Monte Carlo Benchmark Calculations with Revised ^{235,238}U Evaluations

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- Bettis has performed continuous energy Monte Carlo eigenvalue calculations for a variety of geometrically simple uranium fueled benchmarks with ENDF/B-VI.8, JEFF-3.0, JENDL-3.3 or alternative (BRC3, KAPL, LANL, Maslov, ORNL) ^{235,238}U data sets.
  - ENDF/B, JEFF-3.0 and JENDL-3.3 results were recently published in the NS&E ICSBEP special edition, Nucl. Sci. Eng., 145, 213 (2003).

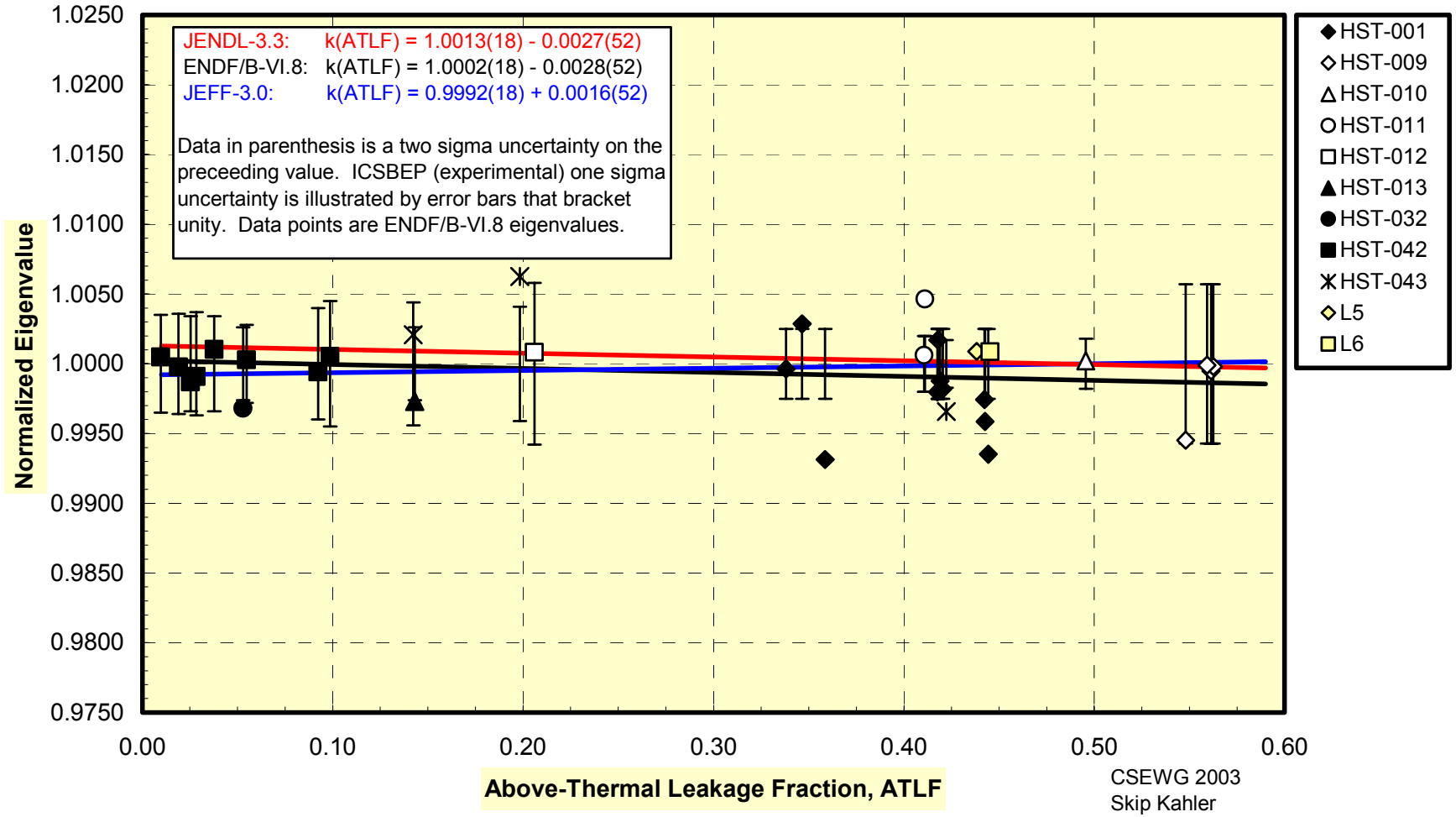
- Eigenvalues presented on subsequent slides are calculated from tracking 50 million neutron histories in ten independent 5 million history jobs.
  - The 95% eigenvalue confidence interval, determined from the variance in the ten independent eigenvalue estimates, is typically less than 0.0005 Δk (i.e., roughly the size of the plot symbol).

- A majority of these calculations use models derived from ICSBEP evaluations, as follows:
  - HEU-SOL-THERM
    - 9 evaluations, 31 critical configurations plus two ORNL experiments (L5, L6) not yet in ICSBEP.
      - 4 evaluations (8 critical configurations) include a H_2O reflector.
  - LEU-COMP-THERM
    - 8 evaluations, 59 critical configurations.
      - 2 evaluations (17 critical configurations) contain metallic reflectors.
  - LEU-SOL-THERM
    - 9 evaluations, 39 critical configurations
      - 4 evaluations (19 critical configurations) include a H_2O reflector.

Selected HEU-SOL-THERM ICSBEP Benchmarks

Benchmark	Description
HEU-SOL-THERM-001 (encompass “RF#”)	Unreflected cylinders (~28cm, ~33cm and ~51cm diameter) containing uranyl nitrate.
HEU-SOL-THERM-009 (Case 3 = ORNL L7)	Water reflected spheres (6.4-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-010	Water reflected sphere (9.7-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-011	Water reflected spheres (17-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-012 (ORNL L10)	Water reflected sphere (91-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-013 (ORNL1)	Unreflected sphere (174-liter) containing uranium nitrate.
HEU-SOL-THERM-032 (ORNL10)	Unreflected sphere (48-inch diameter) containing uranyl nitrate.
HEU-SOL-THERM-042 (encompass ORNL12 through ORNL23)	Unreflected cylinders (~77cm and ~137cm diameter) containing uranium nitrate.
HEU-SOL-THERM-043 (Cases 2 and 3 are ORNL L8 and ORNL L9)	Unreflected spheres (17-liter, 91-liter and 174-liter) containing uranium oxyfluoride solution.
ORNL L5, L6	Unreflected cylinders (13cm diameter) of uranium oxyfluoride. Low $H/^{235}U$ ratios of 27 and 44 lead to large leakage.

HEU-SOL-THERM Eigenvalues



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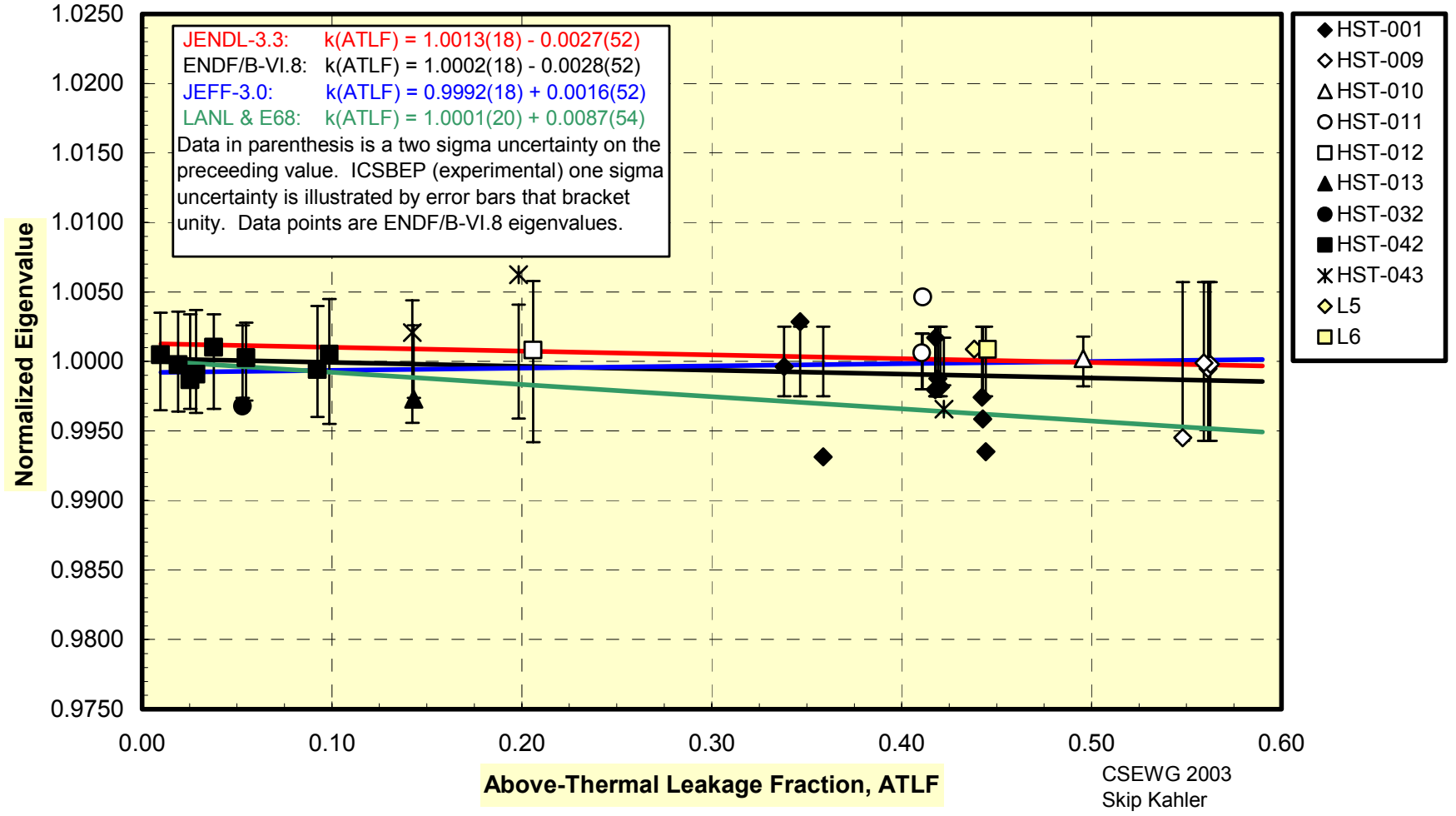
HEU-SOL-THERM Eigenvalues



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HEU-SOL-THERM Observations

- The historical trend in calculated eigenvalue as a function of Above-Thermal Leakage Fraction (ATLF) is statistically insignificant in the latest evaluated cross section libraries.
  - $k_{calc}(ATLF) = 1.0002(18)^{(a)} - 0.0028(52) * ATLF$ (ENDF/B-VI.8)
  - $k_{calc}(ATLF) = 0.9992(18) + 0.0016(52) * ATLF$ (JEFF-3.0)
  - $k_{calc}(ATLF) = 1.0013(18) - 0.0027(52) * ATLF$ (JENDL-3.3)

- The ATLF trend reappears when the latest LANL $^{235,238}U$ data sets are used. The revised ^{235}U fission spectrum is the primary cause for this reappearance.
  - $k_{calc}(ATLF) = 1.0001(20) - 0.0087(54) * ATLF$
  - In the absence of further modifications to eliminate this new trend, the User community will not perceive the latest ^{235}U evaluation to be an improvement over data sets that are already available.

- (a) Read 1.0002(18) as 1.0002 ± 0.0018, where 0.0018 is a two sigma uncertainty on the preceding value.

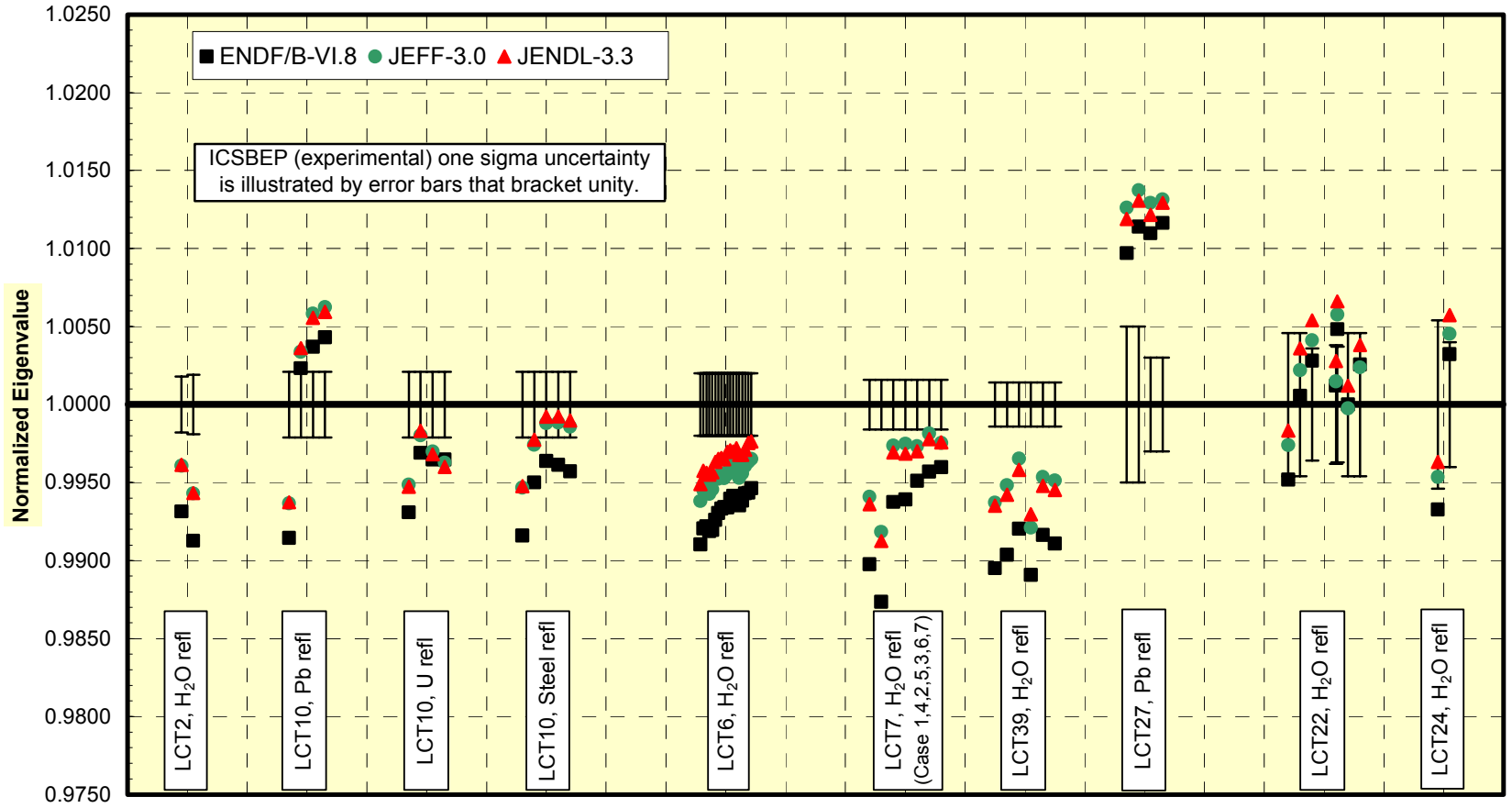
Selected LEU-COMP-THERM ICSBEP Benchmarks

Benchmark	Description
LEU-COMP-THERM-002	Water moderated and reflected U(4.31)O_2 1.415 cm OD fuel rods in 2.54 cm square pitched arrays. Cases 4 and 5 consist of three clusters of 15 x 8 and 13 x 8 rods, respectively.
LEU-COMP-THERM-006	Water moderated and reflected U(2.60)O_2 1.417 cm OD fuel rods in 1.85 cm to 2.29 cm square pitched 15x15 to 21x21 arrays.
LEU-COMP-THERM-007	Water moderated and reflected U(4.74)O_2 0.94 cm OD fuel rods in square and triangular arrays (cases 1 through 7). Pitch varies from 1.26 cm to 2.52 cm.
LEU-COMP-THERM-010	Water moderated U(4.31)O_2 1.415 cm OD fuel rods in 2.54 cm square pitched arrays reflected by two lead, uranium or steel walls at varying distances from the rod clusters. Cases 1 through 13 (mostly 13 x 8 rod clusters with a rod pitch of 2.54 cm) analyzed.
LEU-COMP-THERM-022	Water moderated and reflected U(10)O_2 0.51 cm OD fuel rods in triangular pitched (0.7 cm to 1.85 cm) arrays.
LEU-COMP-THERM-024	Water moderated and reflected U(10)O_2 0.51 cm OD fuel rods in square pitched (0.62 cm and 0.88 cm) arrays.
LEU-COMP-THERM-027	Water moderated and lead reflected U(4.74)O_2 0.94 cm OD fuel rod arrays (1.60 cm square pitch and variable distance to the lead reflector).
LEU-COMP-THERM-039	Water moderated and reflected U(4.74)O_2 0.94 cm OD fuel rods in square 1.26 cm pitch, 21x21 or 22x22 arrays. Arrays contain 1 in *n* missing rods (i.e., water holes), for *n*=5,4,3 and 2.

Selected LEU-SOL-THERM ICSBEP Benchmarks

Benchmark	Description
LEU-SOL-THERM-001	"SHEBA-II". An unreflected UO_2F_2 + H_2O cylindrical (~20 inch diameter) assembly.
LEU-SOL-THERM-002	174-liter spheres of low enriched (4.9%) uranium oxyfluoride solutions. Case 1 is a water reflected solution, case 2 is unreflected.
LEU-SOL-THERM-003	Bare spheres of 10% enriched uranyl nitrate water solutions. Cases 3, 6 and 9 are full spheres with increasing H-to-^{235}U ratio.
LEU-SOL-THERM-004	STACY; Water reflected, 10% enriched uranyl nitrate solution in a 60cm diameter cylindrical tank. Seven cases with varying gU/liter.
LEU-SOL-THERM-007	STACY; Unreflected, 10% enriched uranyl nitrate solution in a 60cm diameter cylindrical tank. Five cases with varying gU/liter.
LEU-SOL-THERM-016	STACY; Water reflected, 10% enriched uranyl nitrate solution in a rectangular (slab, ~28cm x ~69cm) tank. Seven cases with varying gU/liter.
LEU-SOL-THERM-017	STACY; Unreflected, 10% enriched uranyl nitrate solution in a rectangular (slab, ~28cm x ~69cm) tank. Six cases with varying gU/liter.
LEU-SOL-THERM-020	STACY; Water reflected, 10% enriched uranyl nitrate solution in an 80cm diameter cylindrical tank. Four cases with varying gU/liter.
LEU-SOL-THERM-021	STACY; Unreflected, 10% enriched uranyl nitrate solution in an 80cm diameter cylindrical tank. Four cases with varying gU/liter.

LEU-COMP-THERM Eigenvalues



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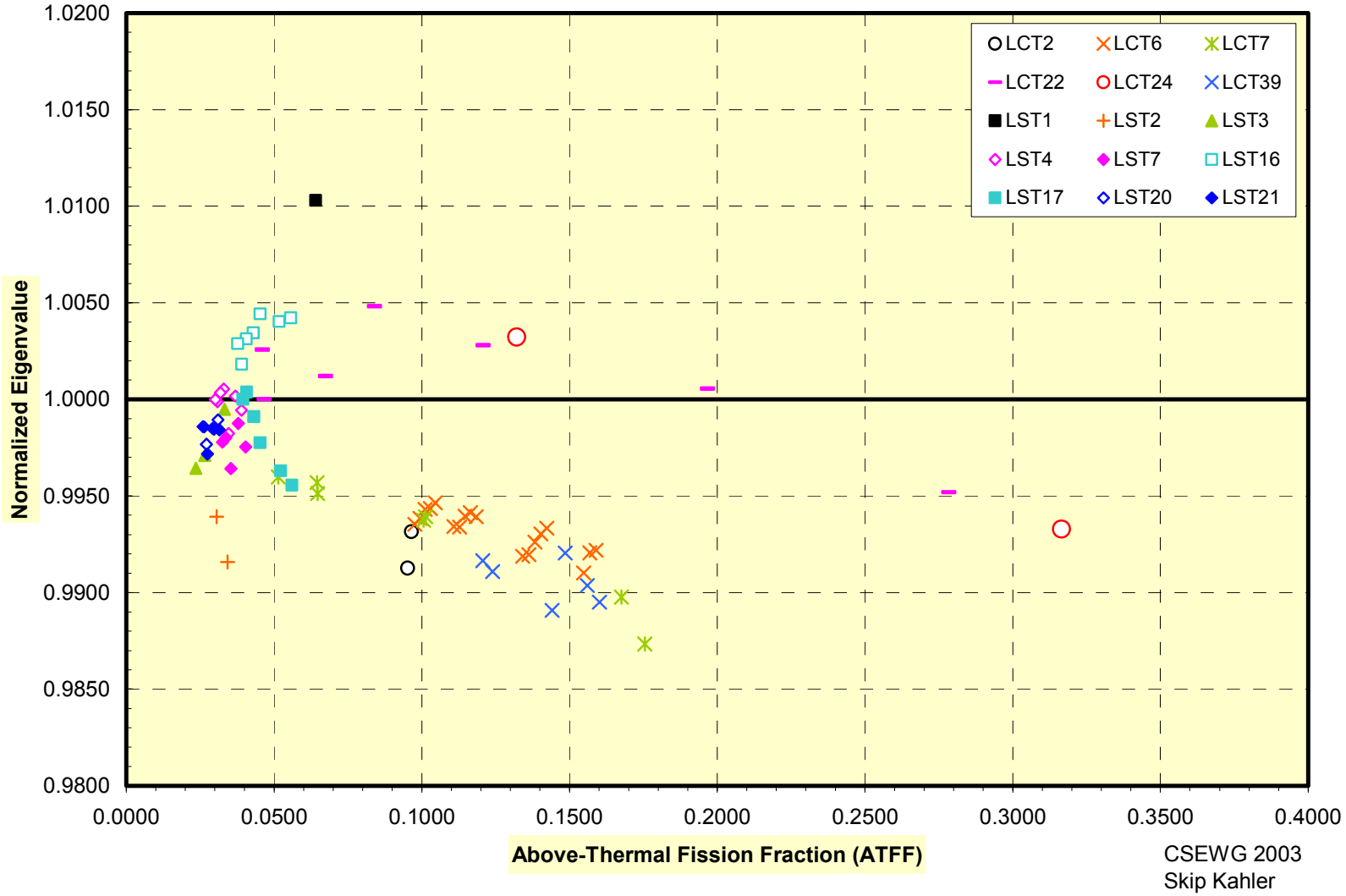
LEU-xxx-THERM Eigenvalues with ENDF/B-VI.8 Cross Sections
Normalized Eigenvalue
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.0000
0.0500
0.1000
0.1500
0.2000
0.2500
0.3000
0.3500
0.4000
Above-Thermal Fission Fraction (ATFF)
LCT2
LCT6
LCT7
LCT22
LCT24
LCT39
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
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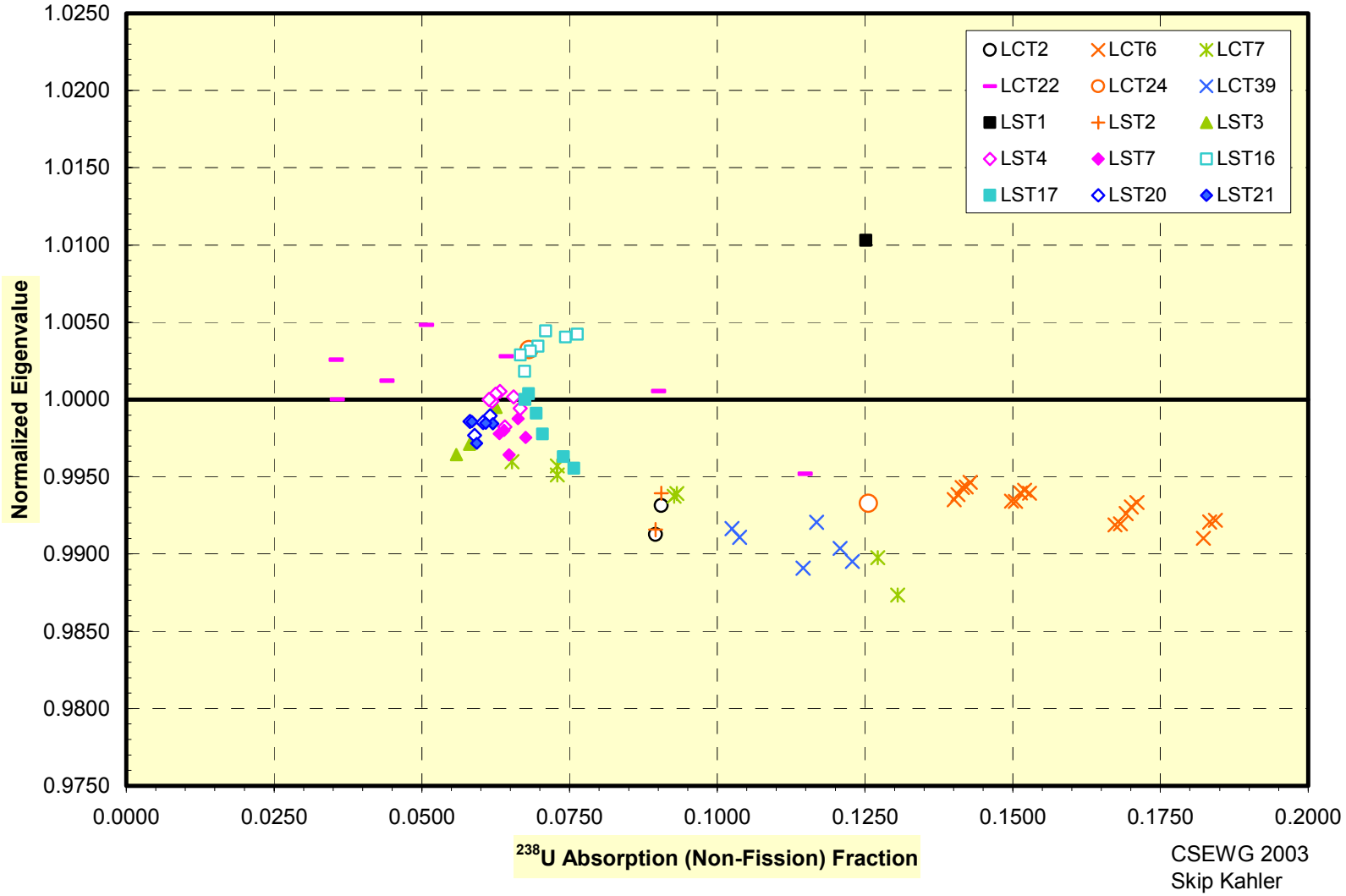
LEU-xxx-THERM Eigenvalues with ENDF/B-VI.8 Cross Sections
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
0.0000
0.0250
0.0500
0.0750
0.1000
0.1250
0.1500
0.1750
0.2000
238U Absorption (Non-Fission) Fraction
LCT2
LCT6
LCT7
LCT22
LCT24
LCT39
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
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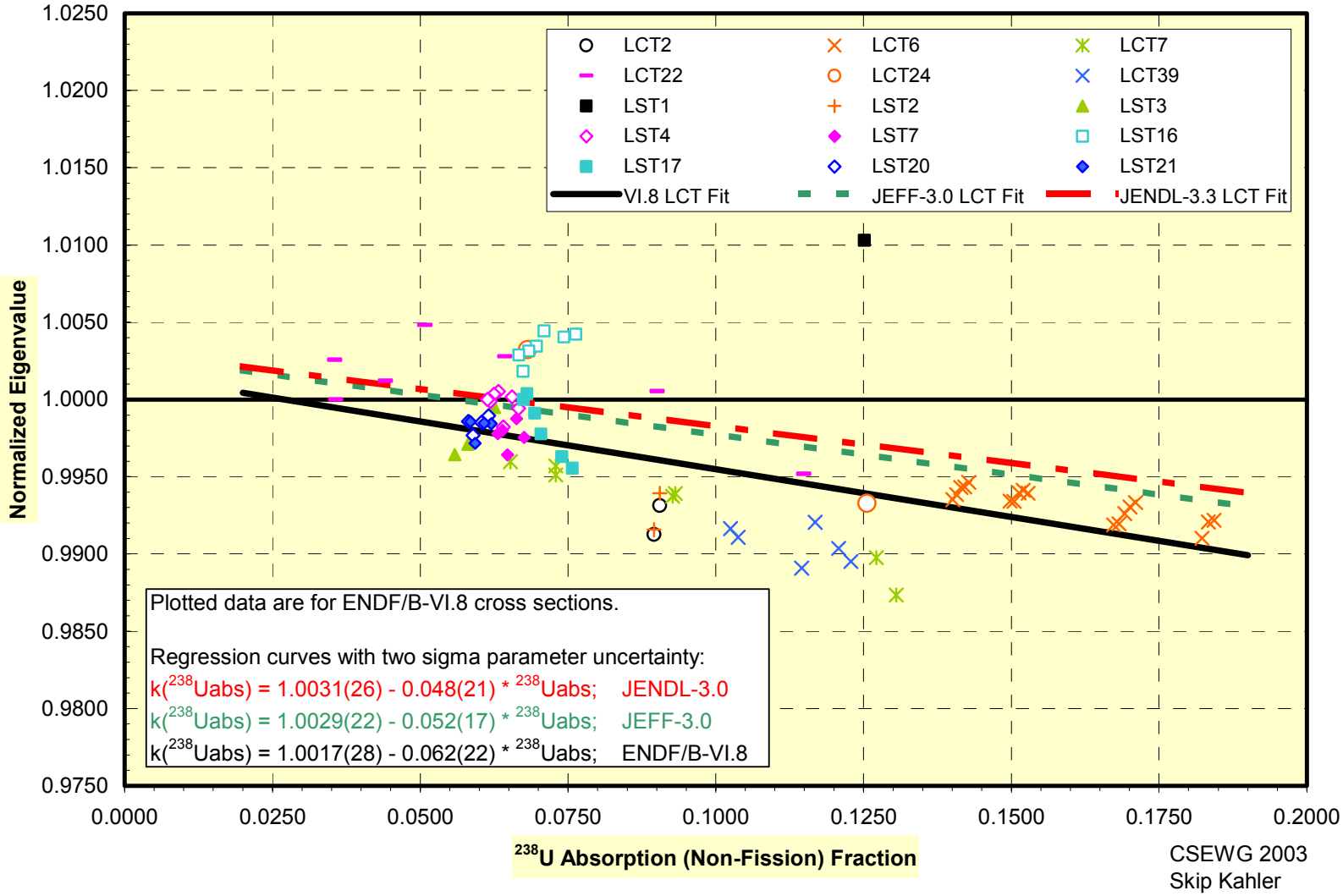
LEU-xxx-THERM Eigenvalues with ENDF/B-VI.8, JEFF-3.0 and JENDL-3.3 Cross Sections
LCT2
LCT6
LCT7
LCT22
LCT24
LCT39
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
VI.8 LCT Fit
JEFF-3.0 LCT Fit
JENDL-3.3 LCT Fit
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
0.0000
0.0250
0.0500
0.0750
0.1000
0.1250
0.1500
0.1750
0.2000
238U Absorption (Non-Fission) Fraction
Plotted data are for ENDF/B-VI.8 cross sections.
Regression curves with two sigma parameter uncertainty:
k(238Uabs) = 1.0031(26) - 0.048(21) * 238Uabs; JENDL-3.0
k(238Uabs) = 1.0029(22) - 0.052(17) * 238Uabs; JEFF-3.0
k(238Uabs) = 1.0017(28) - 0.062(22) * 238Uabs; ENDF/B-VI.8
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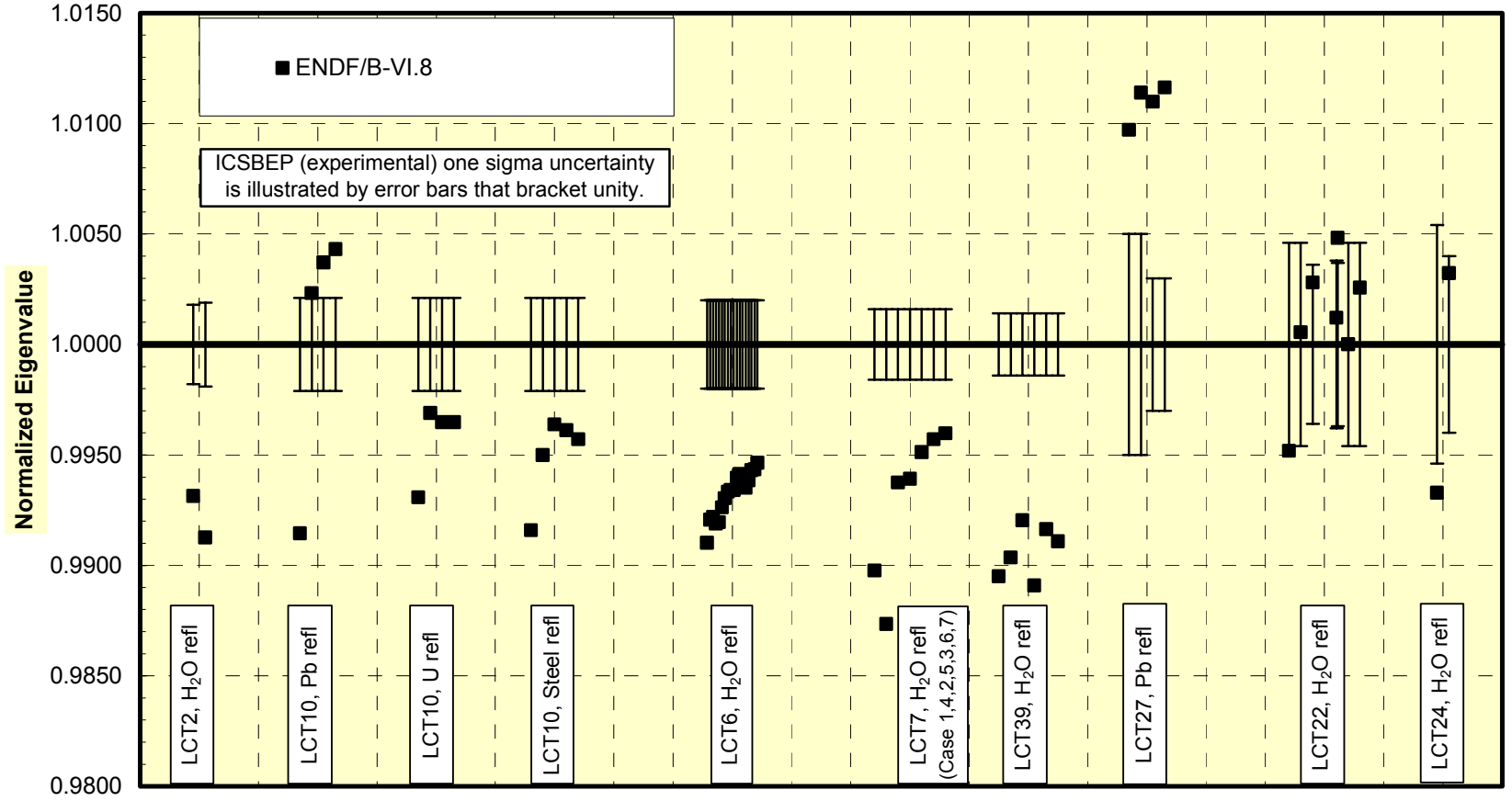
LEU-COMP-THERM Eigenvalues with Selected ^{238}U Data Sets



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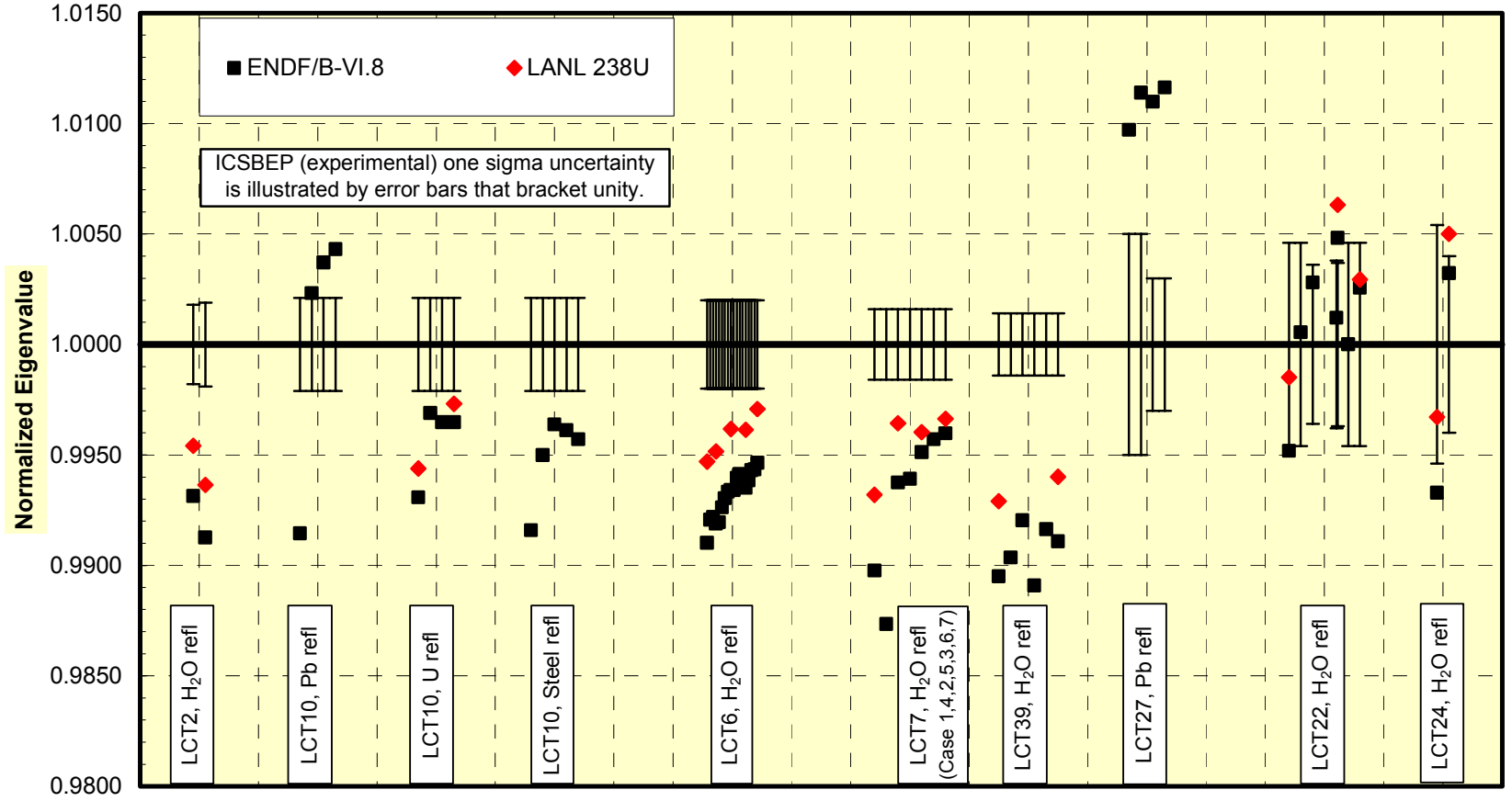
LEU-COMP-THERM Eigenvalues with Selected ^{238}U Data Sets



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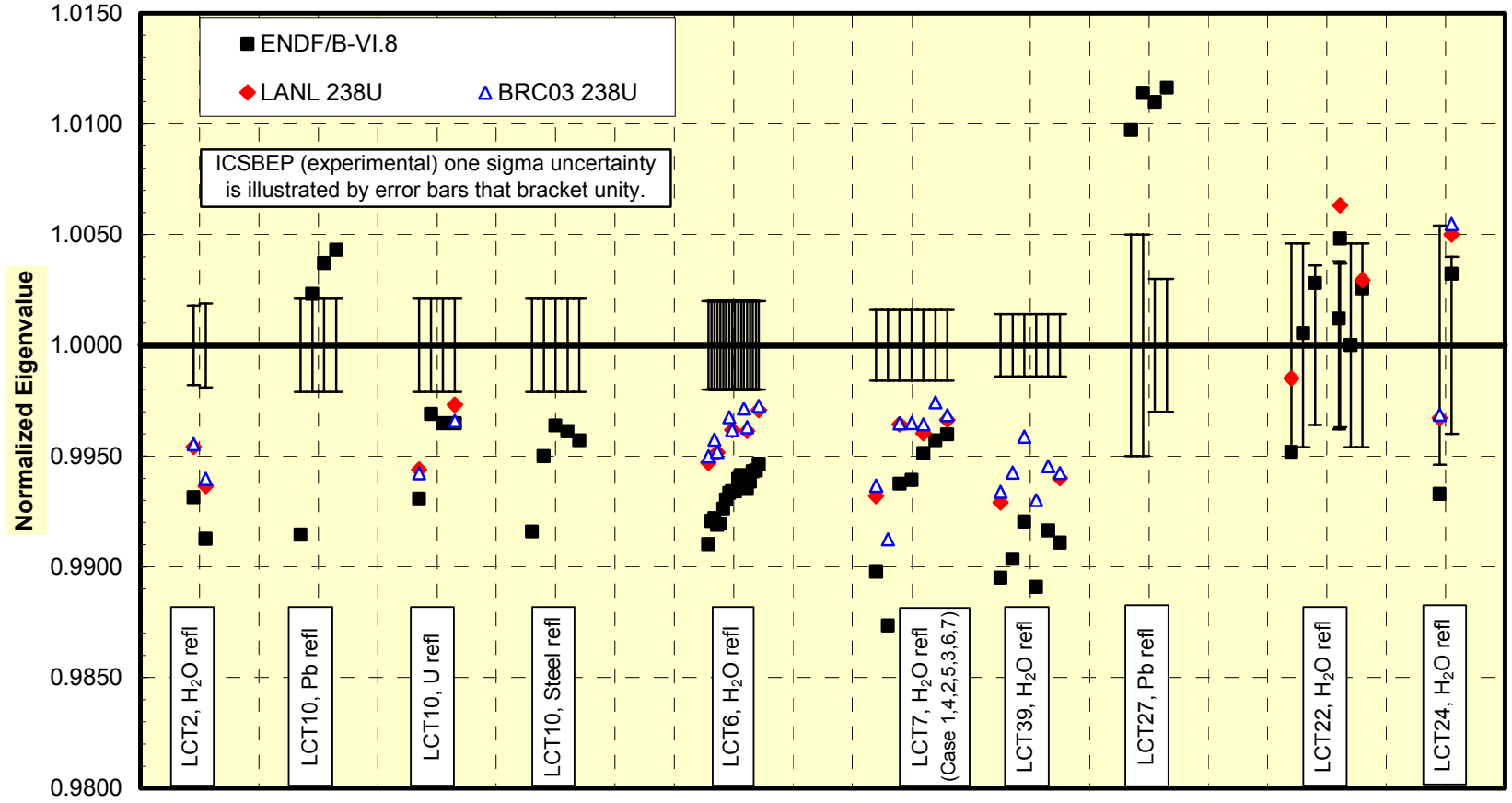
LEU-COMP-THERM Eigenvalues with Selected ^{238}U Data Sets



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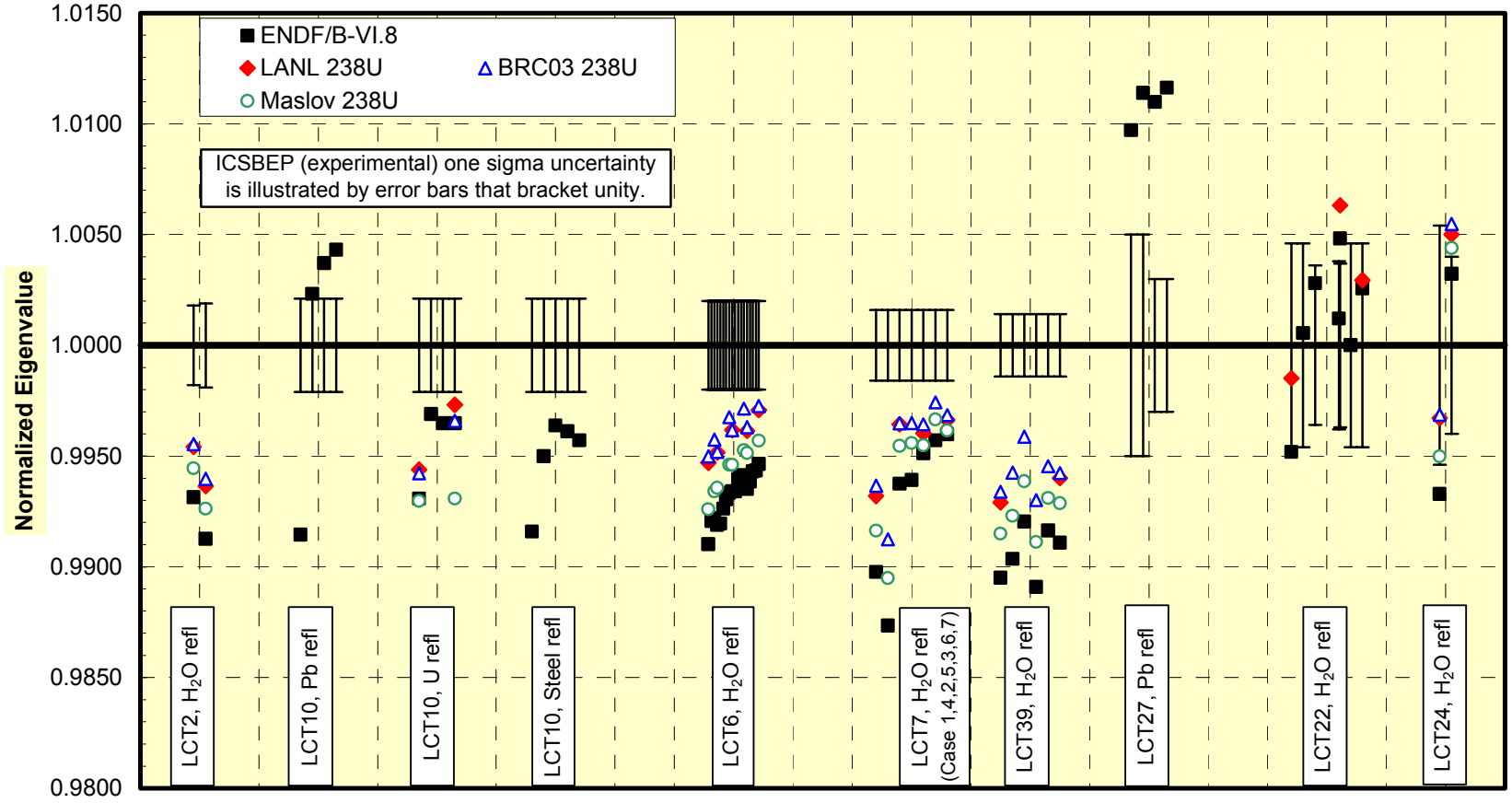
LEU-COMP-THERM Eigenvalues with Selected ^{238}U Data Sets



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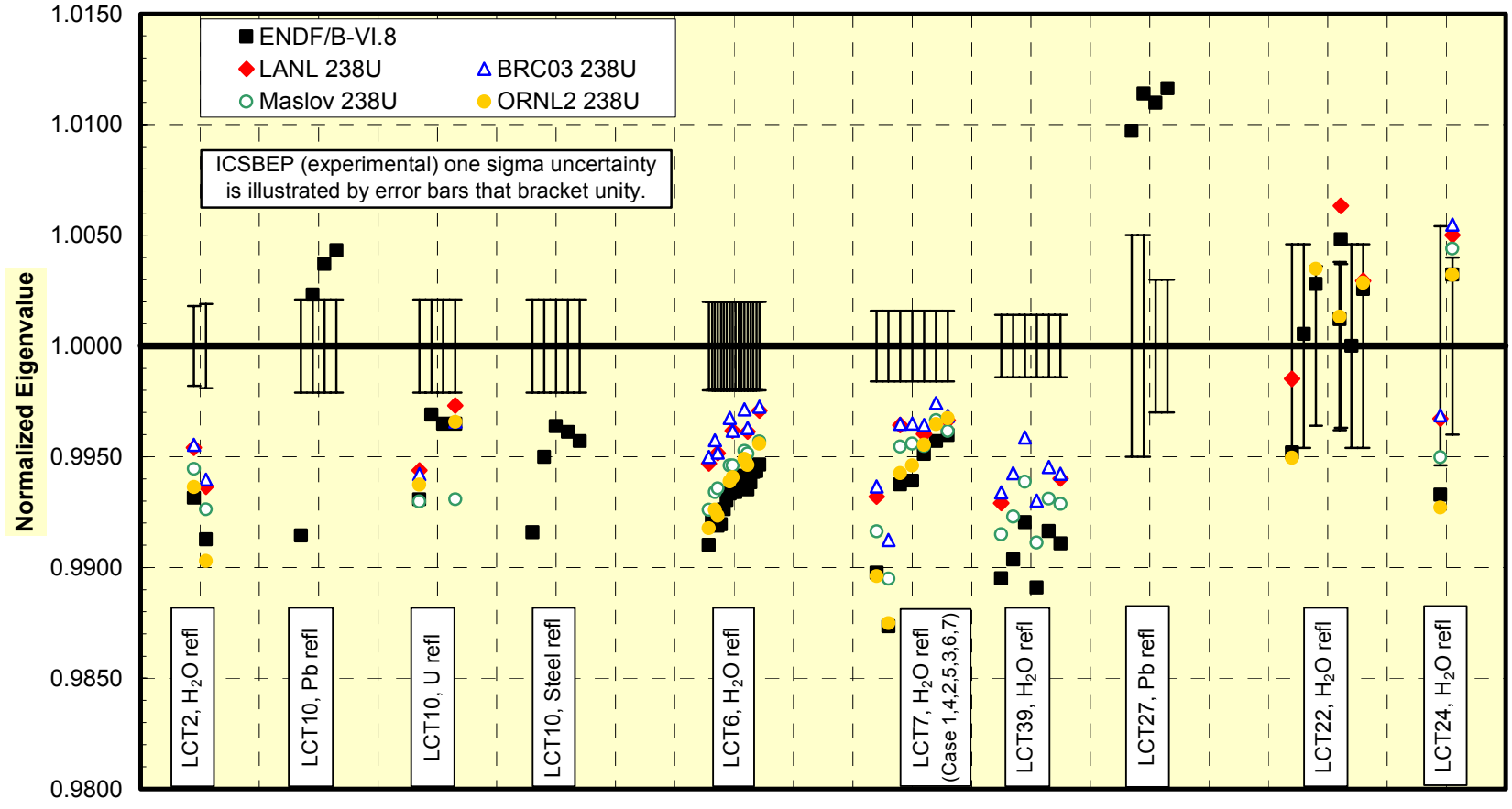
LEU-COMP-THERM Eigenvalues with Selected ^{238}U Data Sets



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LEU-COMP-THERM Observations

- LEU-COMP-THERM eigenvalues are generally low, with a decreasing eigenvalue trend observed as a function of Above Thermal Fission Fraction, ATFF or as a function of ^{238}U absorption fraction.
  - New data sets proposed by BRC03, LANL, Maslov and ORNL all yield larger, but still less than unity, LCT benchmark eigenvalues.
    - The BRC03 and LANL data sets also reduce the magnitude of the eigenvalue trend with ^{238}U capture fraction, but do not eliminate it. Maslov and ORNL changes are too small to draw such a conclusion.
  - Calculations with the KAPL v223 data set, not shown on the previous plots, exhibit an average eigenvalue decrease of ~0.05%, suggesting that the continuum inelastic scattering representation is not a significant contributor to these deficiencies.

Final Observations

- Current (ENDF/B-VI.8, JEFF-3.0, JENDL-3.3) libraries generally perform well for ^{235}U solution systems.
  - HEU-SOL-THERM eigenvalues are virtually unity with no underlying eigenvalue trend as a function of Above-Thermal Leakage Fraction (ATLF).
    - 33 ENDF/B-VI.8 eigenvalues range from 0.9931 to 1.0063, with an average of 0.9994 ± 0.0010 ± 0.0057 (0.0010 and 0.0057 are 95% confidence intervals for the average and for the population, respectively).
  - LEU-SOL-THERM benchmarks, whose ATLF values range from ~0.06 to ~0.24, also exhibit near unity eigenvalues
    - 39 ENDF/B-VI.8 eigenvalues range from 0.9916 to 1.0103, with an average of 0.9994 ± 0.0011 ± 0.0066 (0.0011 and 0.0066 are 95% confidence intervals for the average and for the population, respectively).
- Future data set revisions should strive to maintain these excellent results.