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Data Assimilation of Benchmark Experiments for Homogenous Thermal / Epithermal Uranium Systems

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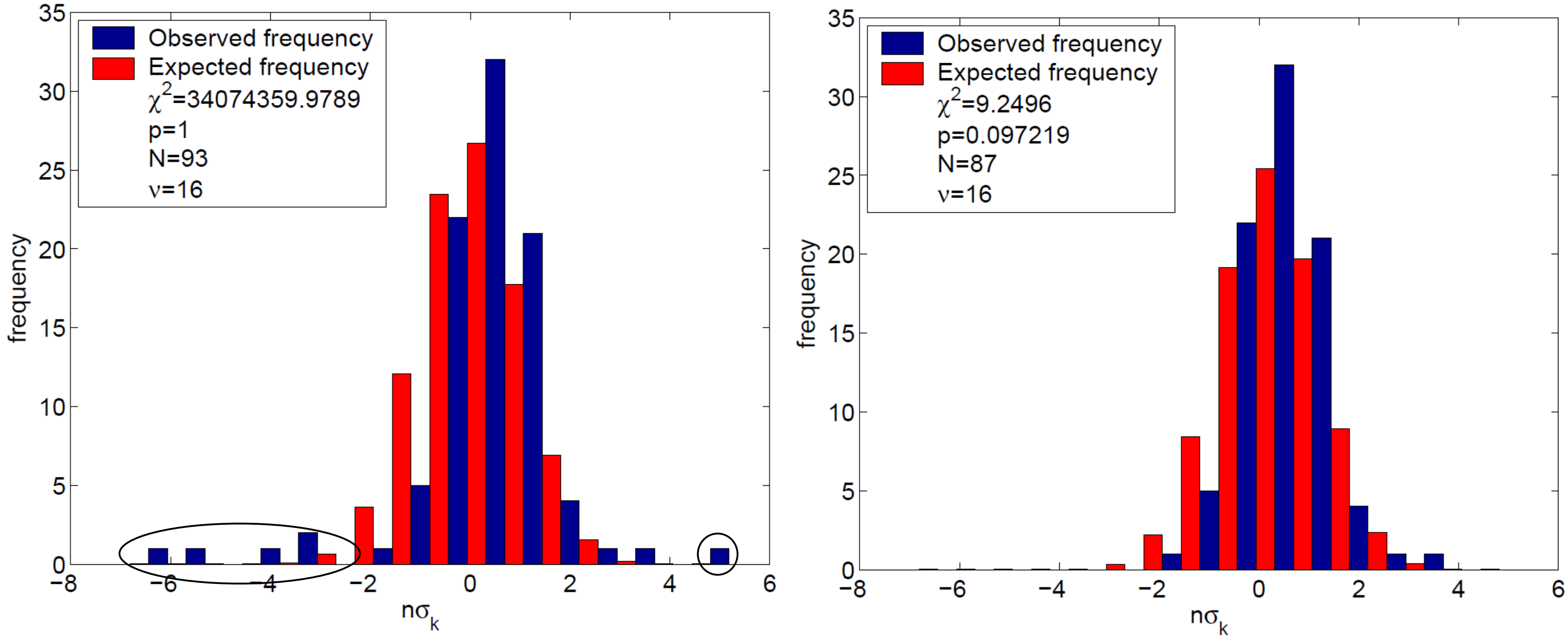
Identification of Similar Benchmark Experiments to new UK IEU Evaluations

Evaluation Identifier (Cross-references)	Evaluation Title	Fuel form	No. cases
LEU-SOL-THERM-001	Unreflected UO_2F_2+H_2O Cylindrical Assembly SHEBA-II	Uranyl Fluoride (5% ^{235}U)	1
LEU-SOL-THERM-002	174 Liter Spheres of Low Enriched (4.9%) Uranium Oxyfluoride Solutions	Uranyl Fluoride (4.9% ^{235}U)	3
IEU-SOL-THERM-002	Bare & Water Reflected Spheres/Hemispheres of Aqueous Uranyl Fluoride Solutions	Uranyl Fluoride (30.45% ^{235}U)	13
IEU-SOL-THERM-003	Bare & Water Reflected Cylinders of Aqueous Uranyl Fluoride Solutions	Uranyl Fluoride (30.3% ^{235}U)	46
HEU-SOL-THERM-009	Water Reflected 6.4-Liter Sphere of Enriched Uranium Oxyfluoride Solutions	Uranyl Fluoride (93.18% ^{235}U)	4
HEU-SOL-THERM-010	Water Reflected 9.7-Liter Sphere of Enriched Uranium Oxyfluoride Solutions	Uranyl Fluoride (93.18% ^{235}U)	4
HEU-SOL-THERM-011	Water Reflected 17-Liter Sphere of Enriched Uranium Oxyfluoride Solutions	Uranyl Fluoride (93.18% ^{235}U)	2
HEU-SOL-THERM-012	Water Reflected 91-Liter Sphere of Enriched Uranium Oxyfluoride Solutions	Uranyl Fluoride (93.18% ^{235}U)	1
HEU-SOL-THERM-034	Water-Moderated and -Reflected Slabs of Uranium Oxyfluoride	Uranyl Fluoride (93.2% ^{235}U)	5
HEU-SOL-THERM-043	Large Unreflected Spheres of Uranium Oxyfluoride Solutions	Uranyl Fluoride (93.13% ^{235}U)	3
HEU-SOL-THERM-050	Unreflected Aluminium Containing Uranyl Fluoride Solutions	Uranyl Fluoride (93.2% ^{235}U)	11
LEU-COMP-THERM-045	Plexiglas or Concrete-Reflected U(4.46)3O8 with H/U=0.77 and Interstitial Moderation	Uranium Oxide (4.46% ^{235}U)	21
LEU-COMP-THERM-049	Maracas Programme: Polythene-Reflected Critical Configurations with Low-Enriched and Low-Moderated Uranium Dioxide Powder U(5)O_2	Uranium Oxide (5% ^{235}U)	18
LEU-COMP-THERM-069	Plexiglas Reflected U(4.48)3O8 with H/U=1.25 or H/U=2.03 and Interstitial Moderation	Uranium Oxide (4.48% ^{235}U)	5
IEU-COMP-THERM-015 (IEU-COMP-INTER-006) (IEU-COMP-MIXED-004)	Single Cores of 30.14% ^{235}U Enriched UO_2-Wax Mixtures Bare and with Single Reflector Materials	Uranium Oxide (30.14% ^{235}U)	32 (1) (6)
IEU-COMP-THERM-016	Single Cores of 30.14% ^{235}U Enriched UO_2-Wax Mixtures with Composite Reflector Materials	Uranium Oxide (30.14% ^{235}U)	45
HEU-COMP-MIXED-001 (HEU-COMP-THERM-001)	Arrays of Cans of Highly Enriched Uranium Dioxide Reflected by Polyethylene	Uranium Oxide (93.15% ^{235}U)	26 (6)
LEU-COMP-THERM-033	Reflected and Unreflected Assemblies of 2 and 3 %-Enriched Uranium Fluoride in Paraffin	Uranium Tetrafluoride (2–3% ^{235}U)	52
IEU-COMP-INTER-003 (IEU-COMP-THERM-011) (IEU-COMP-MIXED-003)	Unreflected UF_4-CF_2 Blocks with 37.5% ^{235}U	Uranium Tetrafluoride (37.5% ^{235}U)	14 (2) (3)
IEU-COMP-MIXED-002 (IEU-COMP-INTER-004)	Unreflected UF_4-CF_2 Blocks with 30, 25, 18.8 and 12.5% ^{235}U	Uranium Tetrafluoride (12.5–30% ^{235}U)	9 (2)
IEU-COMP-THERM-001 (IEU-COMP-MIXED-001)	Critical Arrays of Polyethylene-Moderated U(30)F_4-Polytetrafluoroethylene One-Inch Cubes	Uranium Tetrafluoride (30% ^{235}U)	29 (4)

Rejection of Evaluations

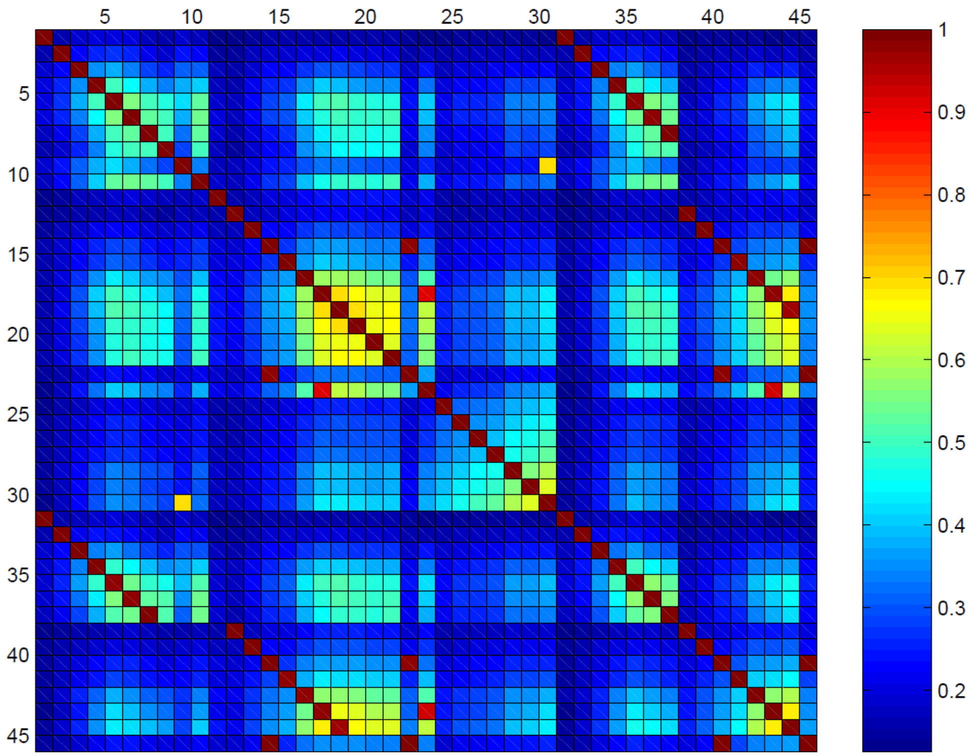
- Uranyl-fluoride solution configurations



5 cases from HEU-SOL-THERM-034 rejected

Experimental Covariance & Correlation

- Correlations for IEU-SOL-THERM-002 (46 cases)



$$cov\{xy\} = \delta k_x \delta k_y \rho_{x,y} = \sum_{i=1}^{n} \delta k_{i,x} \delta k_{i,y} (u_s + u_r \gamma_i^{x,y})$$

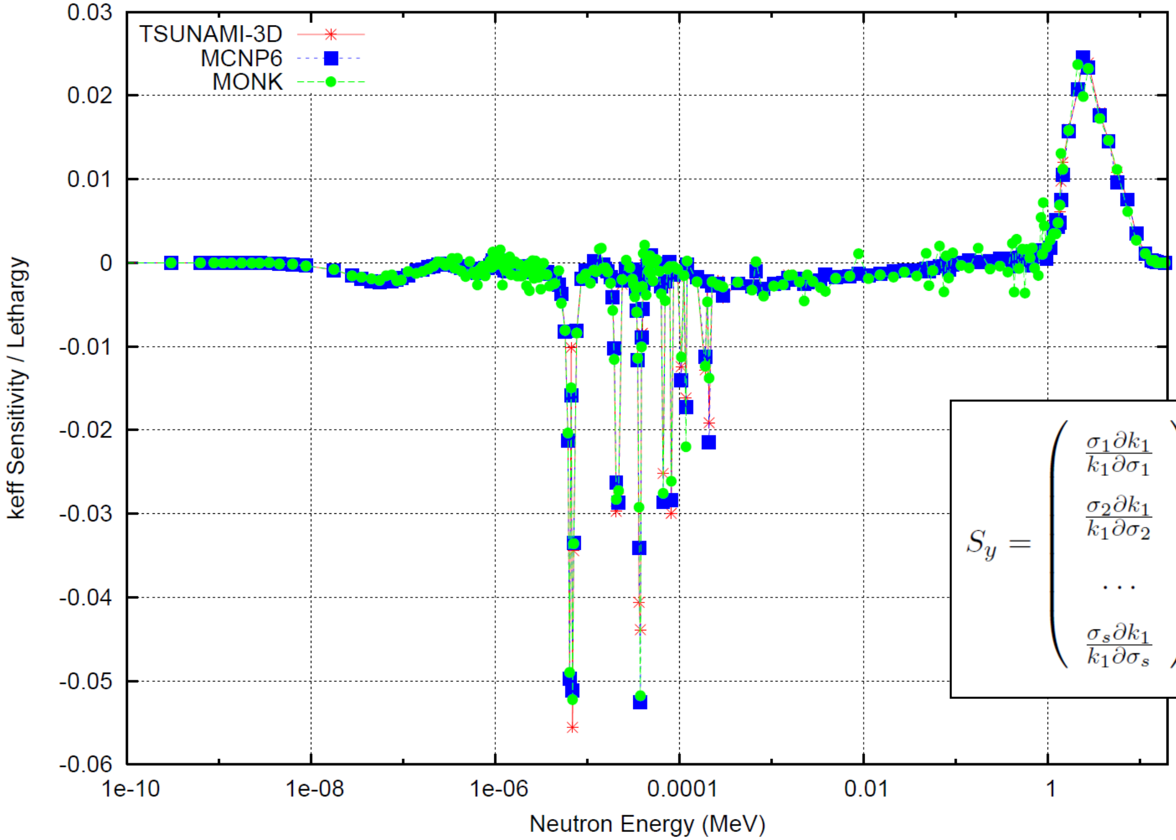
Cases with identical solutions have highly correlated solution measurement uncertainties

Concentration uncertainty dominates total therefore high overall correlation

$\Rightarrow C_Y$

Sensitivity Data (MONK9 – ENDF/B-VII.0)

- MONK uses a DOS Monte Carlo method



Example from UACSA Phase 3.1 Benchmark

^{238}U total sensitivity in SCALE 238 energy

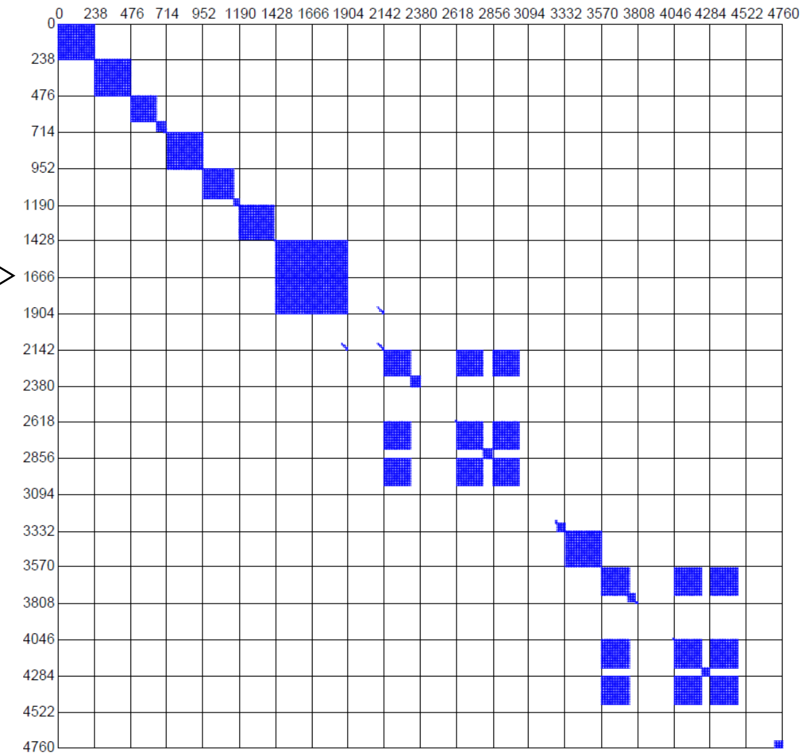
$$S_y = \begin{pmatrix} \frac{\sigma_1 \partial k_1}{k_1 \partial \sigma_1} \\ \frac{\sigma_2 \partial k_1}{k_1 \partial \sigma_2} \\ \cdots \\ \frac{\sigma_s \partial k_1}{k_1 \partial \sigma_s} \end{pmatrix} \rightarrow S_Y = \begin{pmatrix} \frac{\sigma_1 \partial k_1}{k_1 \partial \sigma_1} & \frac{\sigma_1 \partial k_2}{k_2 \partial \sigma_1} & \cdots & \frac{\sigma_1 \partial k_y}{k_y \partial \sigma_1} \\ \frac{\sigma_2 \partial k_1}{k_1 \partial \sigma_2} & \frac{\sigma_2 \partial k_2}{k_2 \partial \sigma_2} & \cdots & \frac{\sigma_2 \partial k_y}{k_y \partial \sigma_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_s \partial k_1}{k_1 \partial \sigma_s} & \frac{\sigma_s \partial k_2}{k_2 \partial \sigma_s} & \cdots & \frac{\sigma_s \partial k_y}{k_y \partial \sigma_s} \end{pmatrix}$$

ENDF/B-VII.1 Covariances

- Dominant 20 reactions available were included

Nuclide-reaction/energy (s)	Nuclide-reaction
1–238	^{1}H(n,γ)
239–476	^{1}H(n,elastic)
477–714	C(n,γ)
715–952	C(n,elastic)
953–1190	^{16}O(n,γ)
1191–1428	^{16}O(n,elastic)
1429–1666	^{19}F(n,γ)
1667–1904	^{19}F(n,elastic)
1905–2142	^{19}F(n,inelastic)
2143–2380	^{235}U(n,γ)
2381–2618	^{235}U(n,2n)
2619–2856	^{235}U(n,F)
2857–3094	^{235}U(n,elastic)
3095–3332	^{235}U(n,inelastic)
3333–3570	^{235}U($\bar{\nu}$)
3571–3808	^{238}U(n,γ)
3809–4046	^{238}U(n,2n)
4047–4284	^{238}U(n,F)
4285–4522	^{238}U(n,elastic)
4523–4760	^{238}U(n,inelastic)

C_X



Kalman Filter Equations

- Minimisation of a combined error cost function

$$F^2 = (\Delta X) C_X^{-1} (\Delta X)^{\mathrm{T}} + (k_c + S\Delta X - k_b) C_Y^{-1} (k_c + S\Delta X - k_b)^{\mathrm{T}}$$

$$\Delta X = -\left(C_X S^{\mathrm{T}}\right)\left(C_Y + S C_X S^{\mathrm{T}}\right)^{-1}(k_c - k_b)$$

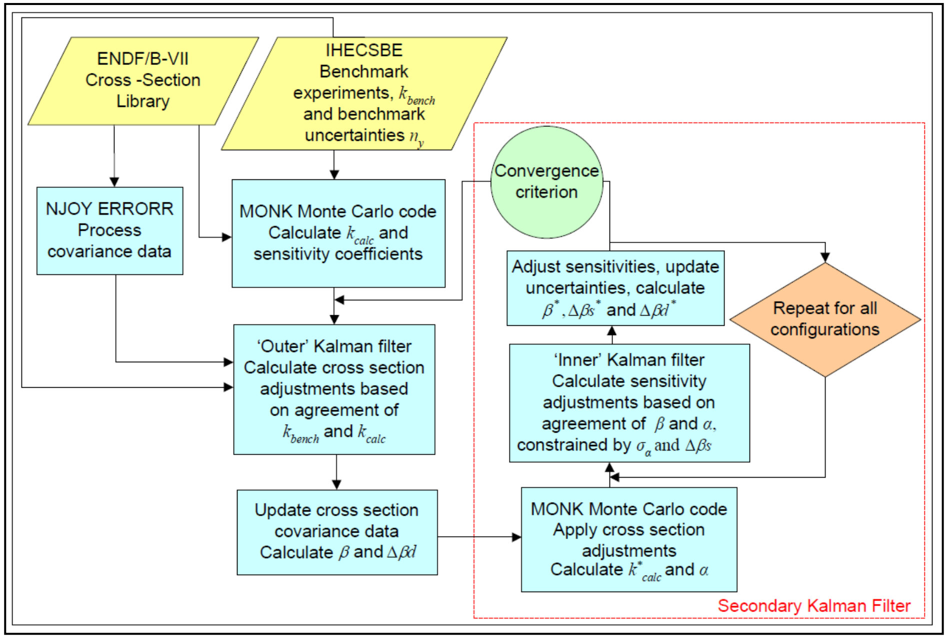
$$\Delta X = -K(k_c - k_b)$$

$$K = \left(C_X S^{\mathrm{T}}\right)\left(C_Y + S C_X S^{\mathrm{T}}\right)^{-1}$$

$$C_X^* = (I - K S_Y) C_X$$

$$\beta_Y = S_Y \Delta X$$

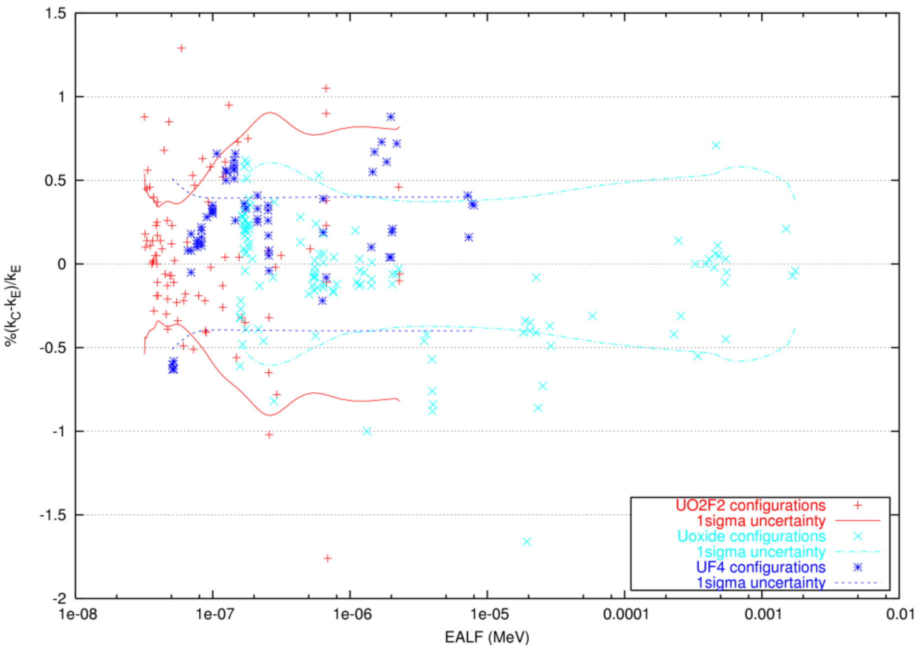
$$\Delta\beta d_Y = \sqrt{[S_Y C_X^* S_Y^{\mathrm{T}}]_{y,y}}$$



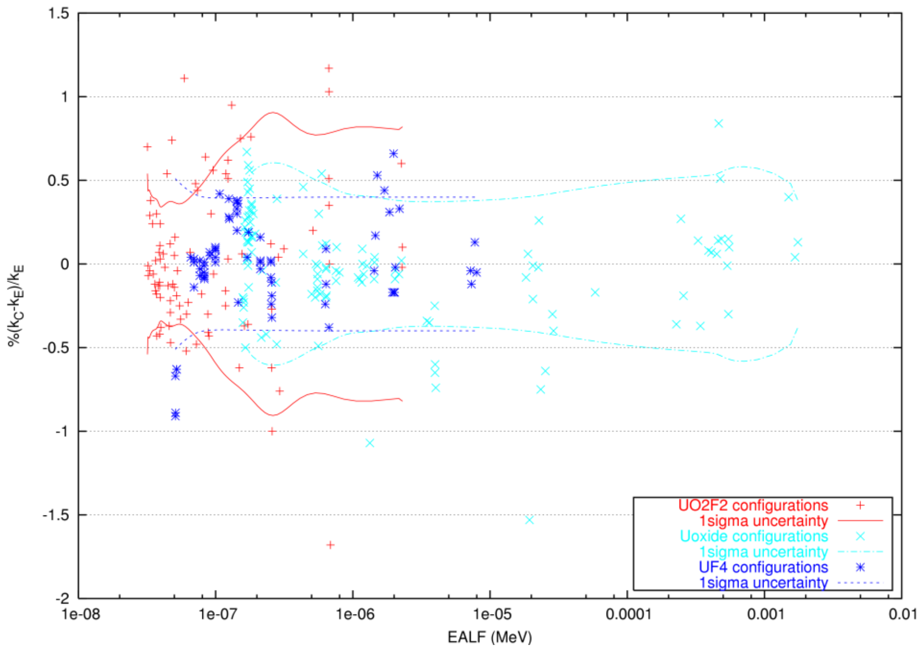
Posterior covariance and bias information

Improvement in (C-E)/E Distribution

- Reduction in RMS (*nσ*) deviation about 0
  - All cross section adjustments propagated



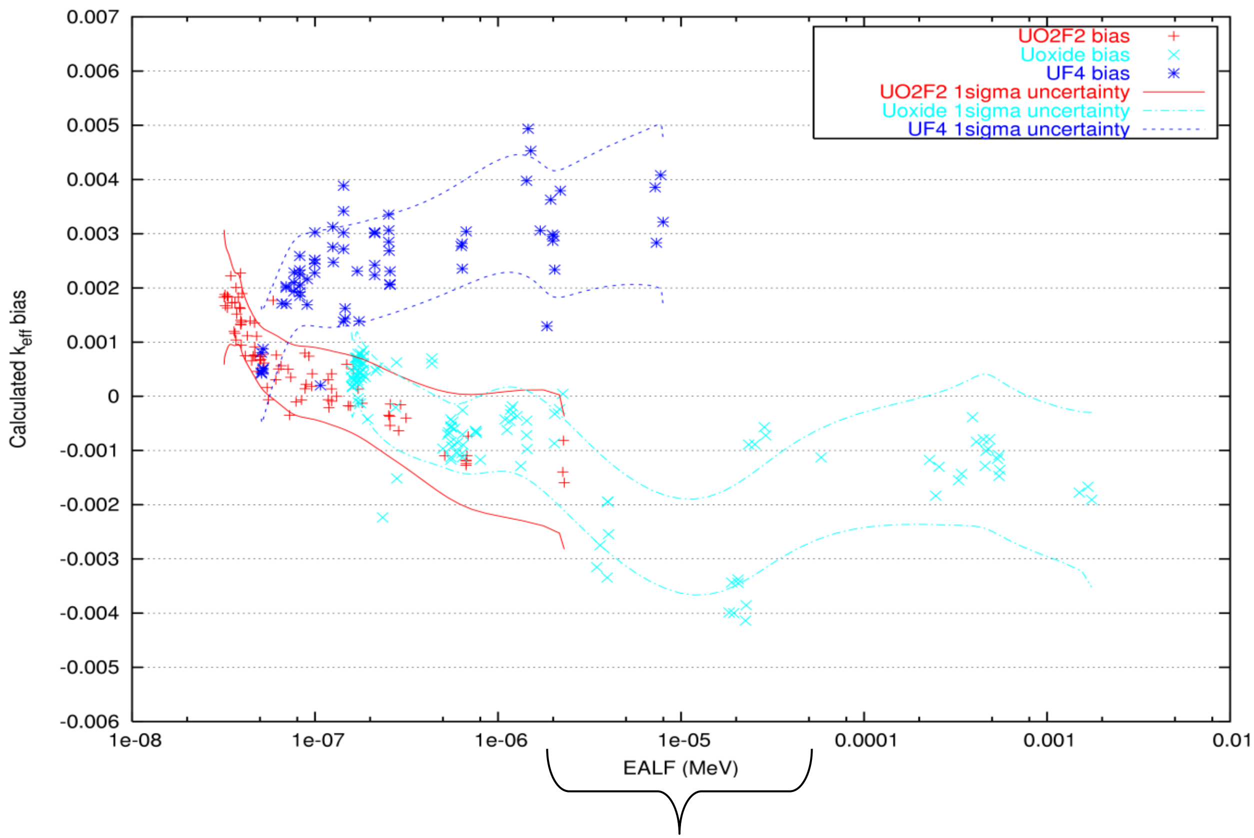
RMS=0.89 σ



RMS=0.74 σ

278 configurations

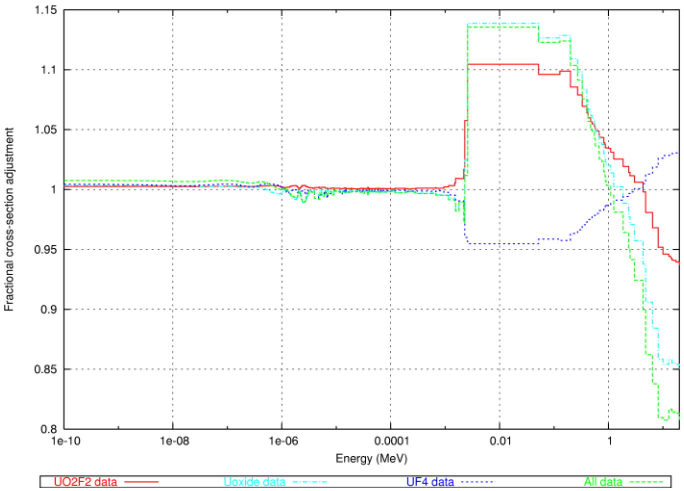
Configuration Biases and Bias Uncertainties



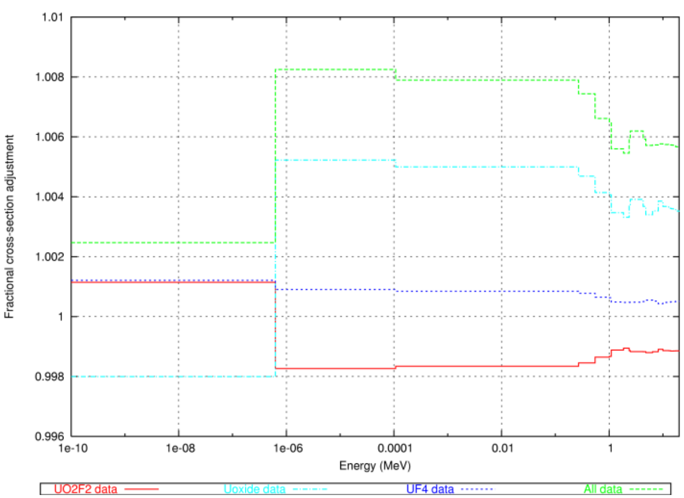
Region relatively sparse of any other integral data (~ 2-50 eV)

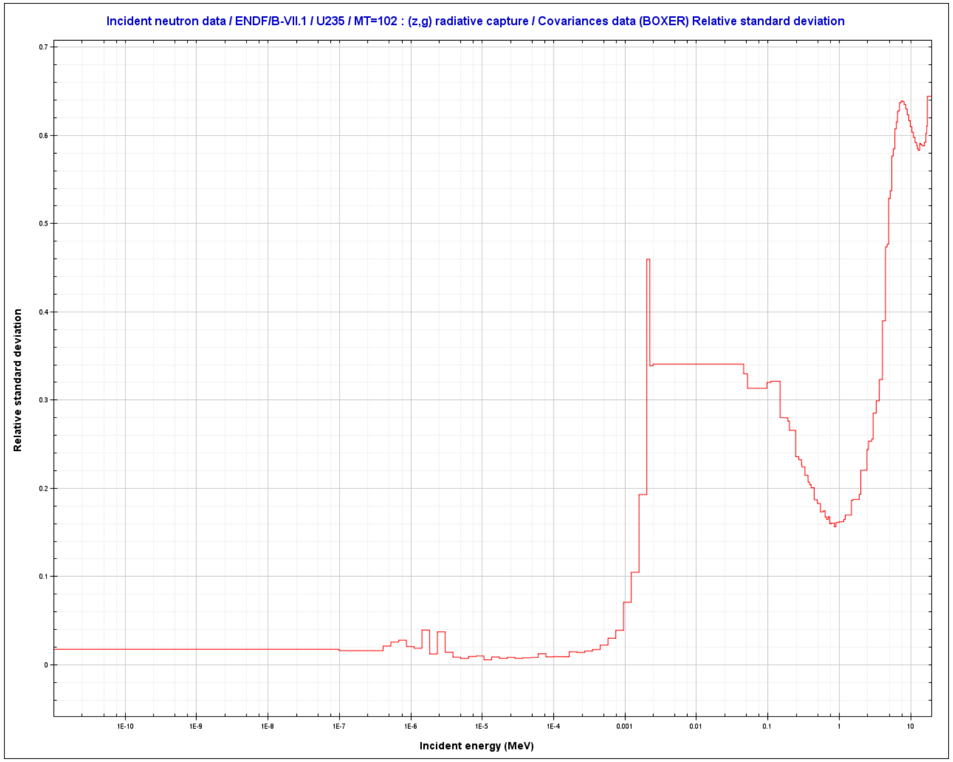
^{235}U Radiative Capture and Nubar

MT=102



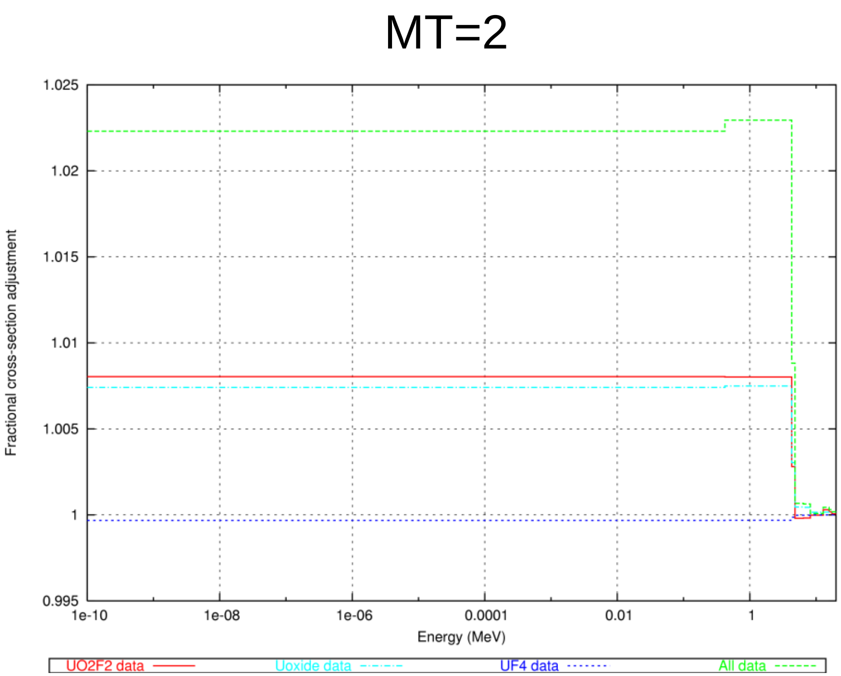
MT=452

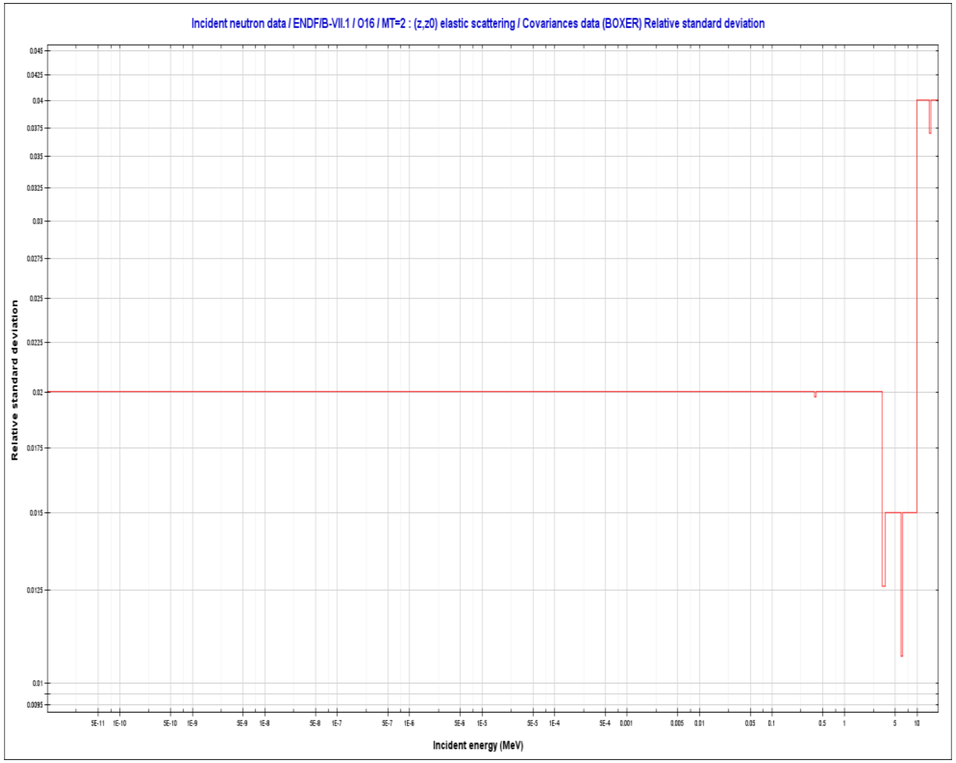




Inconsistency between sets of experiments

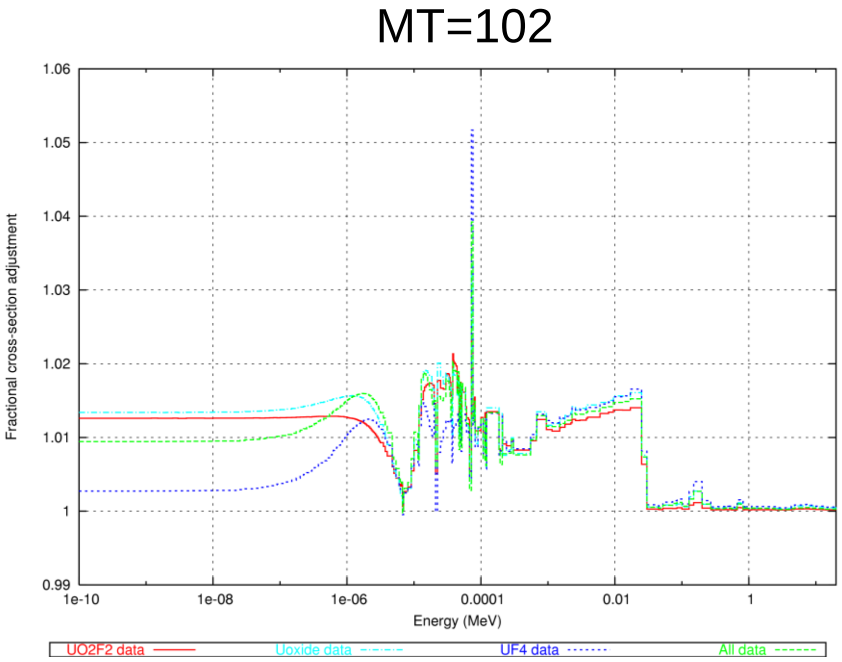
^{16}O Elastic Scatter

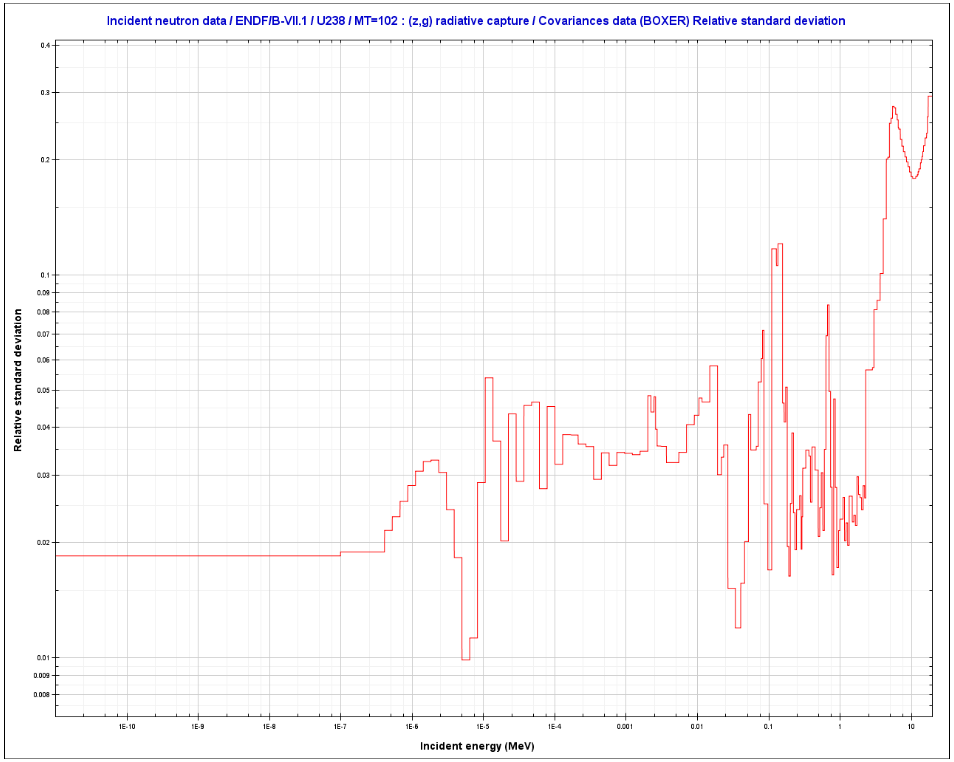




Based upon Caro (1998) cross section evaluation

^{238}U Radiative Capture





Based upon Derrien (2004) cross section evaluation

Included decrease of thermal capture cross section for thermal LEU systems

Conclusions

- Overall improvement in calculation-benchmark agreement when **all** adjustments are incorporated
  - Other parameters neglected – secondary angle/energy distributions
  - Generation of sensitivities and availability of covariance
- Can aid selection of basic data for light scattering nuclei as well as fissile isotopes
  - Compatibility with TMC method results
- Effect of assumed uncertainty correlations
  - EG UACSA Phase IV benchmark seeks to inform further
- Appropriate selection of experiments
  - Adjustment consistency issue
  - Provision of sufficient constraints on adjustable data

Thank you.

Questions?