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Fast neutron reactions with ^{241}Am: a detailed TALYS study

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Introduction - ^{241}Am

- Relatively large abundance in radioactive waste of conventional thermal reactors:

$$^{238}\mathrm{U} \xrightarrow{(n,\gamma)} {}^{239}\mathrm{U} \xrightarrow[23.5\ \mathrm{min}]{\beta-} {}^{239}\mathrm{Np} \xrightarrow[2.3565\ \mathrm{d}]{\beta-} {}^{239}\mathrm{Pu}$$

$$^{239}\mathrm{Pu} \xrightarrow{2(n,\gamma)} {}^{241}\mathrm{Pu} \xrightarrow[14.35\ \mathrm{y}]{\beta-} {}^{241}\mathrm{Am}$$

- Potential hazards for humans: $^{241}\mathrm{Am} \rightarrow {}^{237}\mathrm{Np} + 5\alpha + \gamma$
  - ^{241}Am is mainly concentrated in the bones, liver and lungs
  - α-particles deposit a large amount of equivalent dose
  - γ-rays

Introduction – Motivation

- Fast neutrons will be of central role in 4th generation fission reactors
  - Determine the competitive decay channels of ^{241}Am and the corresponding cross sections
  - How these channels affect neutron flux inside the reactor via *(n,xn)* reactions
- Reduce ^{241}Am abundance in nuclear waste: transmutation following the neutron capture
- Reuse ^{241}Am as a fuel (e.g. RTGs): neutron induced fission
- TALYS calculations not optimally aligned with experimental data

Methodology

- Energy range of interest: 10KeV – 20MeV
  - activated channels: *(n,γ), (n,n'), (n,2n), (n,f)*
- CN reactions dominate → Hauser Feshbach calculations → main ingredients: OMP, NLD, γSF, Fission Barriers
- Cross section data: EXFOR database – *(n,n')* not available
- Large number of models/parameters combinations to run:
  - Divide and conquer → unit testing to focus on smaller energy ranges and affecting models and parameters set
- Automated TALYS runs with various models and parameters combinations – variable energy step
- Automated postprocessing of TALYS output and calculation of residual error (RRMSE) → elimination of combinations, add new combinations, calculate again until minimizing RRMSE

The Models

NLD
1 – CTM & FGM
2 – BFGM
3 – GSM
4 – Microscopic LD (Skyrme) Goriely's tables
5 – Microscopic LD (Skyrme) Hilaire's tables
6 – Microscopic LD (TD HFB, Gogny) Hilaire's tables

Adjusted tabulated densities (c, δ parameters)

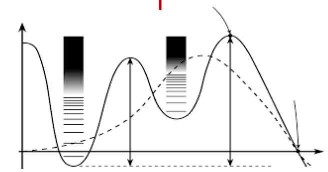
$$\rho(U,J,P)_{renorm} = e^{c\sqrt{(U-\delta)}} \times \rho(U-\delta,J,P)$$

γSF
1 – Kopecky-Uhl generalised Lorentzian
2 – Brink-Axel Lorentzian
3 – Hartree-Fock BCS tables
4 – Hartree-Fock- Bogolyubov tables
5 – Goriely's hybrid model
6 – Goriely T-dependent HFB
7 – T-dependent RMF
8 – Gogny D1M HFB+QRPA

Not significantly affects the calculations of cross section for the *(n,f)* and *(n,2n)* channels. Default model works well for *(n,γ)*, as well

Fission	
Hill-Wheeler + Bohr transition states + double humped	**Experimental barriers**
	RLDM

Adjusted barriers' height/width



OMP
Global Koning & Delaroche

$$V_V(E) = u_1^n[1 - u_2^n(E-E_f^n) + u_3^n(E-E_f^n)^2 - u_4^n(E-E_f^n)^3]$$

$$W_V(E) = w_1^n\frac{(E-E_f^n)^2}{(E-E_f^n)^2+(w_2^n)^2}$$

$$r_V = r_W = 1.3039 - 0.4054A^{-1/3}$$

$$a_V = a_W = 0.6778 - 1.487\cdot 10^{-4}A$$

Adjusted parameters

$$W_D(E) = d_1^n\frac{(E-E_f^n)^2}{(E-E_f^n)^2+(d_3^n)^2}\exp[-d_2^n(E-E_f^n)]$$

$$r_D = 1.3424 - 0.01585A^{1/3}$$

$$a_D = 0.5446 - 1.656\cdot 10^{-4}A$$

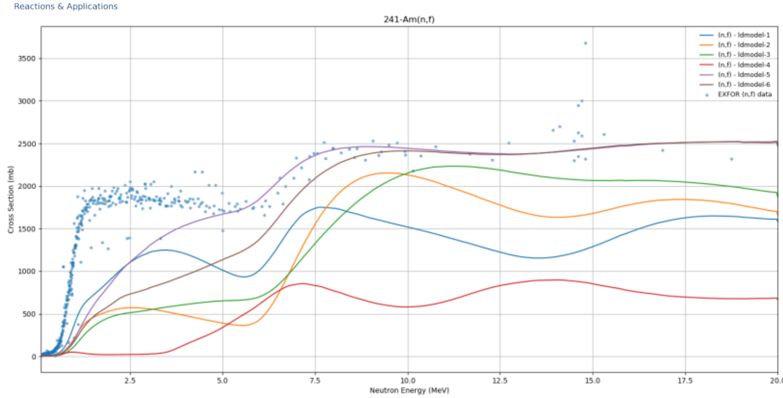
$$V_{SO}(E) = u_{so1}^n\exp[-u_{so2}^n(E-E_f^n)]$$

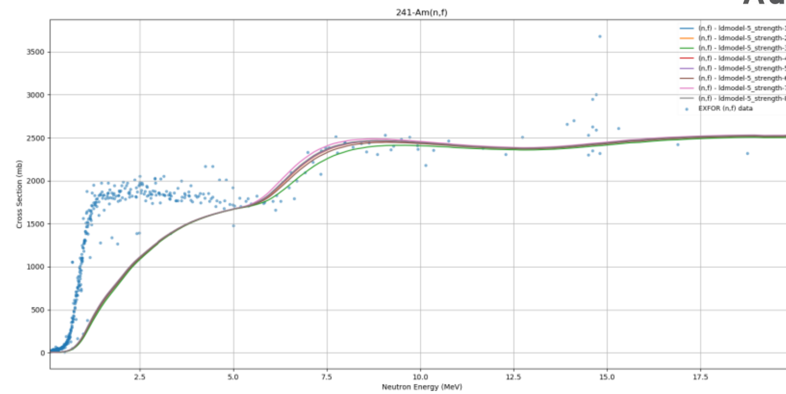
$$W_{SO}(E) = w_{so1}^n\frac{(E-E_f^n)^2}{(E-E_f^n)^2+(w_{so2}^n)^2}$$

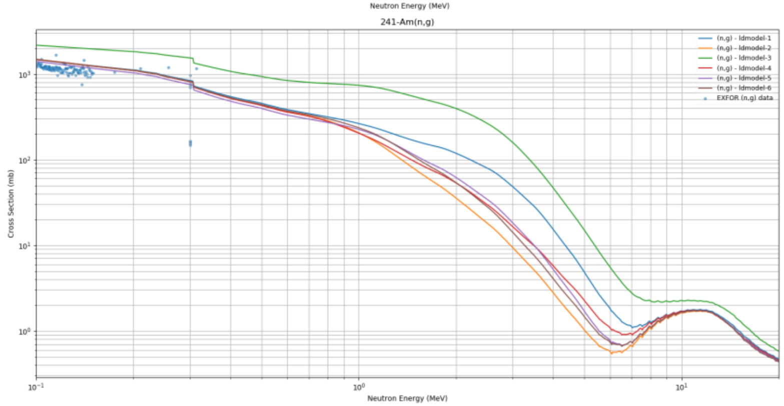
$$r_{VSO} = r_{WSO} = 1.1854 - 0.647A^{-1/3}$$

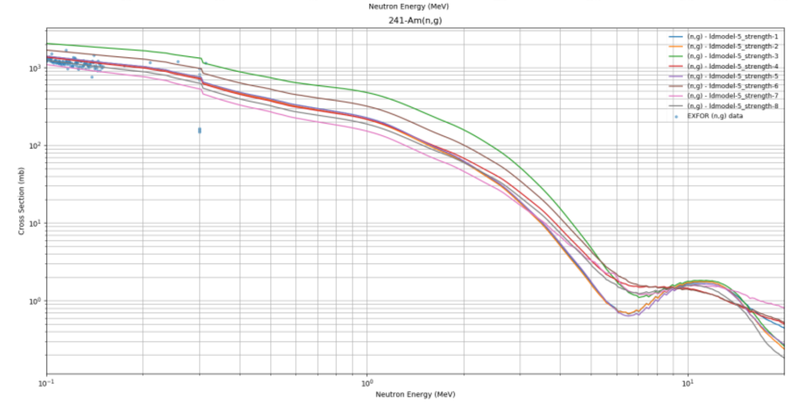
$$a_{VSO} = a_{WSO} = 0.59$$

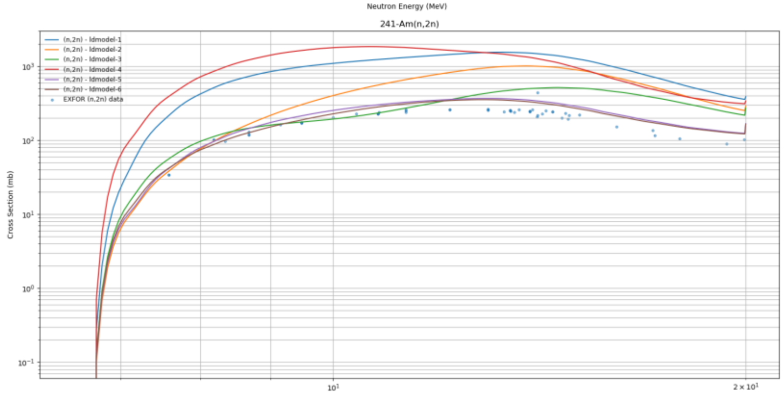
Results – all NLD/γSF models

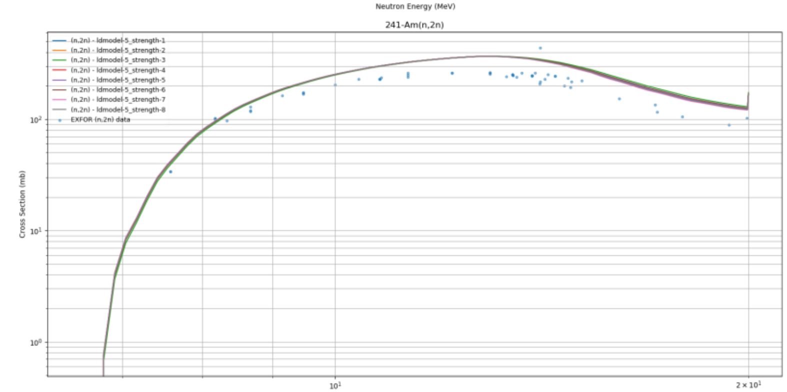




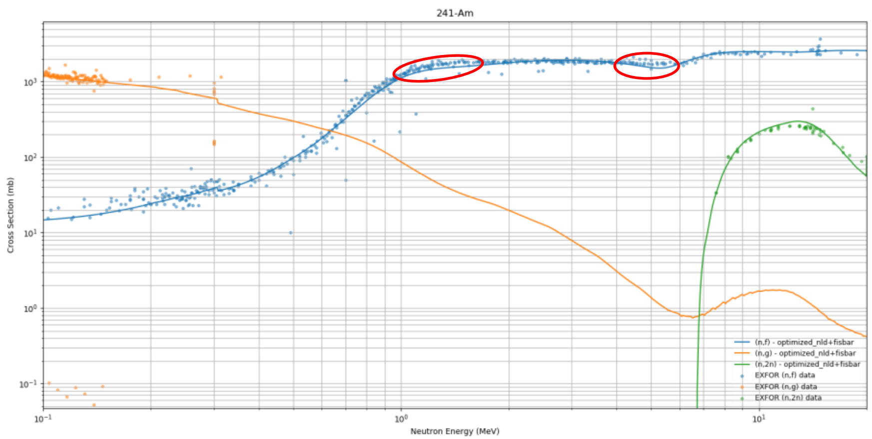




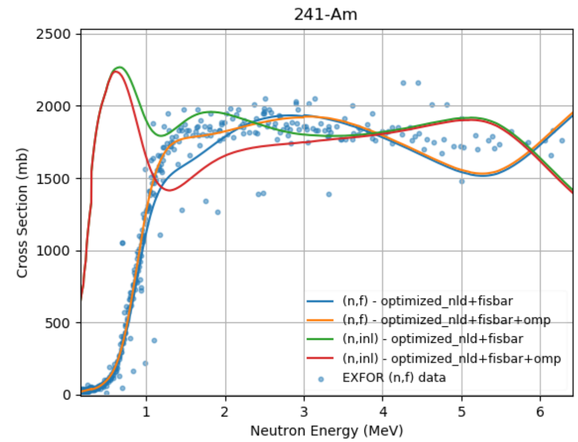


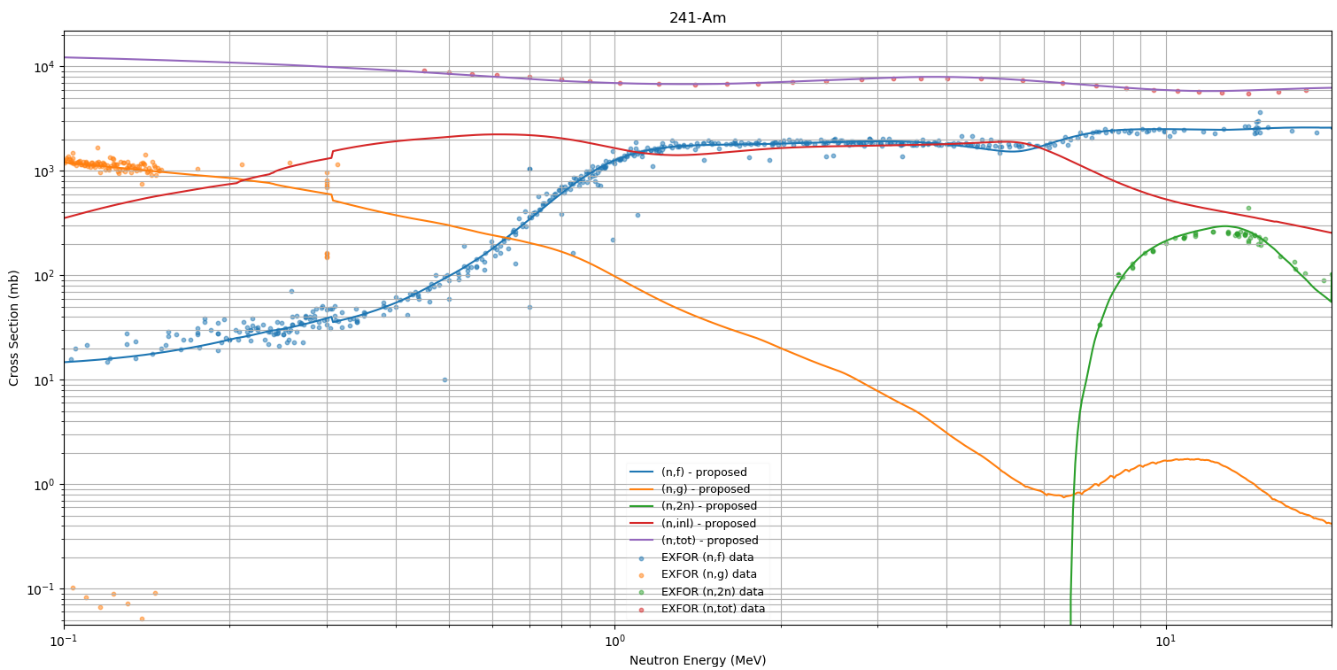


Results – NLD 5/Fission barriers/OMP



OMP adjustments

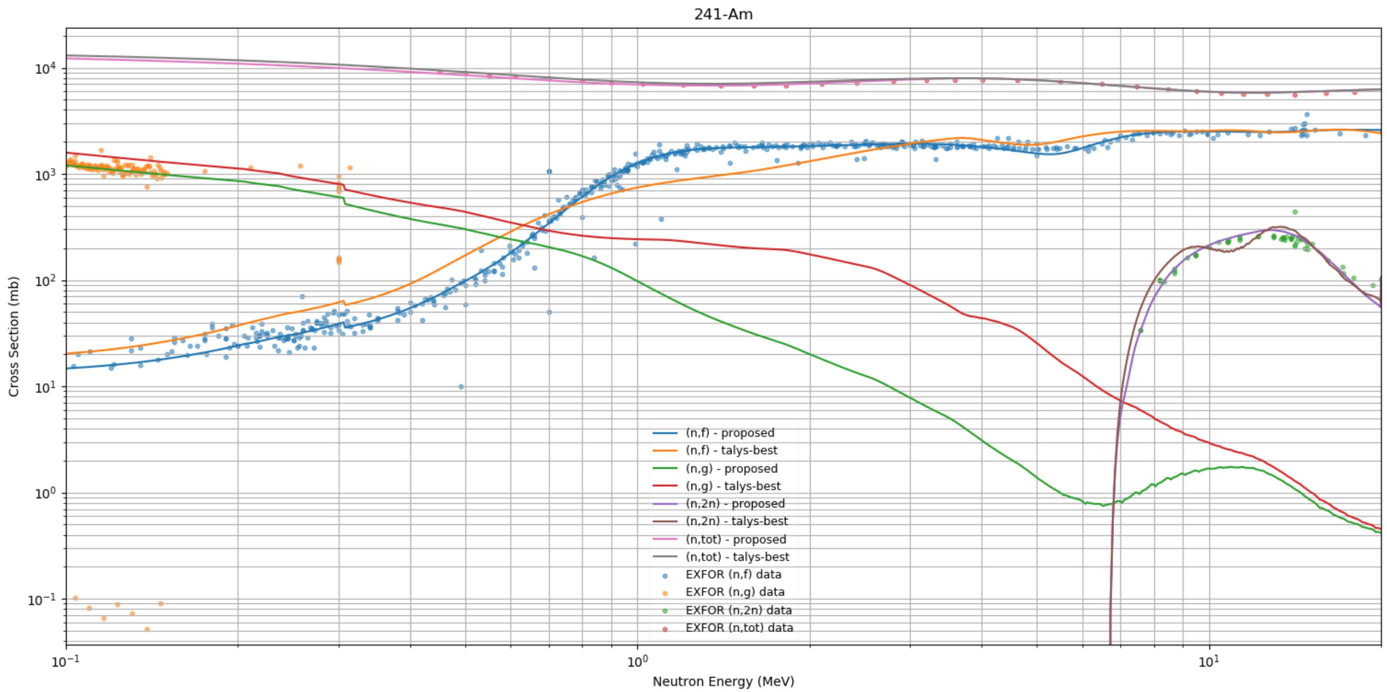




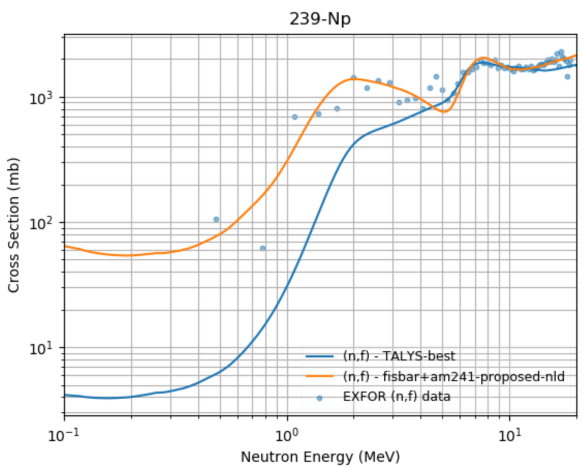
TALYS configuration

```
ldmodel 5
ctable 95 242 -2.000 1
ctable 95 241 -0.100 1
ptable 95 242 -2.000 1
ptable 95 241 0.100 1
ctable 95 242 -0.150 2
ptable 95 241 -0.300 2
ptable 95 242 0.400
fisbar 95 241 5.600 1
fisbar 95 240 5.700 1
fisbar 95 242 5.500 2
fisbar 95 241 4.900 2
fisbar 95 240 5.600 2
rvadjust n 1. 0.4 4.6 1.3 0.98
avadjust n 1. 0.4 4.6 1.3 1.05
w1adjust n 1. 0.4 4.6 1.3 0.5
w2adjust n 1. 0.4 4.6 1.3 0.5
```

Results – TALYS best comparison/^{239}Np



The proposed adjusted NLD successfully applied to the isotone ^{239}Np (+ fission barrier adjustments)



Conclusions

- Very good agreement of adjusted TALYS calculations with experimental data in the 10KeV-20MeV energy range:
  - Adjusted microscopic Skyrme/Hilaire NLD model
  - Proposed fission barrier heights for ^{242}Am, ^{241}Am, ^{240}Am
  - Koning-Delaroche OMP adjustment for the range 1-2MeV
- Proposed excitation function for the inelastic channel
- Adjusted Skyrme/Hilaire NLD successfully applied to the isotone ^{239}Np (similar phase space)