Nuclear model parameter optimisation with TALYS

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Introduction

• TALYS covers
  • All nuclides
  • All projectiles
  • 0-200 MeV
• 6000-7000 citations in all possible fields: neutron fission, medical isotope production, astrophysics, fusion, activation, etc.
• Objective: make the code globally better, regardless of the application
• Global good prediction: better physics, global optimisation to experimental data
• Global good description: nuclide-by-nuclide optimisation to experimental data
Input

- Physical parameters

  - Nuclear Structure (RIPL-3)
    - Masses
    - Discrete levels
    - Level densities
    - Resonance parameters
    - Optical model parameters
    - Fission barrier parameters

  - Phenomenological parameters
  - Microscopic tables

- Other
  - Fission fragment distributions
  - ‘Best’ nuclear model parameters optimised to experimental reaction data

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
    - Reactions
  - Angular distributions
    - Elastic
    - Per level
    - Particle multiplicities
    - Fission yields, neutron observables
  - Astrophysical reaction rates, MACS
  - …etc

Output

- Reaction models
  - Optical model (ECIS)
    - Local/global OMP
    - Phenomenological
    - Semi-microscopic (JLM)

- Direct reaction
  - Spherical OMP
  - DWBA
  - Coupled-channels
    - Rotational
    - Vibrational
  - Giant resonances
  - Weak-coupling

- Compound reactions
  - Hauser-Feshbach
  - Width fluctuations
  - Blatt-Biedenharn angular distribution
  - Particle, photon and fission transmission coefficients

- Pre-equilibrium reactions
  - Exciton model
  - Particle hole level density
  - Kalbach systematics
    - Angular distribution
    - Cluster emission
  - γ-ray emission

TALYS

~ 400 keywords

- projectile n
- element Fe
- mass 56
- energy 14.0

~ 400 keywords
Microscopic global models

Phenomenological global models

Micro/pheno models with adjusted parameters

Micro/pheno models with unphysical parameters or functions

Direct normalisation of model output to experimental data

Prediction of reality

Description of reality = exp. data
TALYS Application to \((n, \gamma)\) cross sections

- Adjust width of the E1 SMLO photon strength function (TALYS: ‘wtable’) to match the best nuclear data library with
  - Best reproduction of MACS, around 30 keV
  - Best reproduction of experimental \((n, \gamma)\) cross section from the top of the RR - 100 keV/1 MeV
- Best nuclear data library before TENDL-2021:
  - JENDL-4.0: 97 target isotopes
  - JENDL-AD: 2 target isotopes
  - CENDL-3.2: 2 target isotopes
  - TENDL-2019: 106 target isotopes
  - JEFF-3.3: 8 target isotopes
  - ENDF/B-VIII.0: 61 target isotopes

n–Eu153.tasman

#Esearch 0.01 0.1 102

#libinclude 102 endfb8.0
Adjusted width parameter does not affect original photon strength function very much.

\[ f_{E1} \left[ \text{MeV}^{-3} \right] \]

\[ E_{\gamma} \left[ \text{MeV} \right] \]

\[ S_n + E_{\text{in}}: \text{range important for } (n, \gamma) \]

\[ \langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) \, d\varepsilon_\gamma \]
Optimization to included exp. data

$^{69}\text{Ga}(n,\gamma)^{70}\text{Ga}$  GOF= 1.037

Cross section [mb]

Incident Neutron Energy [MeV]
$^{160}\text{Gd}(n,\gamma)^{161}\text{Gd}$ \hspace{1cm} GOF = 1.094
Wtable for (n,g) with exp. MACS, fitted to best library

F_{rms} : 12\%
TALYS optimisation to EXFOR

- Two birds with one stone:
  - Exforcism (flag evil data in EXFOR)
    - Add to current database of experimental ‘outliers’ by Alhassan, Gaughan and Dzysiuk
    - ‘Graphical’ outliers
    - Full JSON files available
  - Optimization of TALYS parameters to all cross sections
    - Use of XC5 format of EXFOR (V. Zerkin)
    - Dimension reduction
    - Same parameter set for all nuclides
8400 JSON outlier/inlier files, one per EXFOR subentry

```
"Subentry" : "A0001004",
"Author" : "Skakun",
"Year" : 1975,
"Projectile" : "p",
"Target Z" : 48,
"Target A" : 111,
"Target state" : "0",
"X4 Reaction" : "48-CD-111(P,N)49-IN-111,,SIG",
"Evaluations" : [
  {
    "Evaluator" : "Arjan Koning",
    "Date" : "2022-06-05",
    "Weight" : 0,
    "Comment" : [
      "Excluded from evaluation: graphical outlier"
    ],
  },
  {
    "Evaluator" : "Erwin Alhassan",
    "Date" : "2019-11-08",
    "Weight" : 0,
    "Comment" : [
      "Erwin Alhassan (PSI, 2018) 0",
      "(1 \rightarrow accept and 0 \rightarrow reject)",
      "Reasons for inclusion/exclusion",
      "1) Experimental data set not consistent with other experiments such as Takacs (2005) between about 10 – 15 MeV (The cross sections are systematically lower)"
    ],
  },
  {
    "Evaluator" : "Natalie Gaugan",
    "Date" : "2019-03-15",
    "Weight" : 1,
    "Comment" : [
      "IAEA-TECDOC-1211 – Data selected"
    ],
  }
]
```
# TALYS parameters for optimization

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<tr>
<th>Reaction</th>
<th>Nuclides</th>
<th>Parameter</th>
<th>Parameter</th>
<th>Parameter</th>
<th>Parameter</th>
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<tr>
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<td>278</td>
<td>wtable</td>
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<tr>
<td>(n,f)</td>
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<td>vfiscor</td>
<td>betafiscor</td>
<td>ctable(1)</td>
<td>ptable(1)</td>
<td>ctable(2)</td>
<td>ptable(2)</td>
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<tr>
<td>(n,n', (n,2n), (n,p))</td>
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<td>gₚh(0)</td>
<td>gₚh(n)</td>
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<td>Cstrip(α)</td>
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<td>rv(n)</td>
<td>gₚh(0)</td>
<td>gₚh(n)</td>
<td>ctable(n)</td>
</tr>
</tbody>
</table>

**TASMAN code (AK):** Nelder-Mead optimisation.

**Number of TALYS trials:** N(parameters) x 20
Fitting all actinides at the same time
Fission: WKB (Sin, Capote) + HFB level densities (Hilaire, Goriely)
(p,n): several nuclides with JENDL-5 evaluation
Segal’s law: A man with a watch knows what time it is. A man with two watches is never sure.
$(\alpha,n)$: TENDL rules! (OK OK, because there is nothing else for $A > 20$)
Outlier assignment

Summed over all \((n,g), (n,f), (n,n'), (n,2n), (n,p), (n,a), (p,n), (g,n), (a,n), (d,n)\) reactions we could mine from EXFOR. 6500 accepts, 1000 rejects
Outlier assignment: a learning curve?

Inclusion ratio: 7500 experimental data sets (7 year average)

Other analyses possible:
- per reaction channel
- per author, co-author, lab, etc
- per incident energy (e.g. 14 MeV)
- re-insert this as prior in the next Bayesian update
$^{98}\text{Mo}(n,\alpha)^{95}\text{Zr}$  GOF= 1.058

$^{41}\text{K}(n,\alpha)^{38}\text{Cl}$  GOF= 1.031
Can ML help here for unmeasured nuclides?

Can we discover trends that a human can not see?

We know that for $A < 20$ the physics of TALYS is not good enough

Are 160 nuclides enough to select a 20% training set?

Can an ML algorithm be predictive for nuclides at or close to the valley of stability?
Optical model parameter $rv(a)$ for 2 different level density models

Can we discover trends that a human can not see?

We know that for $A < 20$ the physics of TALYS is not good enough

Are 160 nuclides enough to select a 20% training set?

Can an ML algorithm be predictive for nuclides at or close to the valley of stability?
Summary

- Trying to put human knowledge and opinions in consistent metadata
- Part of the objective to make TALYS more predictive and more descriptive (zeroing in on the truth)
- Accessible experimental database essential
- “Standard” optimisation with Nelder-Mead done for each reaction and target nuclide: scripts running scripts running search code running TALYS
- Per reaction channel: scattered parameters for up to 5 dimensions, for typically 200 nuclides, looking for trend and parameter guesses for unmeasured nuclides closed to the measured ones
Thank you!