60 Years

IAEA Atoms for Peace and Development

Status of (the) TALYS (empire)

Arjan Koning, IAEA

Contents

- Public relations
- Level density and photon strength function validation
- Eric!
- Wild ideas for the future

Eur. Phys. J. A (2023) 59:131
https://doi.org/10.1140/epja/s10050-023-01034-3

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Review

TALYS: modeling of nuclear reactions

This is now the basic reference for TALYS

Arjan Koning[1,a], **Stephane Hilaire**[2,3,b], **Stephane Goriely**[4,c]

[1] Nuclear Data Section, IAEA, Wagrammerstrasse 5, Vienna 1400, Austria
[2] DIF, CEA, Arpajon 91297, France
[3] Université Paris-Saclay, CEA, LMCE, 91680 Bruyères-le-Châtel, France
[4] Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine, CP-226, Brussels 1050, Belgium

Received: 16 February 2023 / Accepted: 6 May 2023

Communicated by Nicolas Alamanos

Abstract TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. A general overview of the implemented physics and capabilities of TALYS is given. The general nuclear reaction mechanisms described are the optical model, direct reactions, compound nucleus model, pre-equilibrium reactions and fission. The most important nuclear structure models are those for masses, discrete levels, level densities, photon strength functions and fission barriers. A wide variety of nuclear reactions simulated with TALYS will be demonstrated, ranging from low-energy neutron cross sections, astrophysics, high-energy charged particle reactions and other reactions. TALYS is a nuclear reaction software which aims to give a complete description of nuclear reaction observables, and to be an important link between fundamental nuclear physics and applications.

TALYS & Related Software

TALYS and the related packages are open source software and datasets (MIT License) for the simulation of nuclear reactions.

60 Years

Atoms for Peace and Development

nds.iaea.org/talys

TALYS

Arjan Koning, Stephane Hilaire, Stephane Goriely

Nuclear reaction model code.

- Download TALYS-2.0 or TALYS-1.97 (equivalent results)
- Previous and Other Versions
- Read Tutorial
- Cite Reference
- Use TALYSworld
- Watch TALYS video lectures
- Access on GitHub

Created at NRG cea ULB UNIVERSITÉ LIBRE DE BRUXELLES IAEA

TASMAN

Arjan Koning

Statistical software for TALYS: Uncertainties, sensitivities and optimization.

- Download TASMAN-2.0
- Read Tutorial
- Cite Reference
- Access on GitHub

TEFAL

Arjan Koning

Code to make ENDF-6 nuclear data libraries from TALYS.

- Download TEFAL-2.0
- Read Tutorial
- Cite Reference
- Access on GitHub

EXFORTABLES

Arjan Koning

Experimental nuclear reaction database based on EXFOR.

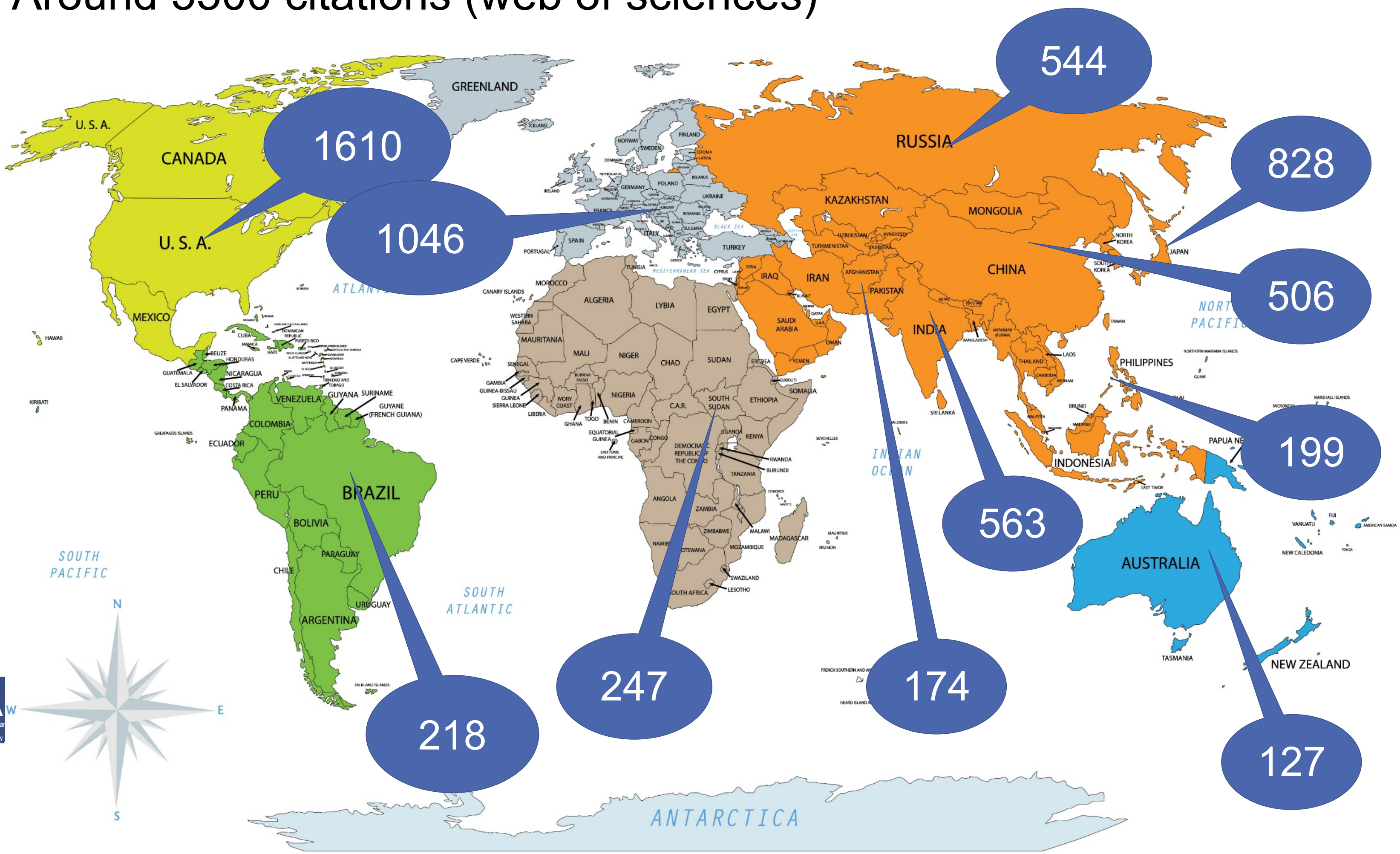
ENDFTABLES

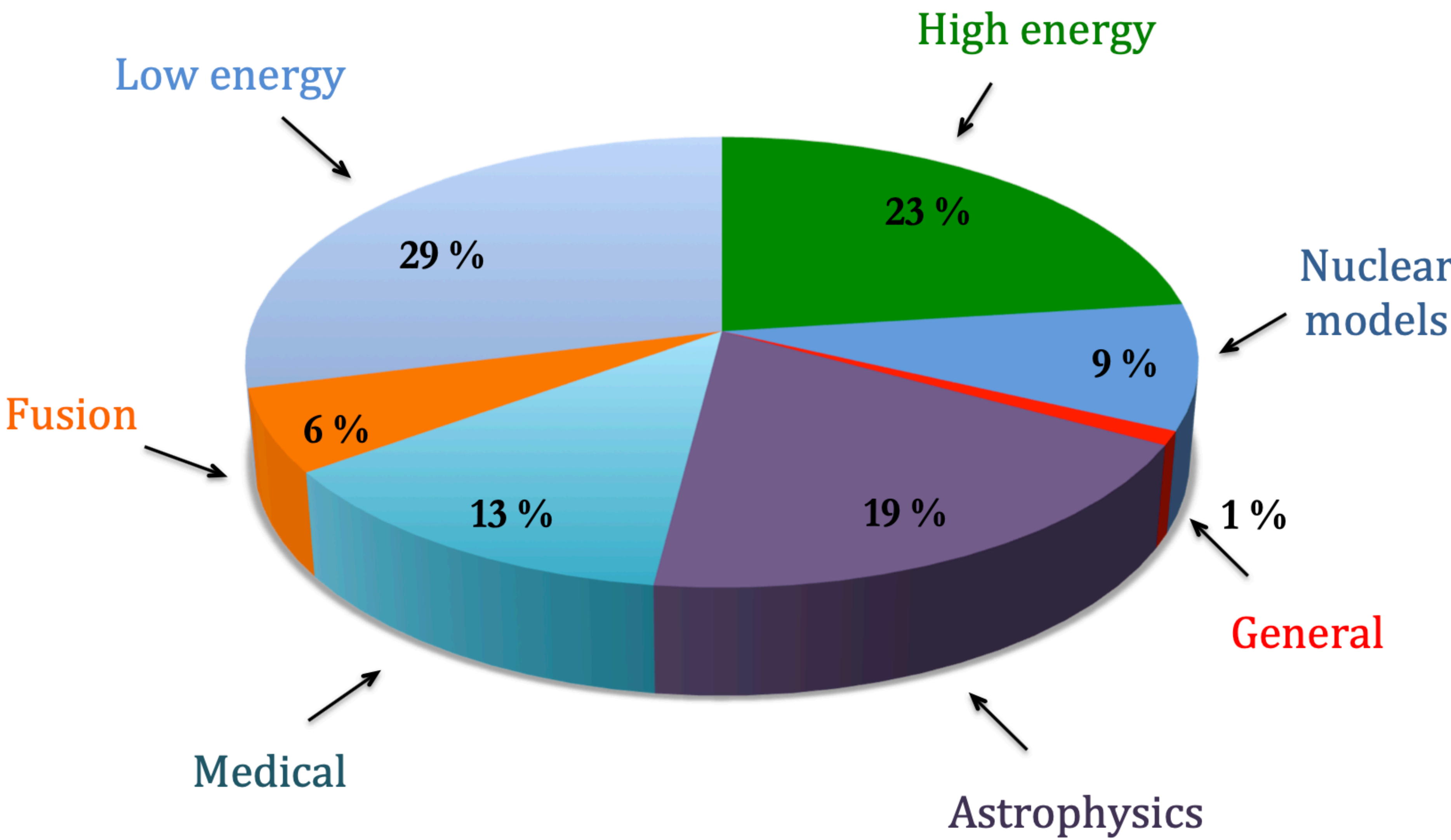
Arjan Koning

Code to translate ENDF nuclear data libraries into tabular format.

TALYS around the World (status 2022)

- Around 5500 citations (web of sciences)




High energy
23 %
Low energy
29 %
Nuclear models
9 %
Fusion
6 %
13 %
19 %
1 %
General
Medical
Astrophysics

https://indico.ictp.it/event/10221/ : 30 hours of TALYS videos

Speakers

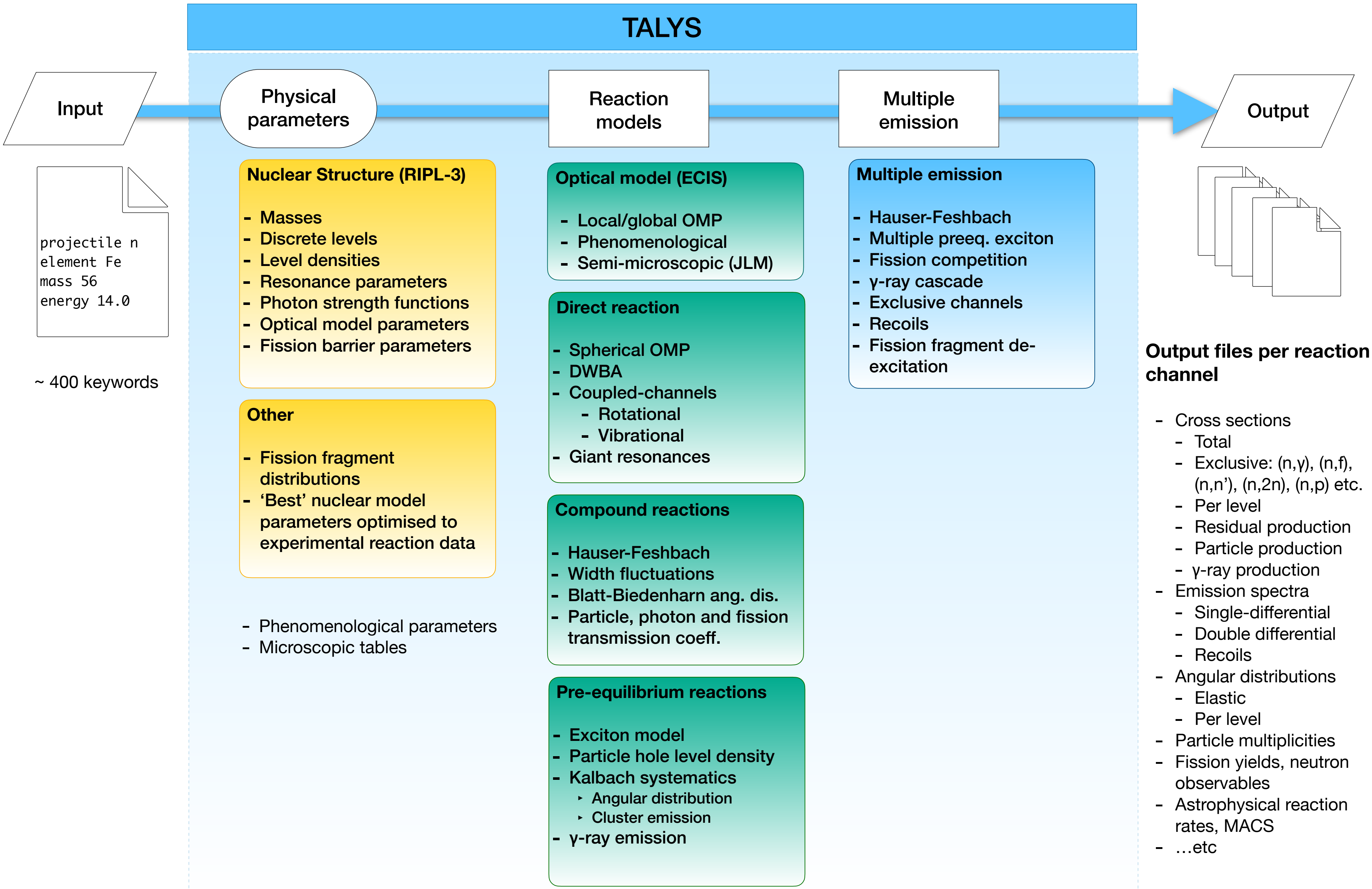
Practical info

Material

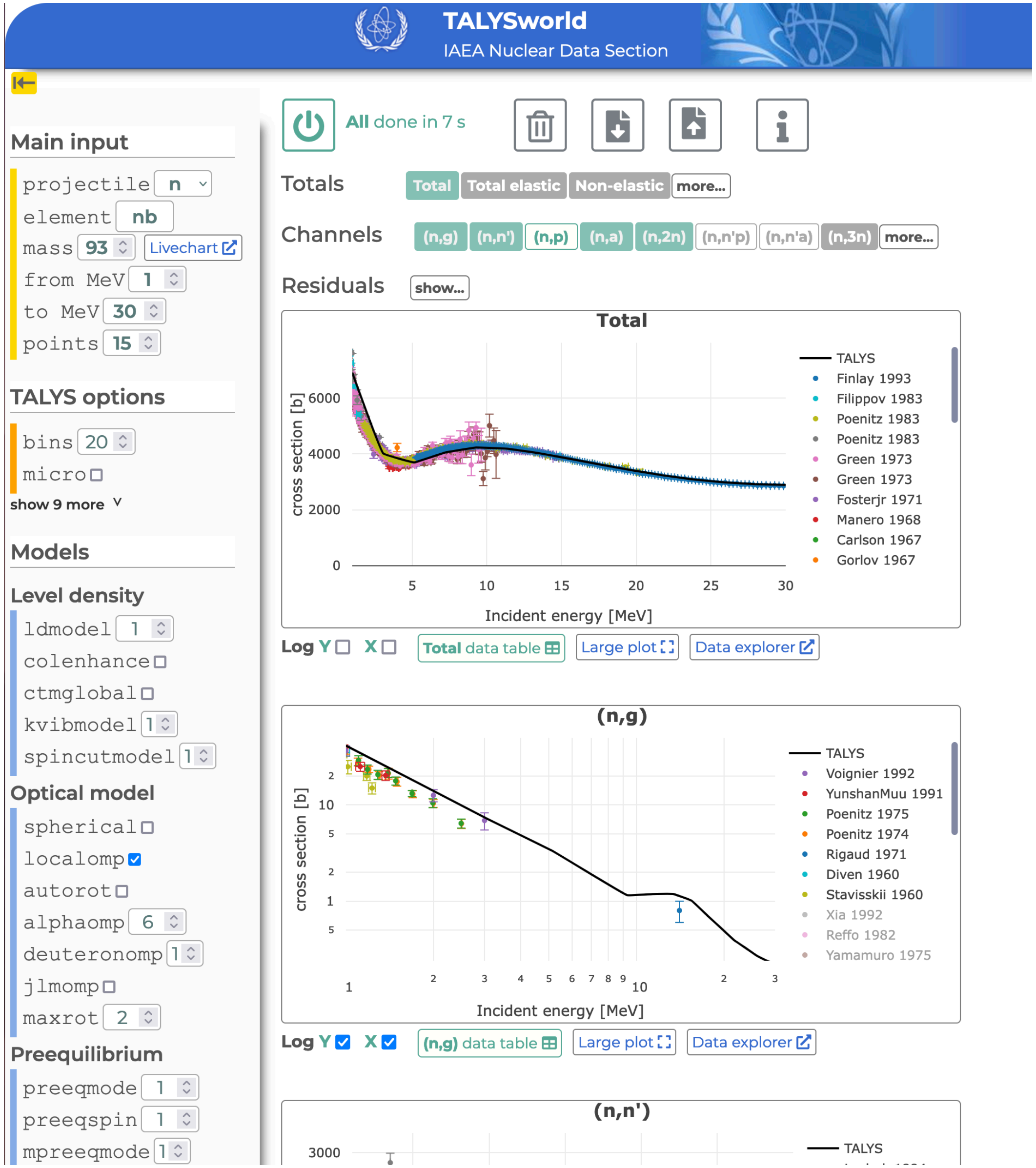
- AGENDA
- AbstractTemplate
- Booklet Participants' talks
- Final list of Participants
- Group photo
- How to choose your Time Zone
- Poster

09:00 - 17:30

09:00	**Introduction to ICTP and the Workshop** *10'* Speakers: Arjan KONING (IAEA, Austria), Nadia BINGGELI (ICTP, Italy) Material: Slides
09:10	**General overview and use of TALYS** *1h20'* Speaker: Arjan KONING (IAEA, Austria) Material: Slides, Video
10:30	**Coffee break** *30'*
11:00	**Nuclear data facilities and measurements I** *1h30'* Speaker: Stephan POMP (University Uppsala, Sweden) Material: Slides, Video
12:30	**Lunch break** *1h30'*
14:00	**Nuclear structure ingredients for reaction models** *1h30'* Speaker: Stephane GORIELY (Université Libre de Bruxelles, Belgium) Material: Slides, Video
15:30	**Coffee break** *30'*
16:00	**Optical model and compound nucleus model** *1h30'* Speaker: Stephne HILAIRE (CEA, DAM, DIF, France) Material: Slides, Video


TALYS
Input
Physical parameters
Reaction models
Multiple emission
Output
projectile n
element Fe
mass 56
energy 14.0
~ 400 keywords
Nuclear Structure (RIPL-3)
- Masses
- Discrete levels
- Level densities
- Resonance parameters
- Photon strength functions
- Optical model parameters
- Fission barrier parameters
Other
- Fission fragment distributions
- 'Best' nuclear model parameters optimised to experimental reaction data
- Phenomenological parameters
- Microscopic tables
Optical model (ECIS)
- Local/global OMP
- Phenomenological
- Semi-microscopic (JLM)
Direct reaction
- Spherical OMP
- DWBA
- Coupled-channels
- Rotational
- Vibrational
- Giant resonances
Compound reactions
- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.
Pre-equilibrium reactions
- Exciton model
- Particle hole level density
- Kalbach systematics
‣ Angular distribution
‣ Cluster emission
- γ-ray emission
Multiple emission
- Hauser-Feshbach
- Multiple preeq. exciton
- Fission competition
- γ-ray cascade
- Exclusive channels
- Recoils
- Fission fragment de-excitation
Output files per reaction channel
- Cross sections
- Total
- Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
- Per level
- Residual production
- Particle production
- γ-ray production
- Emission spectra
- Single-differential
- Double differential
- Recoils
- Angular distributions
- Elastic
- Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …etc

If nothing else works....TALYSworld!!!



TALYS world

https://nds.iaea.org/relnsd/talys/talys.html

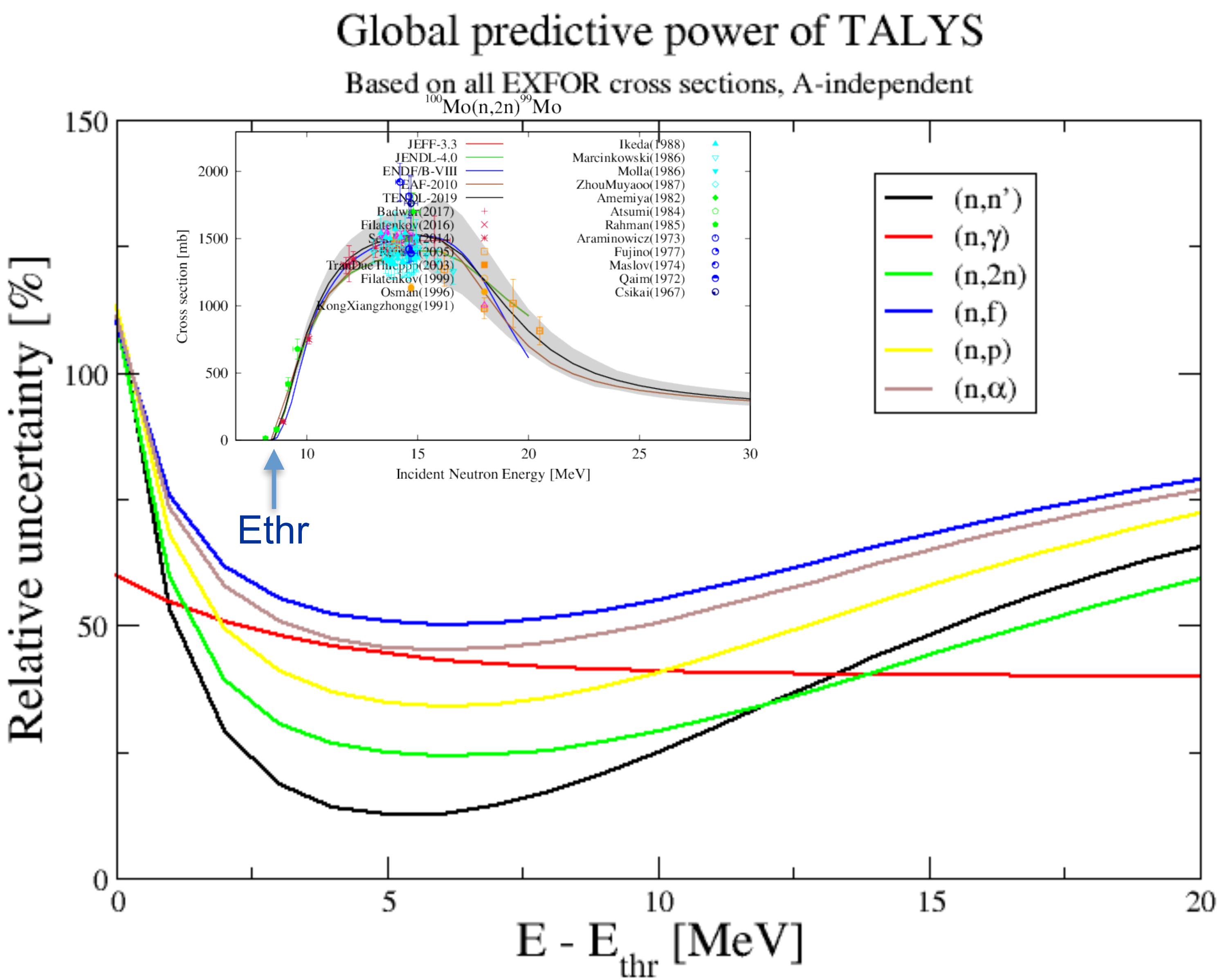
- Run TALYS online
- Direct plots
- EXFORtables included (coverage of EXFOR not complete)
- Status July 2024:
  - First announcement at ICTP Trieste School on TALYS
  - Half of the keywords are implemented
  - Only cross sections

Scan me!

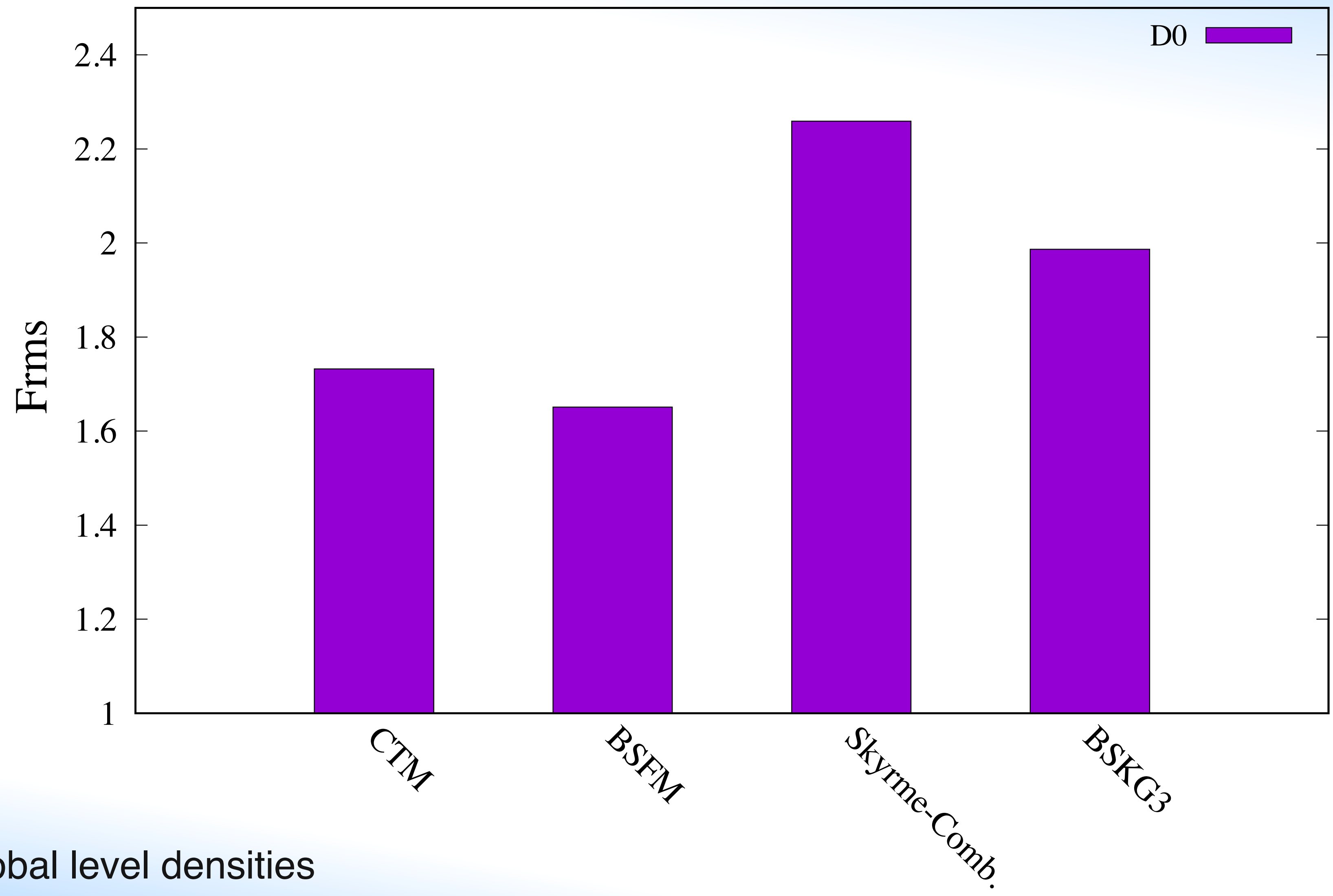
TALYS-2.0

- Some important new features since TALYS-1.96 (Dec 2021)
  - Further refinement of explicit evaporation of fission fragments via Hauser-Feshbach: FY, nubar, nu(A), PFNS, etc. using HF3D, GEF, SPY and 4D-Langevin fission fragment distributions
  - ‘fit y’: read in optimised nuclear model parameters for all nuclides and reaction channels (from TASMAN parameter search to EXFOR), giving the best fits
  - Unifying all TALYS output in YANDF format (Yet Another Nuclear Data Format) for efficient interpretation for processing software - ENDF, GNDS, AI/ML, plotting, astro libraries etc. etc.
- TALYS-1.97/2.0 was released end of December 2023

Long-term goal: Global predictive power

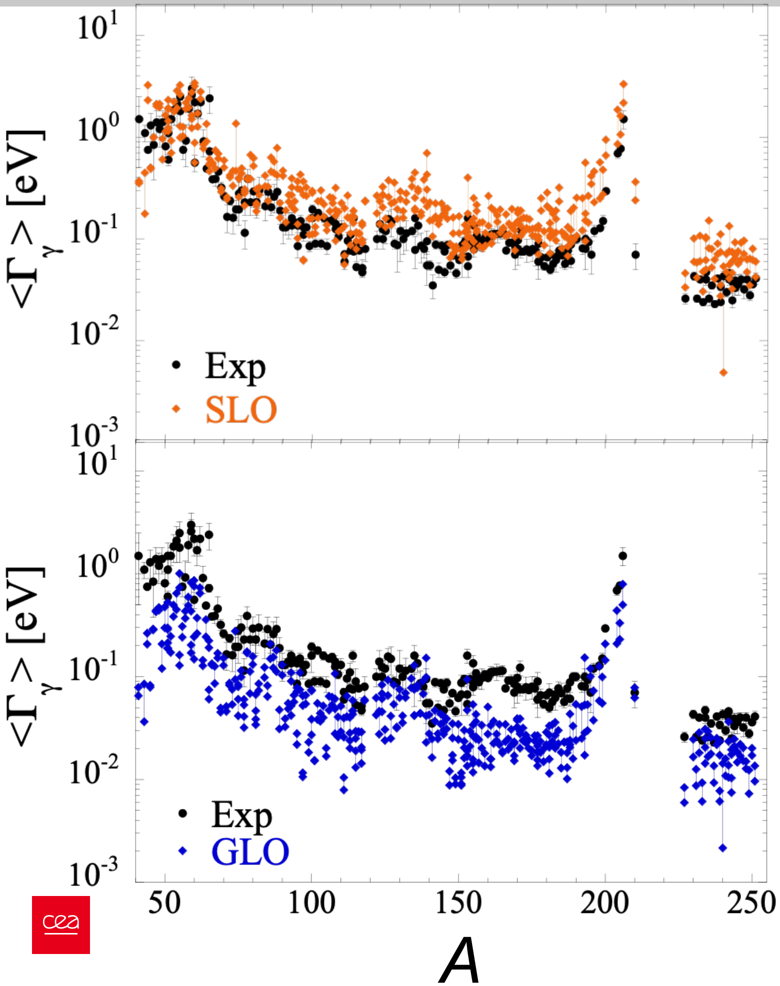


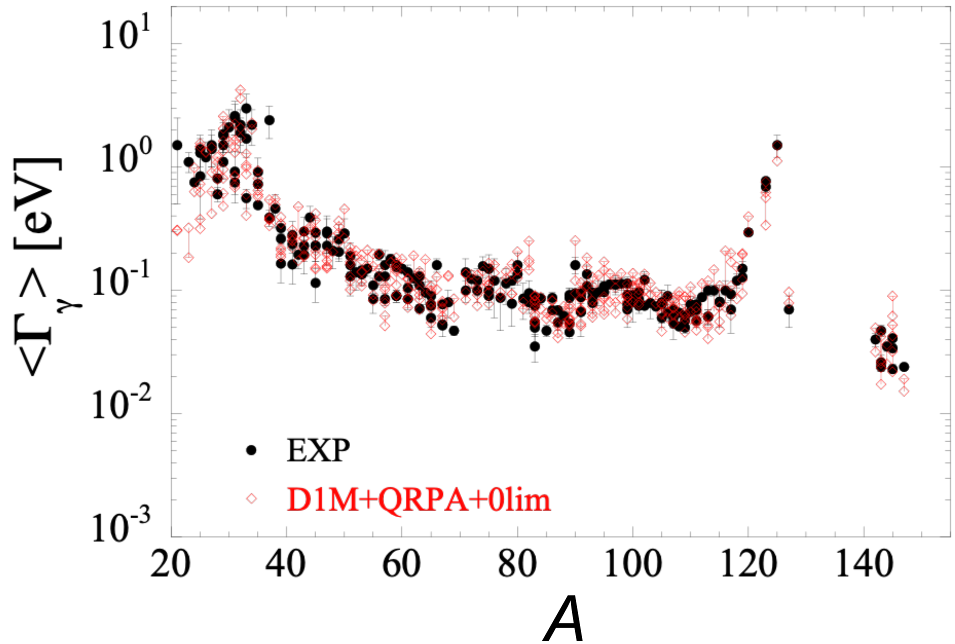
TALYS Average s-wave resonance width (D0) vs. experiment



Global level densities
Nuclides with experimental D0 data: 300 (RIPL-3)

Gamma-ray strengths : Gogny QRPA vs analytical



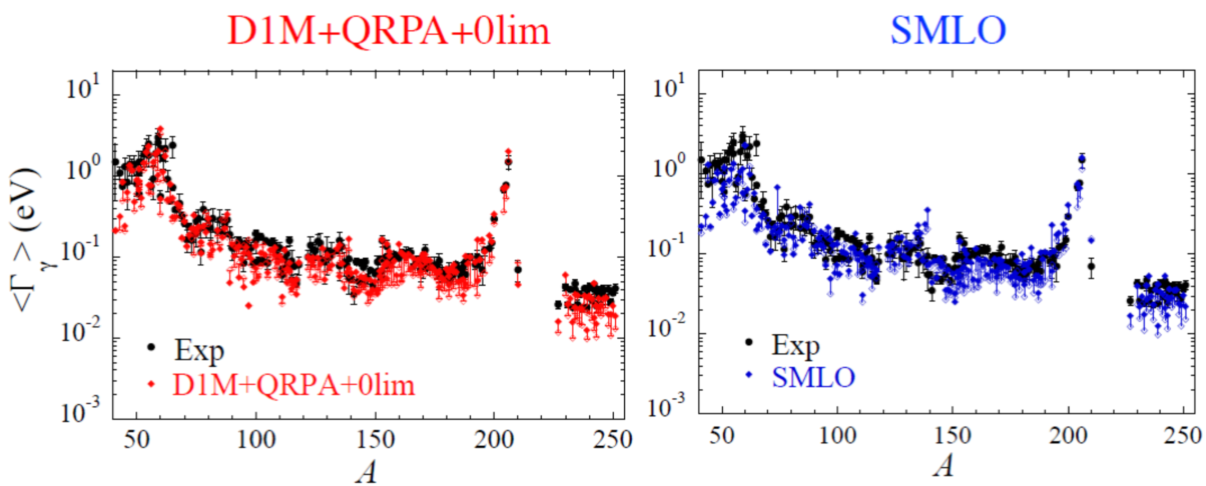


Gamma-ray strengths : Gogny QRPA vs analytical

Disposition : Titre et contenu

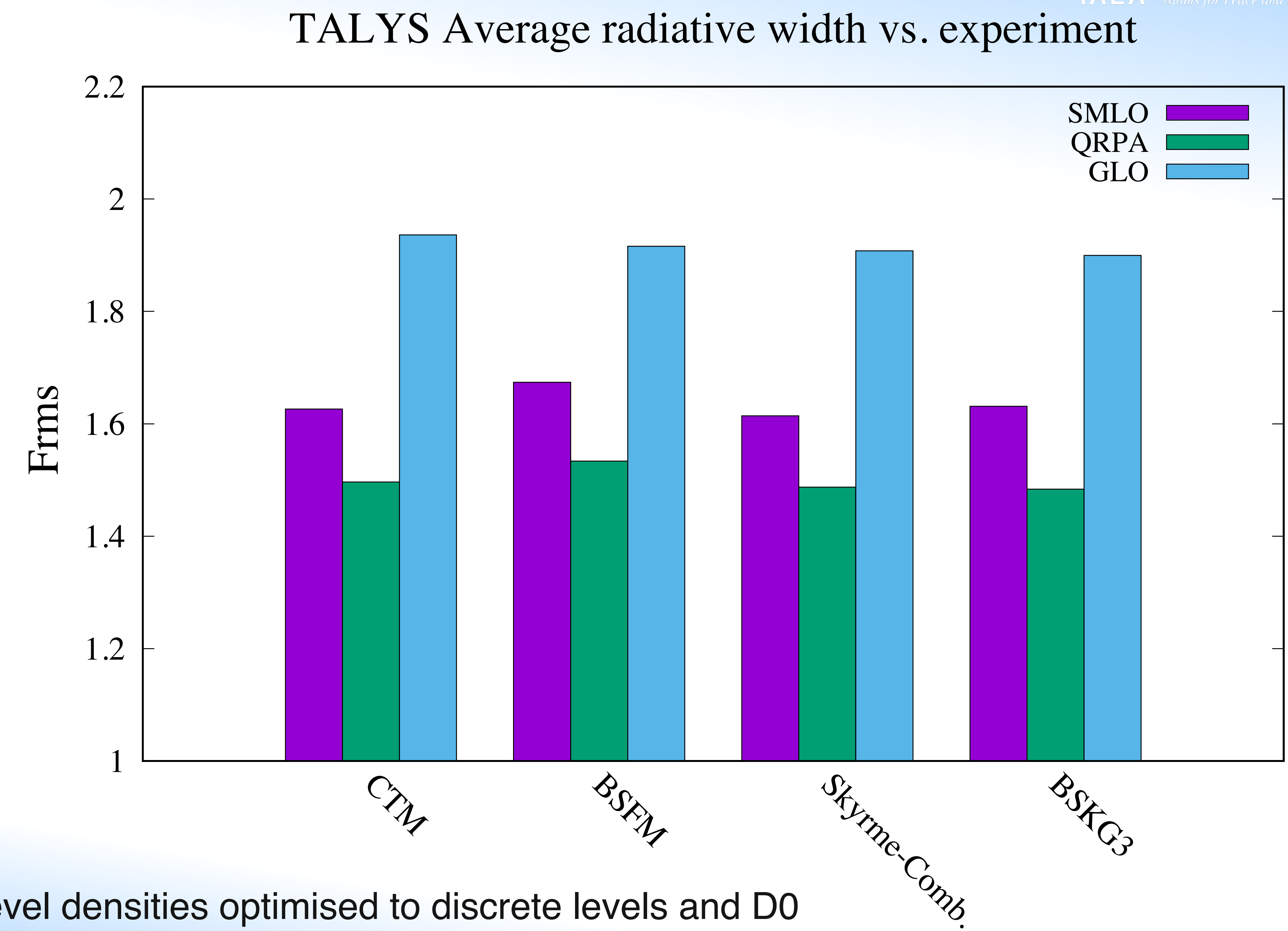
Comparison of D1M+QRPA+0lim and SMLO with $<\Gamma_\gamma>$ data

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



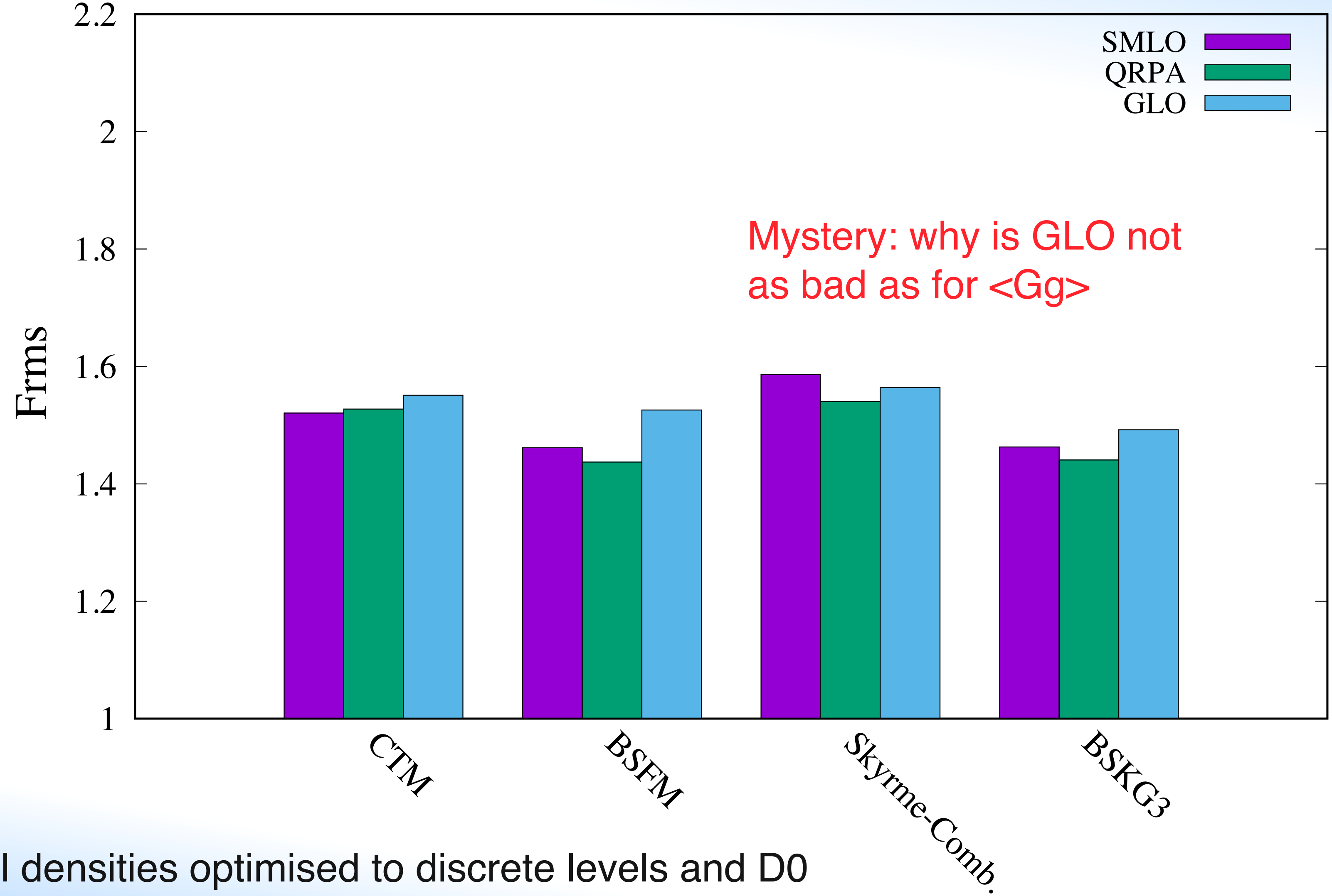
Open diamonds = CT + BSFG
Full diamonds = HFB + Combinatorial

Both PSF models reproduce ~230 $<\Gamma_\gamma>$ within ~ 30-50%



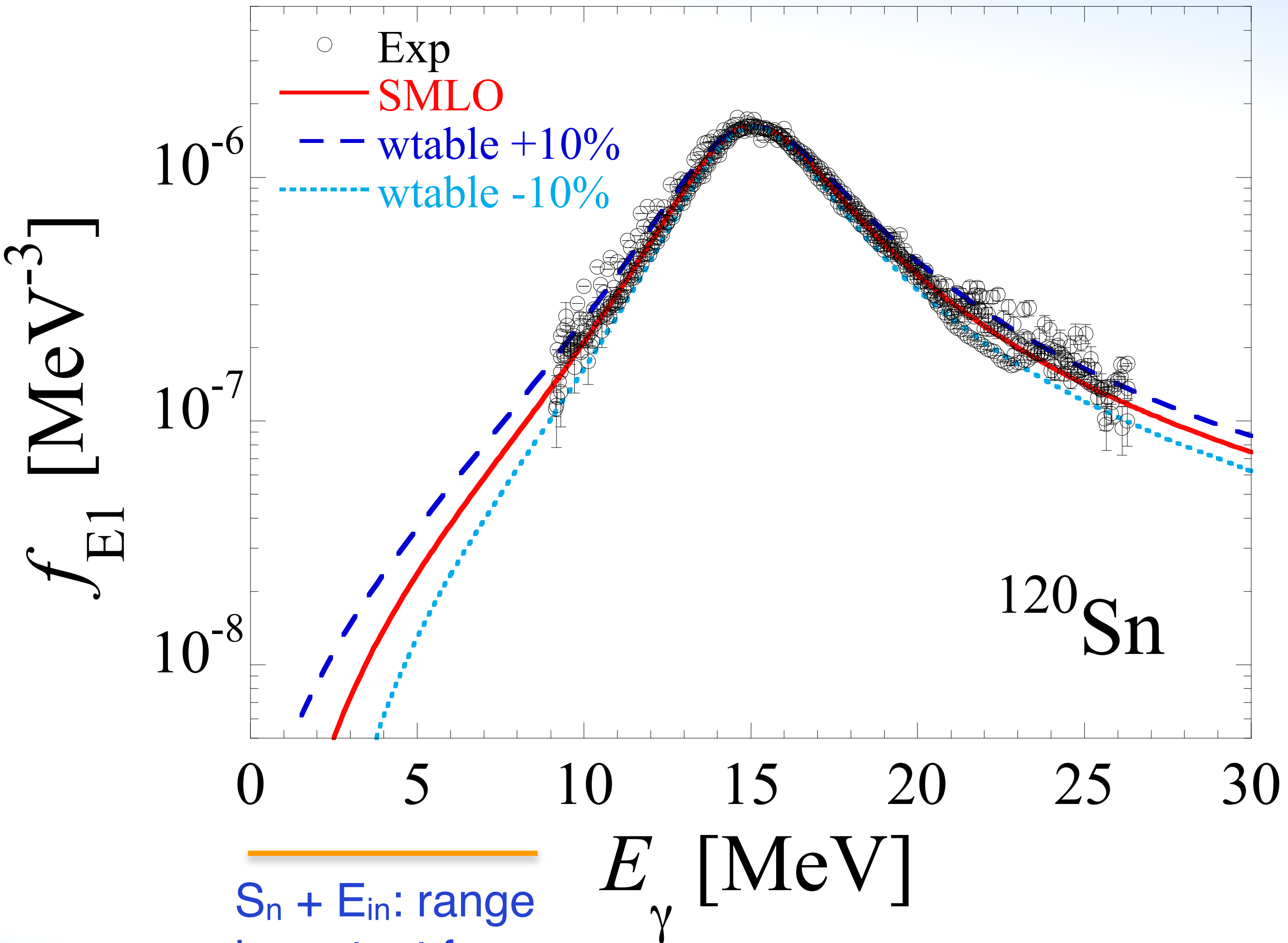
Level densities optimised to discrete levels and D0
Nuclides with experimental <Gg> data: 228

TALYS Maxwellian Averaged cross sections vs. experiment



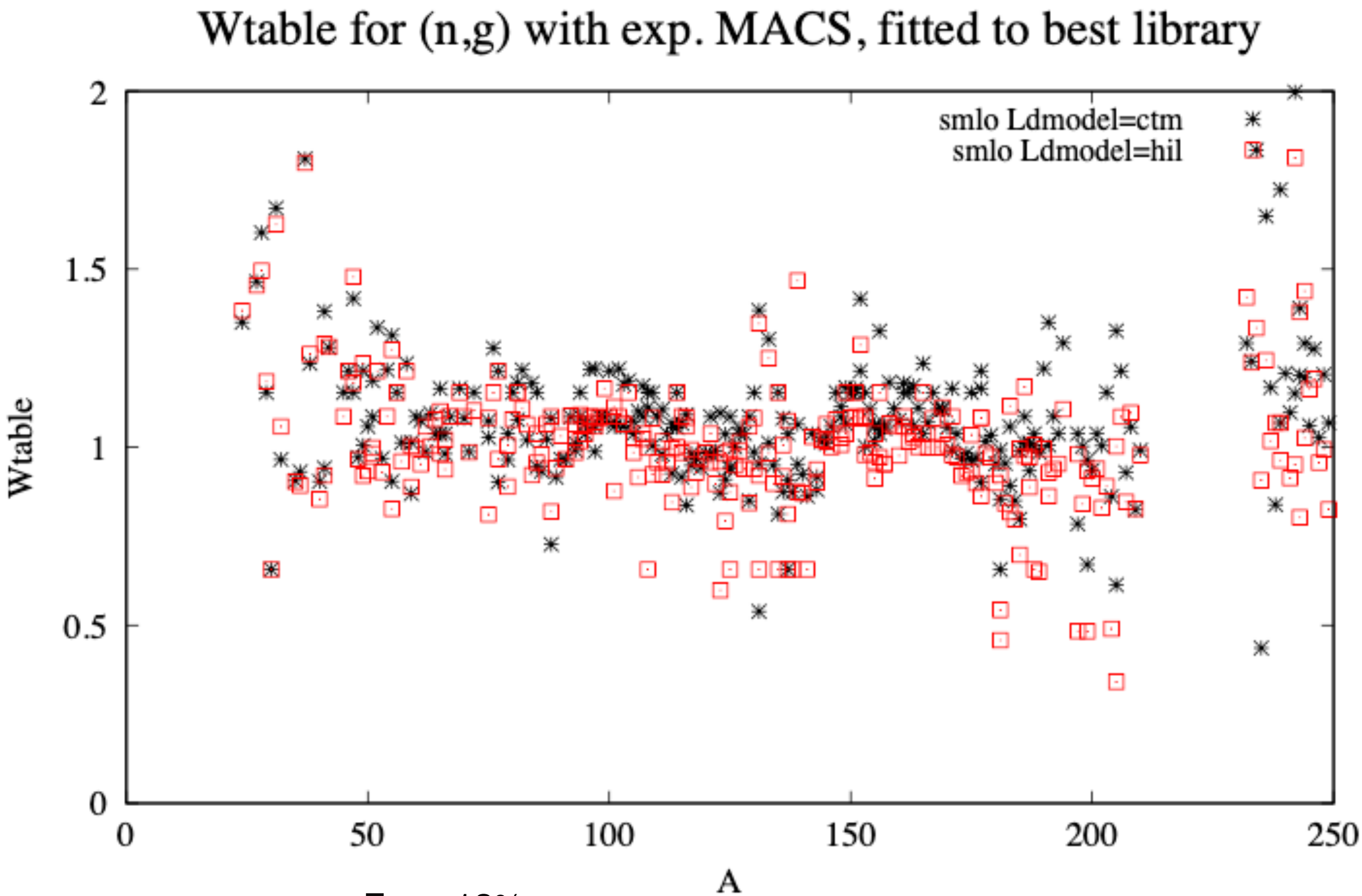
Level densities optimised to discrete levels and D0
Nuclides with experimental MACS data: 277

Adjusted width parameter does not affect original photon strength function very much



S_n + E_{in}: range important for (n,γ)

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



Wtable for (n,g) with exp. MACS, fitted to best library
smlo Ldmodel=ctm
smlo Ldmodel=hil
Wtable
A
0
0.5
1
1.5
2
0
50
100
150
200
250

F_{rms} : 12%

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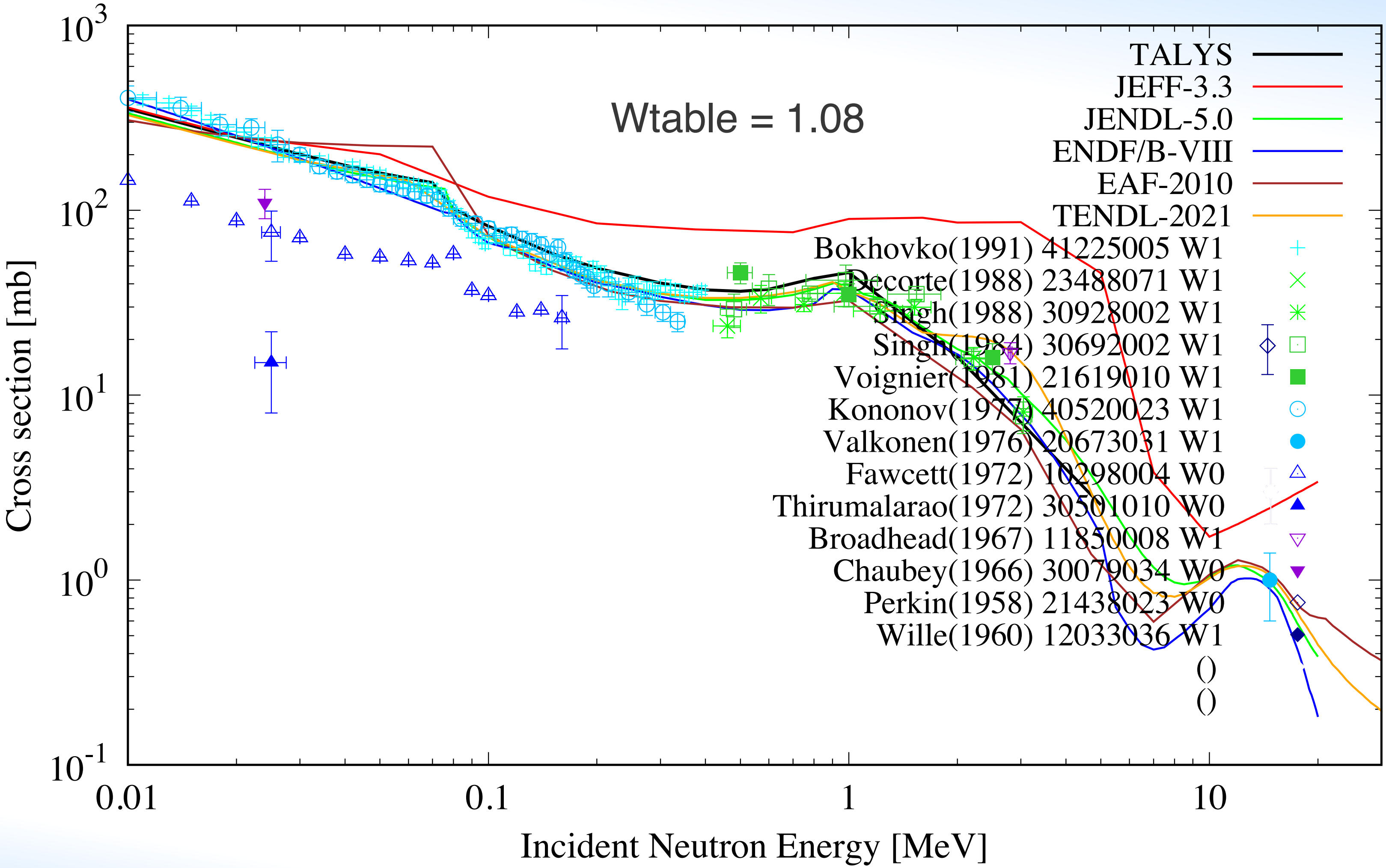
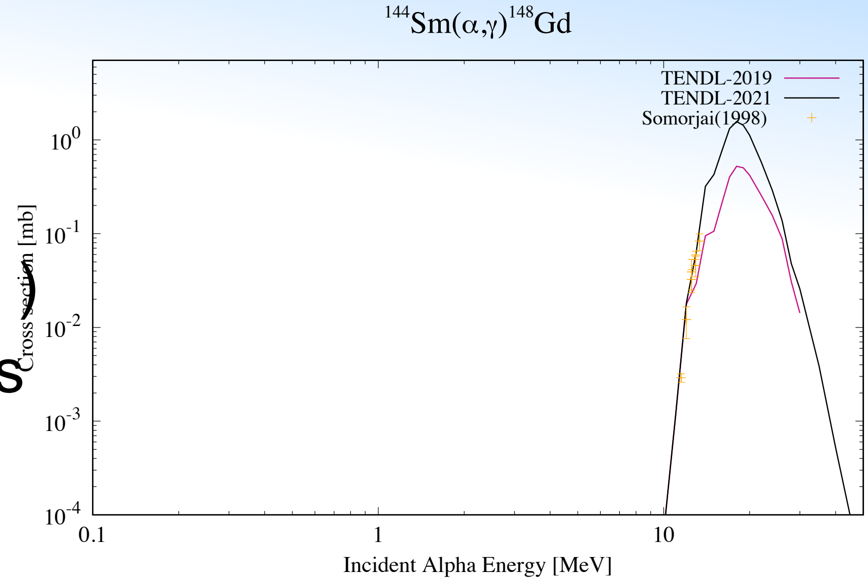
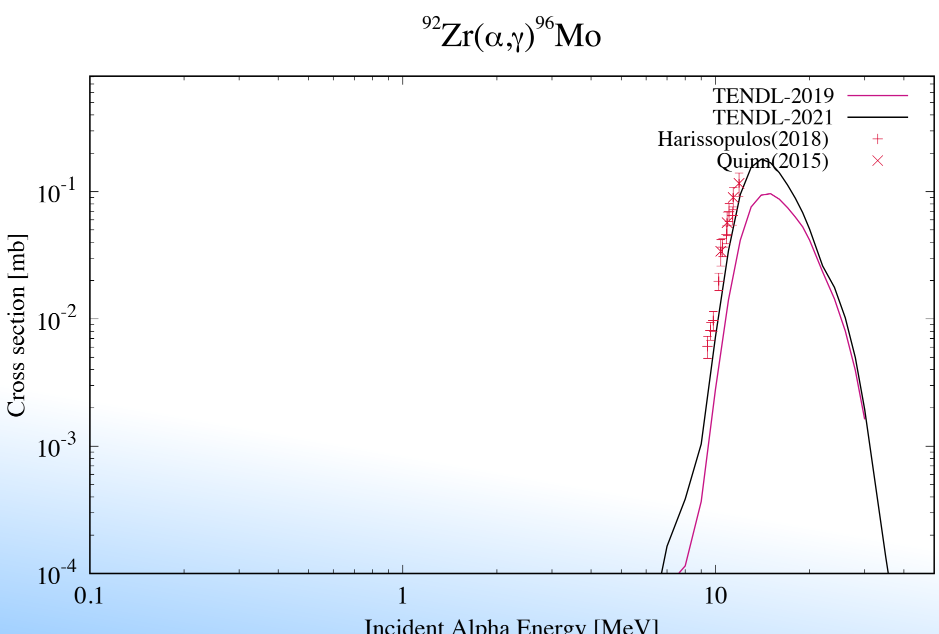
$^{160}Gd(n,\gamma)^{161}Gd$ GOF= 1.094

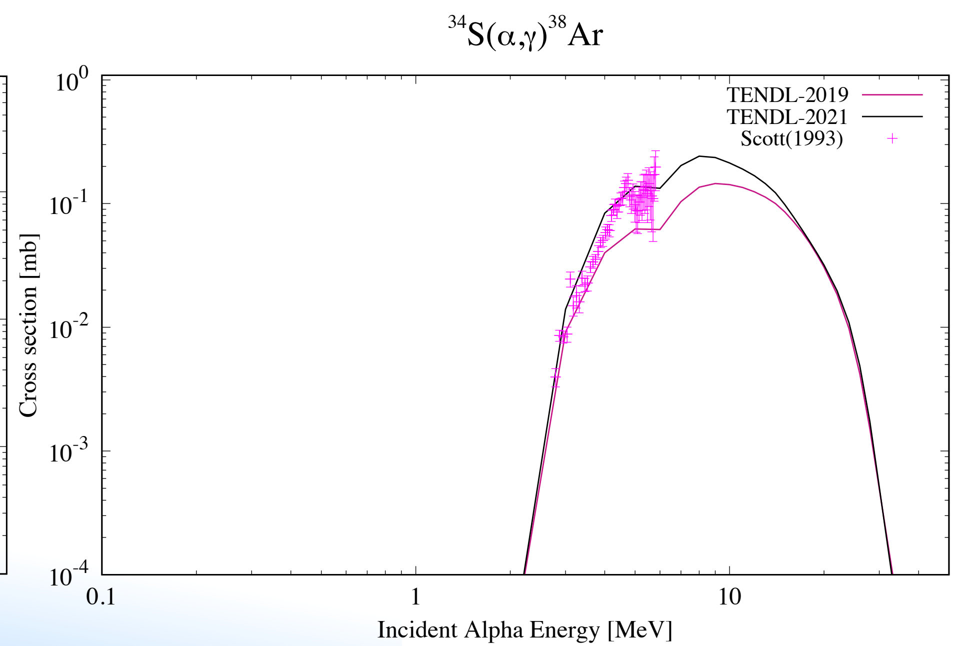


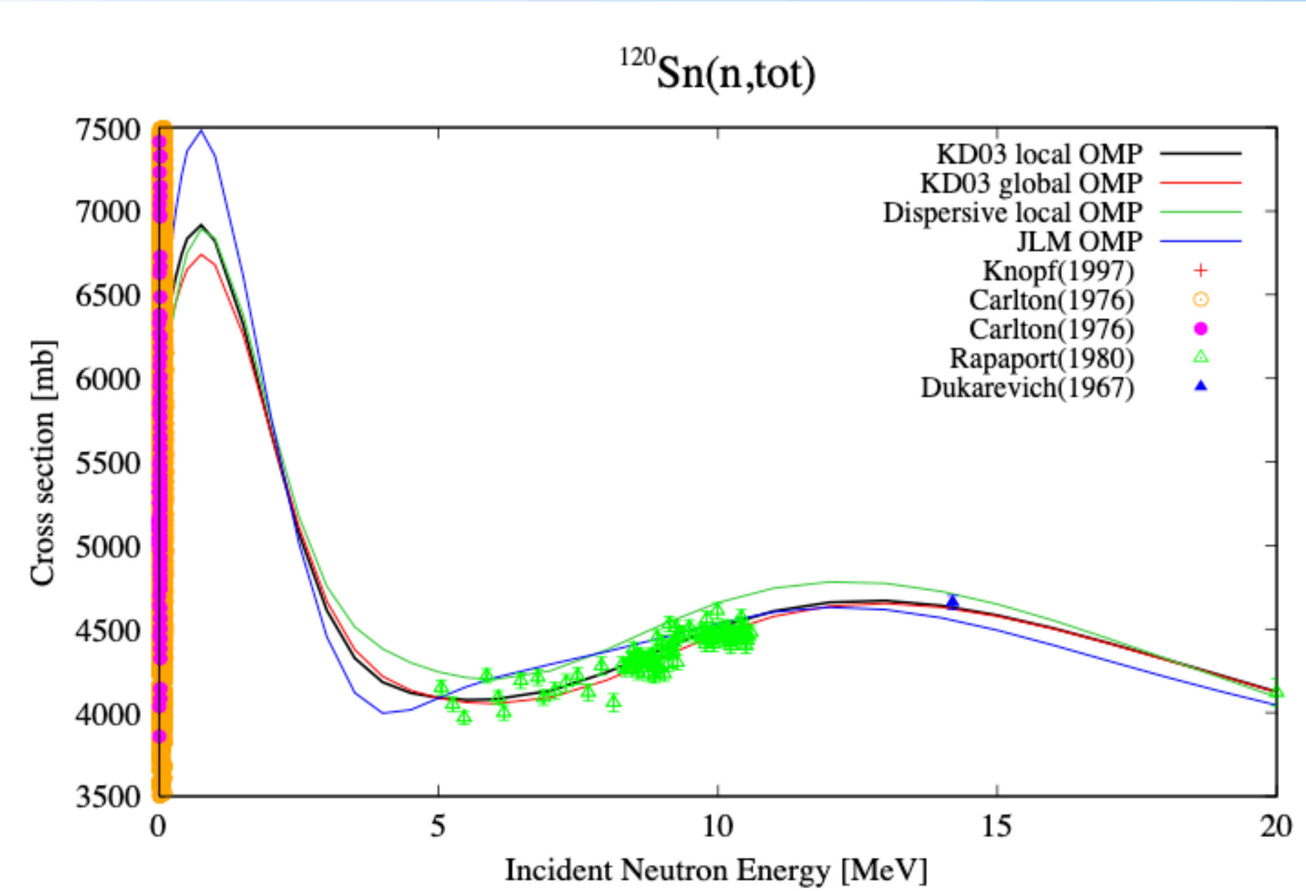
channel: (α , γ)

- New photon strength functions (Plujko & Goriely), SMLO, give better gamma-related data for all reaction channels, including (α ,γ)
- CRP on photon strength functions and photonuclear data, Dimitriou et al (IAEA 2019)









Eric Bauge JMP OMP:
Only 6 parameters

4 different input files

```
#
# n-Sn120-omp-KD03
#
# General
#
projectile n
element    sn
mass       120
energy     energies
```

```
#
# n-Sn120-omp-KD03global
#
# General
#
projectile n
element    sn
mass       120
energy     energies
#
# Parameters
#
localomp n
```

```
#
# n-Sn120-ompKD03disp
#
# General
#
projectile n
element    sn
mass       120
energy     energies
#
# Parameters
#
dispersion y
```

```
#
# n-Sn120-omp-JLM
#
# General
#
projectile n
element    sn
mass       120
energy     energies
#
# Parameters
#
jlmomp y
```

TENDL-2023: Fission yields and fission neutron observables from TALYS

TALYS: reads distribution of excited fission fragments and evaporates them all with Hauser-Feshbach

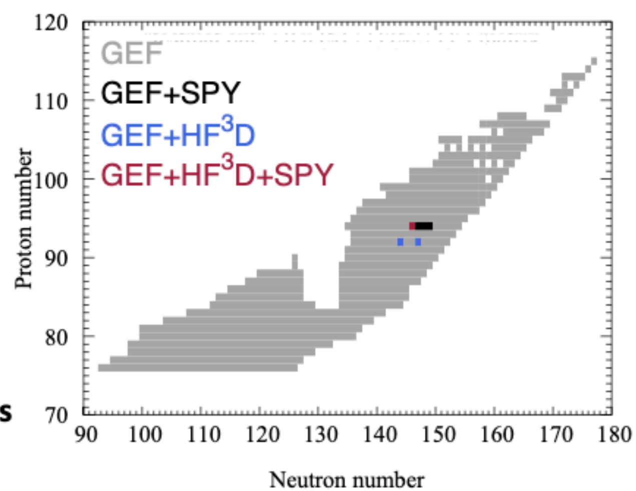
Fission fragment yield models stored in TALYS

GEF Designed with global fitting parameters based on experimental data
F. Nordström, Technical Report UPTEC ES21016, Uppsala university, 2021.
From $_{76}$Os to $_{115}$Mc, 737 nuclides

HF³D Designed with a fully deterministic technique with fitting functions
S. Okumura, T. Kawano, P. Jaffke, P. Talou, and S. Chiba, JNST, 55(9),1009–1023, 2018.
^{236}U, ^{239}U, and ^{240}Pu, 3 nuclides

SPY Designed with a statistical scission point model using microscopic calculation
J.-F. Lemaître, S. Goriely, S. Hilaire, and J.-L. Sida, PRC99, 034612, 2019.
^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{243}Pu, 4 nuclides
(May 2022: 809 nuclides)

Arbitrary fission fragment data provided by users



Tokyo Tech

Univ. Uppsala:
Ali Al-Adili
Fredrik Nordstroem

CEA-DAM Bruyeres:
Jean-Francois Lemaitre

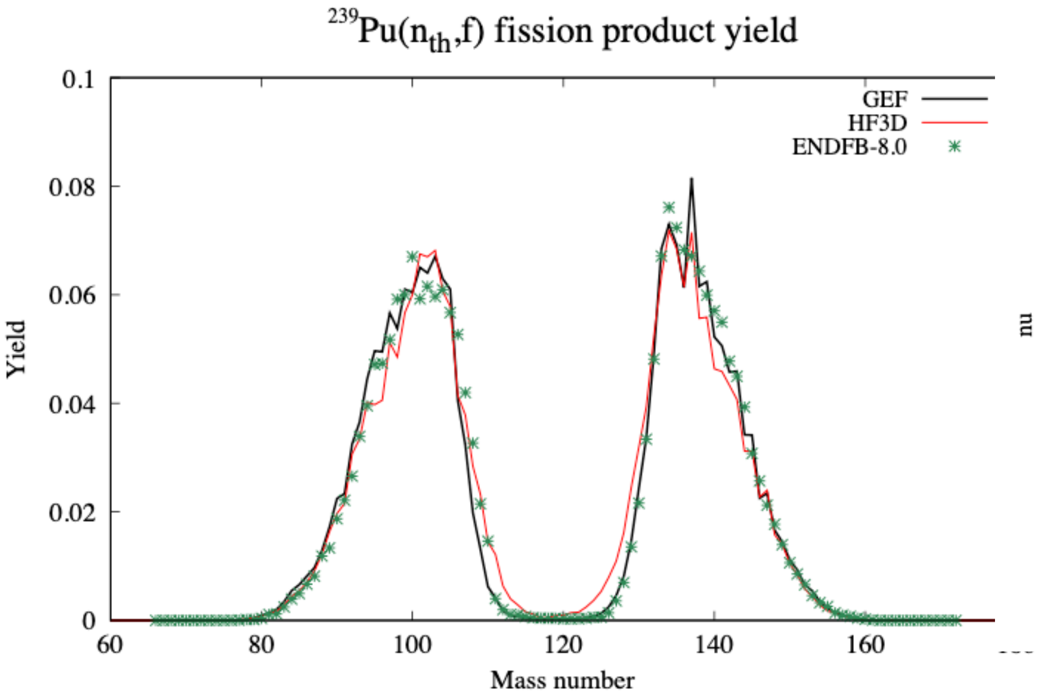
Titech TOKYO:
Kazuki Fujio
Satoshi Chiba

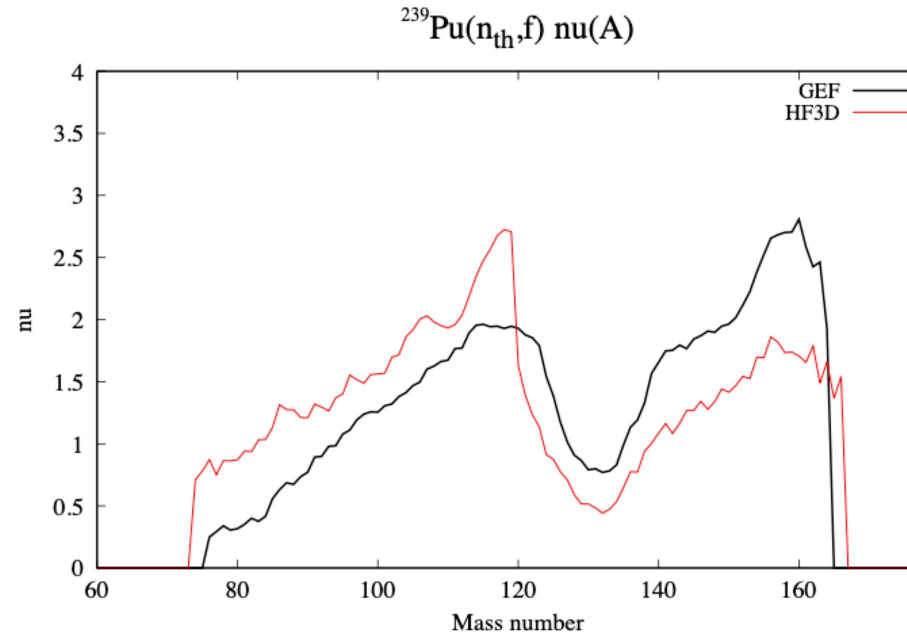
LANL:
Toshihiko Kawano

IAEA:
Shin Okumura
Arjan Koning

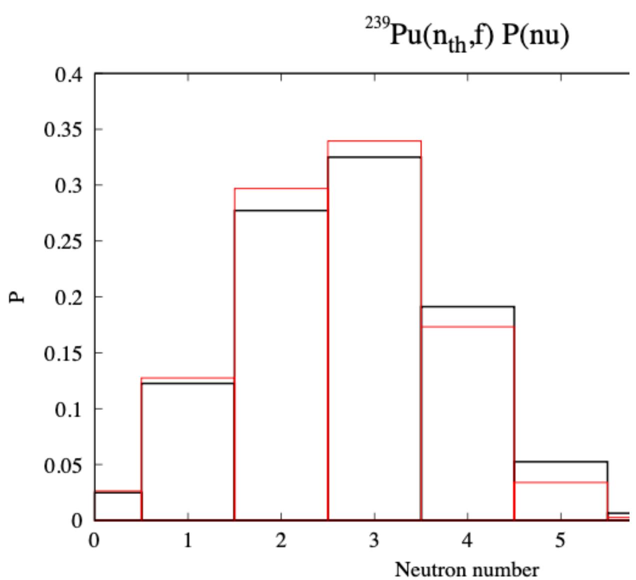
We did:

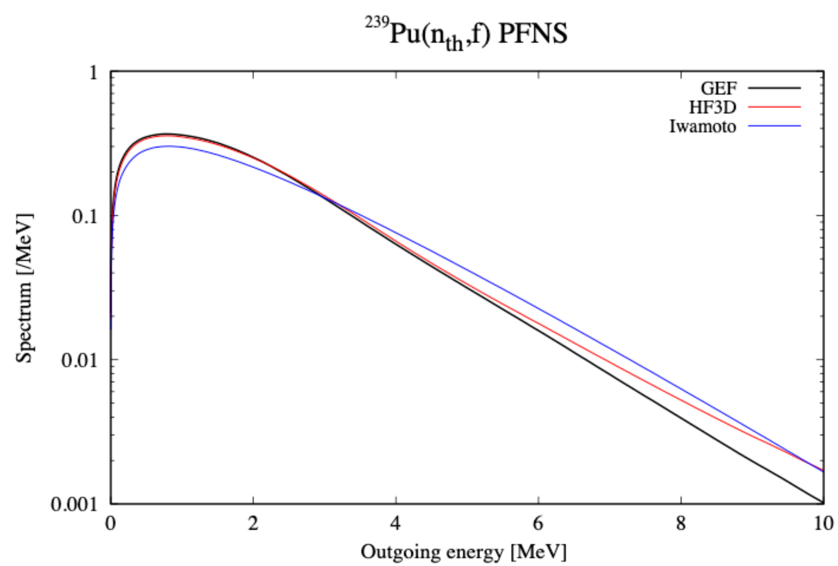
calculations of the de-excitation process for ^{235}U+n with Hauser-Feshbach statistical decay theory and comparison with evaluated and experimental data





TALYS-2 only






```
projectile n
element    Pu
mass       239
energy   2.53e-8
ejectiles g n
massdis y
fymodel 4
ffmodel 1
ldmodel 5
Rfiseps 1.e-5
outspectra y
bins 40
channels y
maxchannel 8
```

TALYS output file: rp039090.L02

```
# header:
#   title: Nb93(n,x)Y90m cross section
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2024-01-11
#   format: YANDF-0.1
# target:
#   Z: 41
#   A: 93
#   nuclide: Nb93
# reaction:
#   type: (n,x)
#   Q-value [MeV]:  4.248473E+00
#   E-threshold [MeV]:  0.000000E+00
#   ENDF_MF: 6
#   ENDF_MT: 5
# residual:
#   Z: 39
#   A: 90
#   nuclide: Y90m
#   mass [amu]:  8.990714E+01
#   level:
#     number: 2
#     energy [MeV]:  6.820100E-01
#     spin:  7.000000E+00
#     parity: 1
#     isomer: 1
#     half-life [sec]:  1.148000E+04
# datablock:
#   quantity: cross section
#   columns: 3
#   entries: 25
##       E              xs        Isomeric ratio
##     [MeV]           [mb]             []
   2.000000E-01   0.000000E+00   0.000000E+00
   4.000000E-01   0.000000E+00   0.000000E+00
   6.000000E-01   0.000000E+00   0.000000E+00
   8.000000E-01   0.000000E+00   0.000000E+00
   1.000000E+00   0.000000E+00   0.000000E+00
   1.200000E+00   0.000000E+00   0.000000E+00
   1.400000E+00   8.135896E-05   0.000000E+00
   1.600000E+00   1.296808E-04   1.266436E-01
   1.800000E+00   2.699952E-04   1.644318E-01
   2.000000E+00   5.832345E-04   2.057970E-01
```


'#' for direct use in various software, e.g. Gnuplot

Without '#': YAMLesque 2 space indentation per level

Parsing to JSON should be easy

Only 5 main attributes for nuclear reactions

TALYS: 2 more main attributes: 'parameters' and 'observables'

EXFOR: All specific metadata may follow after the datablock

Future (?): Extension to 2 GeV

- Challenges:
  - Extension of OMP to 2 GeV
    - folding/microscopic approach, wine-bottle shape
    - Woods-Saxon not appropriate
  - Include pions or good approximation to exclude them
- Existing features:
  - (Multiple) Pre-equilibrium known to work to quite high energies (Mashnik)
  - TALYS has built in multiple loops over itself for residual products (as for fission fragments)
  - The systematic logic of TALYS input, output and reaction flow

Future (?): Extension to heavy ions

- Challenges:
  - Extension of OMP to heavy ions
    - Folding/microscopic approach, Sao Paolo potential
    - Woods-Saxon maybe another option
  - Much higher J-limit in TALYS (more dynamic programming)
- Existing features:
  - Pre-equilibrium known to work for heavy ions (Gadioli)
  - Hauser-Feshbach would be applied as usual
  - Probably easy extension of the arrays
  - The systematic logic of TALYS input, output and reaction flow

Near future: Full particle decay scheme and Monte Carlo

- Challenges:
  - Write complete reaction flow to probability tables: Hauser-Feshbach + Direct + Pre-equilibrium
  - Allows restarting with Monte Carlo scheme
  - Allows direct inclusion in advanced transport codes
  - Finalise “Dicebox-like” capability
- Existing features:
  - Basically there, since we already need it for any TALYS calculation

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Thank you!