Open-source multiple-T ND librararies for MCNP and Serpent applications: fixes, extensions, applications

Dan Roubtsov

Canadian Nuclear Laboratories,
Chalk River, Canada

WONDER 2026
(3 July 2026)

Motivation (1)

- Installing open ND libraries for MCNP, Serpent, and OpenMC applications (ENDF/B-VIII.1, JEFF-4.0, JENDL 5)
- From ENDF/B-VIII.1: developing CNL multiple-temperature ND library for MCNP / Serpent and testing it for PHWRs applications (CANDU), ZED-2, …
- Did some fixes (e.g., O-17, Am-242 / Am-242m), also added some nuclides from JENDL-5 to ENDF/B-VIII.1 to support radio nuclide production
- Discuss "fine tuning" $S(\alpha,\beta)$ for UO_2 (NU) from ENDF/B-VIII.1 and distributed as thermal ACE files by LANL, USA for MCNP6 applications

Motivation (2)

- https://nucleardata.lanl.gov/
- https://nucleardata.lanl.gov/ace/endf81sab

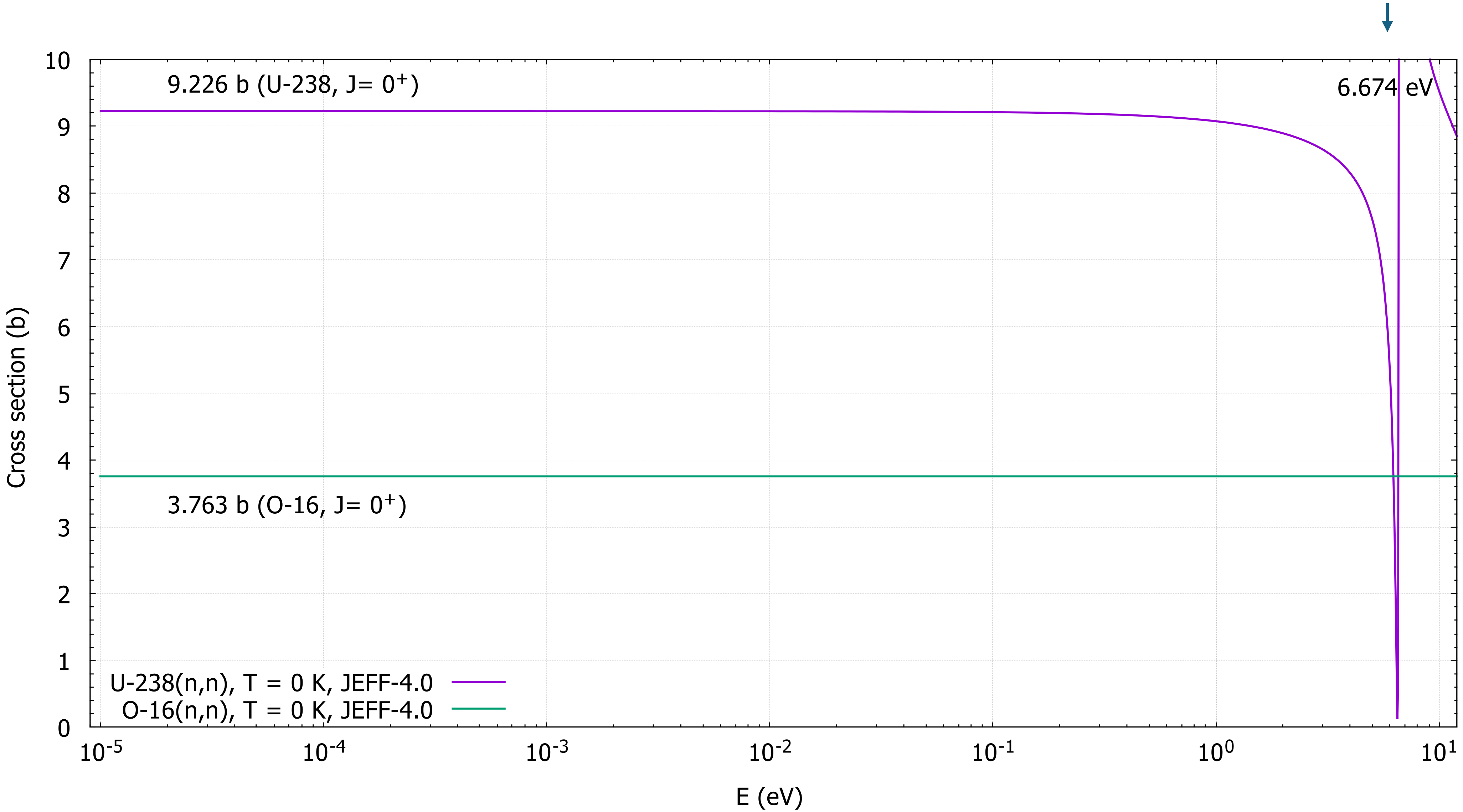
Thermal ACE files u-uo1.70t and o-uo1.70t, read the headers:

```
u-uo1.70t  233.024800  2.5507E-08   10/13/24
U in UO2 (natural U) - ENDF/B-VIII.1 - 296.0 K - October 13, 2024     mat9228
92234        0.  92235        0.  92238        0.     0        0.
...
o-uo1.70t   15.857510  2.5507E-08   10/13/24
O in UO2 (natural U) - ENDF/B-VIII.1 - 296.0 K - October 13, 2024      mat 825
8016         0.     0        0.     0        0.     0        0.
...
```

CNL (Chalk River) TSL for UO2 (NU, SEU): n + U-238 O-16 $_2$

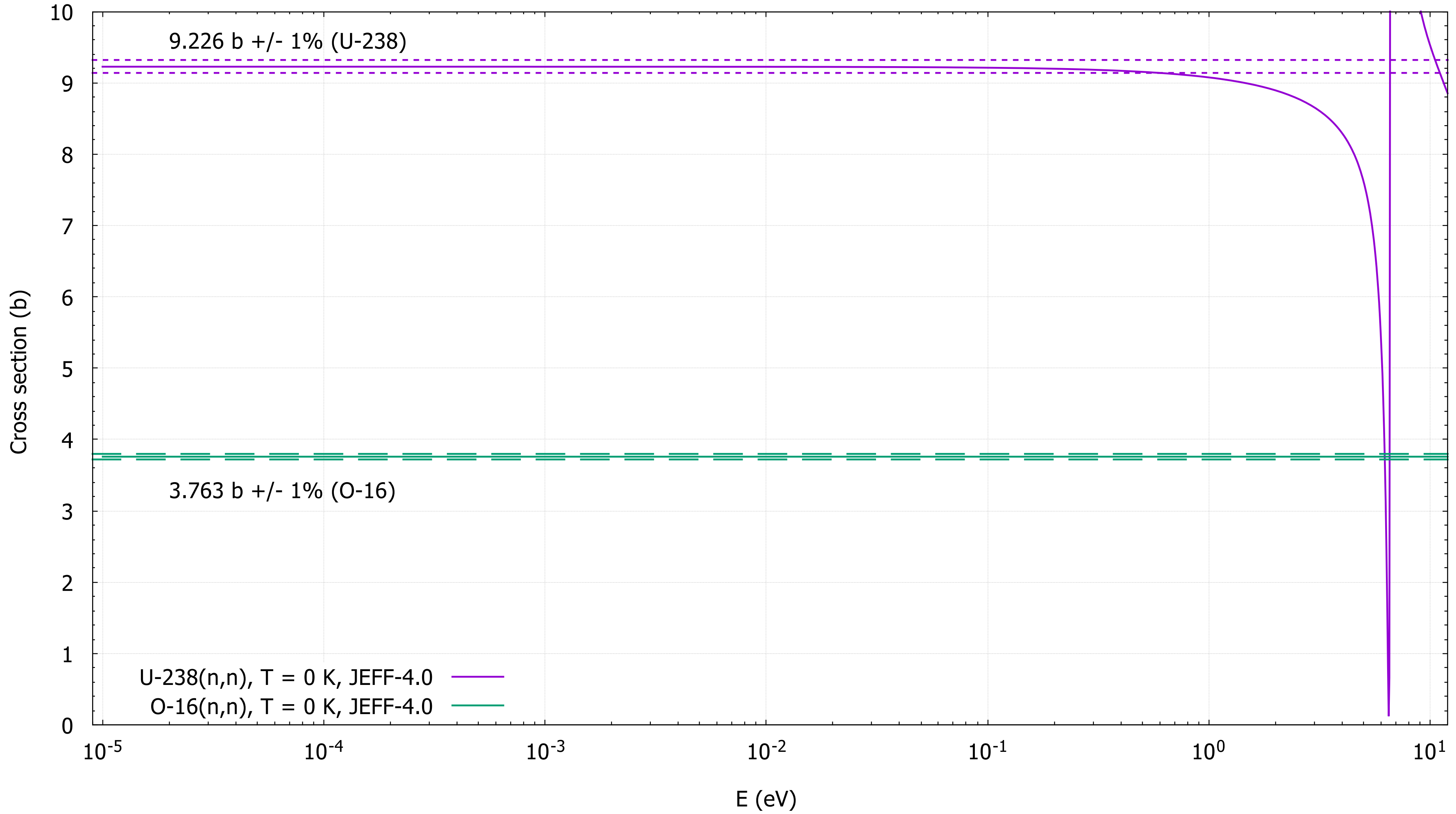
T = 0 K

T – 0 K



U-238 and O-16 (n,n), T = 0 K

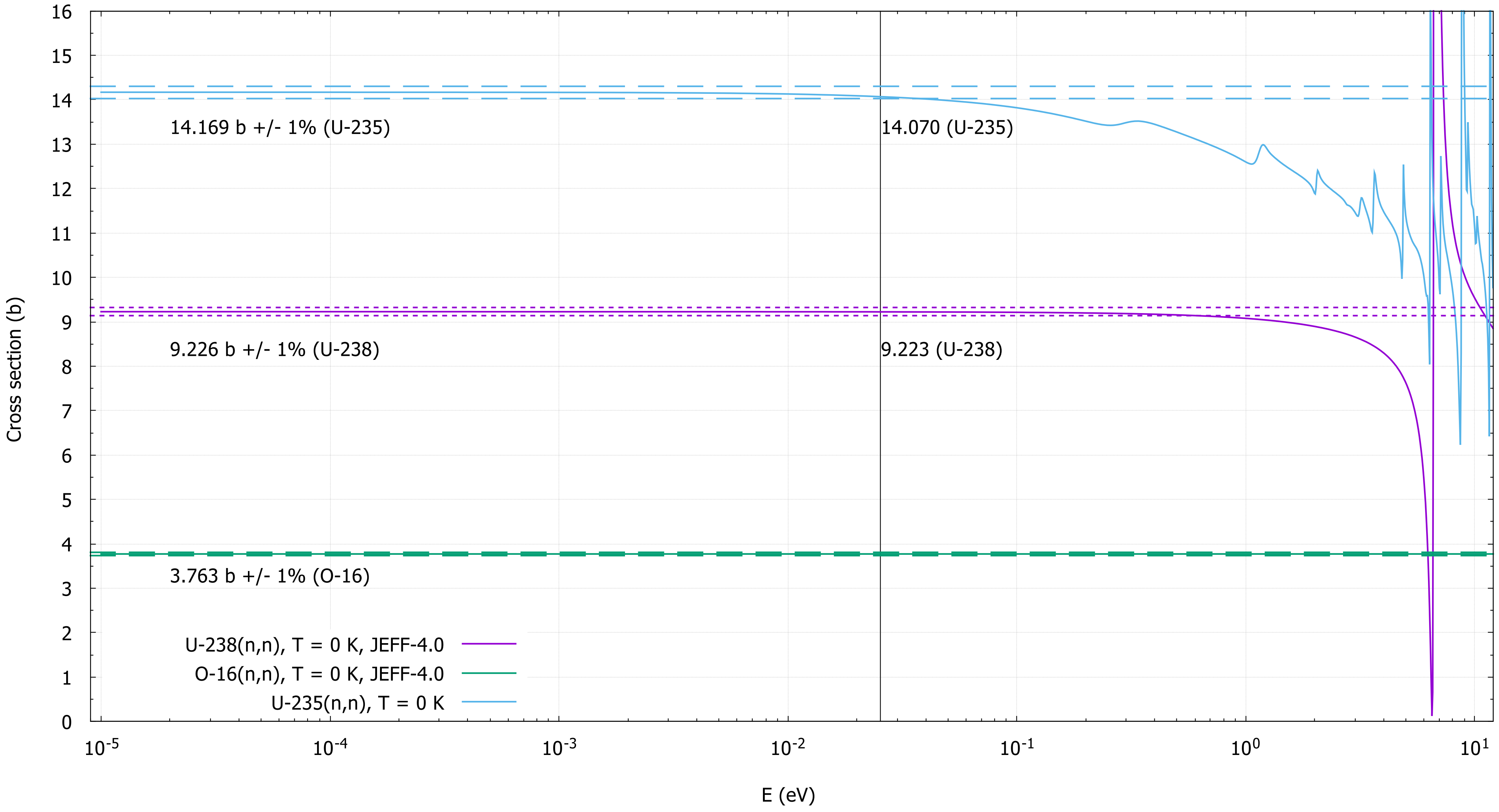
~ ± 1%



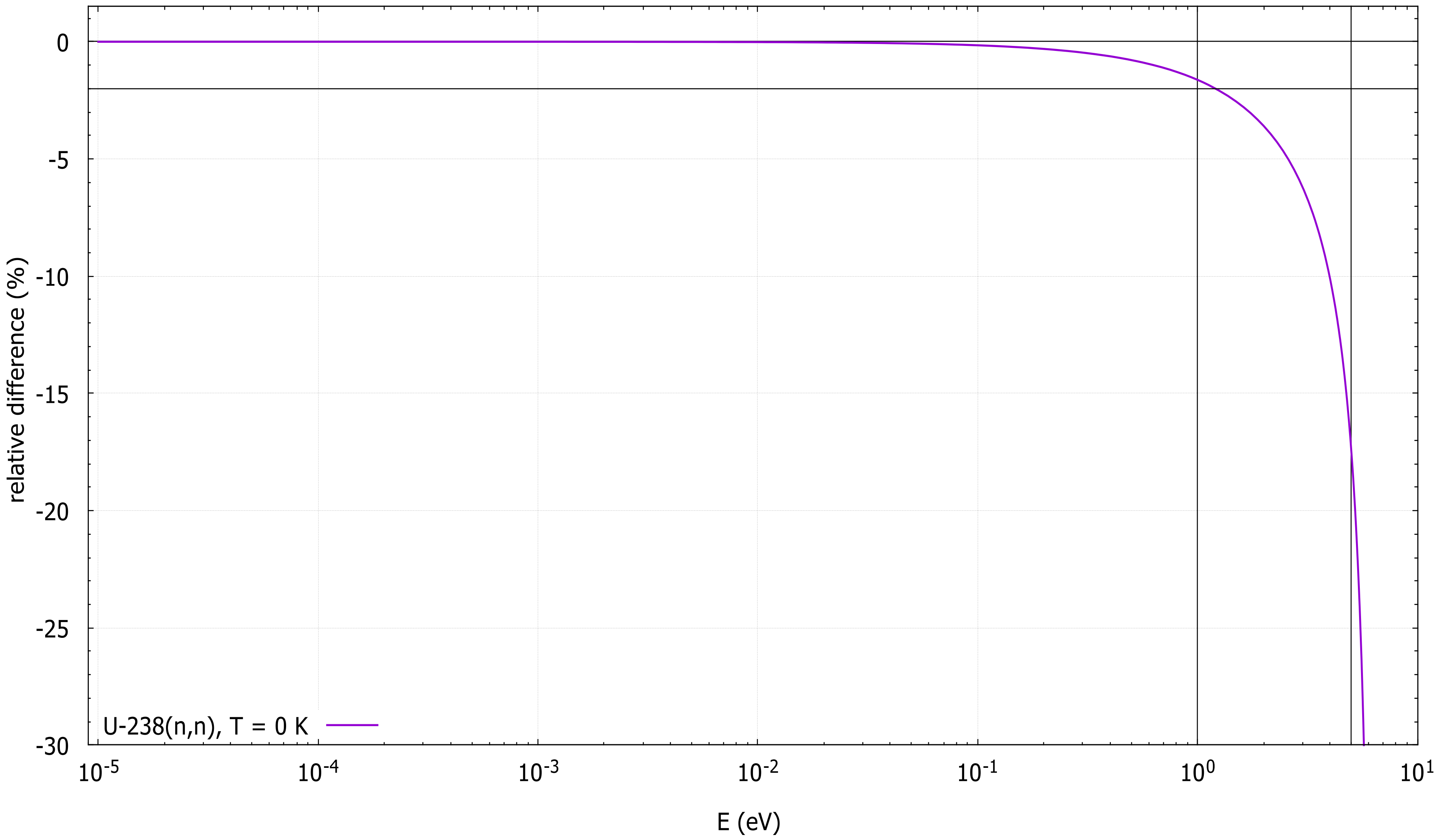
~ ± 1%

L. Leal et al. (2016) : $\sigma_{s,\,th}$ (O-16) = 3.765 ± 0.025 b (±0.7%); in B-VIII.1, 3.794 b, so ~ ±1%.

U-235, U-238 and O-16 (n,n), T = 0 K



U-238, T = 0 K

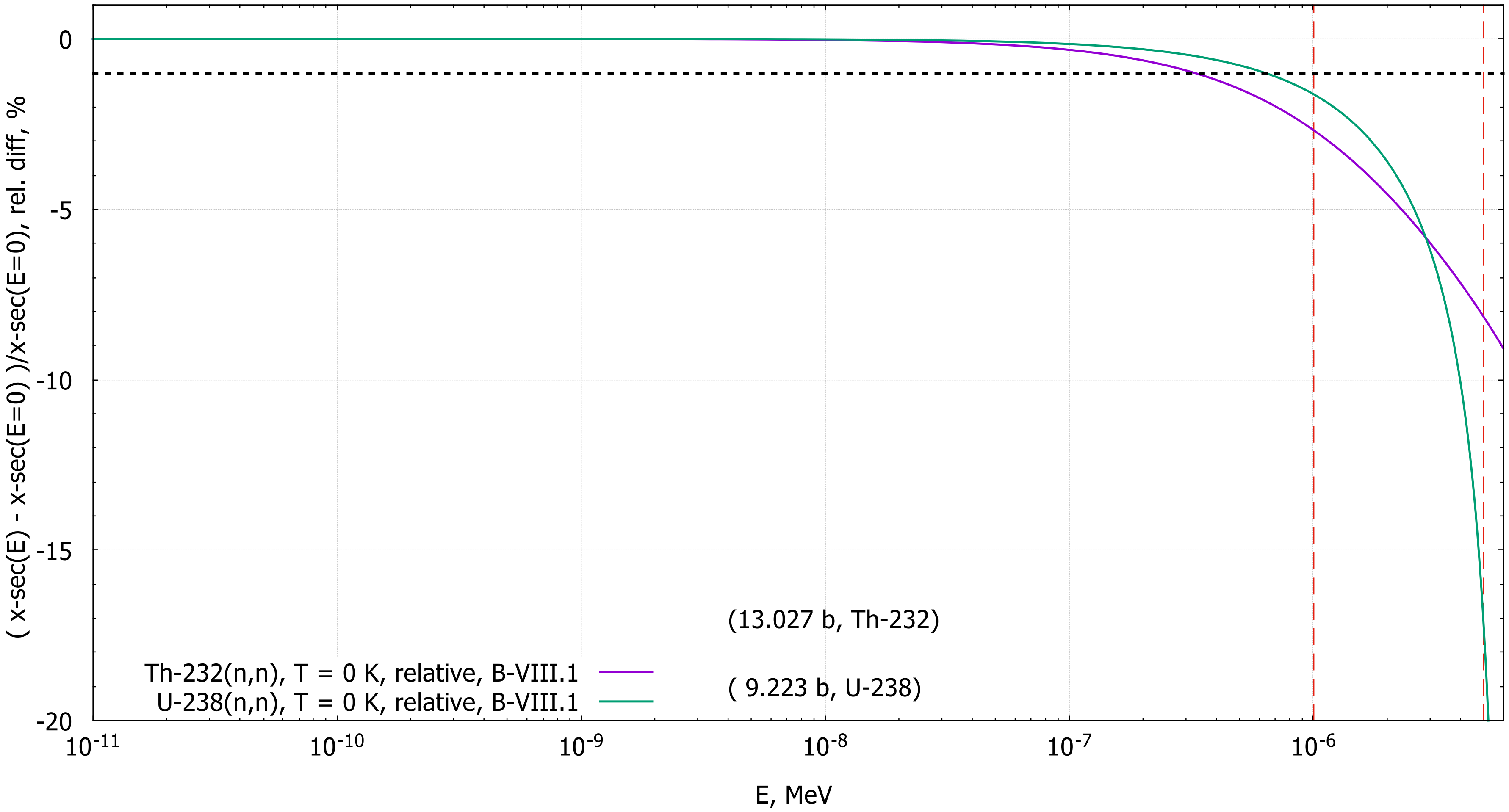


For TSL application,
σ_s(E) vs. E at T = 0 K:
$\sigma_s = 4\pi \times a_s^2$
$(4\pi \times b_s^2)$

proposed "metric" for ND
$100.0 \times$
$(\sigma_s(E) - \sigma_s(E \to 0)) / \sigma_s(E \to 0)$

If the ratio to be ~ 0 with
~ (±) 1%,
then cut-off: ≈ 1 eV for UO_2

U-238 vs. Th-232, (n,n) at T = 0 K

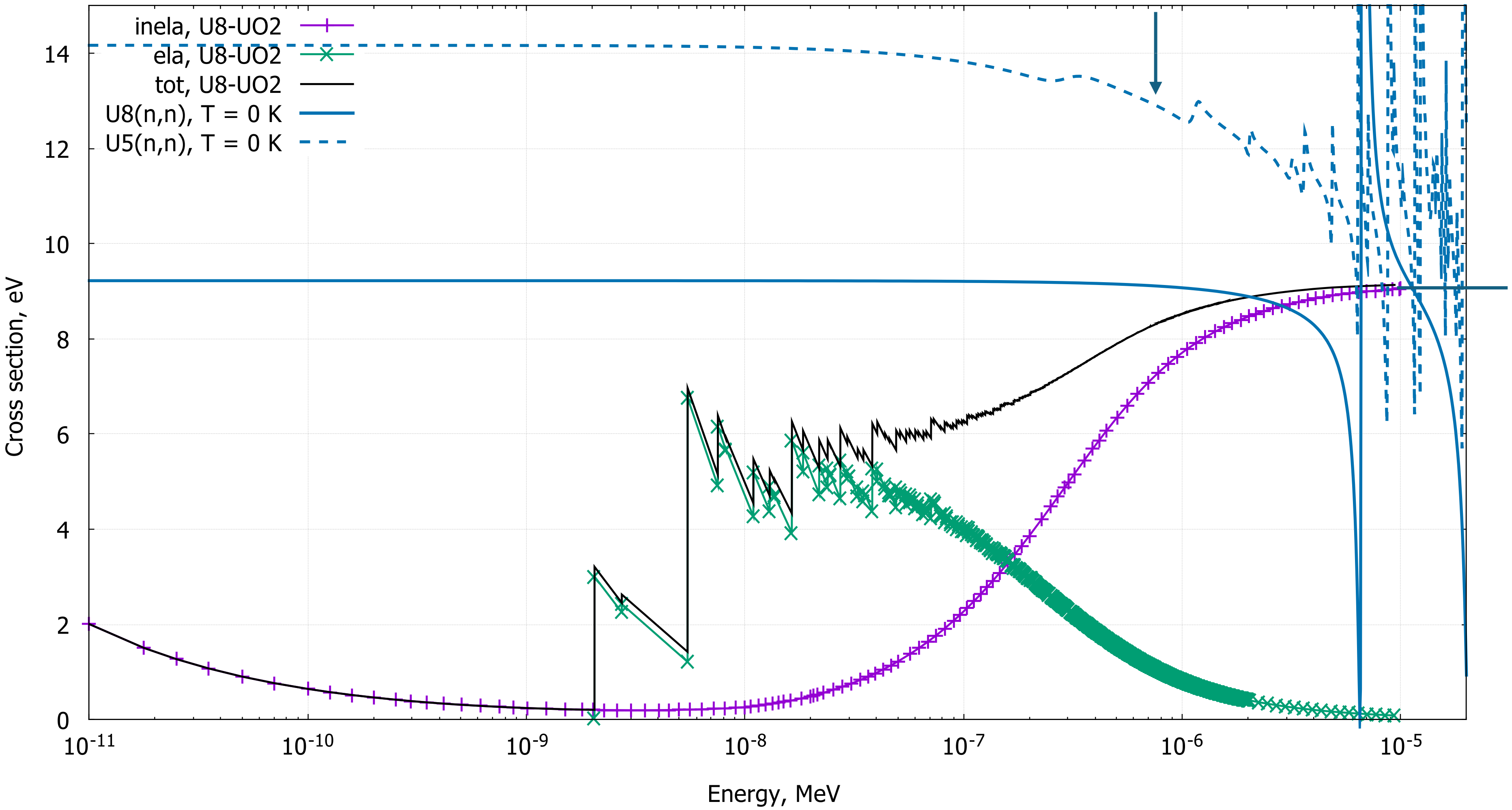


"metric" for ND library x-sections:

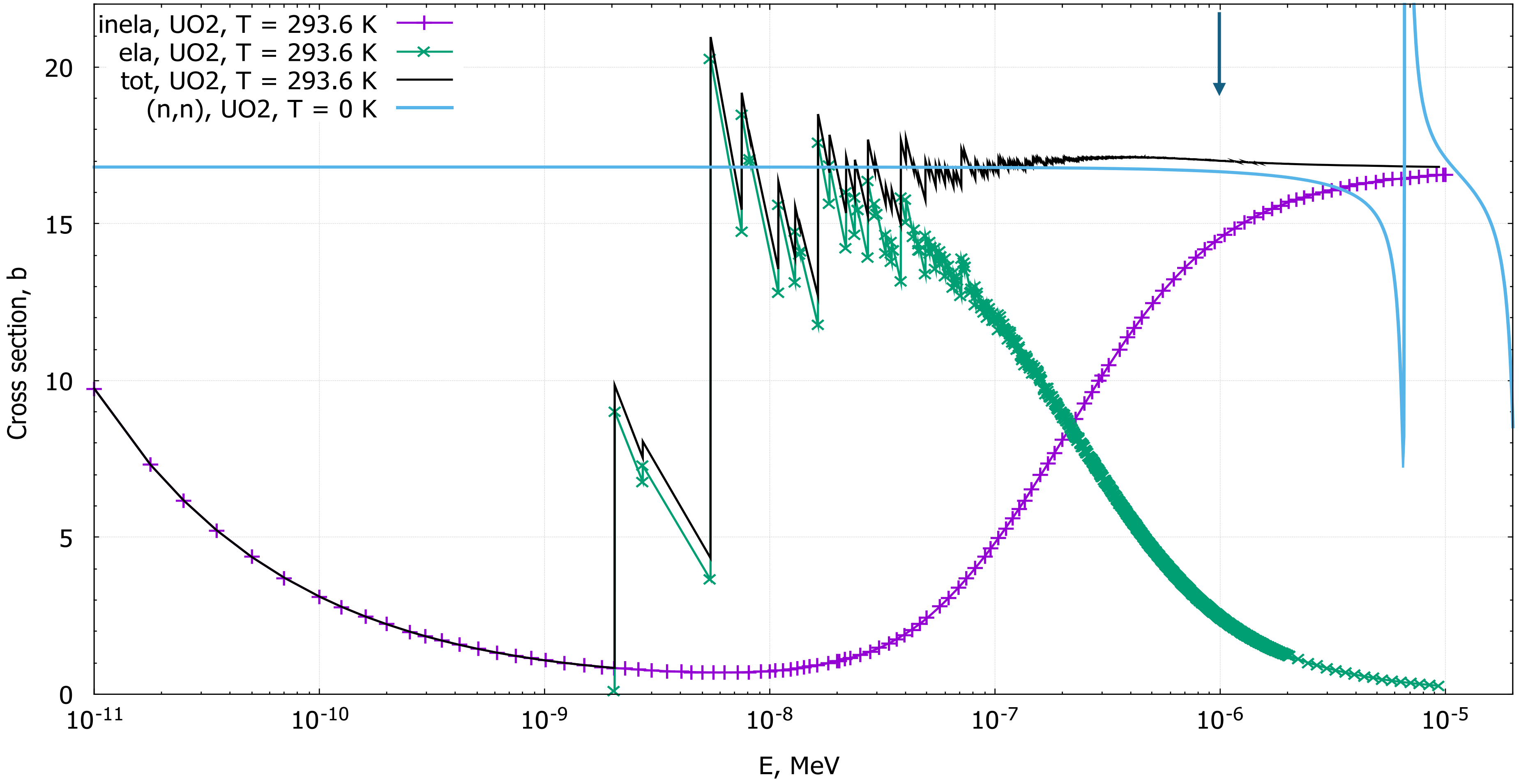
$100.0 \times$
$(\sigma_s(E) - \sigma_s(E \to 0)) / \sigma_s(E \to 0)$

If 0 with ~ 1%,
then TSL cut-off $\approx$ 1 eV
for UO_2 and ThO_2

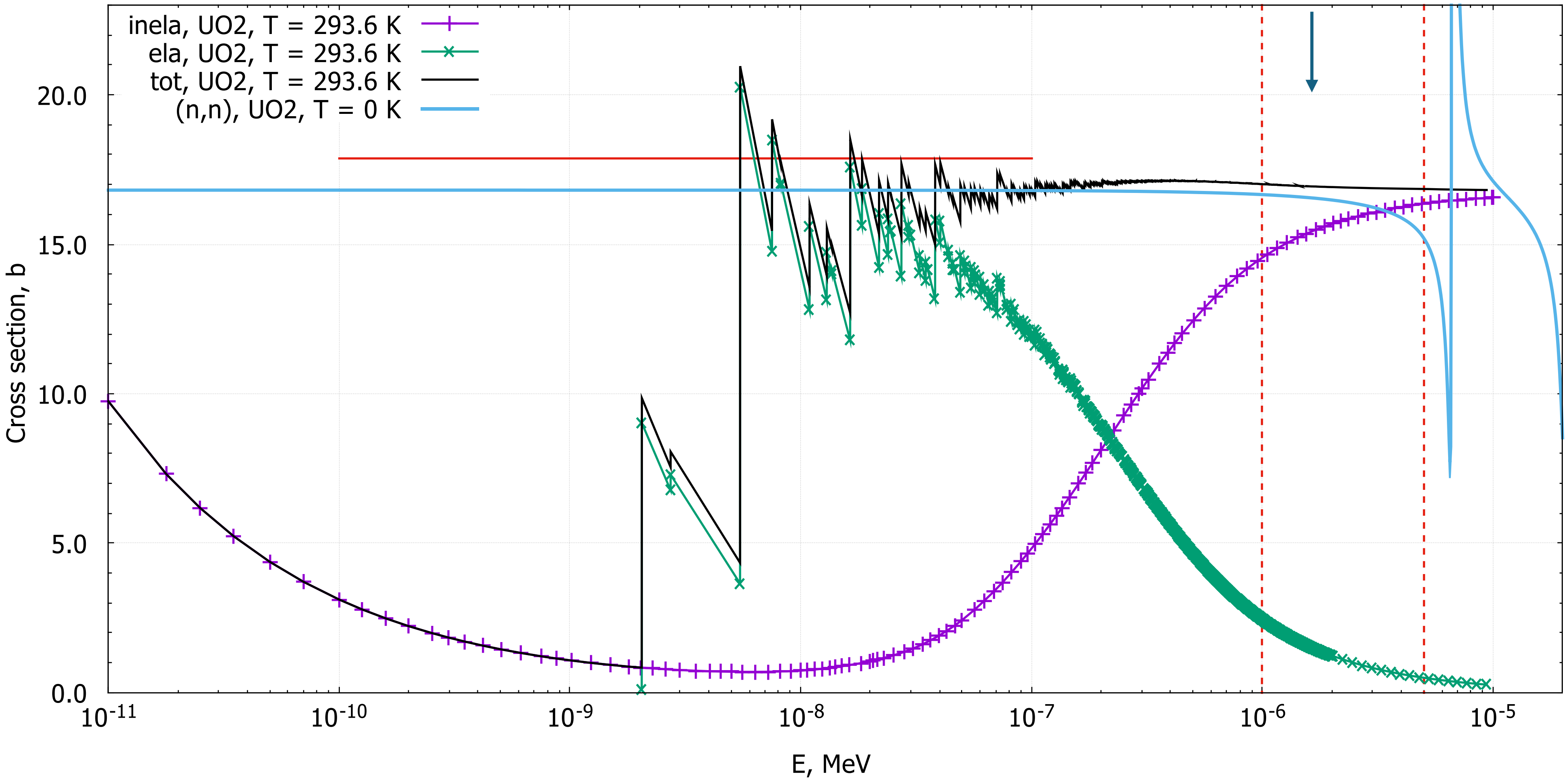
$UO_2 = U\text{-}238\ O\text{-}16\ _2$, $U\text{-}238\text{-}in\text{-}UO_2$



TSL UO_2 (NU) = U-238 O-16 $_2$, E_{cut} = 1.0 eV



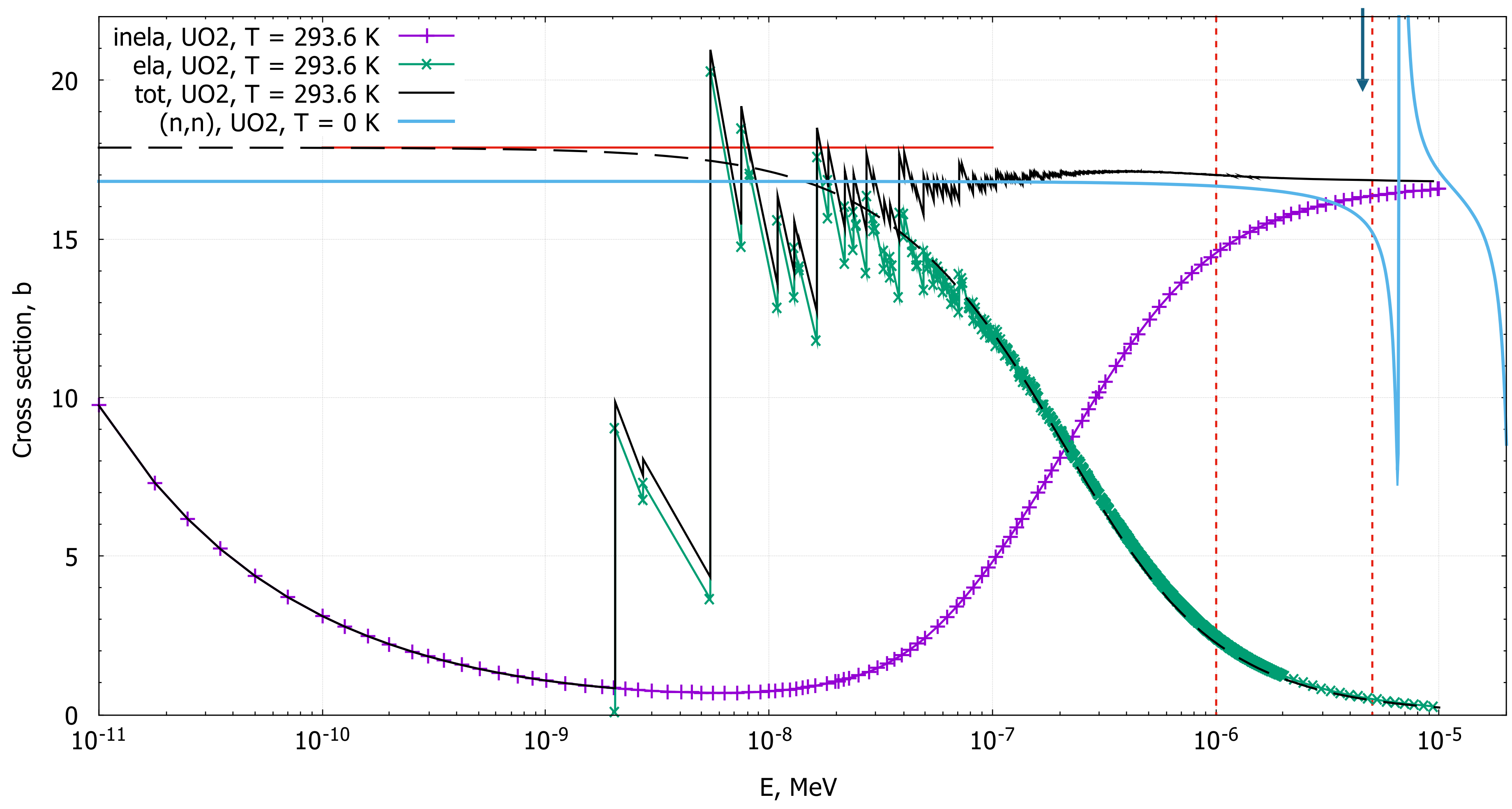
UO_2 = U-238 O-16 $_2$, asymptotic of coh. el. x-sec



$\sigma_{coh} = 4\pi \times b_c^2$

$\sigma_{coh}(E) \propto 1/E$

UO_2 = U-238 O-16 $_2$, asymptotic of coh. el. x-sec



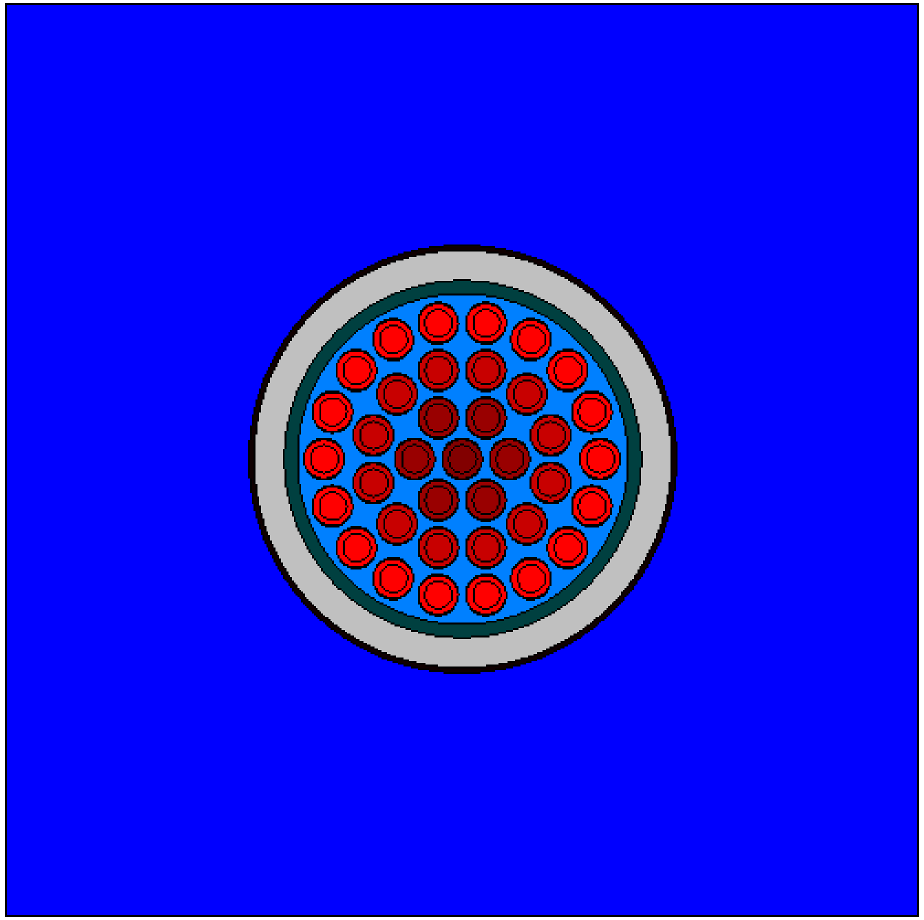
$\sigma_{coh} = 4\pi \times b_c^2$

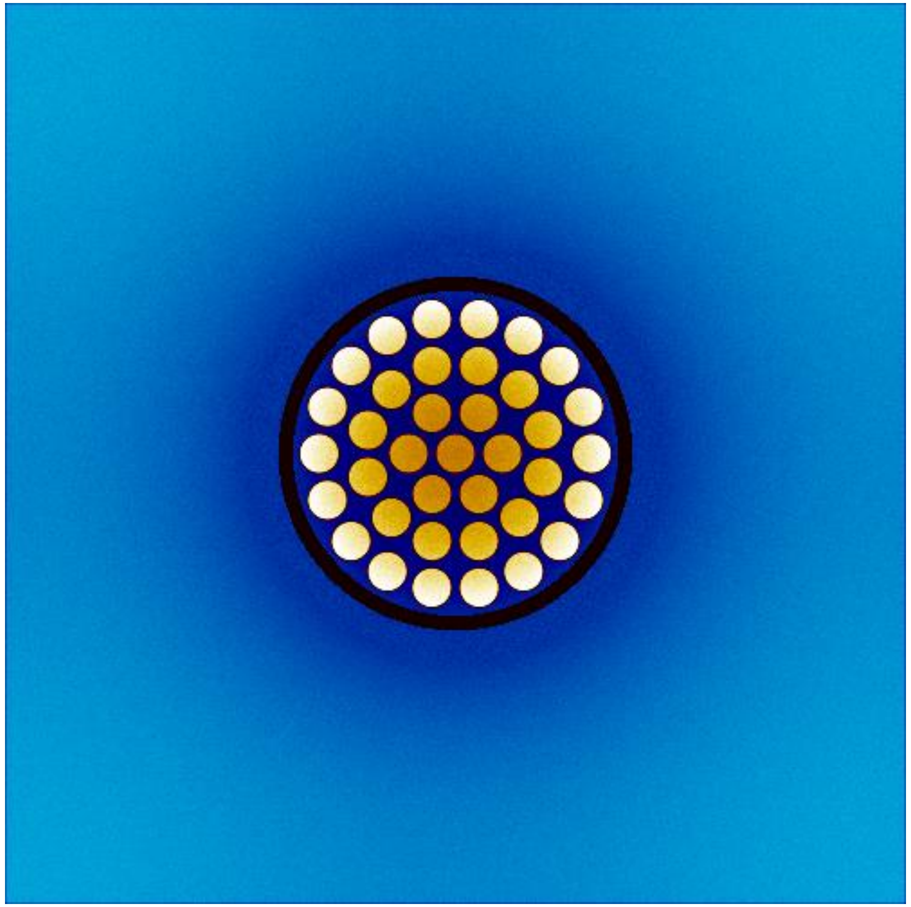
$\sigma(E) = (\sigma_{coh} A / 4E\gamma) \times (1 - \exp(-4E\gamma/A))$

$\sigma(E) \propto 1 / E$
($E >> E_j$, all Bragg edges)

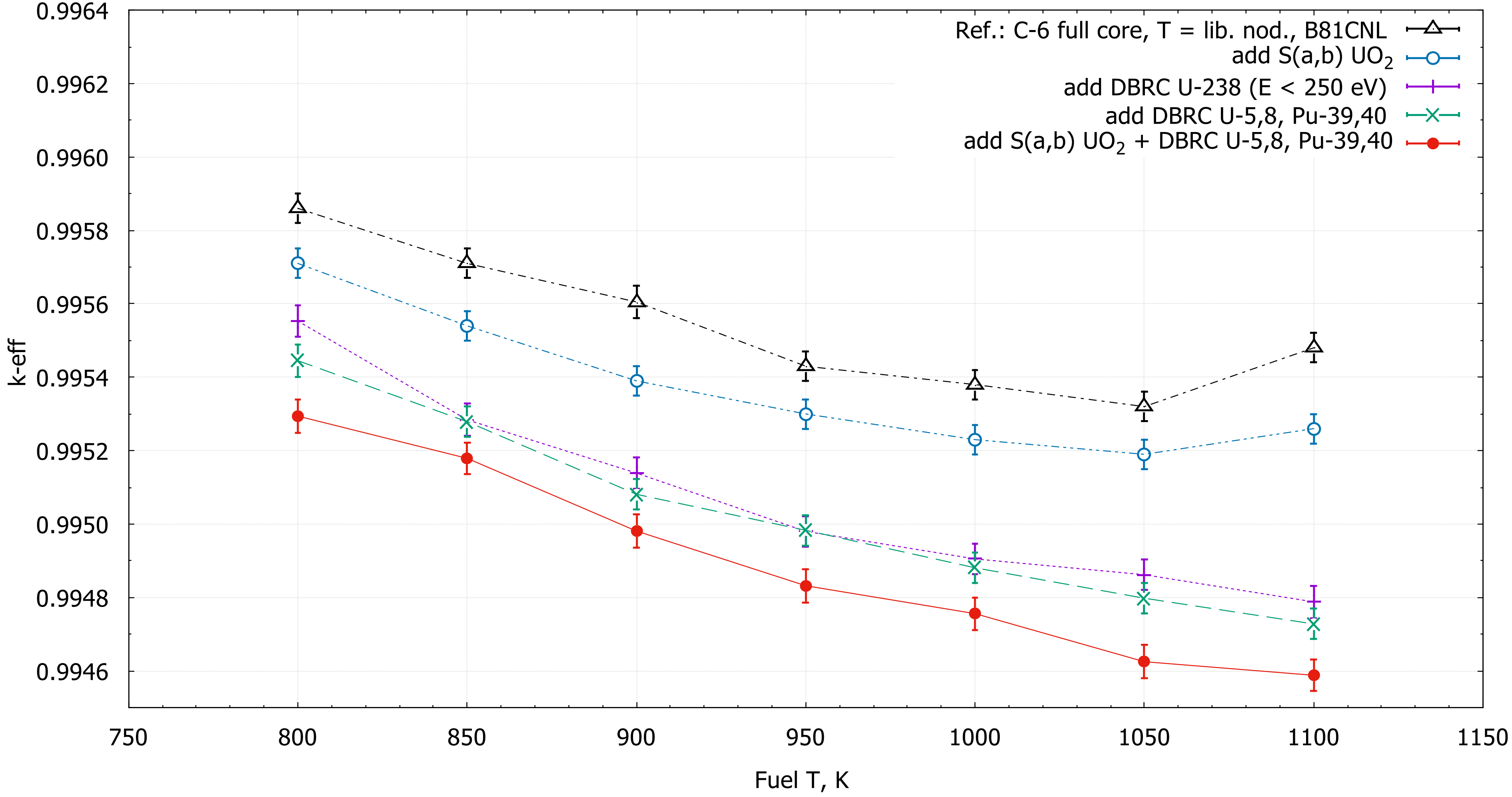
γ = DWI

Applications: PHWR : CANDU





Applications: CANDU, *k*-eff *vs*. T_{fuel}



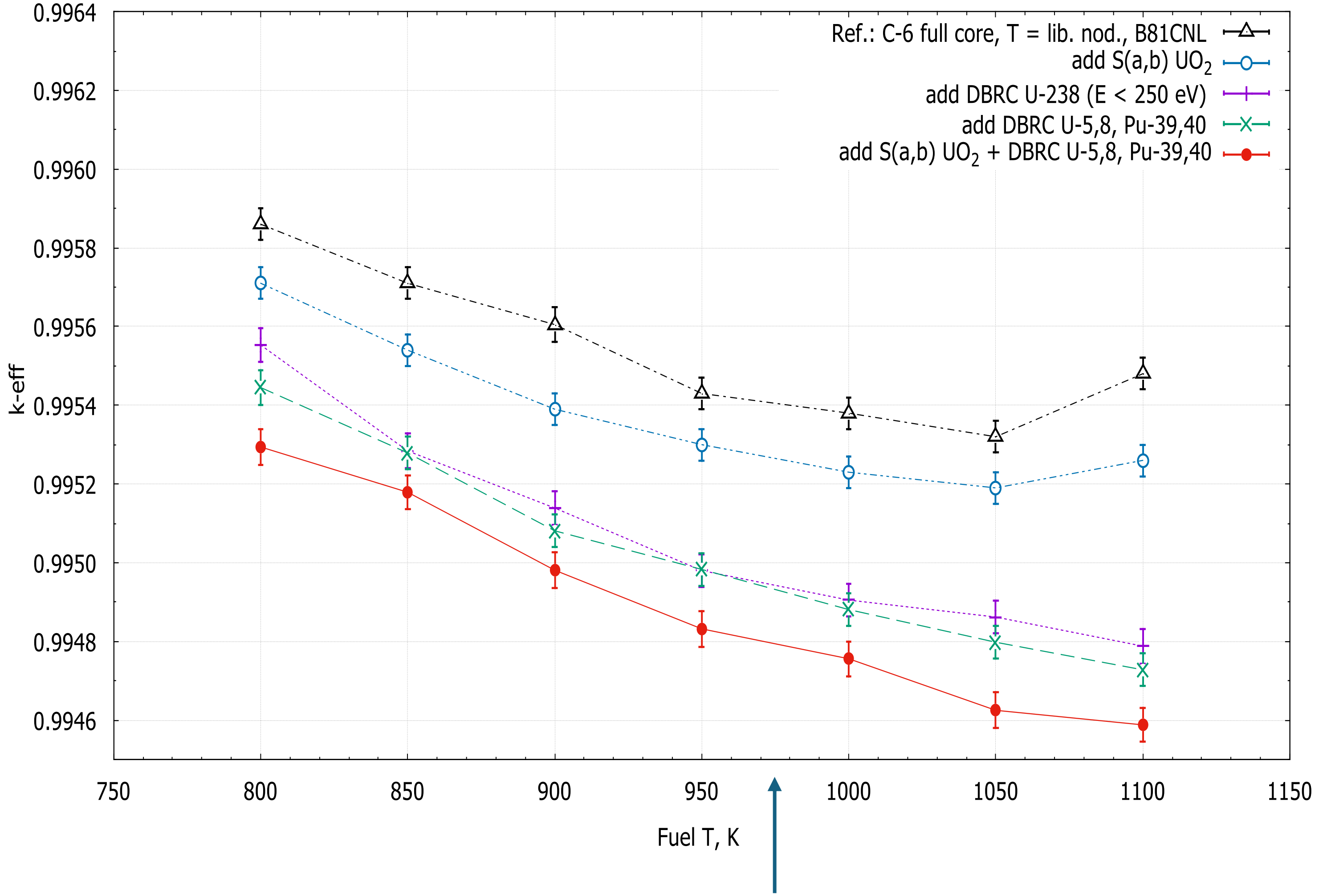
For FTC, we need

$\partial k_{eff}/\partial T_{fuel} \approx$
-2.0 ± 0.3 μk/K
(at the reference T_{fuel})

MCNP6.3
Lib = E81CNL
Library nodes,
ΔT = 50, 100 K

1 mk = 100 pcm
1 μk = 0.1 pcm

Applications: CANDU, *k*-eff *vs.* T_{fuel}

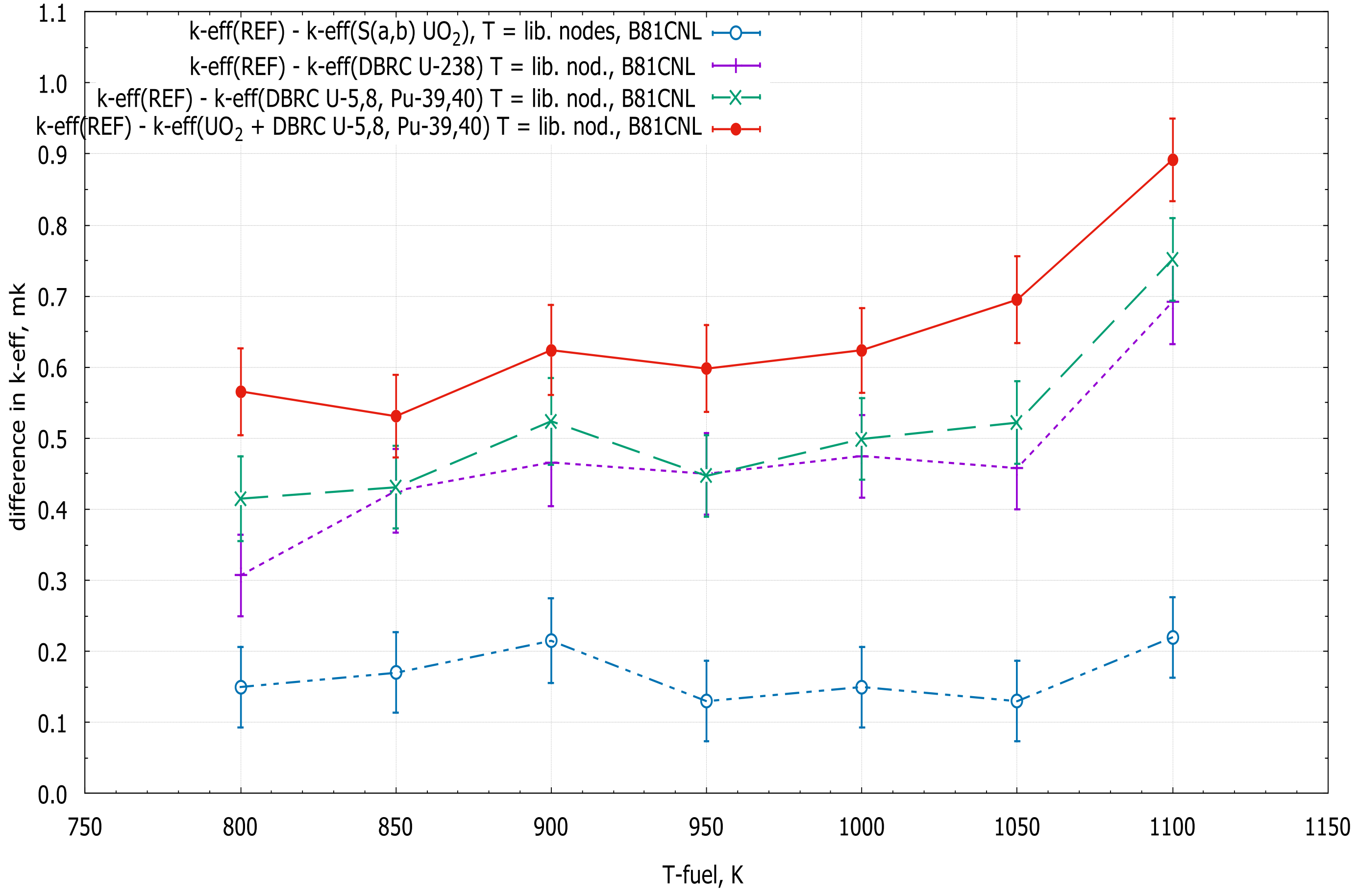


$\partial k_{eff} / \partial T_{fuel} \approx -2.0 \pm 0.3$ μk/K

When DBRC is applied to ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, together with the S(α,β) data for UO_2, from the obtained data ($T_{fuel,i}$, $k_{eff,i}$), the estimated slope becomes

$\partial k_{eff} / \partial T_{fuel} \approx -2.7 \pm 0.2$ μk/K.

Applications: CANDU, *k*-eff *vs.* T_{fuel}



When DBRC is applied to ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, together with the $S(\alpha,\beta)$ data for UO_2, from the obtained data ($T_{fuel,i}$, $k_{eff,i}$), the estimated slope becomes

$$\partial k_{eff} / \partial T_{fuel} \approx -2.7 \pm 0.2\ \mu k/K.$$

Notes on DBRC applications

[MCNP6.3] The DBRC treatment can be extended to multiple actinides,
e.g., ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu, in a straightforward way:

DBRC endf=82 emax=2.5e-4 isos=92235 92238 94239 94240

Here, the keyword “endf=82” instructs MCNP to find and use the nuclear data file "DBRC_endf82.txt".

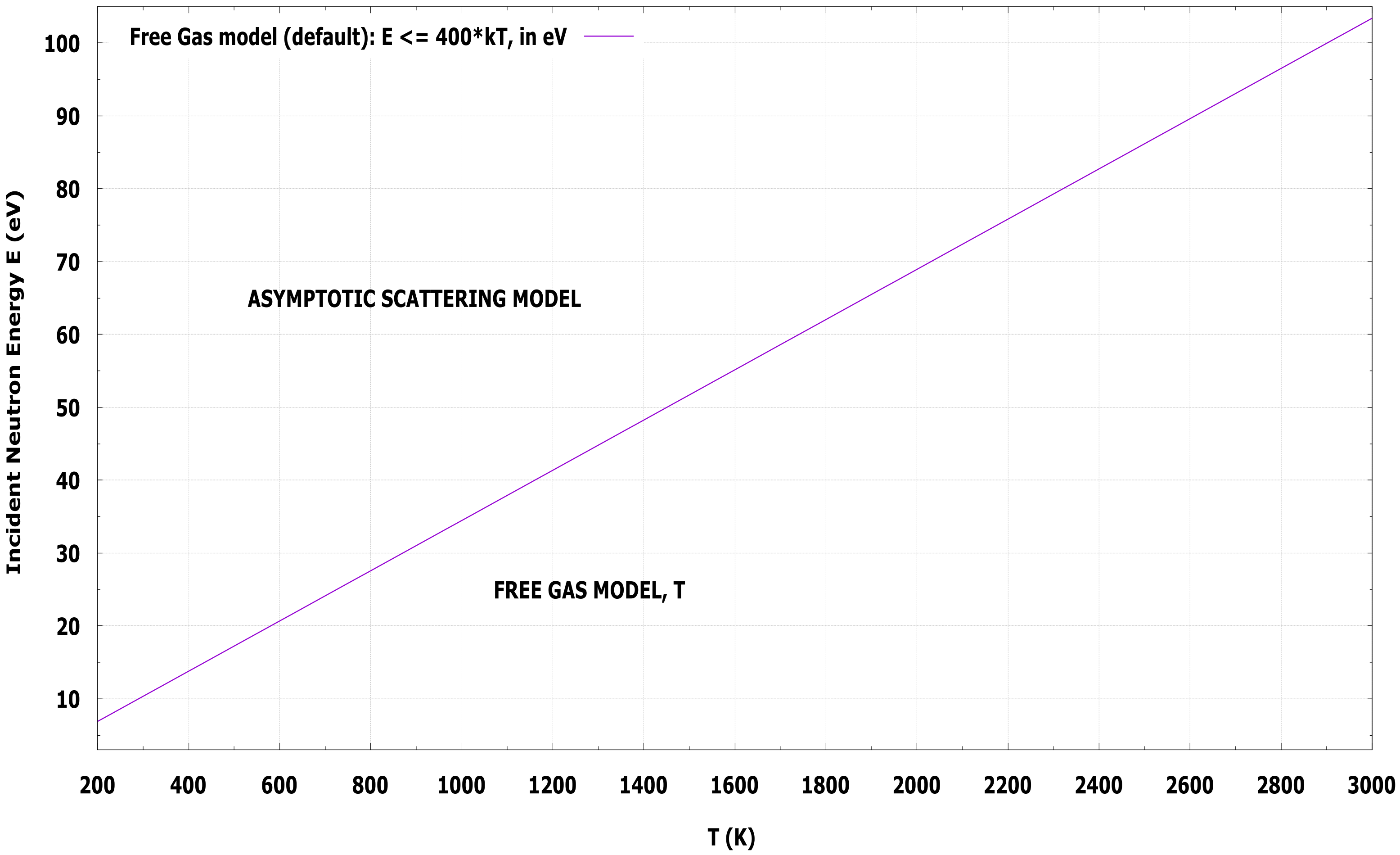
The keyword “emax=2.5e-4” specifies the upper energy cut-off for applying the DBRC treatment,
$E_{max} = 2.5\times10^{-4}$ MeV = 250.0 eV.
The keyword “isos=92238” specifies the nuclide subject of DBRC treatment, in this case ^{238}U…

[Serpent]
for a few selected nuclides (e.g., ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu),
it is straightforward to apply “set dbrc” as follows:

set dbrc 0.01E-6 1.0E-3 92235.00c 92238.00c 94239.00c 94240.00c

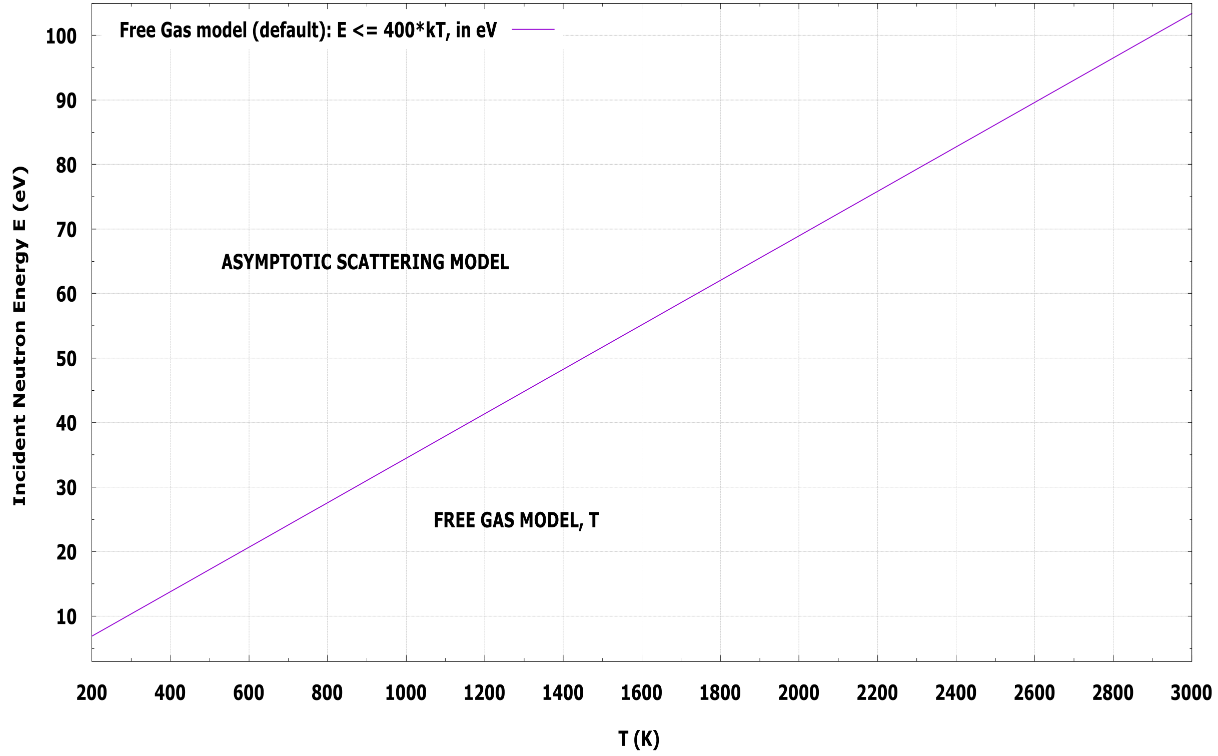
DBRC ND library support for MCNP & Serpent: ?   [MCNP utility dbrc_make_lib, DBRC_endfXX.txt]

Free Gas Model control: cut-off 400×kT → *E*



The default boundary between Asymptotic Scattering Model and Free Gas Model for neutron elastic scattering reaction A(n, n)A, is $E = 400\times\mathrm{kT}$, in MCNP, Serpent, and OpenMC (except H-1)

Free Gas Model control: cut-off 400×kT → E



Serpent

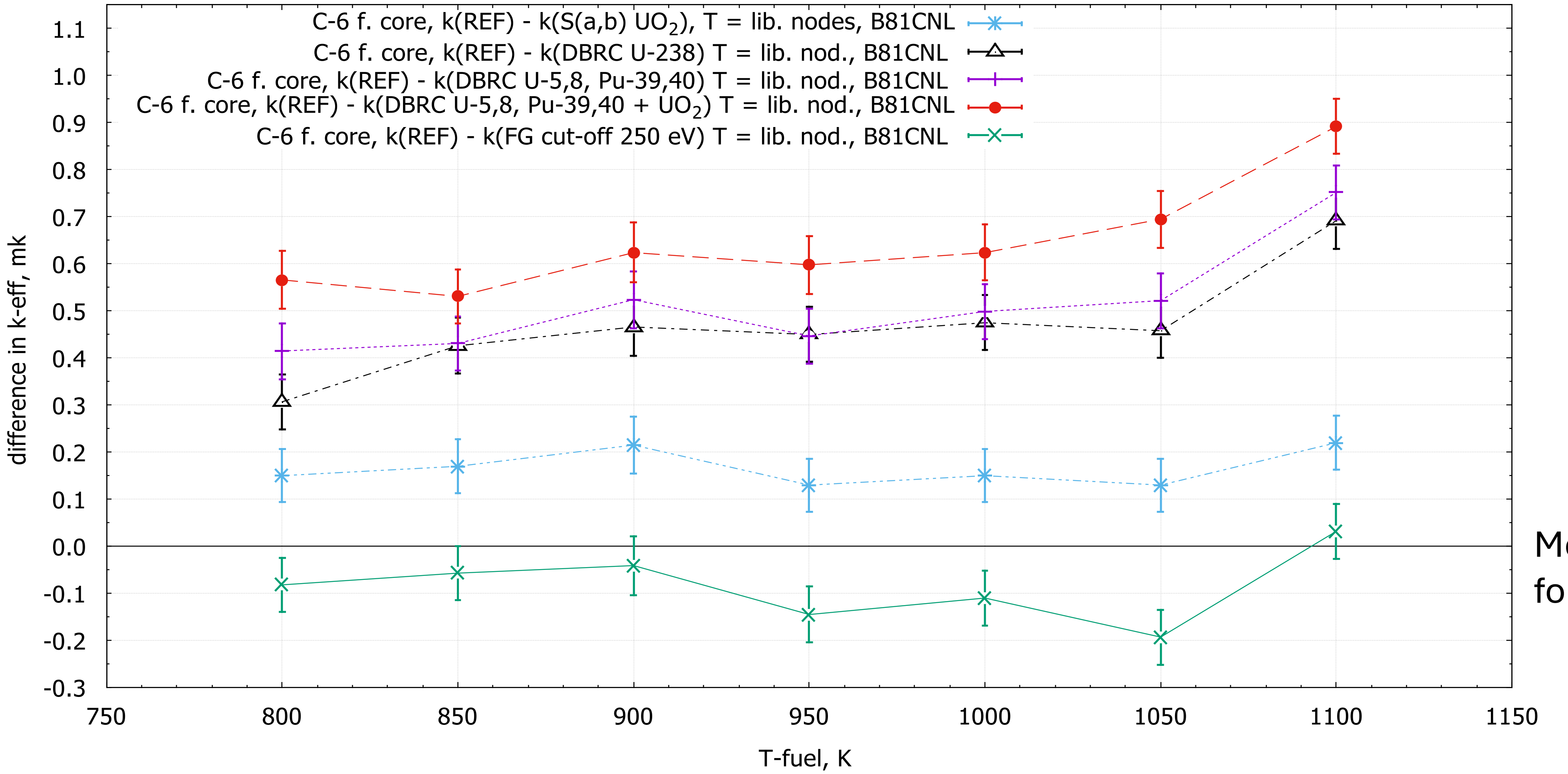
% -- Free Gas Model control: set upper energy cut-off in MeV
set fr 1.0e-3
% --

In MCNP6.3, it is possible to apply the similar increase of E_{max} = 400×kT (Free Gas Model default cut-off) for all nuclides present in the model (except ^{1}H) by applying the DBRC card as follows:

DBRC emax=1.0e-3

In MCNP, the Free Gas Model control (re-set of E_{max}) and the DBRC card (with its main purpose to apply DBRC treatment for the heavy nuclides) are mixed together (?)

Test: FG cut-off = 250 eV (similarly to DBRC cut-off)



More test are left for future studies

Summary

For $S(\alpha,\beta)$ for UO_2 (NU) in ENDF/B-VIII.1,
simplify the model to be ^{238}U-in-UO_2 and ^{16}O-in-UO2

Proposed the cut-off: 1 eV
why? for $E < E_{cut}$, $S(\alpha,\beta)$ data assumptions are satisfied
and to use DBRC for E > 1.0 eV for U-238

Applications for Fuel Temperature Coeffcient of reactivity:
add $S(\alpha,\beta)$ for UO_2 and DBRC for U-238 and Pu-240

ND library support for DBRC : in JEFF-4.0 (?)

Free Gas Model control: increase upper energy cut-off for all (?),
to be consistent with DBRC for actinides (?)