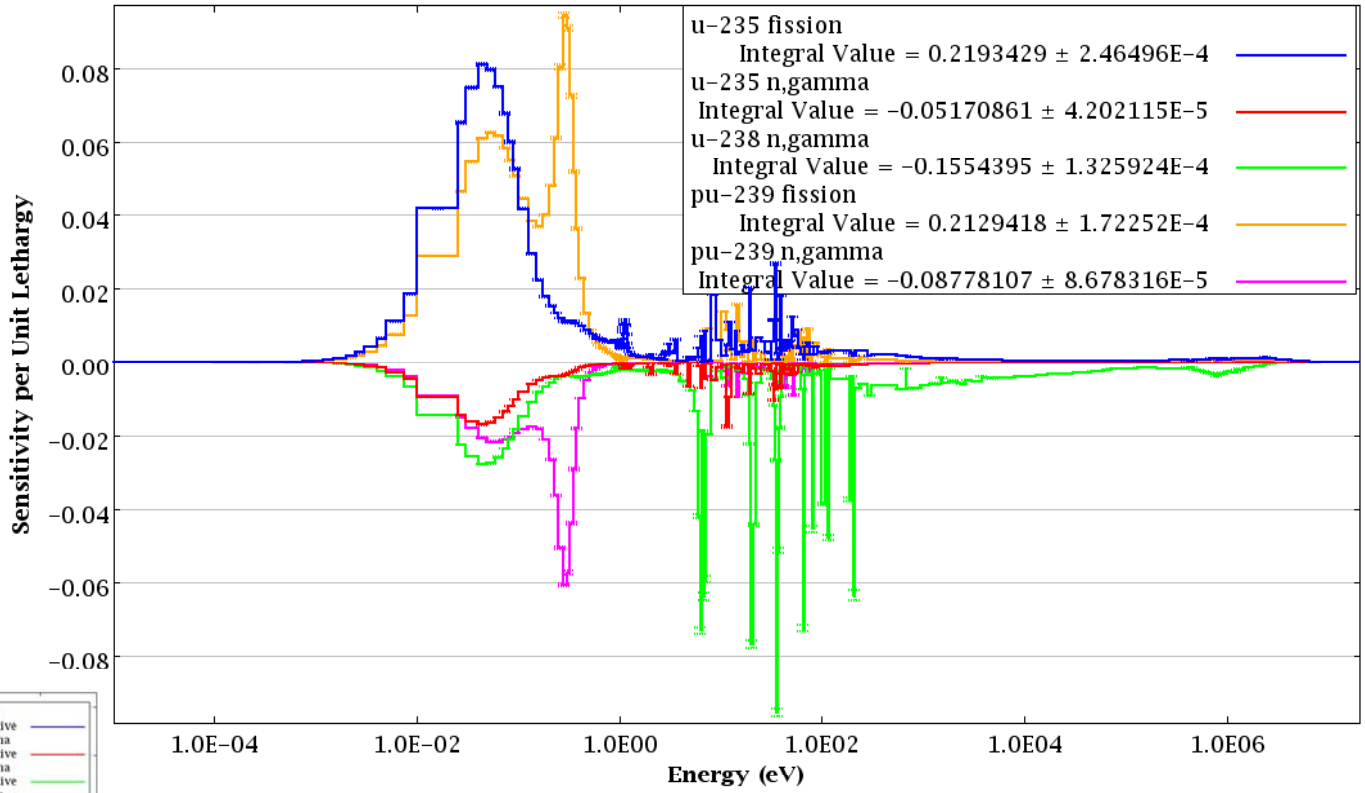
S/U Processing

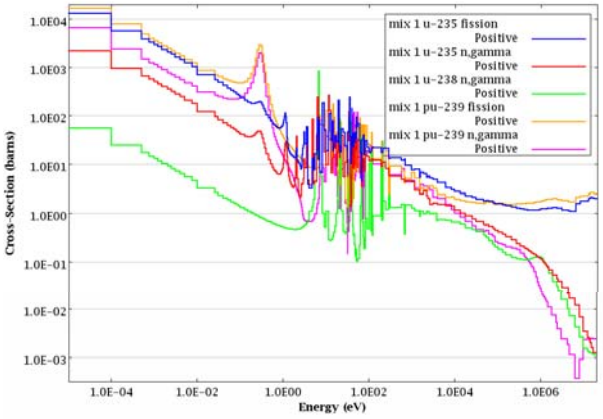
Sensitivity coefficient generation

Uncertainty propagation from cross-section covariance data to k_{eff}

Sensitivities of k_{eff} of Shipping Cask to Cross-Section Data

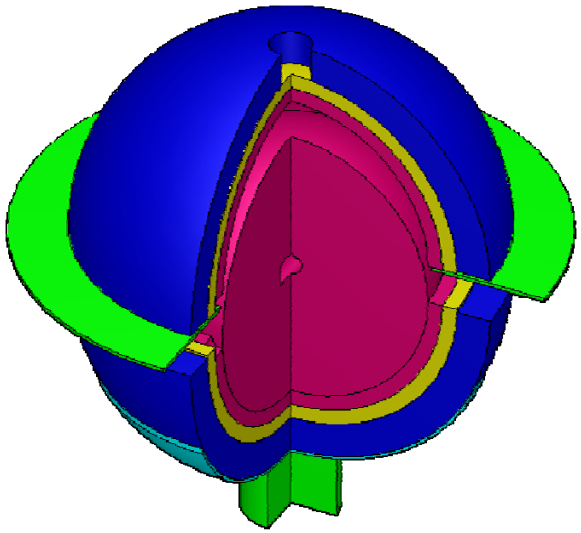


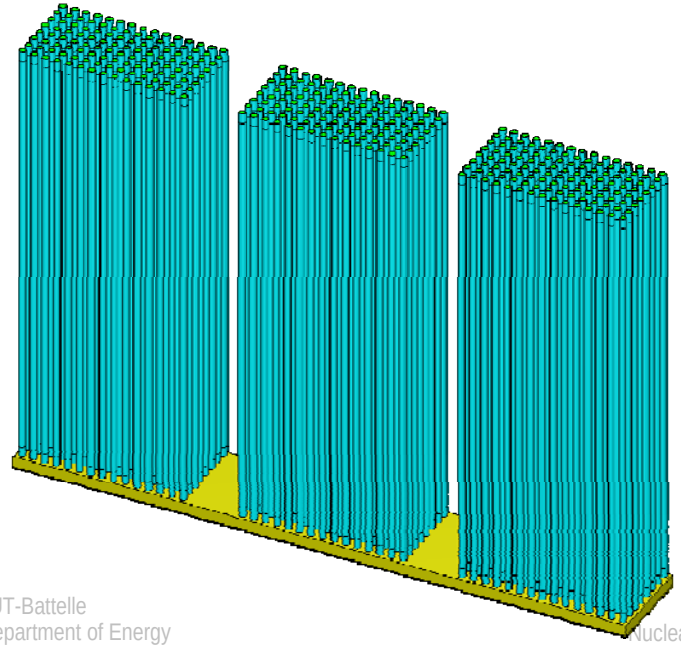




ICSBEP Sensitivity Data

- Under DOE and NRC support, ORNL provides quality-assured SCALE inputs and sensitivity data files for distribution with the ICSBEP
- Files are developed according the SCALE procedure for Verified, Archived Library of Inputs and Data (VALID)





SCALE-CMP-012, Rev. 1

SCALE Procedure for Verified, Archived Library of Input and Data (VALID)

Prepared by
D. A. Reed

Nuclear Modeling, Design, and Safety (NMDS)
Nuclear Science and Technology Division (NSTD)
Energy and Engineering Sciences Directorate (EESD)
Oak Ridge National Laboratory

September 15, 2010

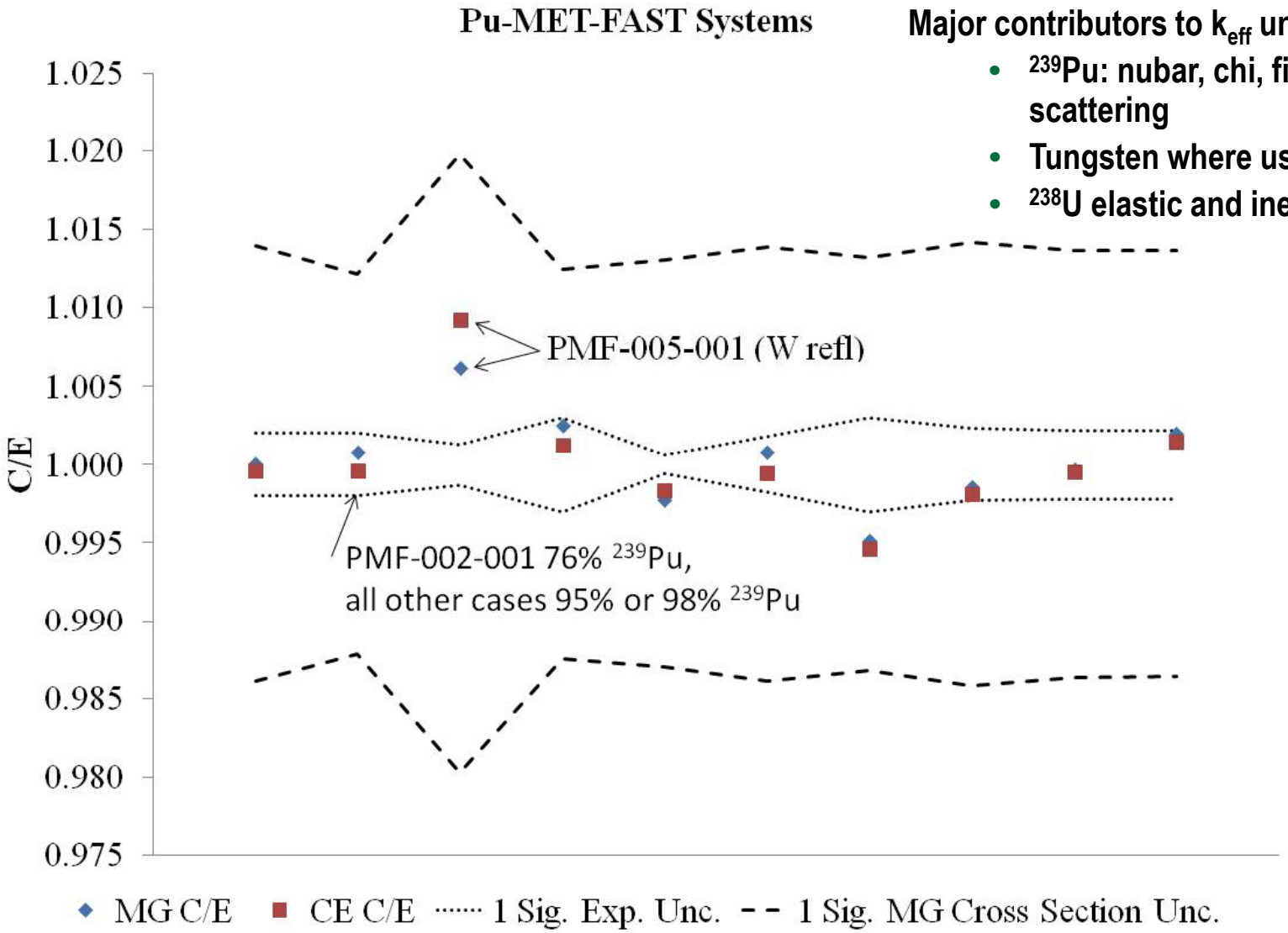
Scale 6 Covariance Library (401 materials)

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	**JENDL-3.3**: evaluated covariance data in JENDL-3.3
ENDF/B-VII-p: recently evaluated data proposed for future release of ENDF/B-VII.1	**BLO approximate data**: lo-fi covariances from BLO project (**B**rookhaven, **L**os Alamos, **O**RNL)
ENDF/B-VI: evaluated covariance data released with ENDF/B-VI	**BLO LANL evaluation**: LANL R-matrix evaluation from BLO project
	SG-26: approximate covariances from WPEC Subgroup-26

KENO Criticality Validation for Scale 6.1

- **Calculation of over 300 total configurations from ICSBEP with ENDF/B-VII.0 238-group and CE libraries**
- **Covers range of fissile material, fissile form, spectrum**
- **All models from verified library**
- **Available as ORNL/TM-2011/450**
- **Calculated-to-expected k_{eff} determined for each case and compared to evaluated experimental uncertainty and multigroup cross section uncertainties**
- **Cross section uncertainties from TSUNAMI-3D**
- **Indication that cross section uncertainties are too large**
- **Only 2 cases (0.6% of cases) outside 2-sigma cross section uncertainty**

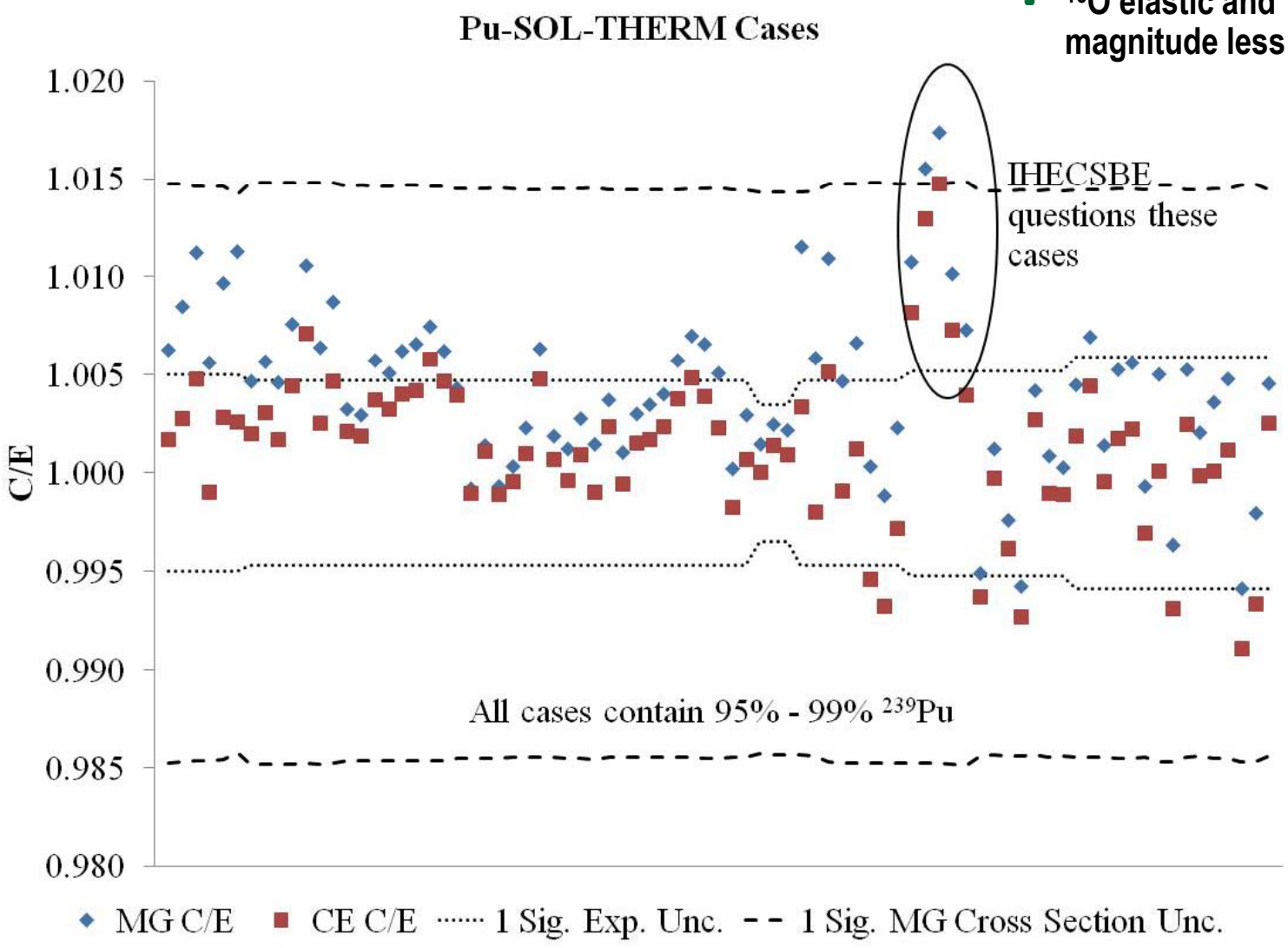


Major contributors to k_{eff} uncertainty:

- **^{239}Pu: nubar, chi, fission and scattering**
- **Tungsten where used as reflector**
- **^{238}U elastic and inelastic scattering**

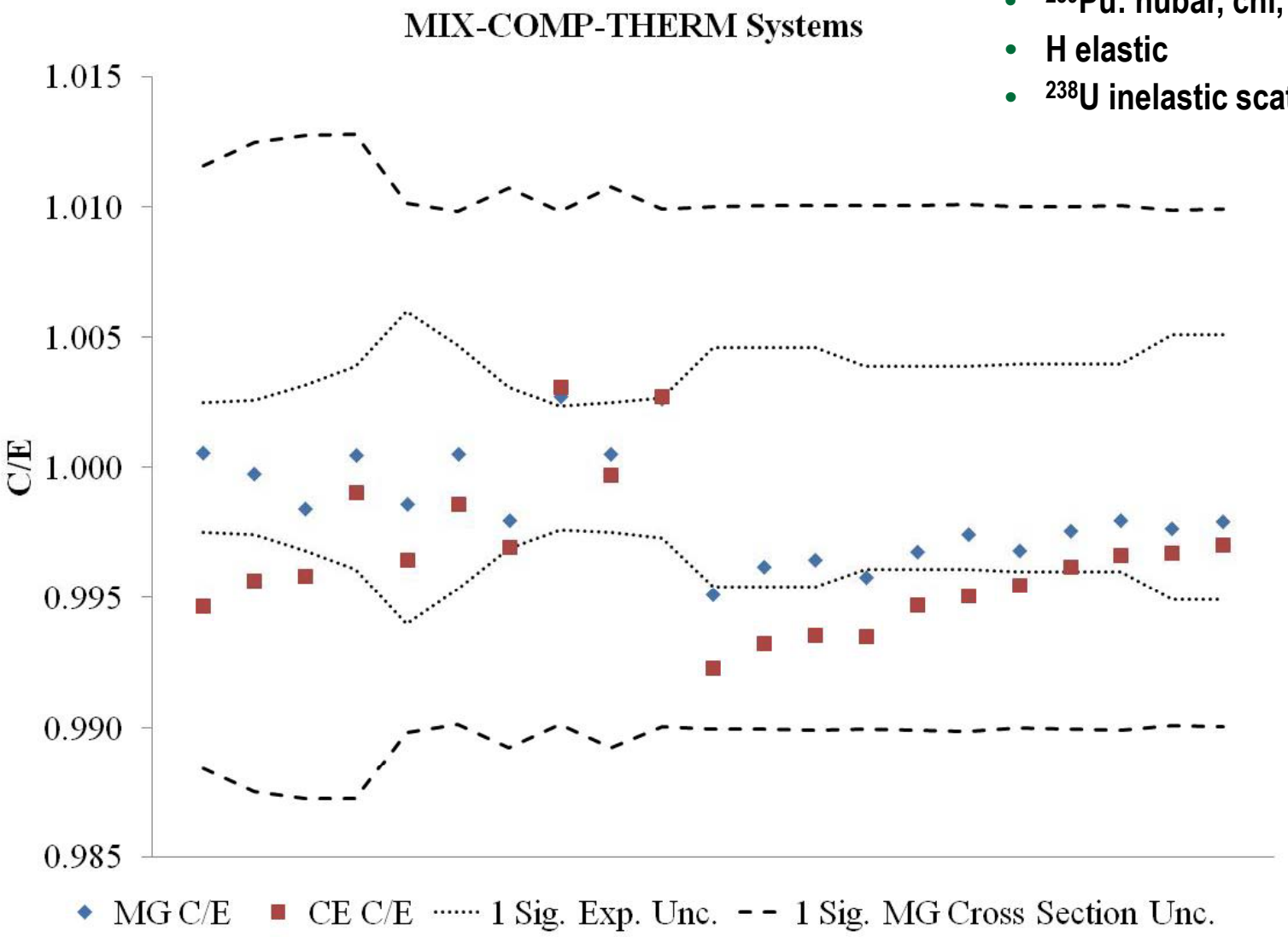
Major contributors to k_{eff} uncertainty:

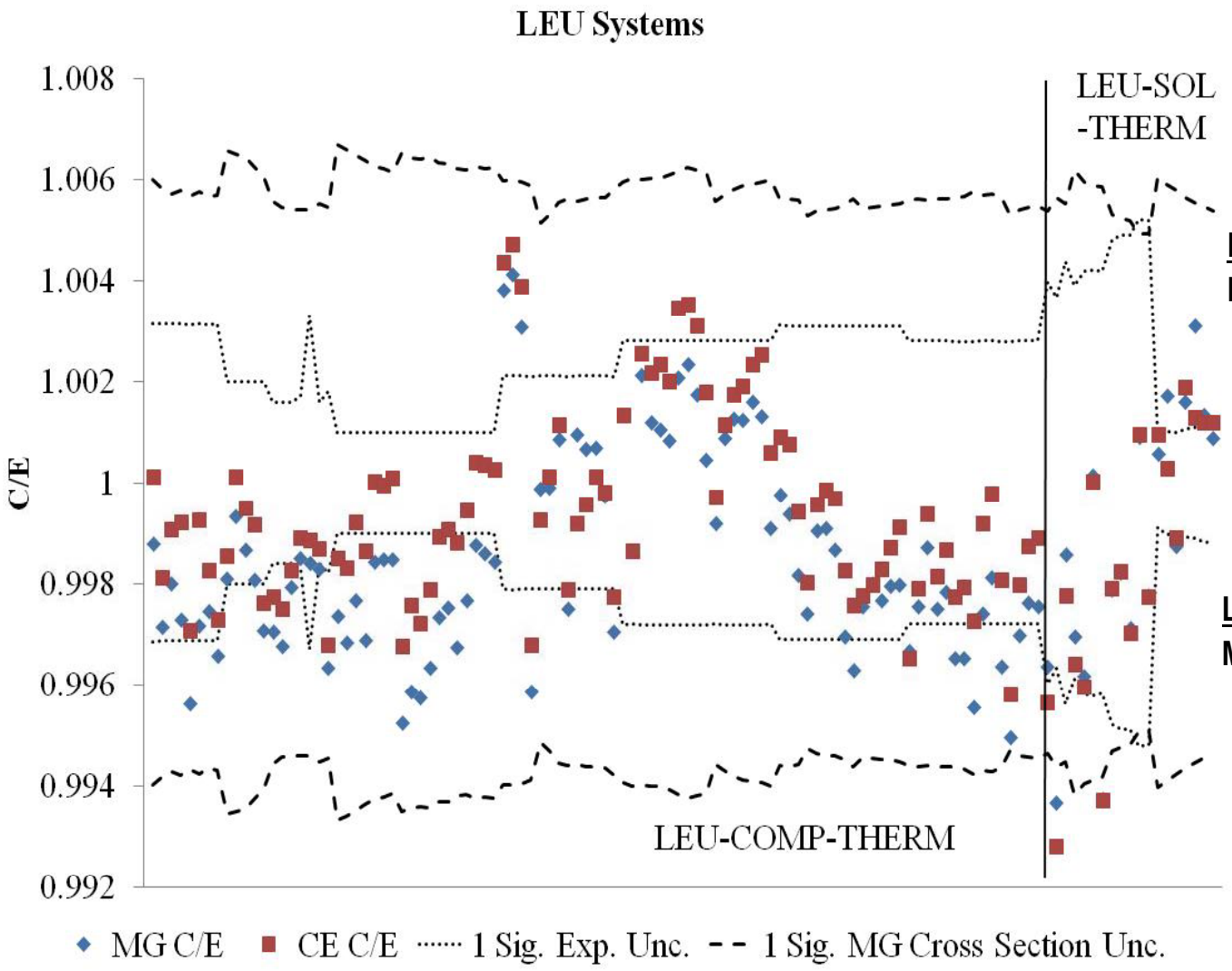
- **^{239}Pu: nubar, chi, fission**
- **H elastic**
- **^{16}O elastic and ^{14}N(n,p): both order of magnitude less relative to ^{239}Pu and H**



Major contributors to k_{eff} uncertainty:

- **^{239}Pu: nubar, chi, fission**
- **H elastic**
- **^{238}U inelastic scattering**





LCT Systems

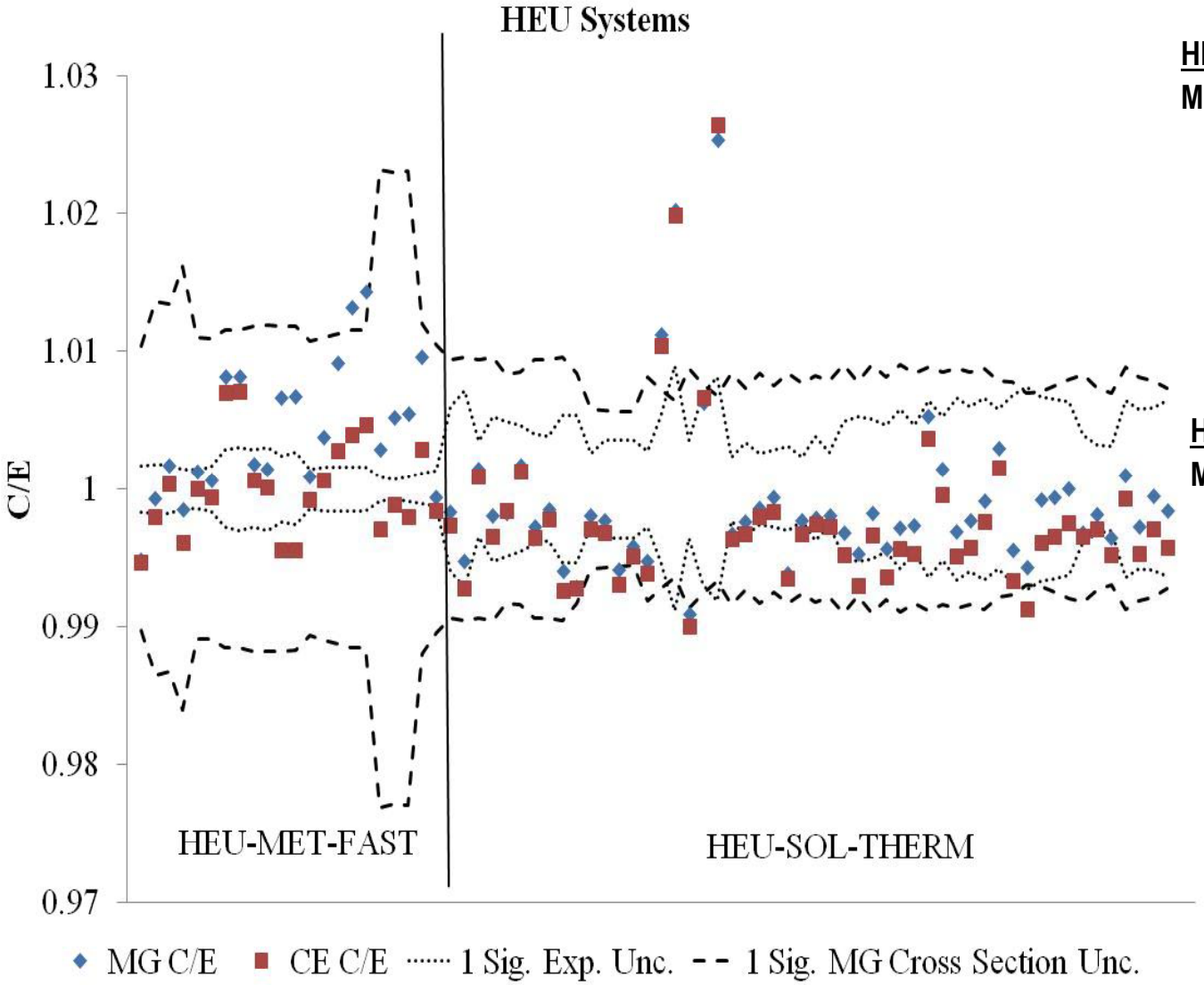
Major contributors to k_{eff} uncertainty:

- **^{235}U: nubar and chi**
- **^{238}U elastic scattering**
- **H elastic**

LST Systems

Major contributors to k_{eff} uncertainty:

- **^{235}U: nubar, chi, fission**
- **H elastic**
- **^{14}N (n,p)**



HMF Systems

Major contributors to k_{eff} uncertainty:

- **^{235}U: nubar, chi, (n,f)**
- **Be-BeO**
- **V elastic**
- **Mo elastic**

HST Systems

Major contributors to k_{eff} uncertainty:

- **^{235}U: nubar and chi**
- **H elastic**

Summary Data

- **Standard deviation of C/E provides estimate of maximum uncertainty**
- **Estimate includes uncertainties in experimental description as another significant component**
- **Cross section uncertainties may be 1.4x – 5x too large**

Category	Ave. C/E	Ave. C/E Unc.	Std. Dev. C/E	Ave. MG XS Unc.	XS Unc. / Std. Dev. C/E
HMF	1.00422	0.00041	0.00488	0.01330	2.7
HST	0.99904	0.00072	0.00587	0.00800	1.4
LCT	0.99851	0.00025	0.00197	0.00583	3.0
LST	0.99871	0.00083	0.00267	0.00556	2.1
MCT	0.99847	0.00087	0.00214	0.01054	4.9
PMF	1.00035	0.00068	0.00298	0.01399	4.7
PST	1.00430	0.00056	0.00432	0.01456	3.4

Summary

- A wide range of different systems were evaluated in the Scale 6.1 validation
- Good confidence in models and results because the models are taken from the verified library (VALID)
- Cross section uncertainties appear to be too large in all cases, though magnitude of over estimate varies
- Standard deviation of C/E values can be used to estimate an upper bound of total uncertainty
- Uncertainties in experiment descriptions are a significant contribution to C/E variation, but are neglected in ratios presented above
- **High quality integral benchmark experiment data available for use**

Acknowledgements

- **U.S. Nuclear Criticality Safety Program (NCSP)**

- **Contact Info:**

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