On sensitivity analysis from first principles (D & ^{16}O neutron scattering)

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Nuclear Data @ BNL, USA

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Introduction (Motivation)

- Nuclear Data (ENDF) ($\mathbf{x}$ = (n,n), (n,γ), etc.)

  $\sigma_x(E) \pm \Delta\sigma_x(E)$, cross-section of reaction channel **x**, in barns

  For a nuclide A without explicit resonance parameters:

  E_j, $\sigma_{x,\,j}$ and E_k, $cov_{x,\,kk'}$ in the nuclear data file (ENDF)

  $(\Delta\sigma_x(E_j))^2 = cov_{x,\,kk}$ (E_j belongs to *k*-th energy bin (E_k ,E_{k+1}))

  Often relative covariance matrices are given,

  $cov_{x,\,kk'} \rightarrow cov_{x,\,kk'}/(\sigma_{x,k}*\sigma_{x,k'})$

  and, from $cov_{x,\,kk}$, we have $\Delta\sigma_x(E_j)/\sigma_x(E_j)$, the relative uncertainty, in %.

  When $\sigma_x(E) \rightarrow \sigma_x(E;T)$, for $\Delta\sigma_x(E;T)$, one can use $\Delta\sigma_x(E_j)/\sigma_x(E_j)$ obtained from $cov_{x,\,kk}$ given in the evaluated data file.

Introduction (Motivation)

- Reactor Physics: k_{eff} [$\sigma_x(E; T)$] , CVR [$\sigma_x(E; T)$], FTC [$\sigma_x(E; T)$]

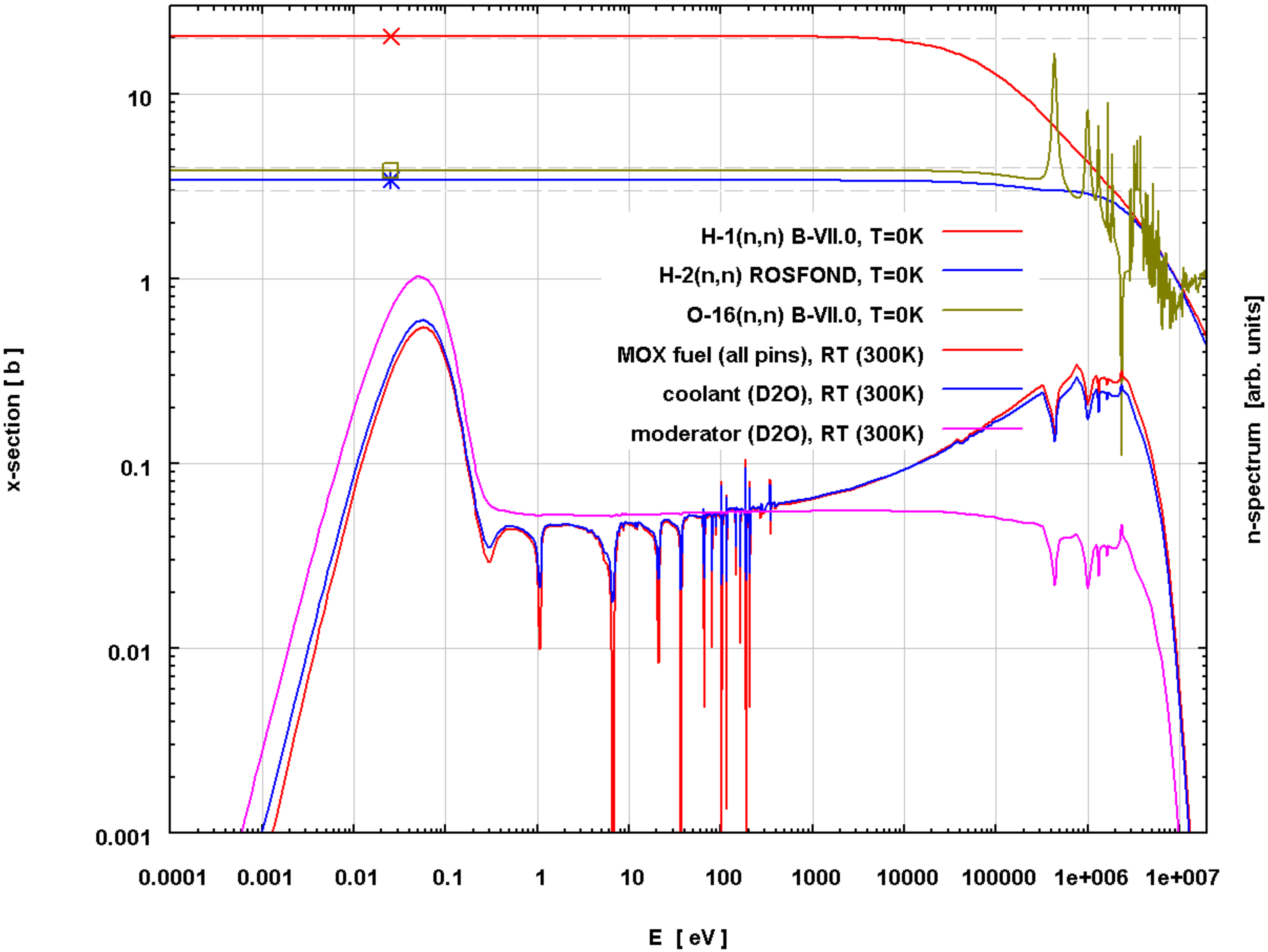
If we know $\Delta\sigma_x(E,T)/\sigma_x(E,T)$ from $cov_{x,\,kk}$ (= $\Delta\sigma_x(E_j)/\sigma_x(E_j)$, in %), then we have $\sigma_x(E,T) \pm \Delta\sigma_x(E,T)$ and ask what is the error propagation: $k_{eff} \pm \Delta k_{eff}$, CVR ± ΔCVR, etc.?

- Observation:

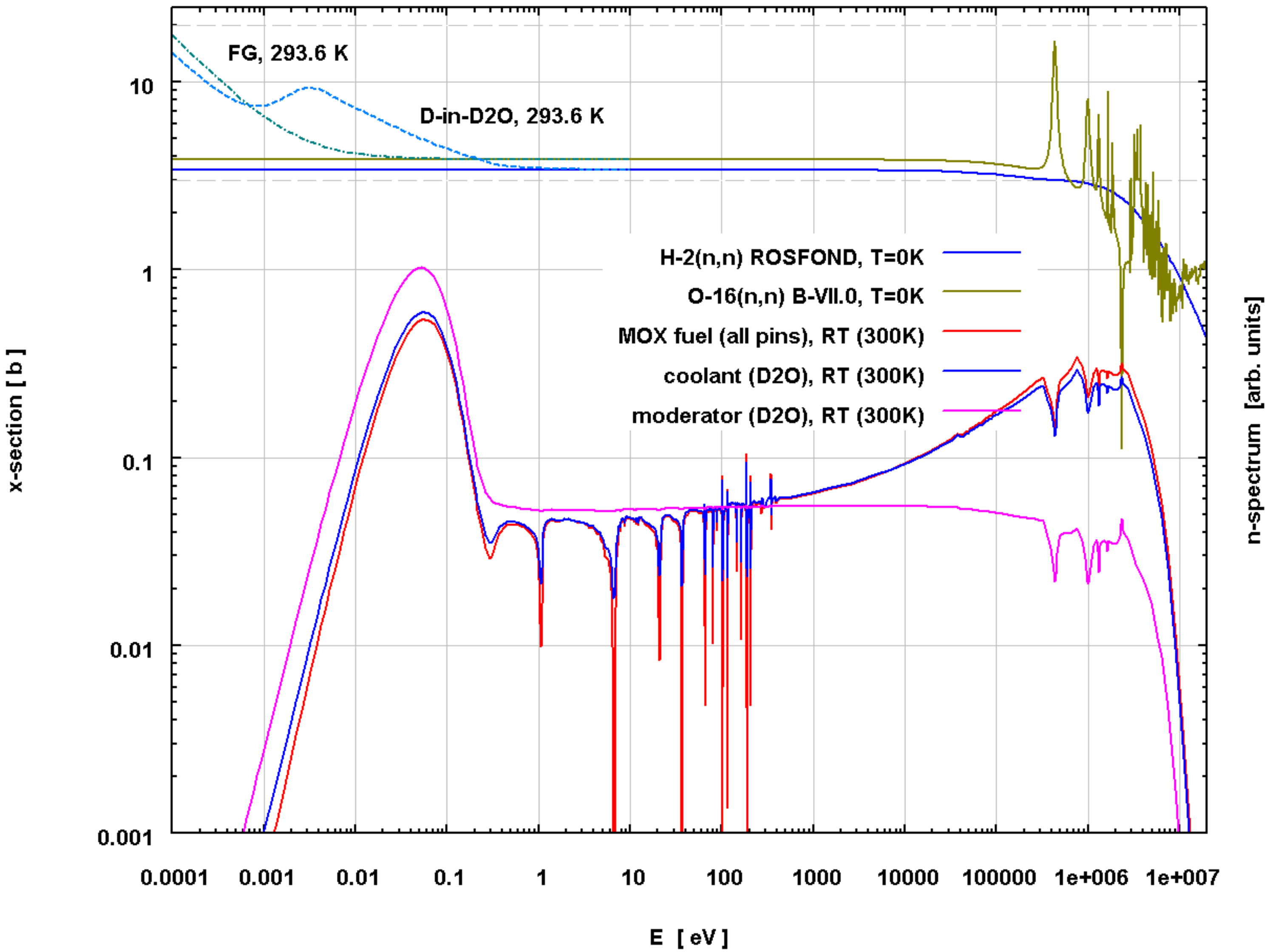
for many light nuclides (H, O, and C, N),
at low neutron energies (E < 1-10 **keV**),
$\sigma_x(E, T = 0\ K)$, x = (n,n), (n,γ), (n,α)
as σ_x vs. E, is simple (and structure-less):

$$\sigma_s(E, T = 0\ K) \sim \text{const} \quad \text{and} \quad \sigma_{n,\gamma}(E) \propto (E)^{½} .$$

Then one parameter, thermal cross section, $\sigma_{x,\,th} = \sigma_x(E = 0.0253\ eV)$, can be used to represent $\sigma_x(E, T)$ at low energies (and at any given T).



(Thermal) Neutron Spectrum of 37-el. bundle (MOX) in ZED-2
A(n,n)A x-sections at T = 0 K



(Thermal) Neutron Spectrum (MOX, ZED-2 reactor, CRL) and A(n,n)A x-sections at T=0 K and at room temperature

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Introduction (Motivation)

- For nuclide A, the **thermal** cross sections are well-known:
  $\sigma_{s,th} \pm \Delta\sigma_{s,th}$ (for scattering, this is T $\rightarrow$ 0 K value)
  $\sigma_{(n,\gamma),th} \pm \Delta\sigma_{(n,\gamma),th}$ (1/v behaviour is invariant under T broadening)

- For many light nuclides, $\sigma_x(E,T) \pm \Delta\sigma_x(E,T)$ is determined by $\sigma_{x,th} \pm \Delta\sigma_{x,th}$, at low neutron energies as E < 1-10 **keV**, i.e., $\sigma_x(E,T)[\,\sigma_{x,th}\,]$

- Reactor Physics: $k_{eff}\,[\,\sigma_x(E;T)\,[\,\sigma_{x,\,th}\,]\,] = k_{eff}\,(\,\sigma_{x,th}\,)$, a function (?), for example, $k_{eff} = k_{eff}\,(\,\sigma_{s,th}, \sigma_{(n,\gamma),th}\,)$

  we can address $\sigma_{x,th} \pm \Delta\sigma_{x,th} \rightarrow k_{eff} \pm \Delta k_{eff}$, $k_{eff} = k_{eff}\,[\,\sigma_x(E;T)\,]$

  if, for a given nuclide, we can calculate **k_{eff} vs. $\sigma_{s,th}$** and **k_{eff} vs. $\sigma_{(n,\gamma),th}$** (and without applying any perturbation theory to neutron transport equation)

Introduction (Motivation)

For a given nuclide A, we propose to construct a set of
trial evaluated nuclear data files
with different $\sigma_{s,th}$ and $\sigma_{(n,\gamma),th}$ chosen from the interval
$(\sigma_{s,th} - 2\Delta\sigma_{s,th}, \sigma_{s,th} + 2\Delta\sigma_{s,th})$ and $(\sigma_{(n,\gamma),th} - 2\Delta\sigma_{(n,\gamma),th}, \sigma_{(n,\gamma),th} + 2\Delta\sigma_{(n,\gamma),th})$

Then we convert each trial ENDF file to the ACE file (at a given non-zero T),
and run an MCNP case (full core / reactor lattice / …) for each trial ACE data file.
We obtain $\mathbf{k_{eff}(\sigma_{s,th}, \sigma_{(n,\gamma),th})}$ on a grid of thermal x-sections (for a nuclide A).

For H-2 and O-16, we have:

$$\sigma_{(n,\gamma),th} \ll \sigma_{s,th}$$

H-2: 0.508 ± 0.015 mb (±2.95%) << 3.390 ± 0.012 b (±0.35%) (Atlas-2006)

O-16: 0.190 ± 0.019 mb (±10.0%) << 3.761 ± 0.006 b (±0.16%) (Atlas-2006)

H-2: $\sigma_{(n,\gamma)}(E) < 10^{-3}$ b $\equiv$ 1 mb at all $E > 10^{-2}$ eV ($E_{th} = 0.0253$ eV)
O-16: $\sigma_{(n,\gamma)}(E) < 10^{-3}$ b $\equiv$ 1 mb at all $E > 10^{-3}$ eV,
we "fix" $\sigma_{(n,\gamma),th}$ (and so $\sigma_{(n,\gamma)}(E)$ at low E) and concentrate on $\mathbf{k_{eff} = k_{eff}(\sigma_{s,th})}$

Problems with thermal x-sections for H-2 and O-16

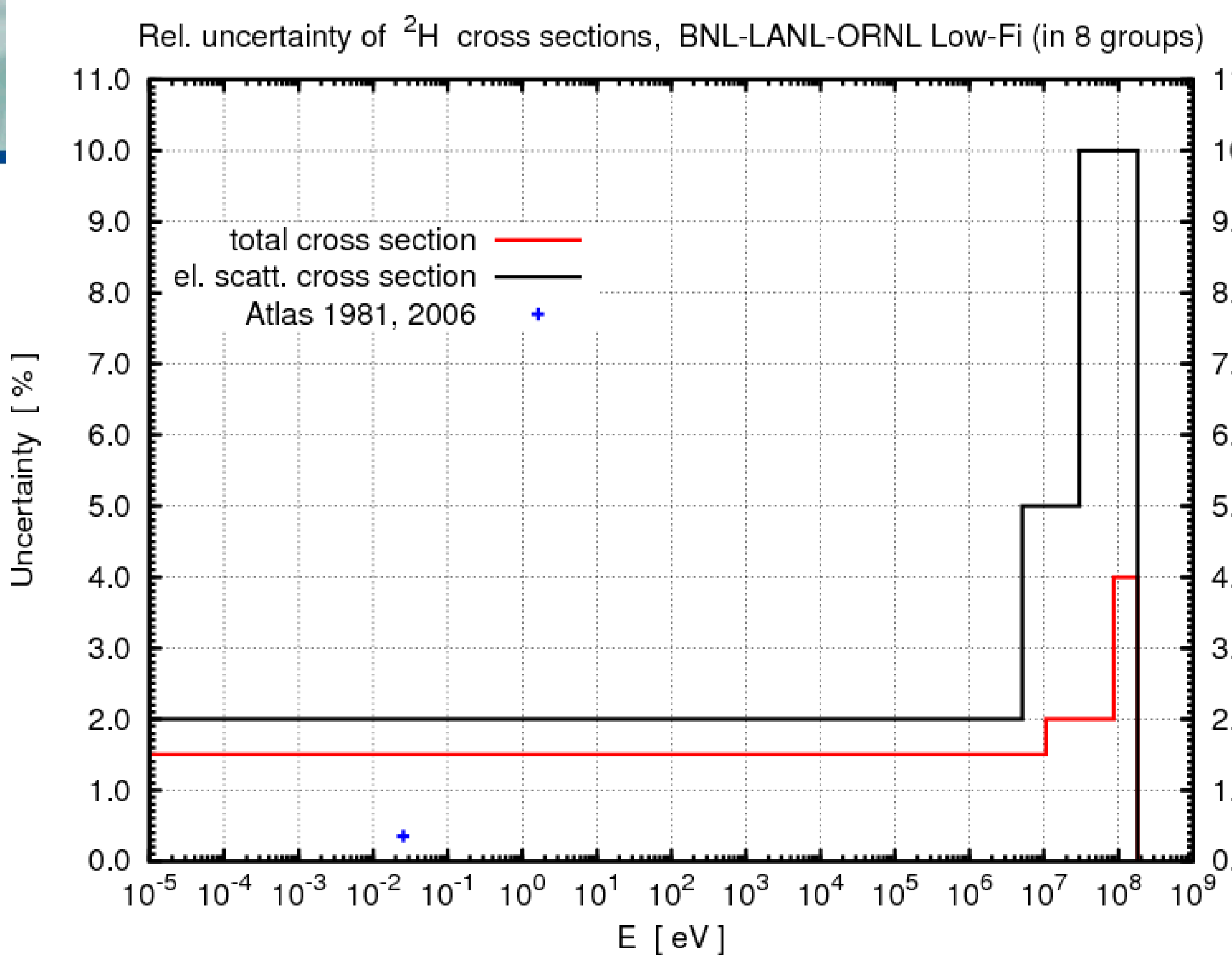
H-2: $\sigma_{s,th}$ = 3.390 ± 0.012 b (±0.35%), Atlas- 2006
$\sigma_{tot,th}$ = 3.3905 ± 0.0120 b (±0.35%), estimated by us from Atlas

$\sigma_{s,th}$ = 3.3950 ± 0.068 b (±2.0%) (ENDF/B-VII.1beta)
$\sigma_{tot,th}$ = 3.3955 ± 0.051 b (±1.5%) (ENDF/B-VII.1beta)

O-16: $\sigma_{s,th}$ = 3.761 ± 0.006 b (±0.16%) Atlas- 2006
$\sigma_{tot,th}$ = 3.7612 ± 0.006 b (±0.16%), estimated by us from Atlas

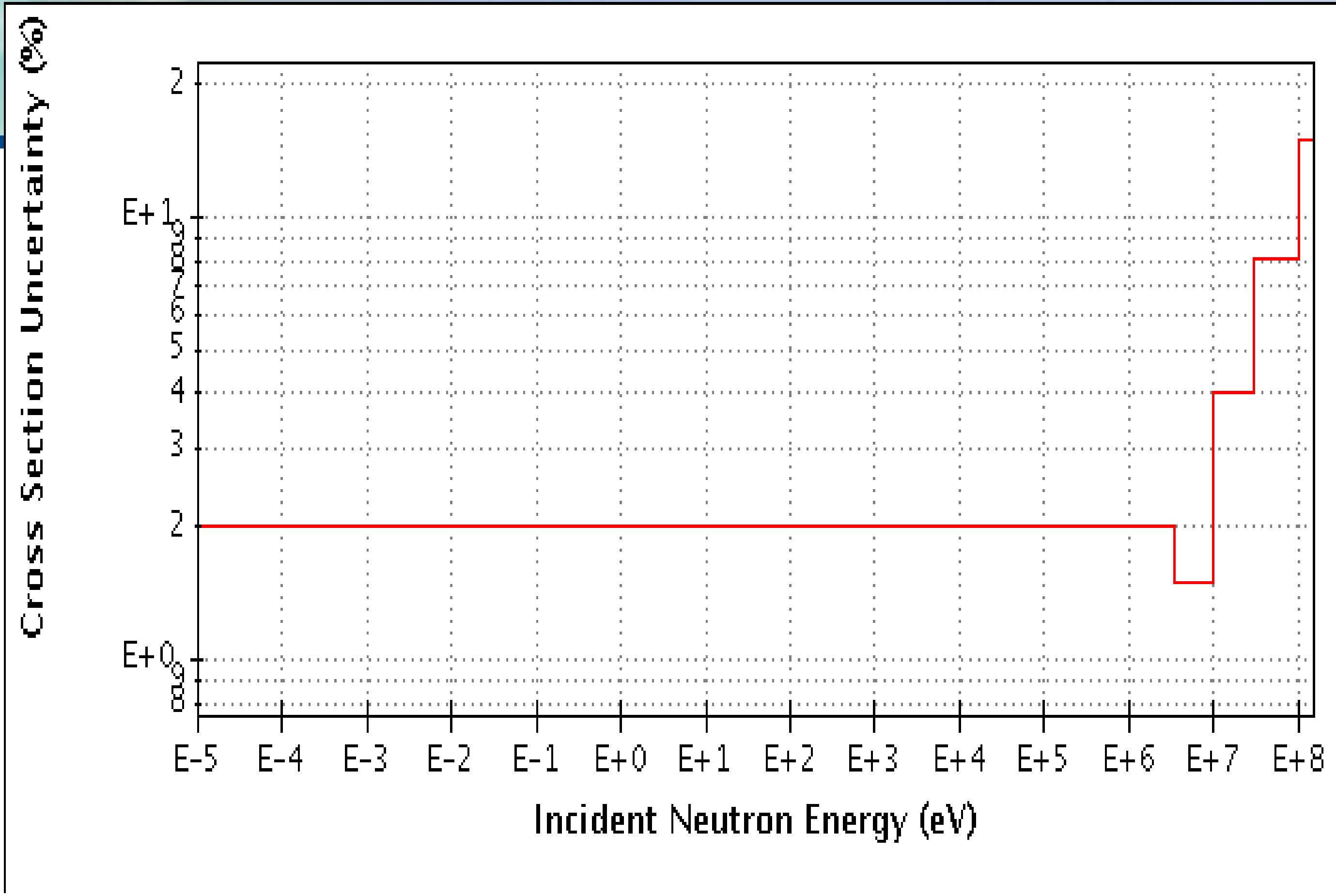
$\sigma_{s,th}$ = 3.85181 ± 0.077 b (±2.0%) (ENDF/B-VII.1beta)
$\sigma_{tot,th}$ = 3.85200 ± 0.077 b (±2.0%) (ENDF/B-VII.1beta;
Optical Theorem at $E \rightarrow 0$ (?))

$\sigma_{s,th}$ = 3.8408 ± 0.038 b (±1.0%) (JENDL 4.0 total is ±1.0%)

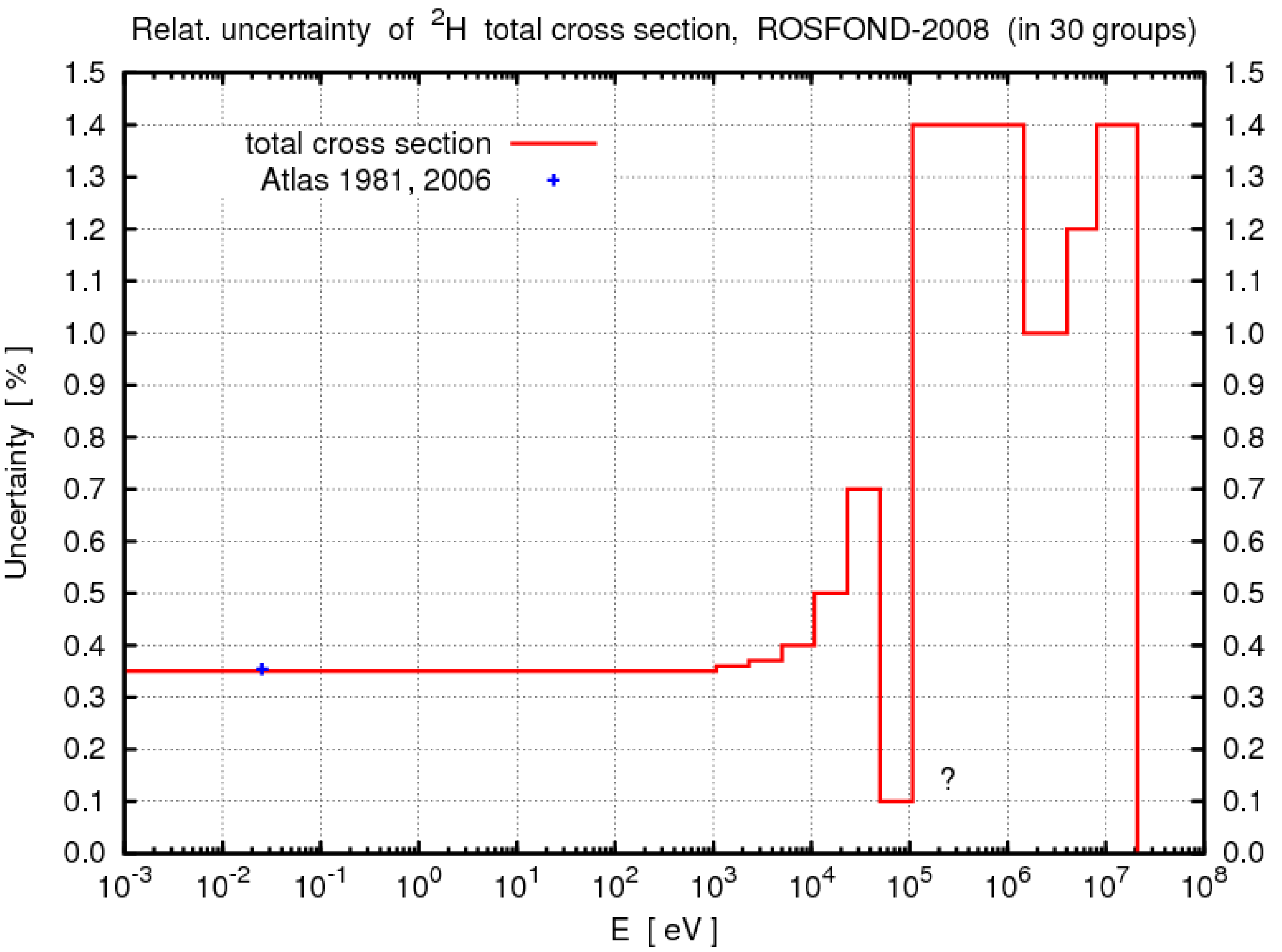


H-2: relative uncertainty of σ_{tot} and σ_s in BOLNA Low-Fidelity library, now in H-2 covariance file in ENDF/B-VII.1beta

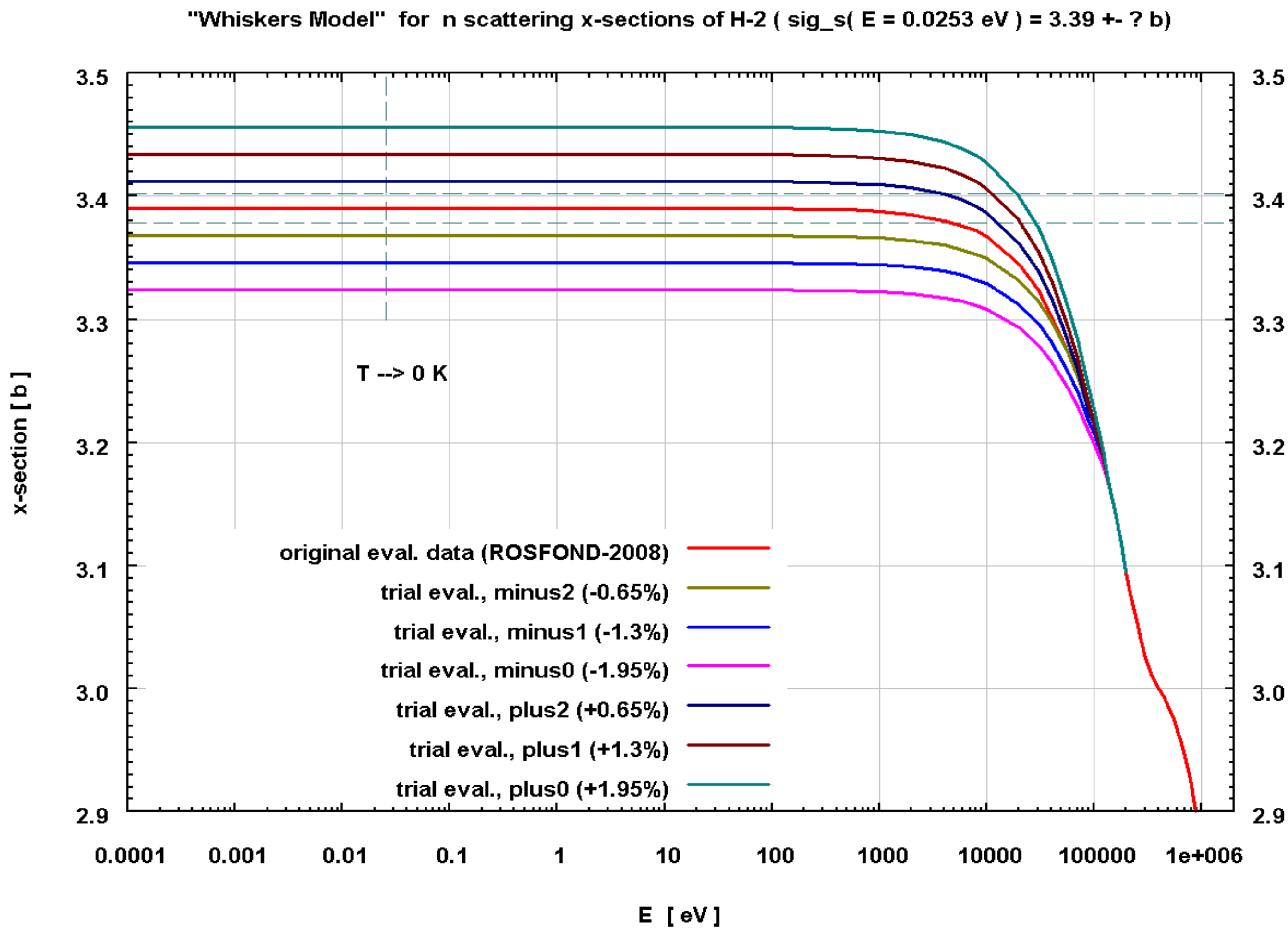
At 10^{-2} eV < E < 3.3 MeV, $\sigma_{tot}(E) \approx \sigma_s(E)$ for deuterium, but $\Delta\sigma_s/\sigma_s \approx 1.3*\Delta\sigma_{tot}/\sigma_{tot}$ in BOLNA (?)



O-16: relative uncertainty of $\sigma_s(E)$,
from O-16 covariance file in ENDF/B-VII.1beta4,
± 2% at E < 1 MeV
± 1% at E < 1 MeV (JENDL 4.0, JENDL 3.3)

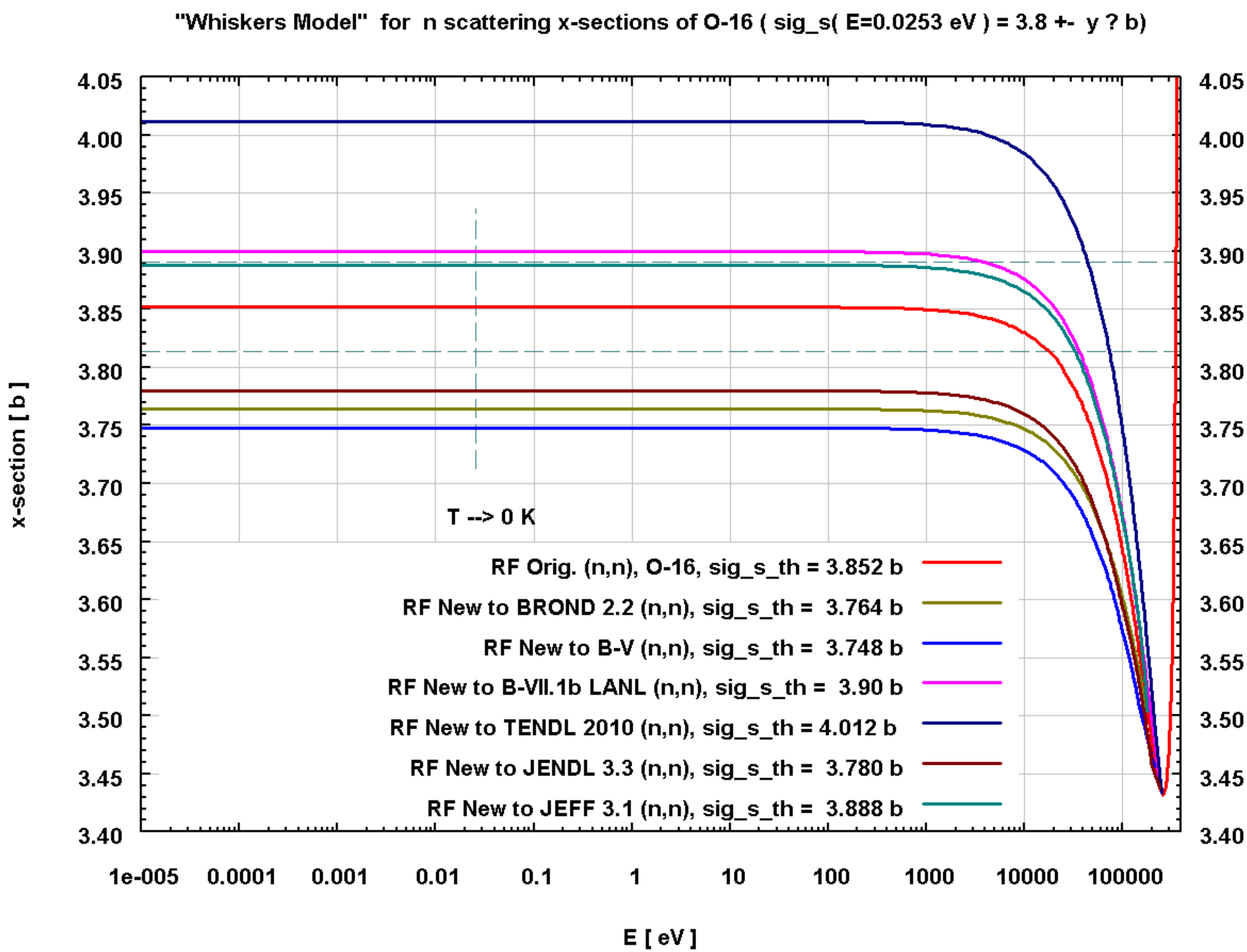


H-2: relative uncertainty of σ_{tot} in ROSFOND-2008, and $\Delta\sigma_s/\sigma_s \approx \Delta\sigma_{tot}/\sigma_{tot}$ at E < 3 MeV.



σ_s(E) for ^{2}H(n,n)^{2}H reaction in our trial nuclear data files at low energies (T $\rightarrow$ 0 K, E < 0.2 MeV): "Whiskers model"

To address the propagation of uncertainty of $\sigma_{s,\,th} = \sigma_s$(E = 0.0253 eV, T= 0 K) of a light nuclide to k_{eff} of critical assemblies/nuclear reactors, a **method of trial evaluations** (*replica method*) can be used; any trial σ_s(E; T= 0 K) is a continuous function of E.



$\sigma_s(E)$ for $^{16}O(n,n)^{16}O$ reaction in our trial nuclear data files, $T \rightarrow 0$ K, $E < 0.3$ MeV $< E_n = 0.43$ MeV: "Whiskers model"

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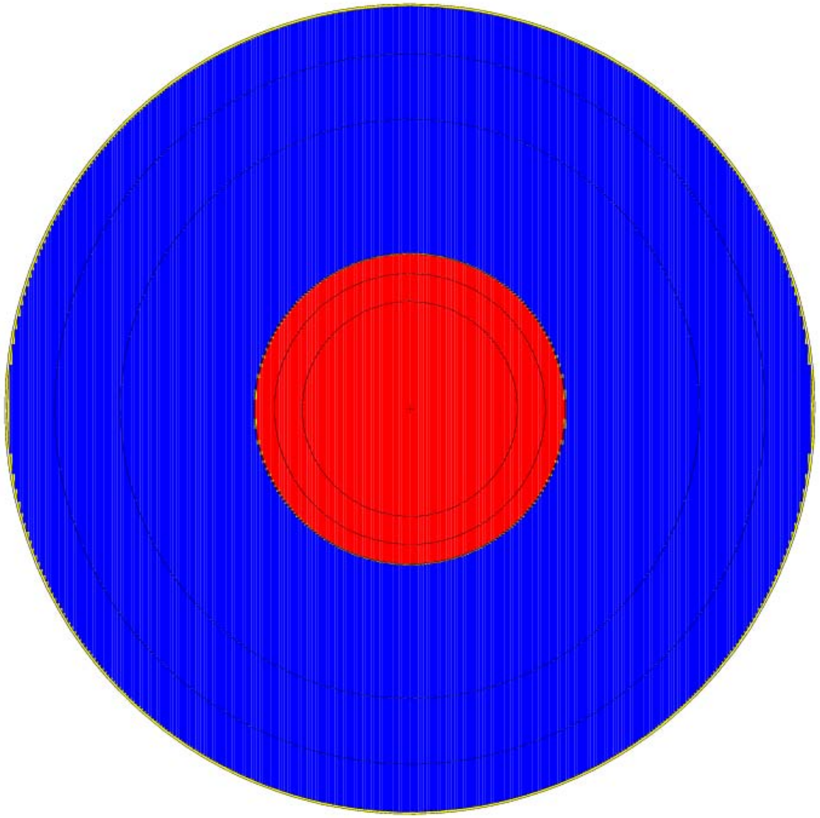
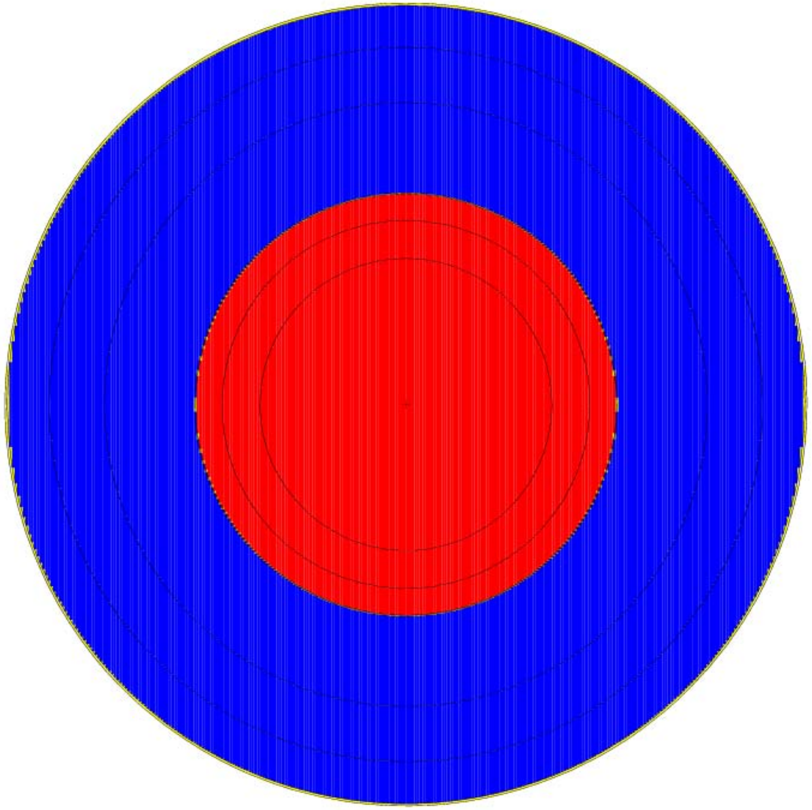
HEU-SOL-THERM-004 benchmark: highly enriched U solution in SS sph., reflector: D_2O





case 1, n(D)/n(U-235) ≈ 34
$R_1 \approx 17$ cm, $R_2 \approx 44$ cm, at RT

case 6, n(D)/n(U-235) ≈ 430
$R_1 \approx 23$ cm, $R_2 \approx 44$ cm, at RT

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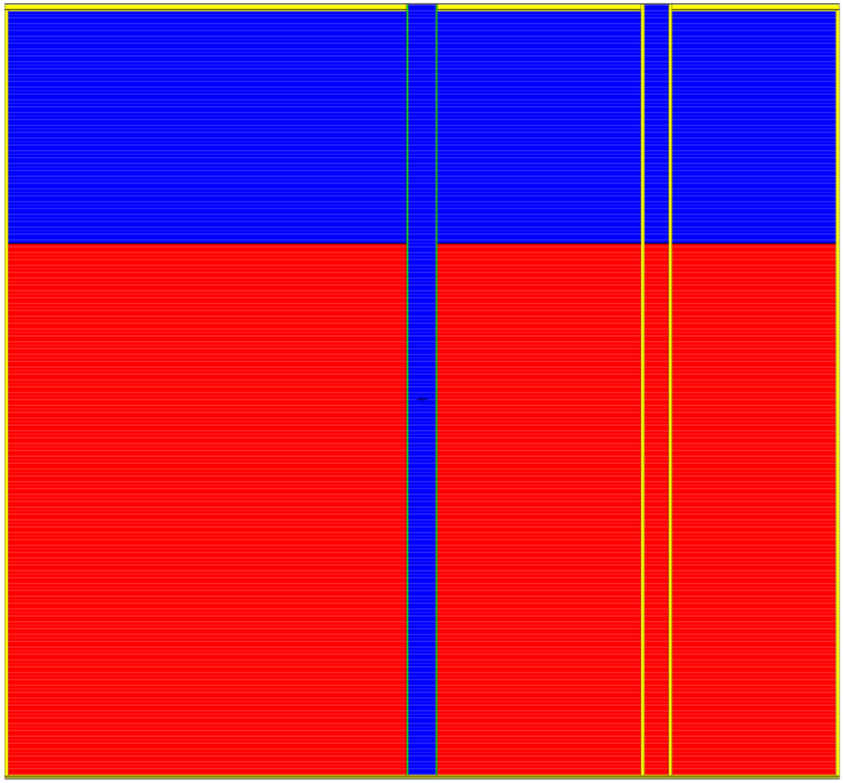
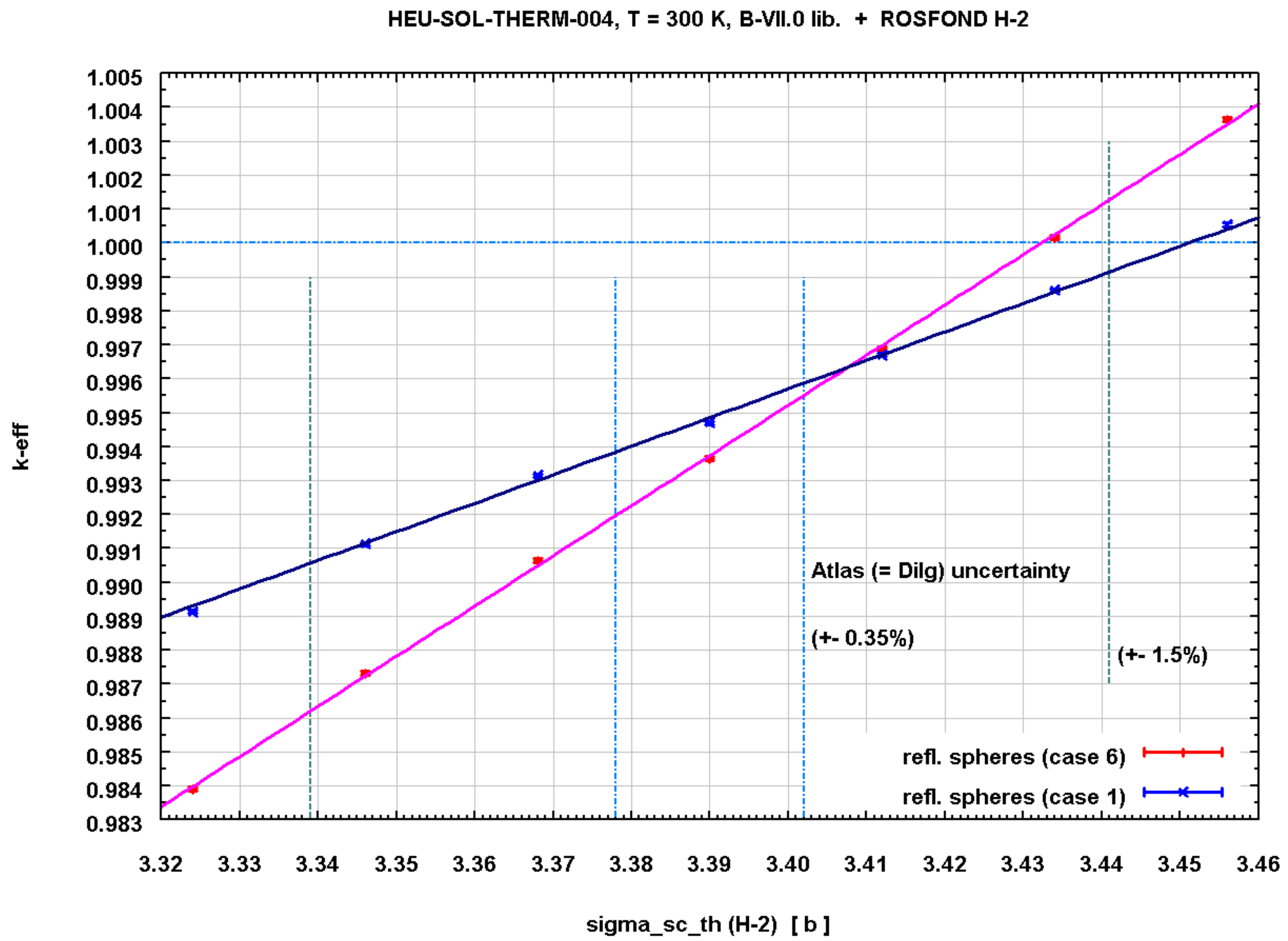
UO_2F_2 & D_2O

HEU-SOL-THERM-020 benchmark: highly enriched U solution (UO_2F_2) in SS cylinder

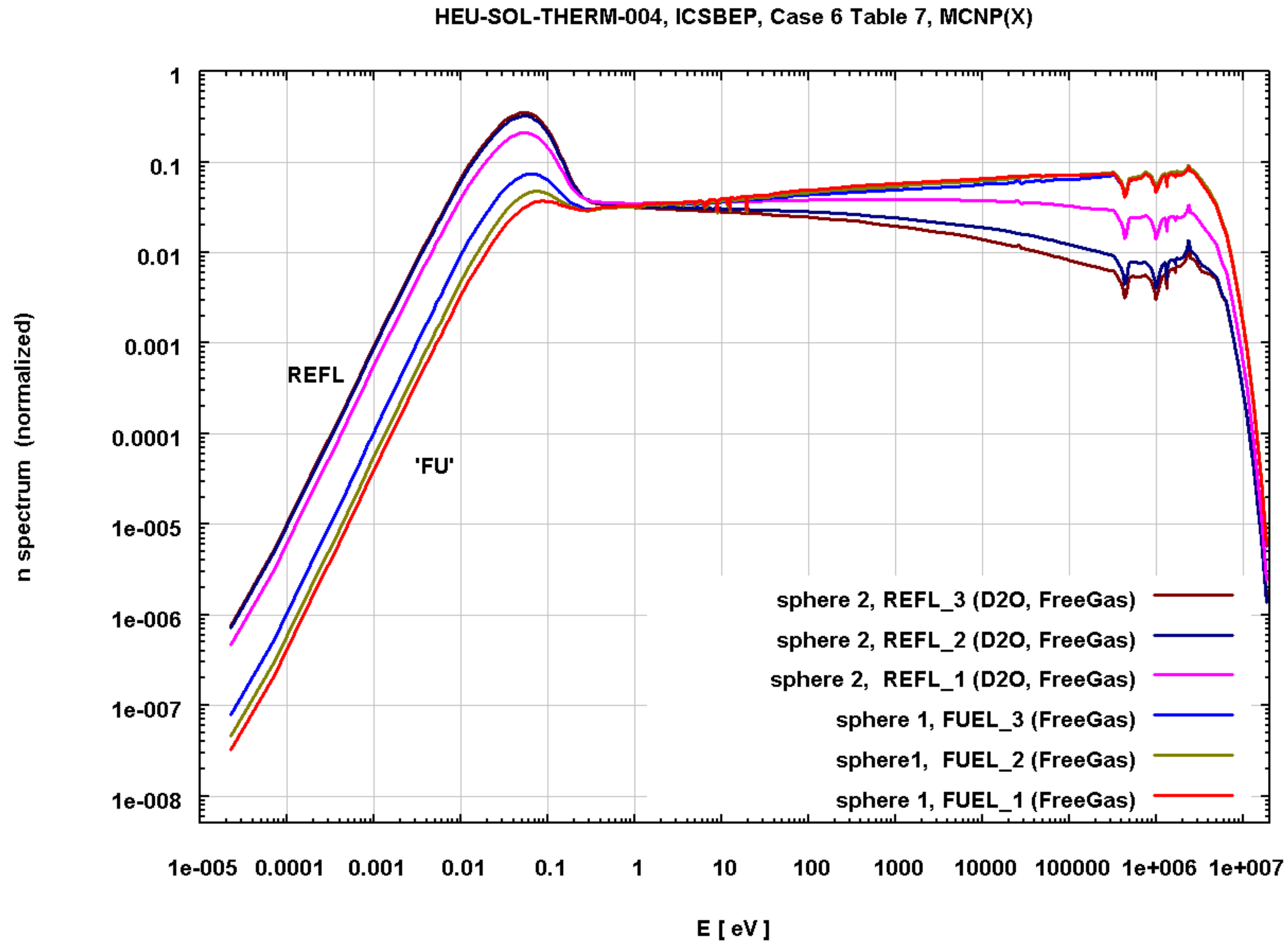


- case 5: n(D)/n(U-235) = 2081 in solution

  $R_1 \approx 1.4$ cm, $R_2 \approx 38$ cm, $H_{cr} \approx 84.7$ cm



^2H: k_{eff} vs. $\sigma_{s,\,th} = \sigma_s(E= 2.53*10^{-2}$ eV, $T = 0$ K)
using "Whiskers model" for $\sigma_s(E, T = 0$ K),
MCNP5 results, HEU-SOL-THERM benchmarks (spheres).



Neutron spectrum of 'case 6' of HEU-SOL-THERM-004

$R_1 \approx 23$ cm, $R_2 \approx 44$ cm, U-235 = 93.7% (at)

n(D)/n(U235) = 430 (in sphere 1 of R_1)

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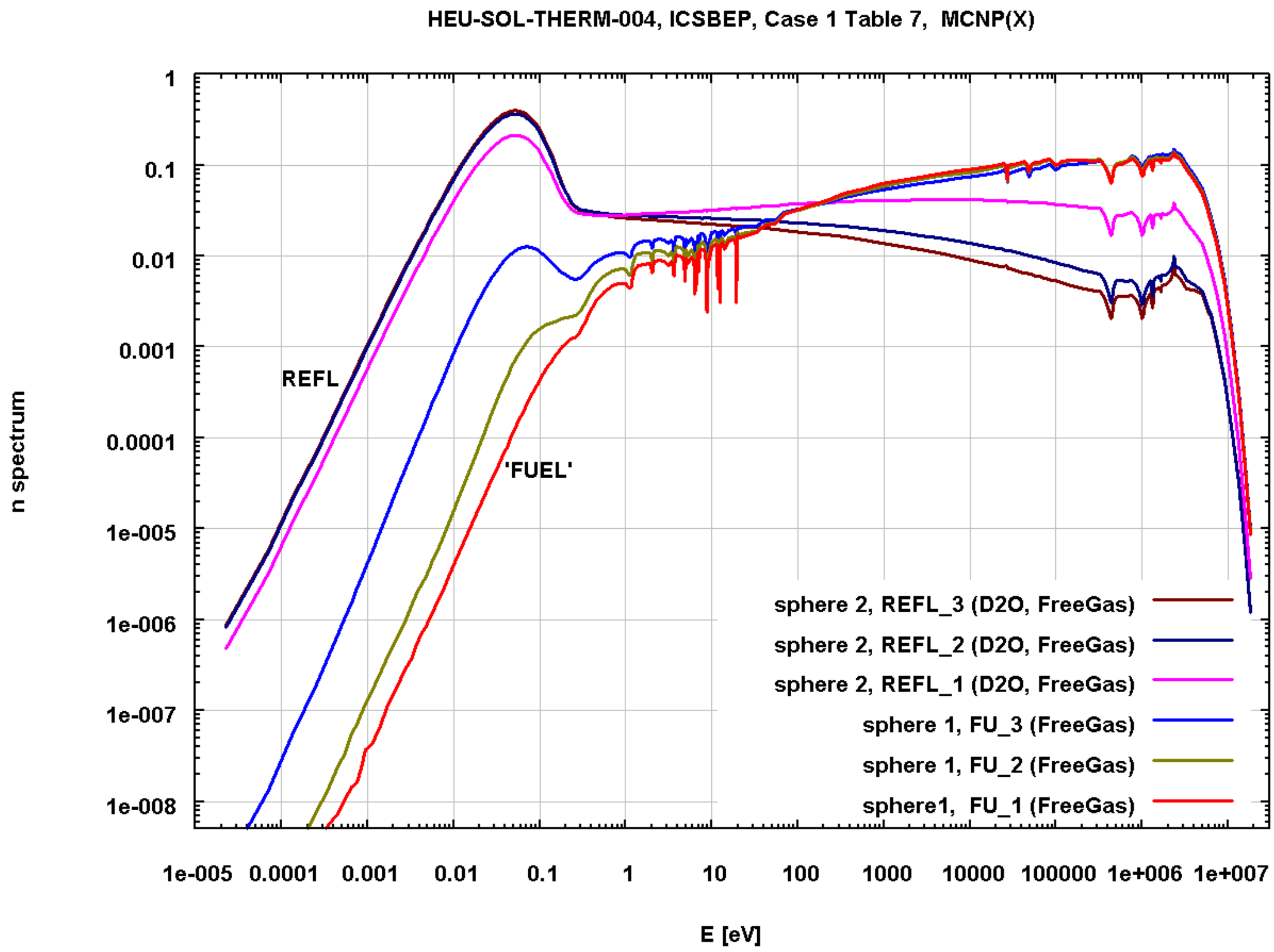
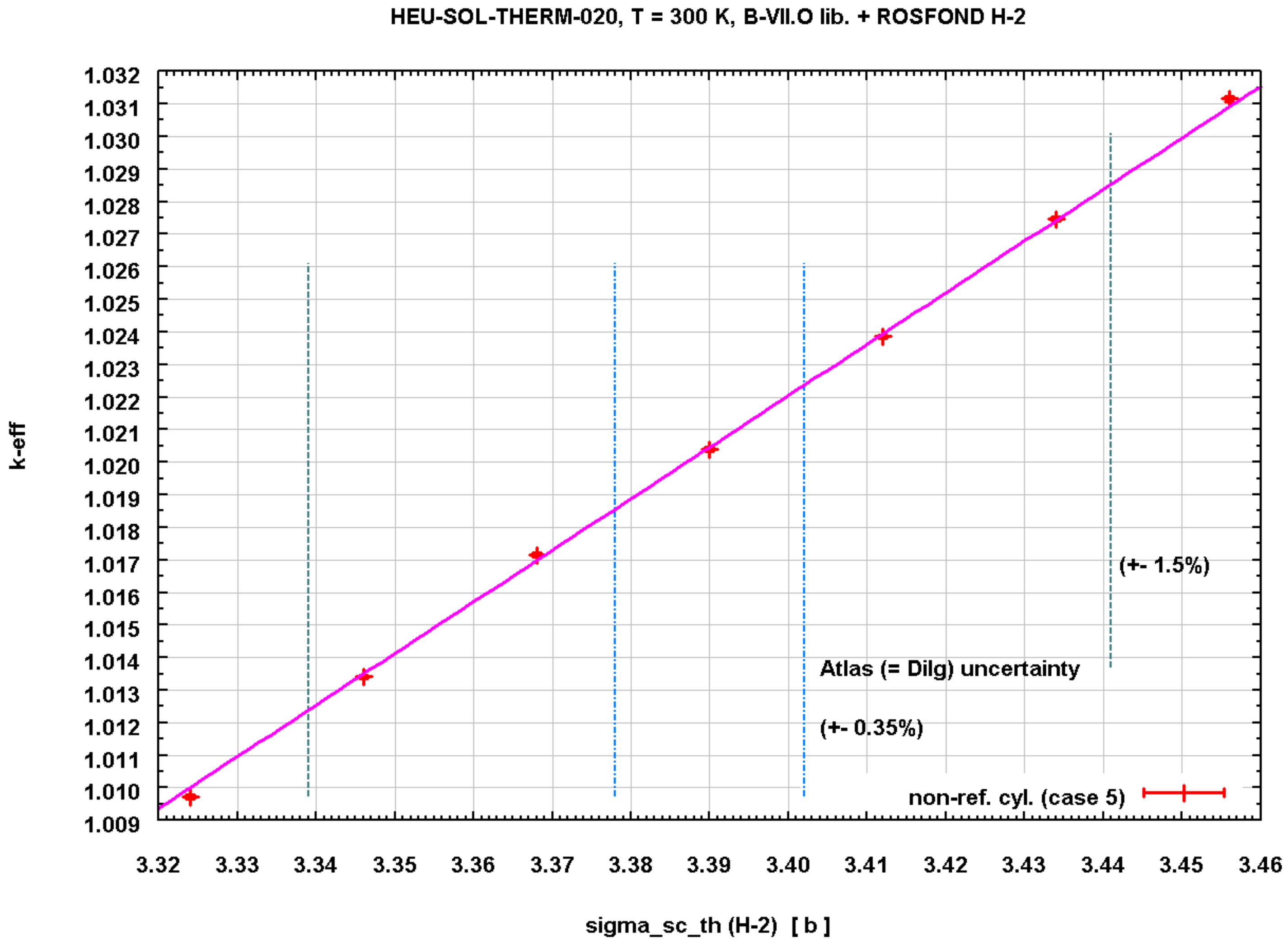


Neutron spectrum of 'case 1' of HEU-SOL-THERM-004

R_1 ≈17 cm, R_2 ≈ 44 cm, U-235 = 93.7 (at%)

n(D)/n(U235) = 34 (in sphere 1 of R_1)



k_{eff} *vs.* $\sigma_{s,\,th} = \sigma_s(\,E = 2.53*10^{-2}$ eV, T = 0 K) of ^{2}H,
using "Whiskers model" for ^{2}H,
MCNP5 results, HEU-SOL-THERM benchmarks: non-reflected cylinder(s))

case 5: U-235 = 93.7 % (at), n(D)/n(U-235) = 2085 (in solution)

Sensitivity to thermal scattering x-section (H-2)

- $k_{eff} = k_{eff}[\ \sigma_s(E;T)\ ] \rightarrow k_{eff} = k_{eff}(\ \sigma_{s,\,th}\ )$, one-parameter model

H-2:

$k_{eff} = k_{eff}(\ \sigma_{s,\,th}\ )$ is a **linear function** of $\sigma_{s,\,th}$ within $\Delta\sigma_{s,\,th}/\sigma_{s,\,th} \approx \pm 1.5\%$ near $\sigma_{s,\,th} = 3.390$ b (the reference value for ^2H)

$$k_{eff} \approx a * \sigma_{s,\,th} + b$$

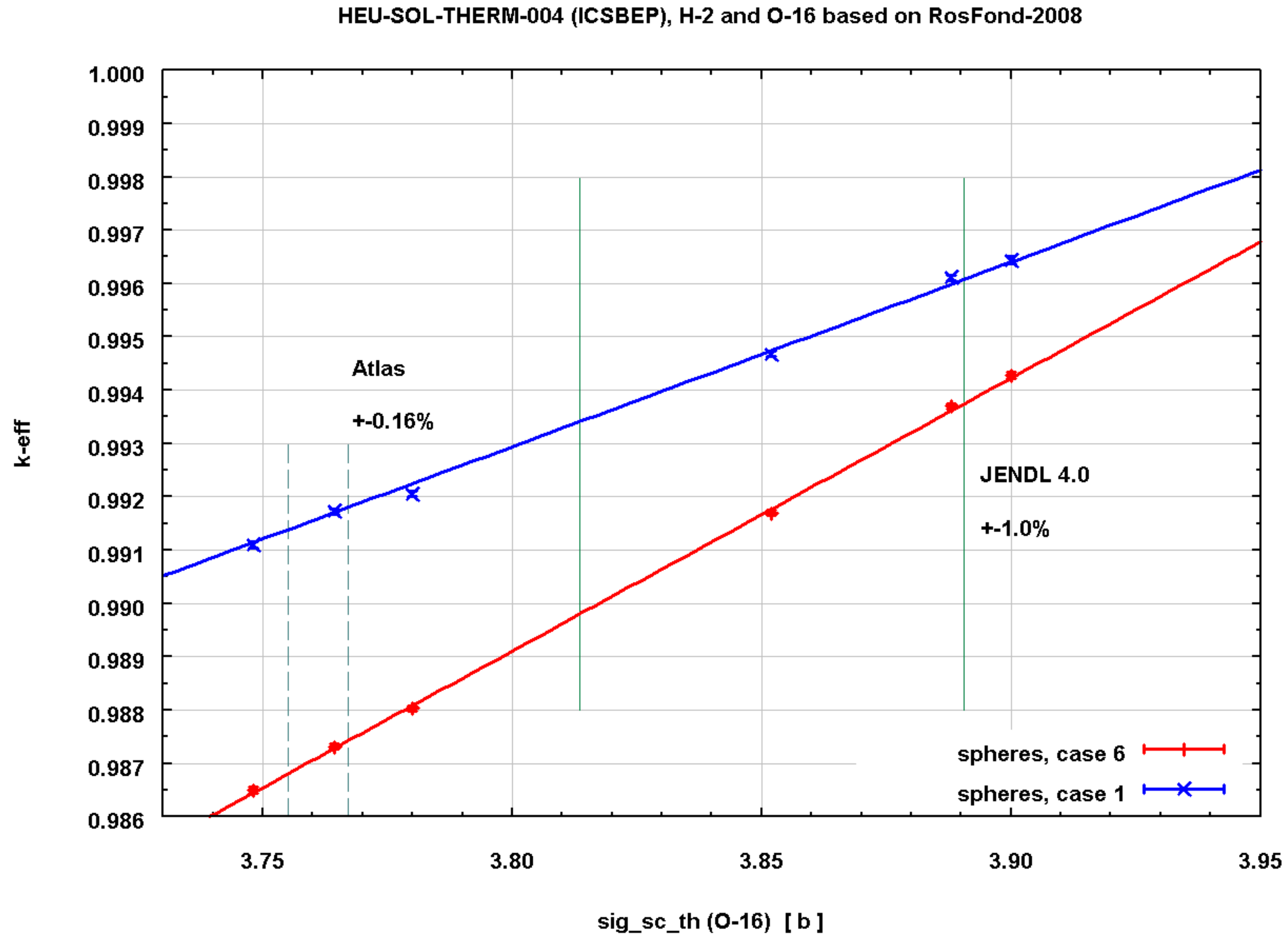
Sensitivity to $\sigma_{s,\,th}$ (dimensional) =
change in k_{eff} per 1% change in $\sigma_{s,\,th}$, in *mk per percent* or *pcm per percent*

Results for reflected spheres (HEU-SOL-THERM-004):

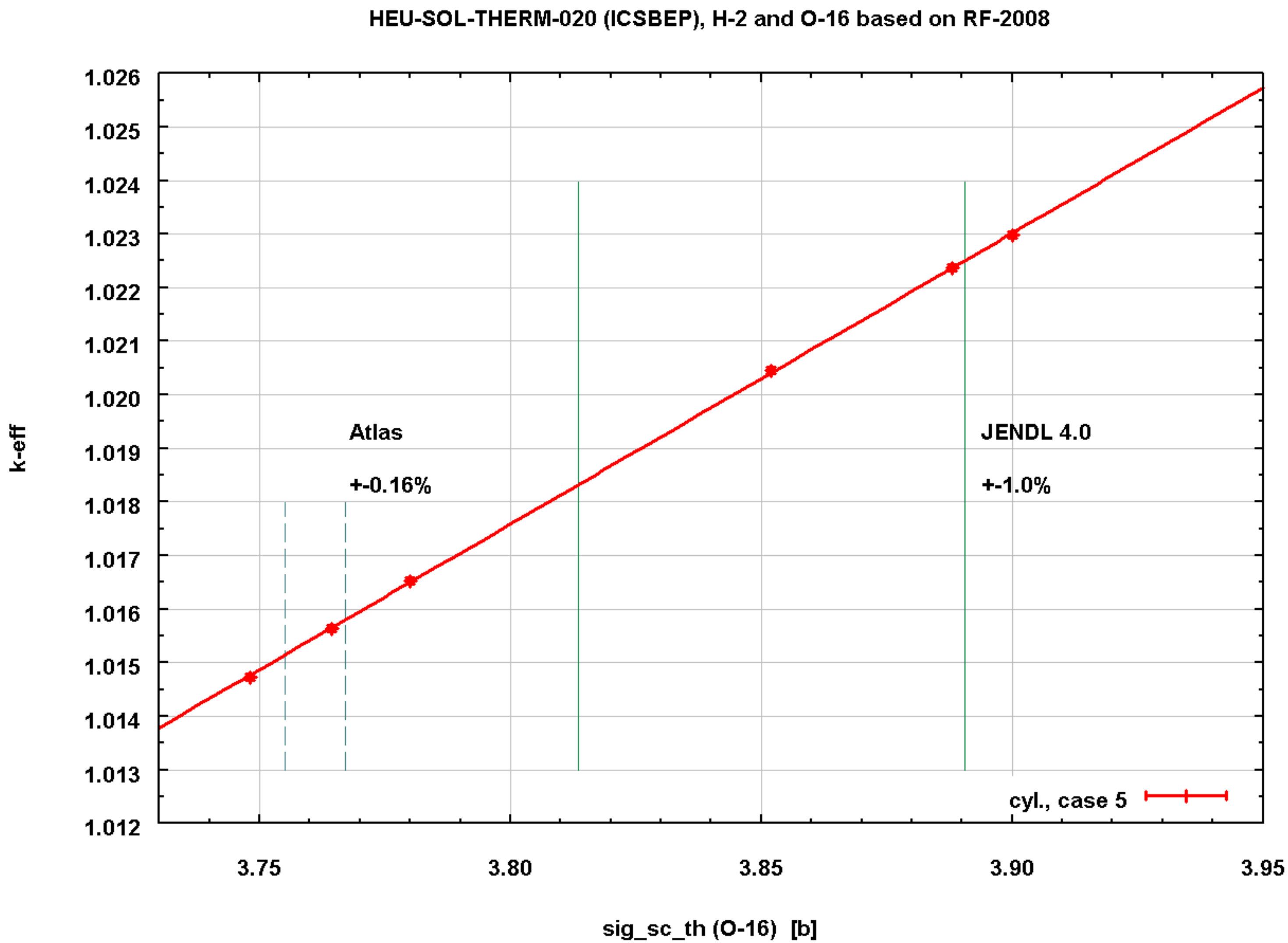
- Case 6 ($R_1 \approx 23$ cm, $R_2 \approx 44$ cm): 5.0 mk per % $\sigma_{s,\,th}$ 1 mk = 100 pcm
- Case 1 ($R_1 \approx 17$ cm, $R_2 \approx 44$ cm): 2.8 mk per % $\sigma_{s,\,th}$

Results for non-reflected cylinders (HEU-SOL-THERM-020):

- Case 5 ($R \approx 38$ cm) : 5.3 mk per % $\sigma_{s,\,th}$



^{16}O: k_{eff} vs. $\sigma_{s,\,th} = \sigma_s(\,E = 2.54{*}10^{-2}$ eV, $T = 0$ K $)$ using "Whiskers model" for $\sigma_s(E)$. MCNP5, HEU-SOL-THERM, reflected spheres



^{16}O: k_{eff} vs. σ_s(E= $2.54*10^{-2}$ eV)
using "Whiskers model" for $\sigma_s(E)$.
MCNP5, HEU-SOL-THERM, non-reflected cylinder(s)

Sensitivity to thermal scattering x-section (O-16)

- $k_{eff} = k_{eff}[\,\sigma_s(E;\,T)\,] \;\rightarrow\; k_{eff} = k_{eff}(\,\sigma_{s,\,th}\,)$, one-parameter model

- We expect $k_{eff} = k_{eff}(\,\sigma_{s,\,th}\,)$ to be a **linear function** of $\sigma_{s,\,th}$ within $\Delta\sigma_{s,\,th}/\sigma_{s,\,th} \approx \pm 1\text{-}2\%$ near $\sigma_{s,\,th} = 3.852$ b (the modern reference value for ^{16}O was chosen, ROSFOND = ENDF/B-VII.0).
  $k_{eff} \approx a' * \sigma_{s,\,th} + b'$

- Sensitivity (dimensional) = change in k_{eff} per 1% change in $\sigma_{s,\,th}$, in *mk per percent* or *pcm per percent*, 1 mk = 100 pcm
- Results for reflected spheres (HEU-SOL-THERM-004).
- Case 6 ($R_1 \approx 23$ cm, $R_2 \approx 44$ cm): ~ 2 mk per % $\sigma_{s,\,th}$
- Case 1 ($R_1 \approx 17$ cm, $R_2 \approx 44$ cm): ~ 1.3 mk per % $\sigma_{s,\,th}$

  Result for non-reflected cylinders (HEU-SOL-THERM-020)
- Case 5 ($R \approx 38$ cm) : ~ 2 mk per % $\sigma_{s,\,th}$

approx. 2-2.5 times smaller than for the sensitivity for $\sigma_{s,\,th}$ (H-2)

On uncertainty of k-eff

- to address the problem of propagation of x-section uncertaintines, in particular,

  $\sigma_{s,th} \pm \boldsymbol{\Delta\sigma_{s,th}} \rightarrow k_{eff} \pm \boldsymbol{\Delta k_{eff}}$

  using $k_{eff} \approx a * \sigma_{s,\,th} + b$

  or (dimensional) sensitivity of k_{eff} to $\sigma_{s,th}$ in *mk per percent*,

  we need a realistic estimate of $\Delta\sigma_{s,th}$

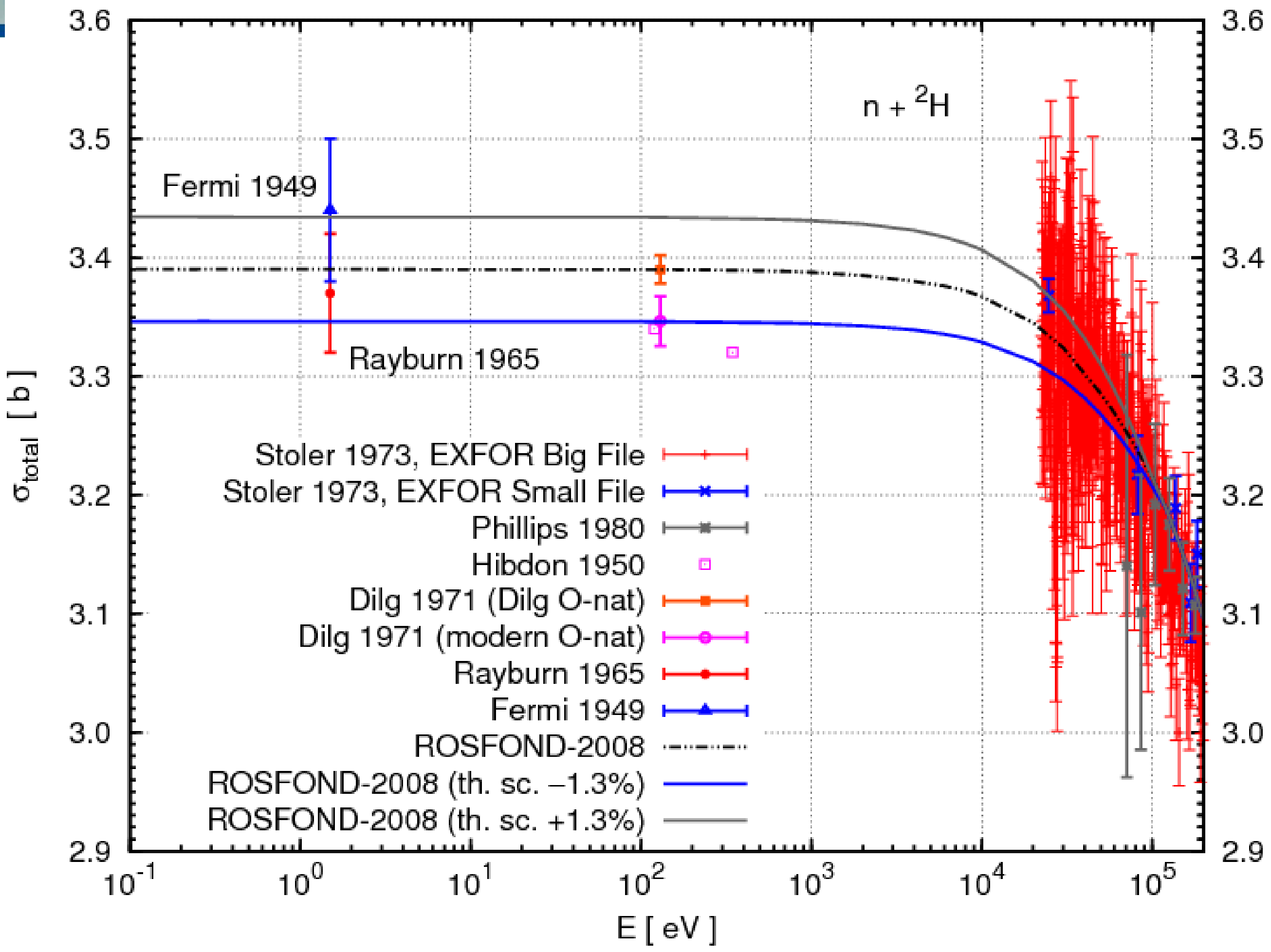
- If $\Delta\sigma_{s,th} \sim \pm 1$-2% for an important nuclide, we can obtain

  $\Delta k_{eff} \sim \pm 1$ mk (± 100 pcm), say, $\pm$ several mk
- If, in fact, $\Delta\sigma_{s,th} \sim \pm 0.1$-0.2% for this important nuclide, we have

  $\Delta k_{eff} \sim \pm\ 0.1$ mk (± 10 pcm),

thanks to the linearity of the problem, $k_{eff} = k_{eff}(\sigma_{s,th})$ within $\Delta\sigma_{s,th} \sim \pm 1$-2%

H-2: realistic estimates of $\sigma_{s,th}$ and $\Delta\sigma_{s,th}$



Asymptotic behavior of $\sigma_{tot}(E)$ of our trail evaluations of ^2H based on ROSFOND-2008 in comparison with low-energy experimental data.

$\sigma_{s,\,\mathbf{th}}(^2H)$ = 3.390 ± 0.012 b in ROSFOND-2008 (= Atlas-2006 ±0.35%)

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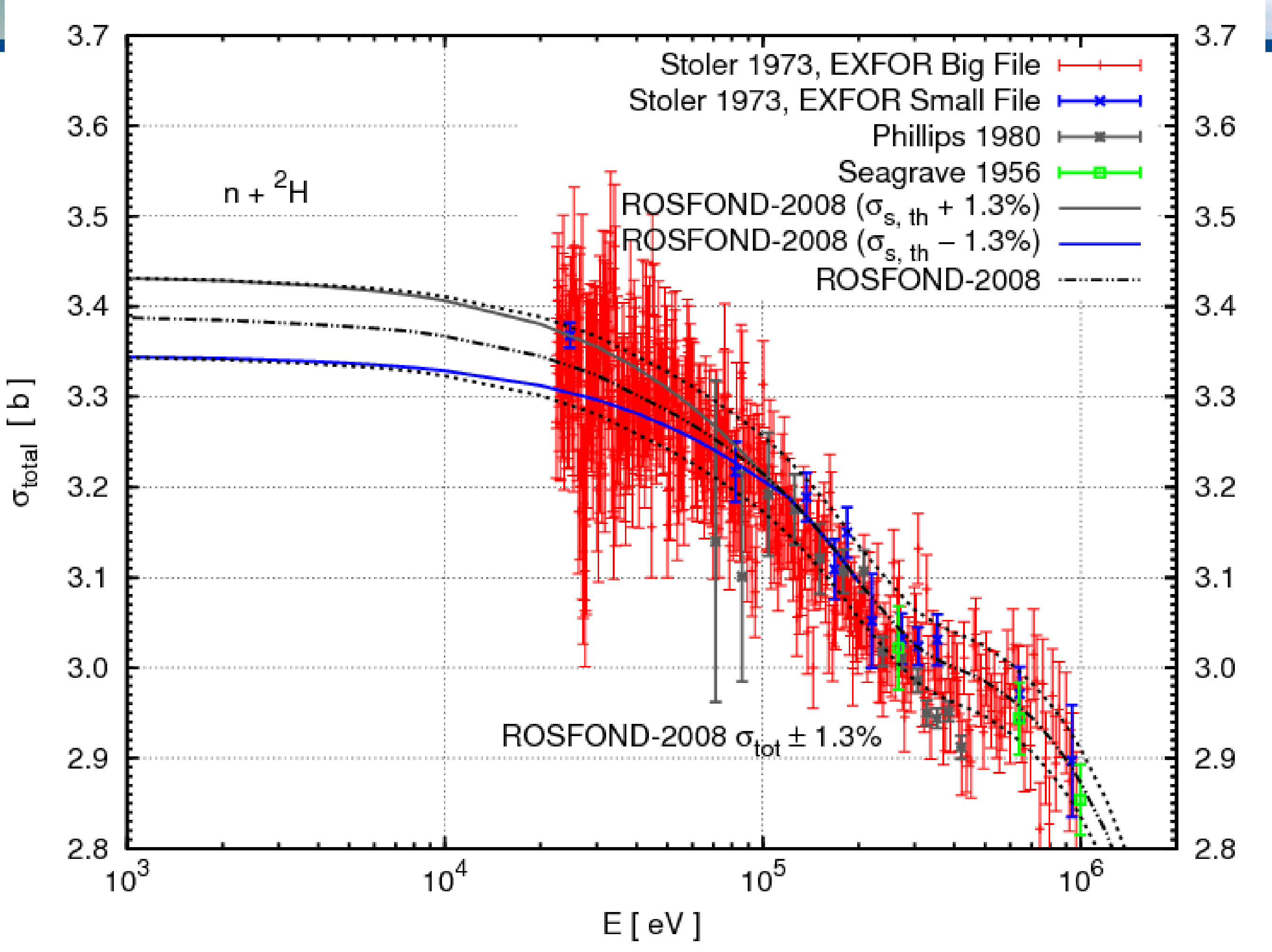
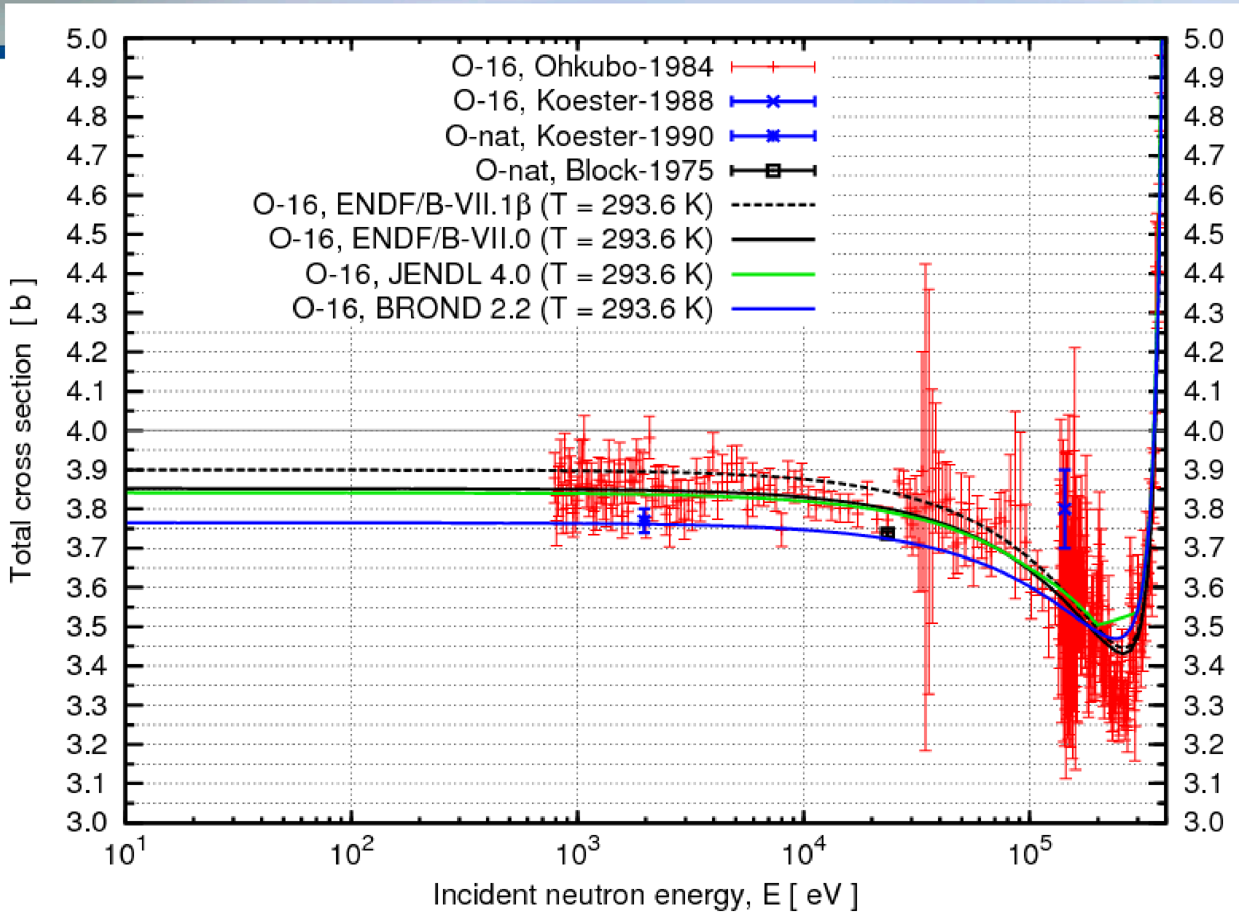
H-2: realistic estimates of $\sigma_{s,th}$ and $\Delta\sigma_{s,th}$



Asymptotic behavior of σ_{tot}(E) of our trail evaluations of ^{2}H based on ROSFOND-2008 in comparison with experimental data

at fast neutron energies (±1.0-1.4%).

O-16: realistic estimates of $\sigma_{s,th}$ and $\Delta\sigma_{s,th}$



$\sigma_{tot}(^{16}O)$ and σ_{tot}(O-nat) from EXFOR data base and different evaluations of ^{16}O.

$\sigma_{sc,\ th}(^{16}O)$ = 3.76440 b in BROND 2.2, compare with

$\sigma_{s,\ th}$ = 3.761 ± 0.006 b of Atlas-2006 and $\sigma_{s,\ th}$ = 3.8408 b ± 0.038 b of JENDL 4.0

Lowest Ohkubo-1984 data points: ±0.064 b (~ ±1.65%), but …

O-16: realistic estimates of $\sigma_{s,th}$ and $\Delta\sigma_{s,th}$, and $b_{coh} \pm \Delta b_{coh}$ (scattering length)

- On the other hand, the evaluation of the ^{16}O **thermal** values is the same in both the Mughabghab-1982 and Mughabghab-2006 editions of the well-known *Atlas of Neutron Resonances*:
- $\sigma_{n,\gamma}$ (^{16}O) = $1.90*10^{-4} \pm 0.19*10^{-4}$ b,
- σ_{sc}(^{16}O) = 3.761 ± 0.006 b (≈ ±0.16%),
- **b_{coh}(^{16}O) = 5.805 ± 0.005 fm**, and

a_{pot} = 4.8 ± 0.1 fm assuming –3.27 MeV local level E_n (fictitious *s*-resonance).

- Note the **consistency of Mughabghab's estimates of σ_{sc} and b_{coh} of ^{16}O:**

$b_{coh} = (A+1/A)*a_{coh} + Z*b_{n,e}$, A = 15.85751, Z = 8, $b_{n,e} \approx -1.38*10^{-3}$ fm

and

$\sigma_{sc} = \sigma_{coh} = 4\pi*a_{coh}^2$. (For ^{16}O and ^{18}O, $I^{\pi} = 0^+$.)

- The estimate of b_{coh}(O-nat) = 5.805 ± 0.004 fm is used in neutron optics, e.g., in the latest measurements of b_{coh}(H) and b_{coh}(D) for oxygen correction.

but σ_{sc}(^{16}O) = 3.852 ± 0.038 b → b_{coh}(^{16}O) = 5.875 ± 0.029 fm

Conclusion

- Sensitivity of k-eff to the **thermal** scattering cross section (of nuclide A):

"Whiskers model" and the trial evaluations for H-2 and O-16

it works for HEU heavy water benchmarks;

it also works for more realistic applications (ZED-2 cores, etc.)

- Uncertainty of k-eff due to the uncertainty of **thermal** scattering cross sections:

one needs realistic estimates of $\Delta\sigma_{s,th}$

for reactors/critical assemblies with **the thermal neutral spectrum**.

the target uncertainty, $\Delta\sigma_{s,th}$, for important nuclides ~ $\pm$0.1% (not ~ $\pm$1%)

What are reliable (consistent) values for $\sigma_{sc,th}(^{16}O)$ and $b_{coh}(^{16}O)$?

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