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What to expect from microscopic calculations on k_{eff} ?

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JEFDOC-2324

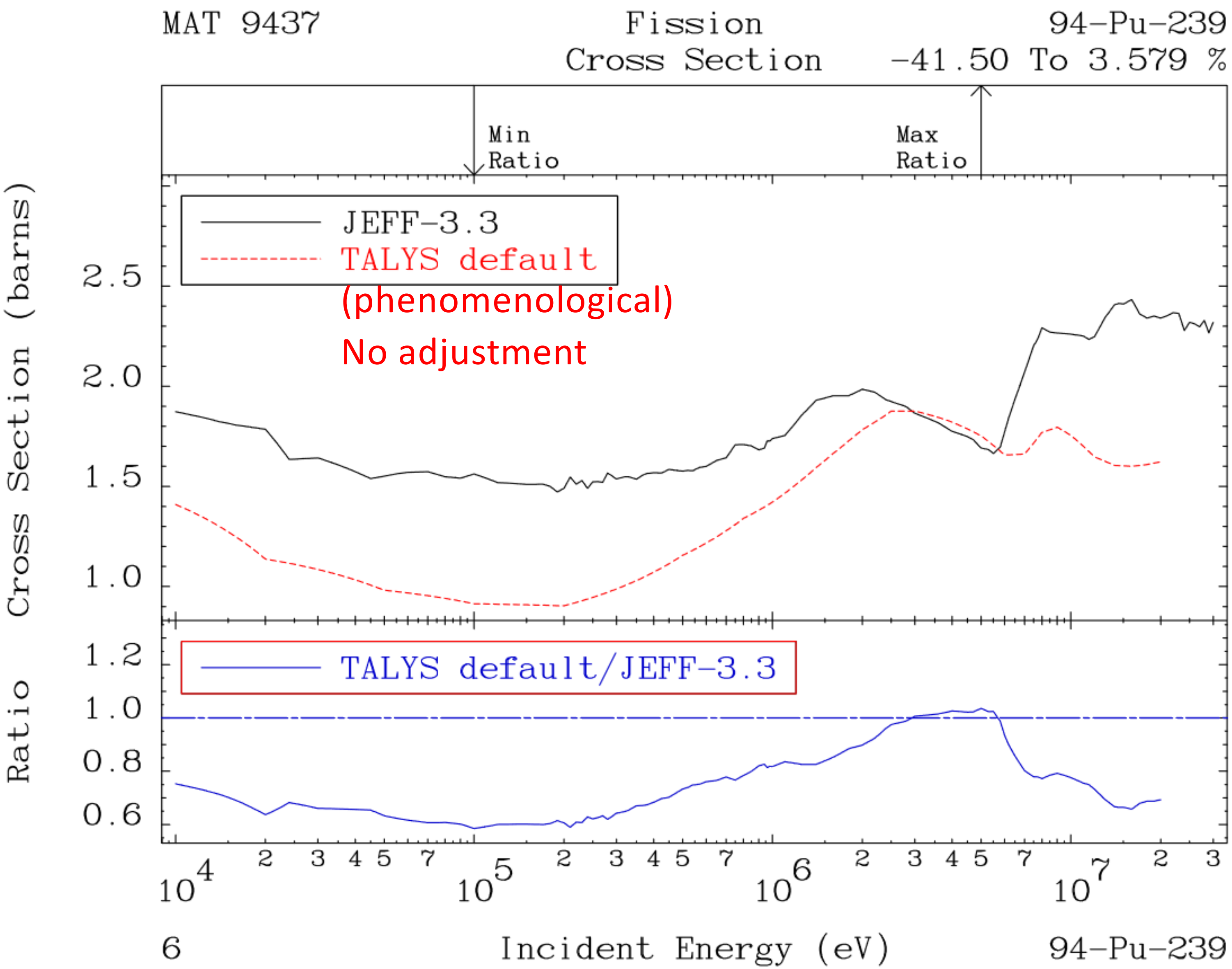
Motivation & approach

- Motivation:
  - Nuclear data of relevance for criticality-safety can be adjusted in existing libraries
  - What happens if we consider non-adjusted nuclear data ?
  - What happens if we consider microscopic models ?
  - What is the impact on criticality-safety benchmarks ?
- Approach:
  - 195 k_{eff} benchmarks (hmf, pmf, imf and mmf, list at the end of the presentation)
  - Isotopes: U, Pu, Cu, Fe, Ni, W, Ni, Cr, Ga, Mo, Ti, Mn, Mg, F
  - Consider JEFF-3.3 (maybe adjusted) and also TALYS pure microscopic model(s)
  - TALYS models: many, from phenomenological to microscopic approach

TALYS models

	Default (phenomenological)	Microscopic (theoretical)
E1 strength	SLMO	Gogny D1M HFB+QRPA
Level density	Constant temperature + Fermi gas model	Gogny-Hartree-Fock-Bogoluybov level densities
OMP	KD (local)	JLM microscopic optical model potential
M1 strength	Hartree-Fock BCS tables	
Collective enhancement LD	No	
Width fluctuation mode	Moldauer	
Mass model	Goriely HFB-Skyrme table + Exp. masses	Goriely HFB-Skyrme table, no Exp. masses
Alpha OMP	Avrigeanu	
Fission barriers	"experimental"	Theoretical, WKB approximation for fission path model
Discrete level	RIPL	Theoretical levels
Best + fit	Yes	No
Global parametrization PSF	No	Yes
Global systema. level den.	No	Yes

^{239}Pu(n,f) cross section



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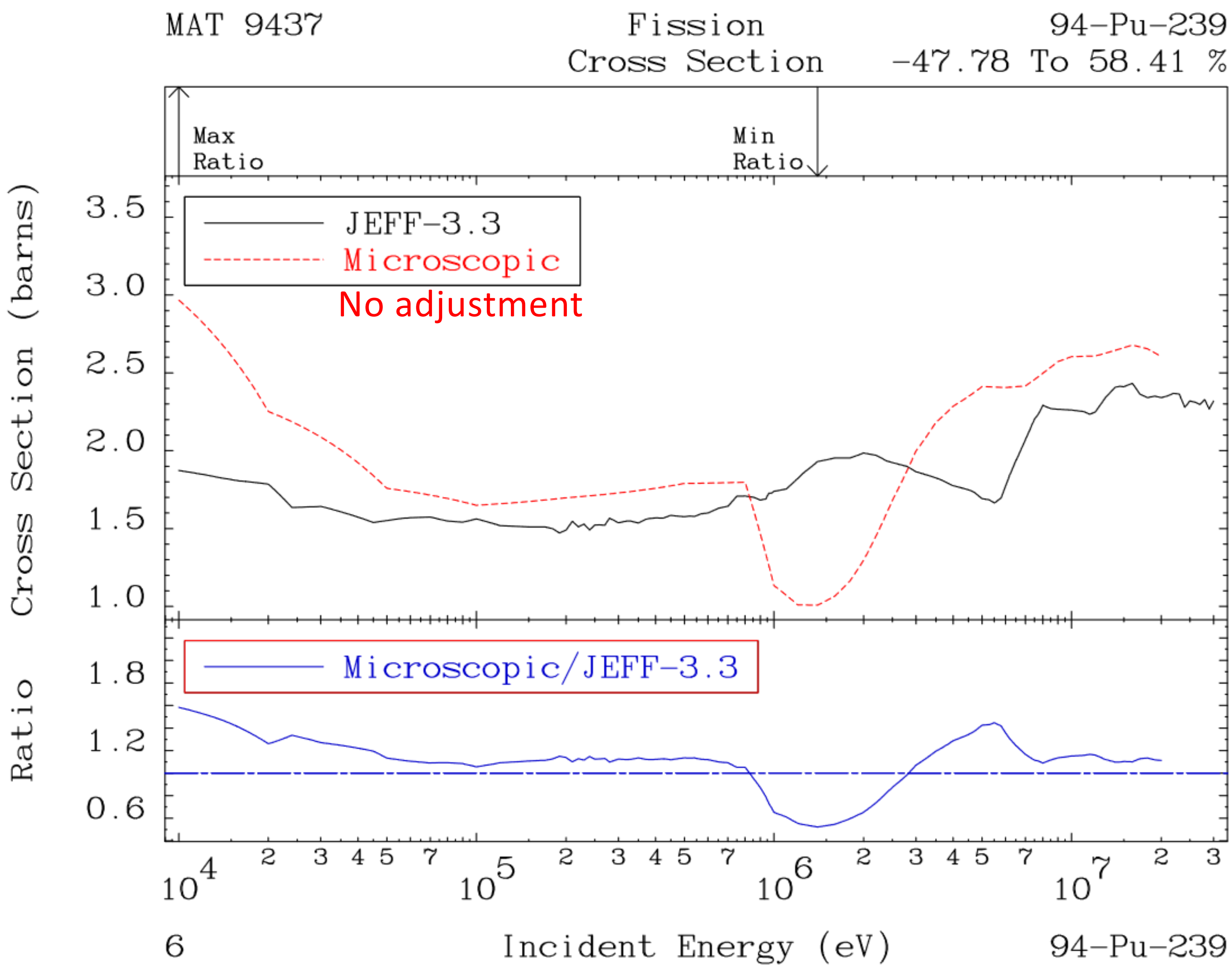
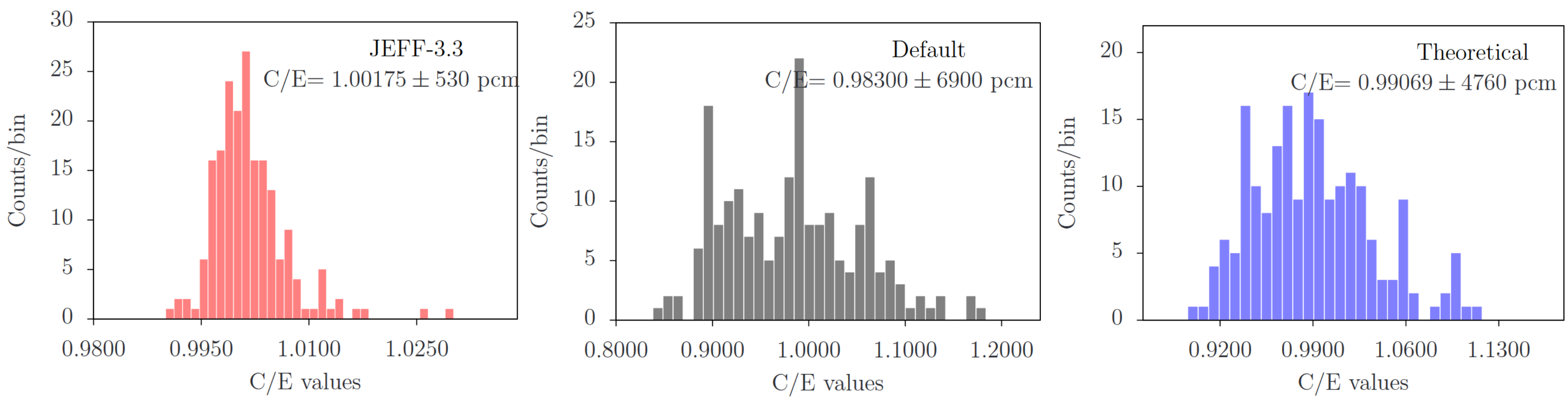


Results

- 195 benchmarks

- JEFF-3.3: C/E= 1.00175 ± 530 pcm
- Default phenomenological models: C/E= 0.98300 ± 6900 pcm
- Microscopic (theoretical) models: C/E= 0.99069 ± 4760 pcm



- This quantifies the evaluation efforts:
  - Reduce the bias from ≈2000 pcm to ≈200 pcm
  - Reduce the spread from ≈5000 pcm to ≈500 pcm

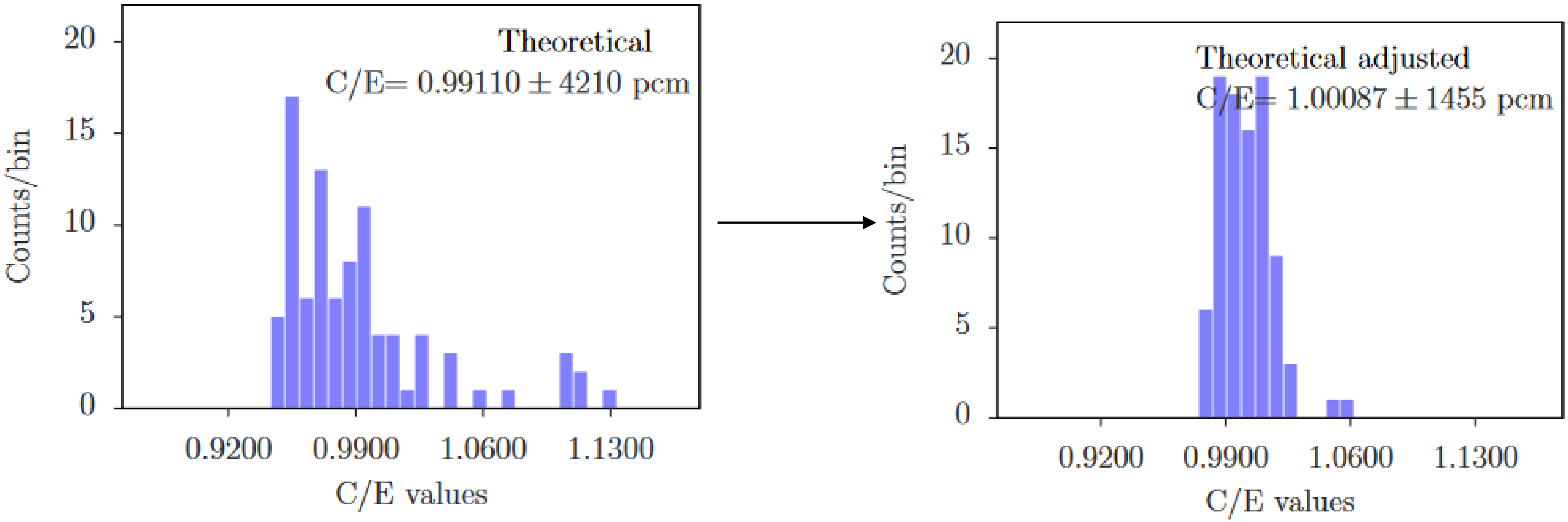
Results with adjusted microscopic ^{239}Pu

- What if we adjust parameters of microscopic models for ^{239}Pu (all other isotopes from JEFF-3.3)
- 90 pmf, imf and mmf benchmarks (no hmf benchmarks)

Results with adjusted microscopic ^{239}Pu

- What if we adjust parameters of microscopic models for ^{239}Pu (all other isotopes from JEFF-3.3)
- 90 pmf, imf and mmf benchmarks (no hmf benchmarks)

- JEFF-3.3: C/E= 1.00179 ± 480 pcm
- Default phenomenological models: C/E= 0.91740 ± 4430 pcm
- Microscopic (theoretical) models: C/E= 0.99110 ± 4210 pcm
- Adjusted microscopic (theoretical) models C/E= 1.00087 ± 1450 pcm



Other models in TALYS

- TALYS contains many models. Variations are applied in TENDL-astro 2023

TENDL-astro 2023

Cross sections, reaction rates and MACS for astrophysics

Recommended quantities

Cross sections

1. (n,g) (n,p), (n,a),
2. (p,g) (p,n), (p,a),
3. (a,g) (a,n), (a,p),

Reaction rates

1. (n,g) (n,p), (n,a),
2. (p,g) (p,n), (p,a),
3. (a,g) (a,n), (a,p),

Normalized partition function G(T)

30 keV Laboratory Maxwellian Averaged (n,g) Cross Sections MACS

Description of TALYS models

Below are various links to 8892 isotopes for astrophysics applications (cross sections, reaction rates and MACS) based on TALYS calculations (version 1.96).

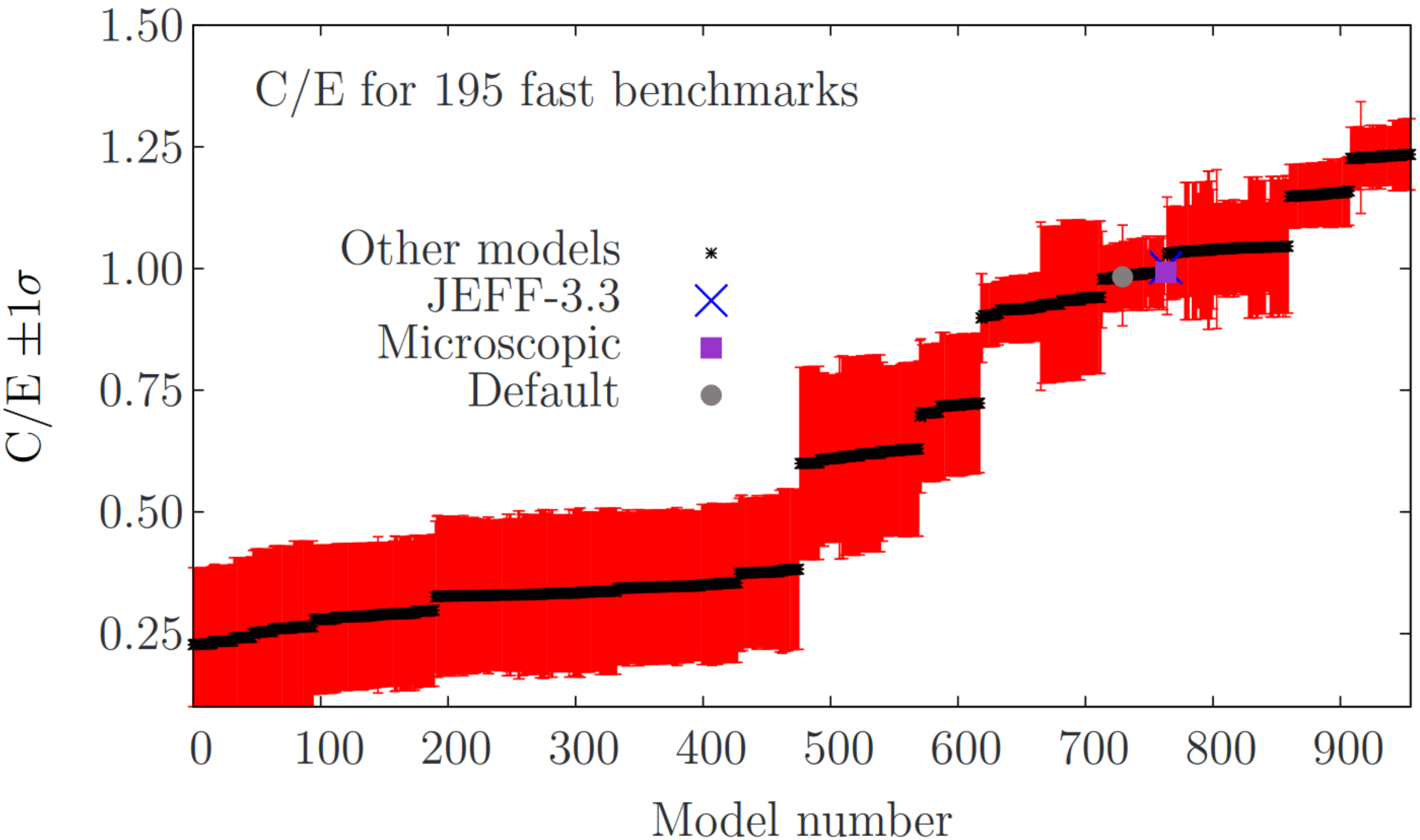
Different reaction "model sets" were used: "a model set" represents a combination of 9 TALYS models:

1. Gamma strength function (values 8 or 9): either Gogny D1M HFB+QRPA, or SMLO
2. Level density (values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables
3. JLM microscopic optical model potential or KD optical model (values y or n)
4. Gamma strength function for M1 (values 3 or 8): Hartree-Fock BCS tables or Gogny D1M HFB+QRPA
5. Collective enhancement (values y or n): yes or no
6. Width fluctuation (values 0, 1 or 2): Moldauer model, or Hofmann-Richert-Tepel-Weidenmueller model
7. Mass model (values 0, 1, 2 or 3): Duflo-Zuker formula, Moeller table, Goriely HFB-Skyrme table, or HFB-Gogny D1M table (except for known masses, where the experimental value is used)
8. Alpha optical model (values 5 or 6): Demetriou/Goriely, or Avrigeanu
9. Fission model (values 1 or 5): "experimental" fission barriers, or WKB approximation for fission path model.

Each of the set models is named with 9 values, such as "91n3n1261" (default TALYS model), or 85n8n1261. These values correspond to the ones in the TALYS manual.

- In total, more than 960 model variations

Other models in TALYS



Conclusion

- 195 fast benchmarks considered (hmf, pmf, imf, mmf)
- Nuclear data from (non adjusted) models

- Average C/E:
  - Default models: C/E= 0.98300 ± 6900 pcm
  - Microscopic models: C/E= 0.99069 ± 4760 pcm
  - Other models: C/E from 0.22700 to 1.23400

  - JEFF-3.3: C/E= 1.00175 ± 530 pcm

- Microscopic model can possibly be adjusted.

- This quantifies the evaluation efforts: gain a factor 10 in precision and accuracy
  - Reduce the bias from ≈2000 pcm to ≈200 pcm
  - Reduce the spread from ≈5000 pcm to ≈500 pcm

Wir schaffen Wissen – heute für morgen

List of the 195 k_{eff} benchmarks

- hmf: 82 cases

hmf1.1, hmf3.1, hmf3.3-hmf3.12, hmf4.1, hmf5.1-hmf5.6, hmf7.1-hmf7.9, hmf8.1, hmf9.1, hmf9.2, hmf11.1, hmf12.1, hmf13.1, hmf15.1, hmf18.1, hmf19.1, hmf20.1, hmf21.1, hmf22.1, hmf24.1, hmf25.1-hmf25.5, hmf26.11, hmf27.1, hmf28.1, hmf34.1-hmf34.3, hmf41.1-hmf41.6, hmf43.1-hmf43.5, hmf44.1-hmf44.5, hmf48.1, hmf48.3, hmf48.5, hmf48.7, hmf48.9, hmf56.1, hmf57.1-hmf57.6

- pmf: 72 cases

pmf1.1, pmf2.1, pmf3.101-pmf3.105, pmf4.207-pmf4.215, pmf5.1, pmf6.1, pmf8.1, pmf9.1, pmf10.1, pmf11.1, pmf12.1, pmf13.1, pmf14.1, pmf15.1, pmf16.1-pmf16.6, pmf17.201-pmf17.205, pmf18.1, pmf19.1, pmf20.1, pmf21.1, pmf22.1, pmf23.1, pmf24.1, pmf25.1, pmf26.1, pmf27.1, pmf28.1, pmf29.1, pmf30.1, pmf31.1, pmf32.1, pmf33.1, pmf35.1, pmf36.1, pmf37.1, pmf38.1, pmf39.1, pmf40.1, pmf41.1, pmf44.1-pmf44.5, pmf45.1-pmf45.5, pmf46.1, pmf46.2

- imf: 23 cases

imf1.1-imf1.4, imf2.1, imf3.1, imf3.2, imf4.1, imf5.1, imf6.1, imf7.1, imf10.1, imf12.1, imf13.1, imf14.1, imf14.2, imf20.1-imf20.7, imf22.1

- mmf: 18 cases

mmf1.1, mmf2.1-mmf2.3, mmf3.1, mmf7.1, mmf7.3, mmf7.5, mmf7.9, mmf7.11, mmf7.13, mmf7.15, mmf8.1, mmf11.1-mmf11.4

List of the considered isotopes

- Actinides: $^{234,235,236,238}U$, $^{239,240,241}Pu$

- Others: $^{63,65}Cu$, $^{54,56,57,58}Fe$, $^{58,60,61,62,64}Ni$, $^{180,182,183,184,186}W$, $^{28,29,30}Si$, $^{50,52,53,54}Cr$, $^{69,71}Ga$, $^{92,94,95,96,97,98,100}Mo$, $^{46,47,48,49,50}Ti$, ^{55}Mn, $^{24,25,26}Mg$, ^{19}F

Typical TALYS inputs

Default

```
#
# TALYS input file generated by Autotalys
#
projectile n
element    Th
mass       232
Ltarget    000
energy     energies
partable y
bins 60
#
# Do not use best parameters from database
#
best n
#
# Set multi-preequilibrium switch lower for actinides
#
multipreeq 6.
isomer 0.1
#
# Produce files for processing into ENDF and
# increase required precision
#
endf y
endfdetail y
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
#
# Output of extra channels
#
channels y
filechannels y
#
# Recoils
#
recoil y
recoilaverage y
urr 20
Upbend y
Ngfit y
strength 9
ldmodel 1
jlmomp n
strengthM1 3
colenhance n
widthmode 1
massmodel 2
alphaomp 6
fismodel 1
disctable 1
```

Microscopic

```
#
# TALYS input file generated by Autotalys
#
projectile n
element    Th
mass       232
Ltarget    000
energy     energies
partable y
bins 60
#
# Do not use best parameters from database
#
best n
#
# Set multi-preequilibrium switch lower for actinides
#
multipreeq 6.
isomer 0.1
#
# Produce files for processing into ENDF and
# increase required precision
#
endf y
endfdetail y
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
#
# Output of extra channels
#
channels y
filechannels y
#
# Recoils
#
recoil y
recoilaverage y
urr 20
strength 8
ldmodel 5
disctable 3
jlmomp y
fit n
best n
fismodel 5
psfglobal y
asys y
localomp n
expmass n
```