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RREFPOS data for the activation library

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USNDP Meeting, Nuclear Data Week
November 2, 2026

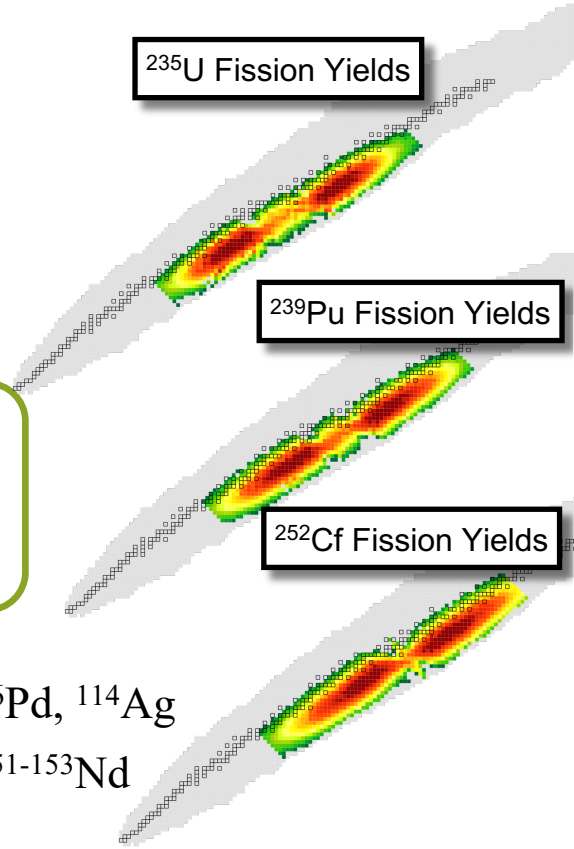
Realistic Reaction Evaluations for Fission Products Off Stability

NA-22-funded 3-year project: FY25-FY27

- Applications such **nonproliferation, post-detonation forensics, spent-fuel assay, reactor burnup and design**, as well as **astrophysics**, rely on the accurate description of the neutron interaction with unstable fission products.
- Current cross-section descriptions of these nuclei are either non-existent or based on simplified assumptions, leading to unquantified impacts on predicted cross-sections.
- By project completion, more **predictive/realistic** new nuclear data will be produced, improving the **reliability** of applications involving **fission products off stability!**

Project Goals and Objectives

To provide evaluated files for neutron-induced reactions on fission products off-stability and submit them to the ENDF/B nuclear data library



The **primary-goal nuclei** (mostly produced by ^{235}U fission):

- 1st Fission yield bump: $^{87\text{-}89}$Br, $^{88\text{-}92}$Kr, $^{91\text{-}94}$Rb, $^{92\text{-}97}$Sr, $^{95\text{-}99}$Y, $^{97\text{-}102}$Zr, $^{101\text{-}103}$Nb
- 2nd Fission yield bump: $^{131\text{-}133}$Sb, $^{132\text{-}136}$Te, $^{135\text{-}138}$I, $^{136\text{-}141}$Xe, $^{139\text{-}143}$Cs, $^{141\text{-}146}$Ba, $^{144\text{-}145}$La, $^{147\text{-}148}$Ce

Secondary goal (main fission products from ^{239}Pu and ^{252}Cf):

- 1st Fission yield bump: ^{94,100}Y, ^{96,103}Zr, ^{99,100,104,105}Nb, $^{102\text{-}108}$Mo, $^{105\text{-}110}$Tc, $^{107\text{-}112}$Ru, $^{110\text{-}114}$Rh, $^{112\text{-}116}$Pd, ^{114}Ag
- 2nd Fission yield bump: ^{131}Te, ^{134}I, ^{135}Xe, ^{137,138,144}Cs, ^{140}Ba, $^{143,146\text{-}148}$La, ^{145,146,149,150}Ce, $^{149\text{-}152}$Pr, $^{151\text{-}153}$Nd

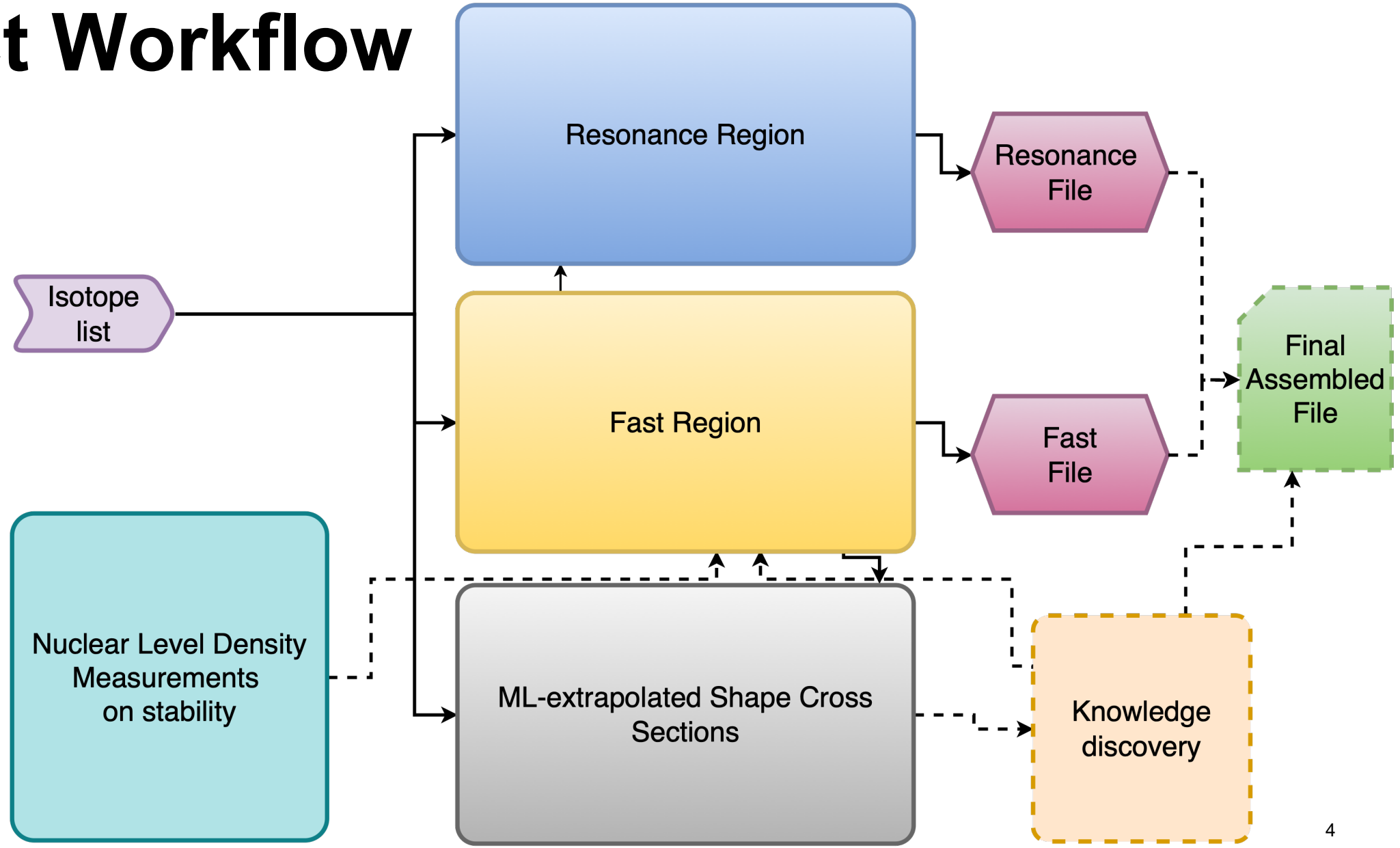
Stretch goal (whole isotopic chain of fission products from ^{235}U, ^{239}Pu, and ^{252}Cf):

- ^{66}V, $^{66\text{-}67}$Cr, $^{66\text{-}71}$Mn, $^{66\text{-}75}$Fe, $^{66\text{-}77}$Co, $^{66\text{-}80}$Ni, $^{66\text{-}82}$Cu, $^{66\text{-}85}$Zn, $^{68\text{-}87}$Ga, $^{70\text{-}90}$Ge, $^{72\text{-}92}$As, $^{75\text{-}95}$Se, $^{77\text{-}98}$Br, $^{79\text{-}101}$Kr, $^{81,83\text{-}103}$Rb, $^{83\text{-}106}$Sr, $^{87\text{-}109}$Y, $^{88\text{-}112}$Zr, $^{91\text{-}114}$Nb, $^{93\text{-}117}$Mo, $^{97\text{-}119}$Tc, $^{98\text{-}121,124}$Ru, $^{101\text{-}125}$Rh, $^{103\text{-}126,128}$Pd, $^{106\text{-}132}$Ag, $^{108\text{-}134}$Cd, $^{111\text{-}137}$In, $^{113\text{-}139}$Sn, $^{118\text{-}140}$Sb, $^{120\text{-}143}$Te, $^{123,125,126,128\text{-}145}$I, $^{125,128,130\text{-}148}$Xe, $^{131\text{-}151}$Cs, $^{132\text{-}153}$Ba, $^{135,137\text{-}155}$La, $^{137\text{-}157}$Ce, $^{139\text{-}159}$Pr, $^{142\text{-}161}$Nd, $^{144\text{-}163}$Pm, $^{147\text{-}165}$Sm, $^{149,151\text{-}168}$Eu, $^{152\text{-}170}$Gd, $^{155\text{-}172}$Tb, $^{157\text{-}172}$Dy, $^{161\text{-}172}$Ho, $^{162\text{-}172}$Er, $^{165\text{-}172}$Tm, $^{168\text{-}172}$Yb, $^{171\text{-}172}$Lu

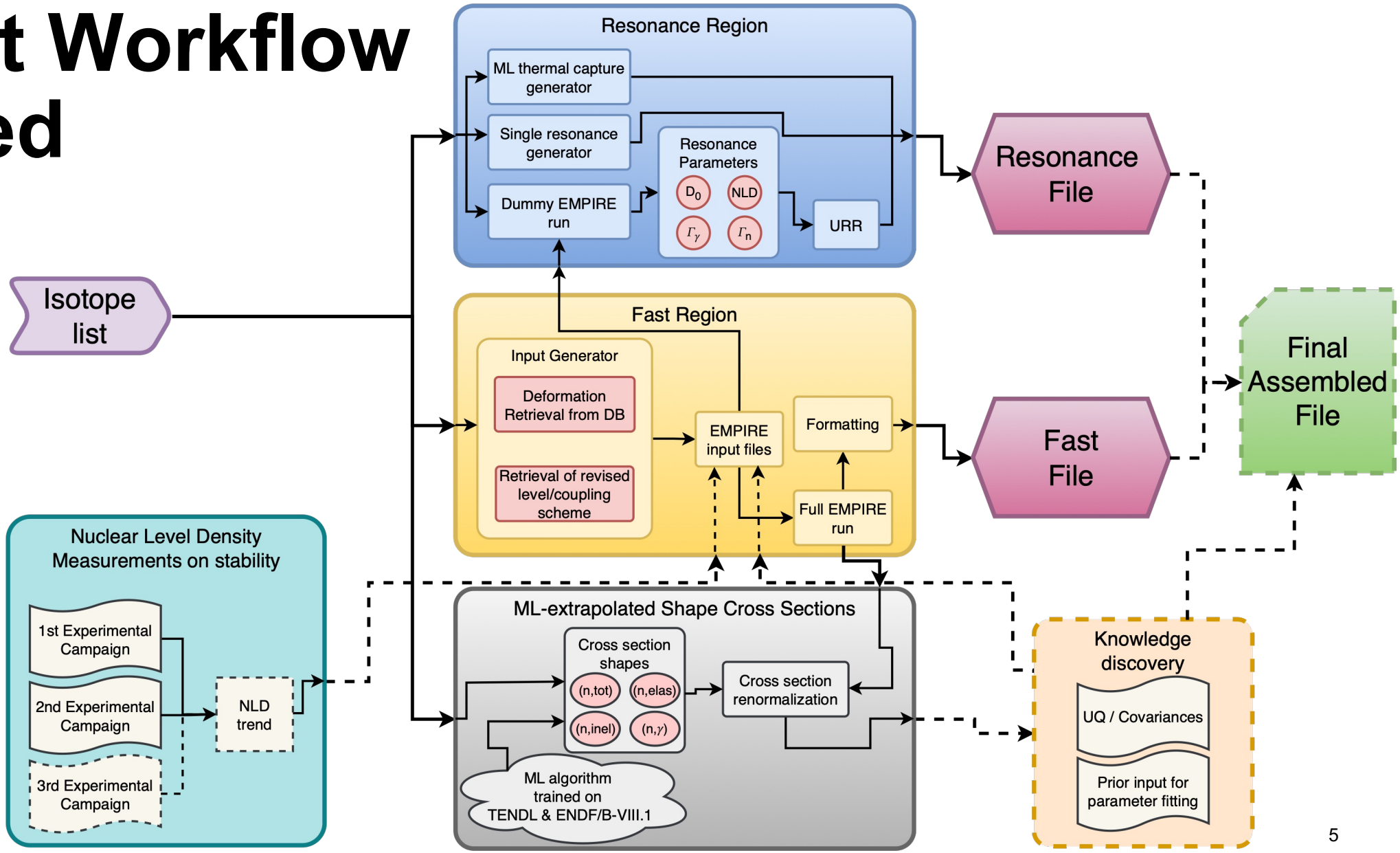
Project will be successful if primary goal is achieved. *However*, when the methods are well-established, generalization to secondary and stretch goals should be possible with relative low effort.

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Project Workflow

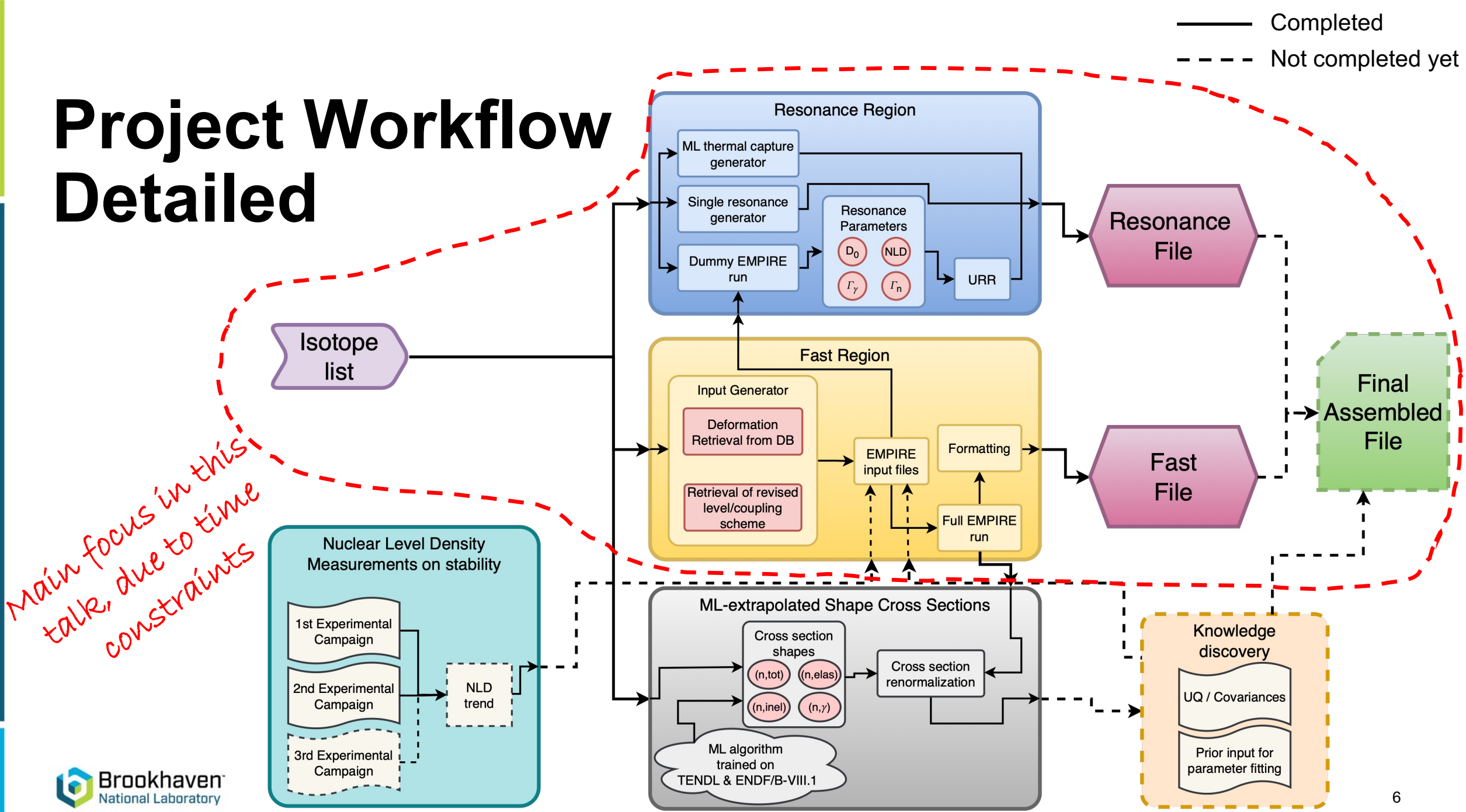


Project Workflow Detailed



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Project Workflow Detailed

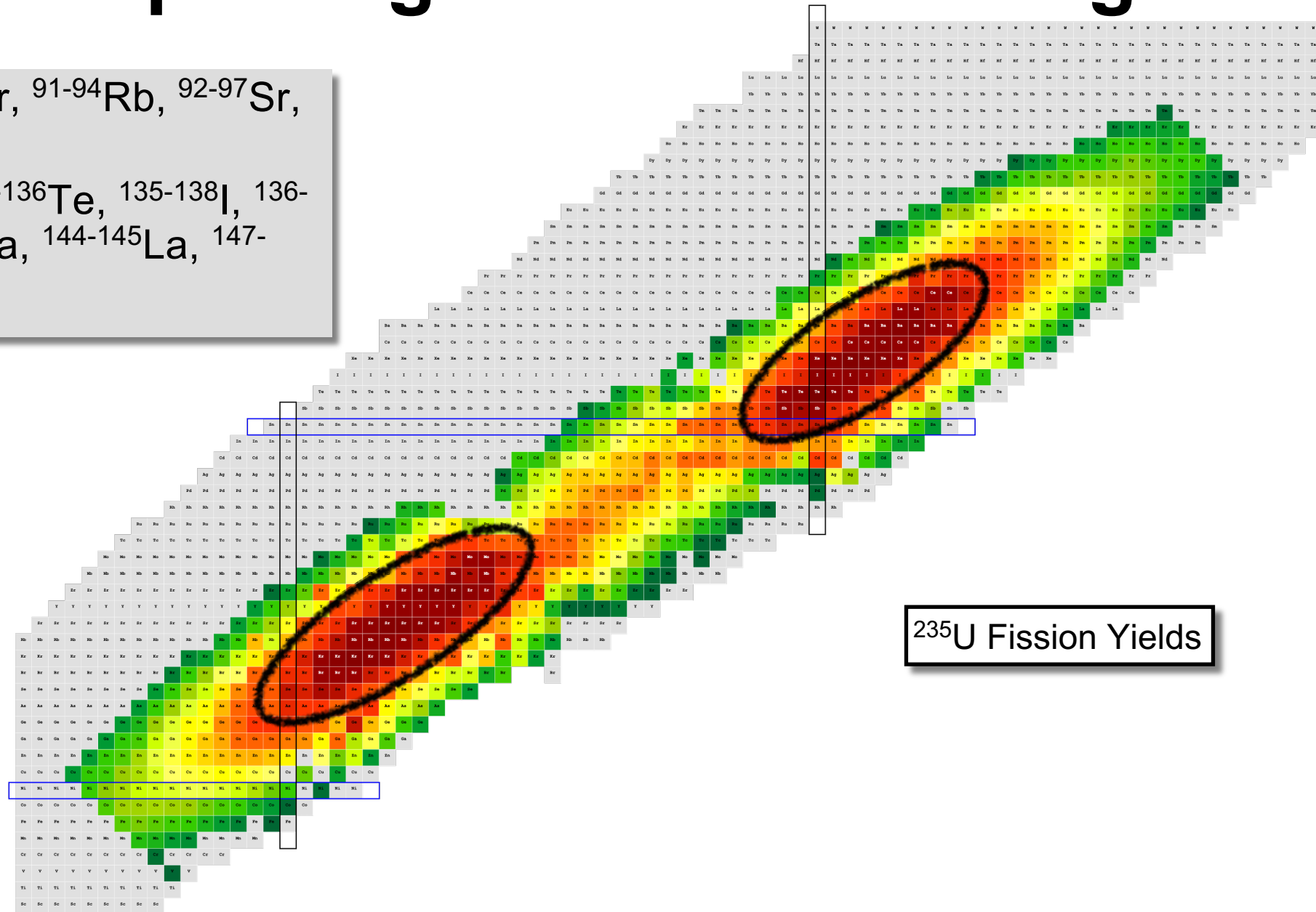


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Approach in fast region

Specificities impacting fast-neutron range

- 1st Hump: $^{87-89}$Br, $^{88-92}$Kr, $^{91-94}$Rb, $^{92-97}$Sr, $^{95-99}$Y, $^{97-102}$Zr, $^{101-103}$Nb
- 2nd Hump: $^{131-133}$Sb, $^{132-136}$Te, $^{135-138}$I, $^{136-141}$Xe, $^{139-143}$Cs, $^{141-146}$Ba, $^{144-145}$La, $^{147-148}$Ce



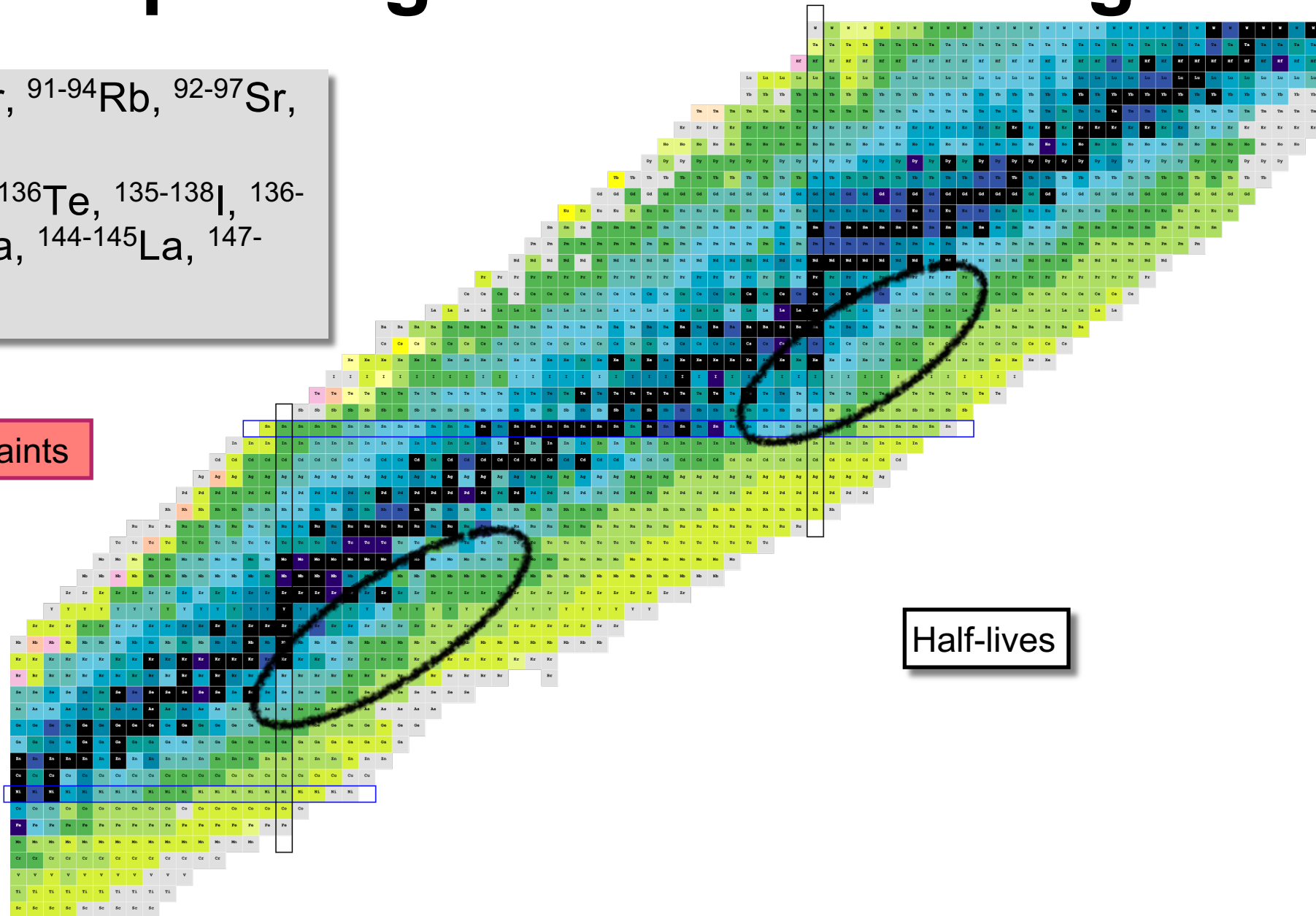
^{235}U Fission Yields

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Specificities impacting fast-neutron range

- 1st Hump: $^{87-89}$Br, $^{88-92}$Kr, $^{91-94}$Rb, $^{92-97}$Sr, $^{95-99}$Y, $^{97-102}$Zr, $^{101-103}$Nb
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Off-stability = few data constraints



Half-lives

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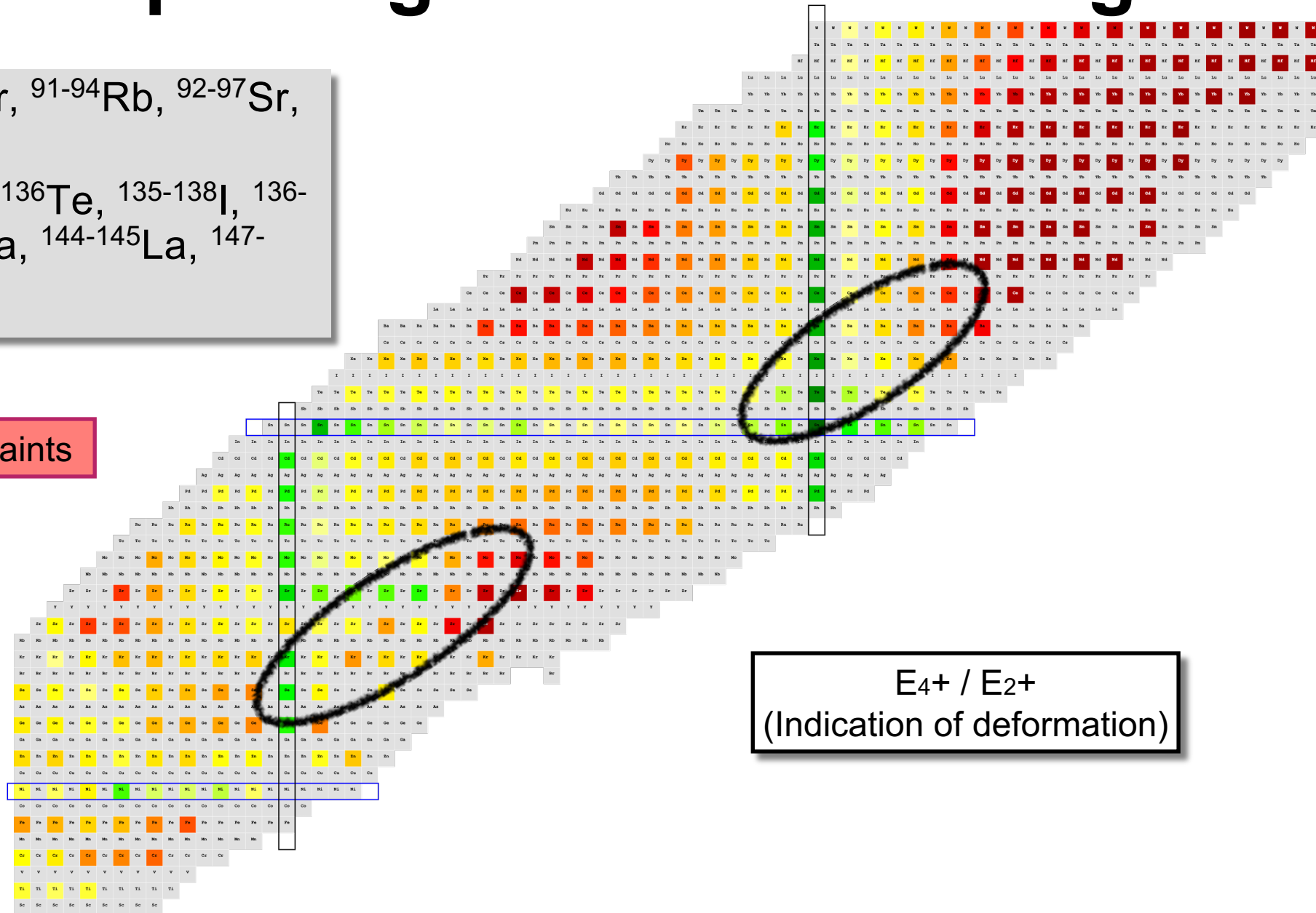
Specificities impacting fast-neutron range

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Off-stability = few data constraints

Most are (highly-)deformed!

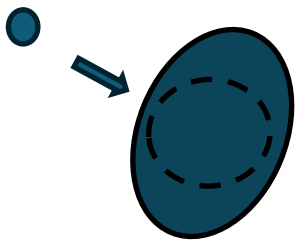
We employ an adiabatic approach, which has been successfully applied to deformed rare-earths



E_{4+} / E_{2+}
(Indication of deformation)

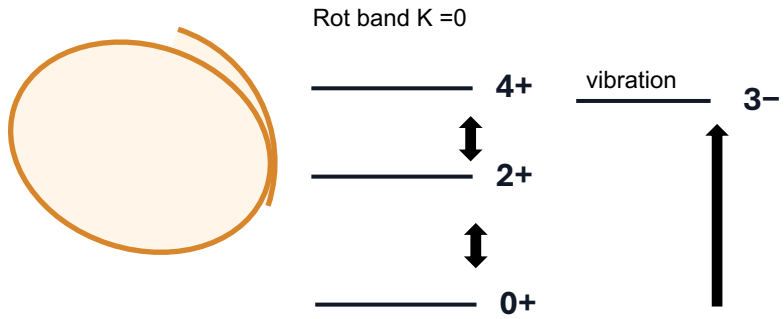
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Automated EMPIRE workflow, accounting for deformation



Adiabatic: Interaction is fast enough that the target looks frozen (during the reaction) (High moment of inertia and consequent low excitation energies of the ground-state band members of the statically deformed nuclei)

3 Rigid Rotor + vibration



static β_2, β_4 define the whole band coupling
but dynamic β_3 are still used for DWBA

- Coupled rotor-band equations; elastic and inelastic amplitudes feed each other
- Deformed nuclei with a ground-state band; extra uncoupled states may be DWBA.

Mini-library

standardized nuclear deformation inputs

main ▾ rrefpos / data / deformations / + ▾ Loc

Readme file explaining where data cames from
echimansk authored 1 year ago

Code owners Assign users and groups as approvers for specific file changes. Learn more.

Name	Last commit
..	
README.md	Readme file explaining where data cames from
collectedData_CEA_5DCH.csv	collected nuclear deformations
collectedData_CEA_HFB.csv	collected nuclear deformations
collectedData_RIPL.csv	collected nuclear deformations
collectedData_RIPL_mass-frdm95.csv	collected nuclear deformations

README.md

- Many nuclei are expected to be deformed
  - Away from closed shells and magic numbers
  - Proton-Neutron asymmetry
- A scripted pipeline reads the deformation library, prepares isotope-specific EMPIRE inputs, runs calculations, formats outputs, and builds ENDF files.

SOURCES

CEA 5DCH
triaxial collective model

CEA HFB
Gogny DS1 mean field

RIPL
Exp. deformations
FRDM95 mass model gs properties

deformations/ • CSV library • reaction-model inputs

Updating level information for the coupled channel calculations

Not everything can be automated…

Model selection requires nuclear-structure information and physics judgment

- Worst cases so far include incomplete level schemes, no spin/parity assignments …

^{87}Br ($t_{1/2}$ ~56 s) ^{91}Kr ($t_{1/2}$ ~9 s), ^{95}Sr ($t_{1/2}$ ~24 s), ^{97}Sr ($t_{1/2}$ ~431 ms)

- For ^{87}Br, for example - negative parity adopted for low-lying states:
  - GS is expected to be 5/2−. Several excited states decay directly to this negative-parity ground state. We took the lowers spin suggestion by ENSDF and E2 transition preserves parity which supports a negative-parity assignment.

ADOPTED LEVELS, GAMMAS for ^{87}Br

Authors: T.D. Johnson and W.D. Kulp | Citation: Nucl. Data Sheets 129, 1 (2015) | Cutoff date: 27-Jul-2015

Full ENSDF file | Adopted Levels (PDF version)

Q(β-)=6818 keV 3 S(n)= 6331 keV 4 S(p)= 10677 keV 4 Q(α)= -6647 keV 4
Reference: 2012Wa38

References:
A ^{87}Se β$^-$ decay

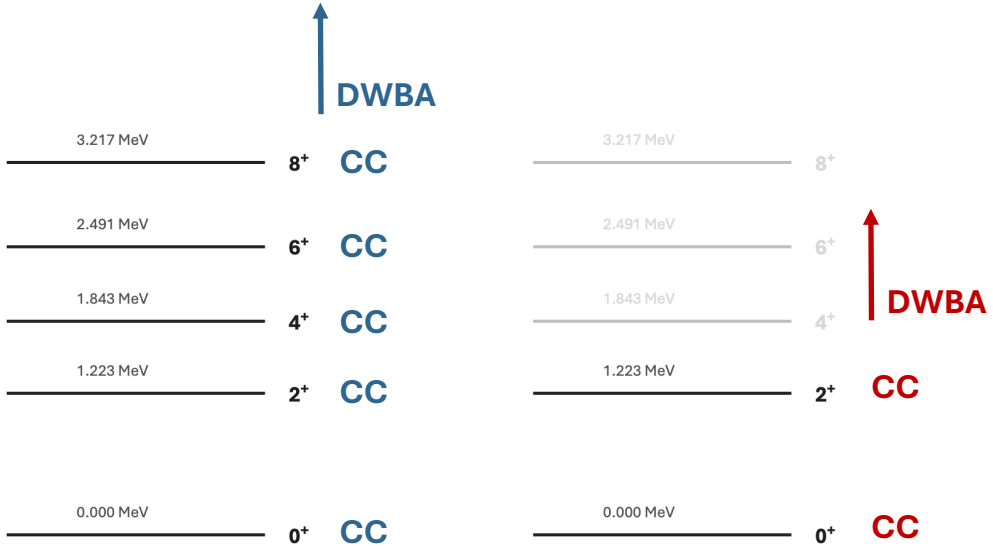
General Comments:

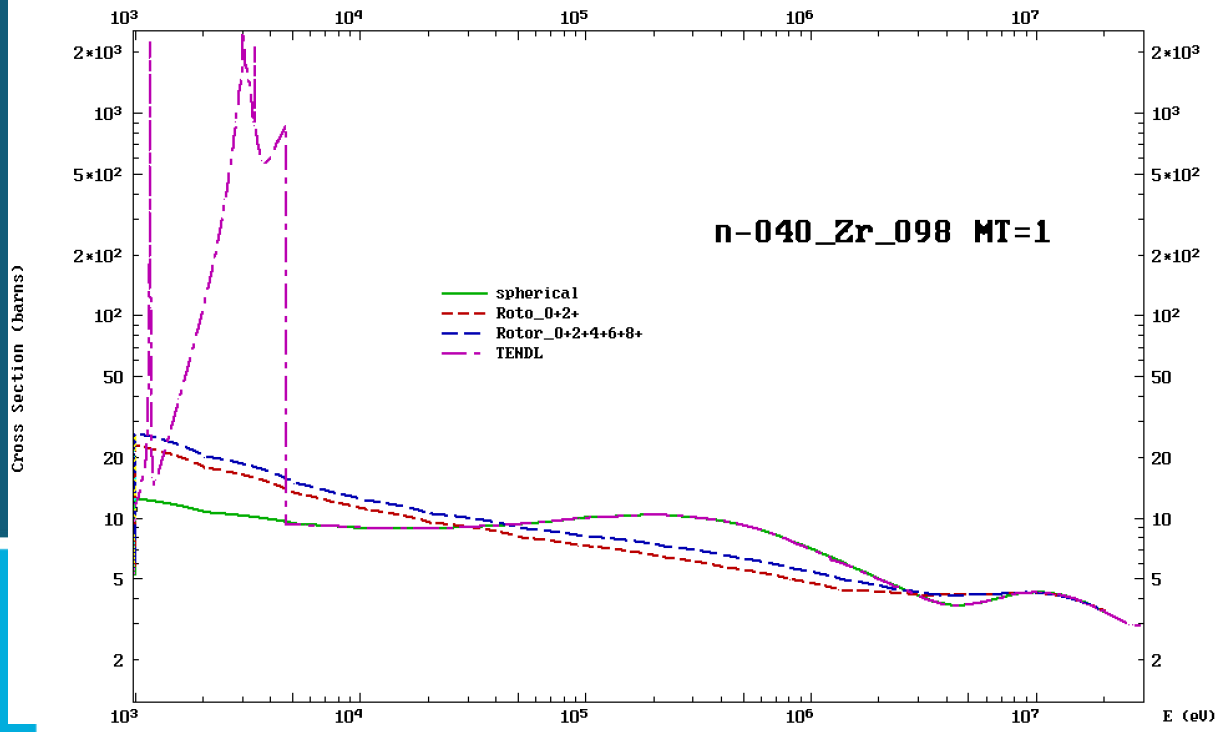
Jπ ☑		T1/2/Decay ☑	E(γ) ☑		I(γ) ☑	Final Levels ☑	
E(level) (keV)	XREF	Jπ(level)	T1/2(level)	E(γ) (keV)	I(γ)	Final Levels	
0.0	A	(5/2-)	55.68 s 12 % β$^-$ = 100 % β$^-$n = 2.60 4				
242.51 23	A	(1/2,3/2,5/2)		242.5 3	100	0.0	(5/2-)
334.0 3	A	(1/2,3/2,5/2)		334.0 3	100	0.0	(5/2-)
573.17 24	A	(1/2,3/2,5/2)		573.2 3	100	0.0	(5/2-)
710.51 21	A	(1/2,3/2,5/2)		468.0 3 710.5 3	100 40.9	242.51 0.0	(1/2,3/2,5/2) (5/2-)
1035.5 6	A	(1/2,3/2,5/2)		701.5 5	100	334.0	(1/2,3/2,5/2)
1878.14 21	A	(1/2,3/2,5/2)		1167.6 3 1305.0 3 1878.1 3	78.0 75.4 100	710.51 573.17 0.0	(1/2,3/2,5/2) (1/2,3/2,5/2) (5/2-)
3926.4 4	A	(1/2,3/2,5/2)		3683.8 5 3926.3 5	57.1 100	242.51 0.0	(1/2,3/2,5/2) (5/2-)
3987.1 6	A	(1/2,3/2,5/2)		3744.5 5	100	242.51	(1/2,3/2,5/2)

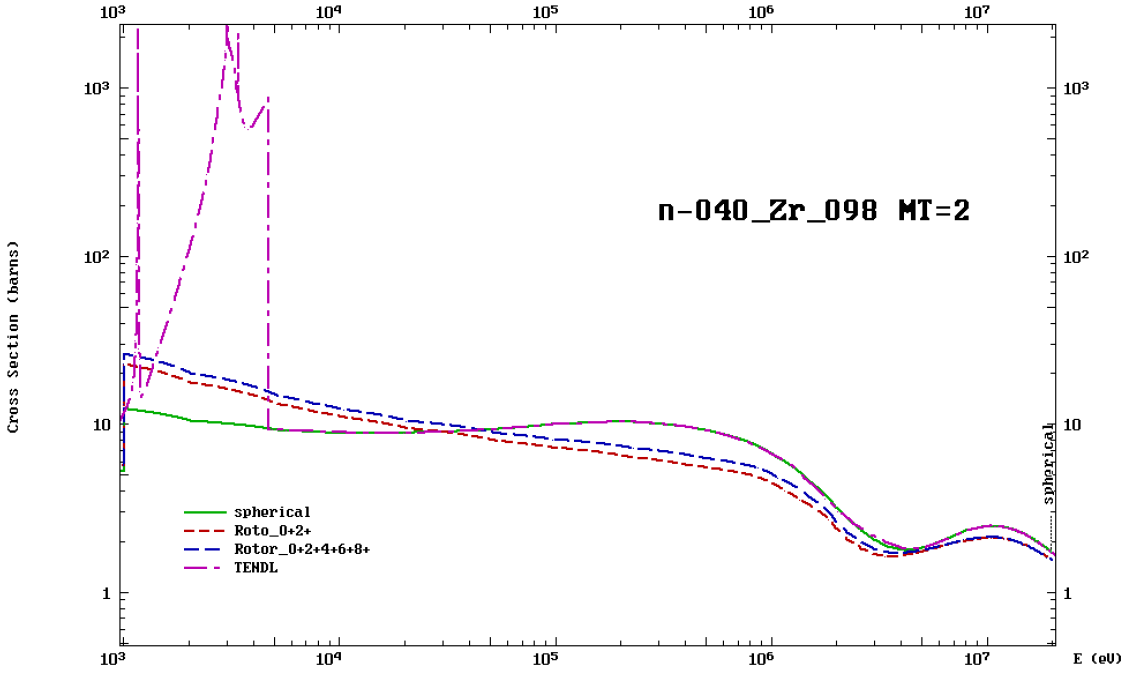
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^{98}Zr

Preliminary results!

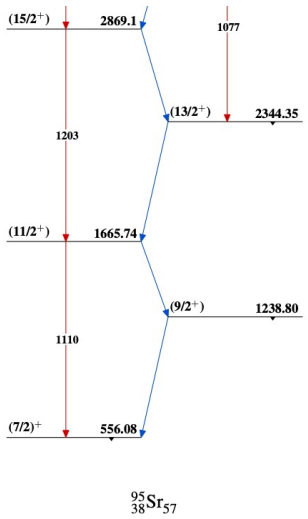






^{95}Sr (Z=38)

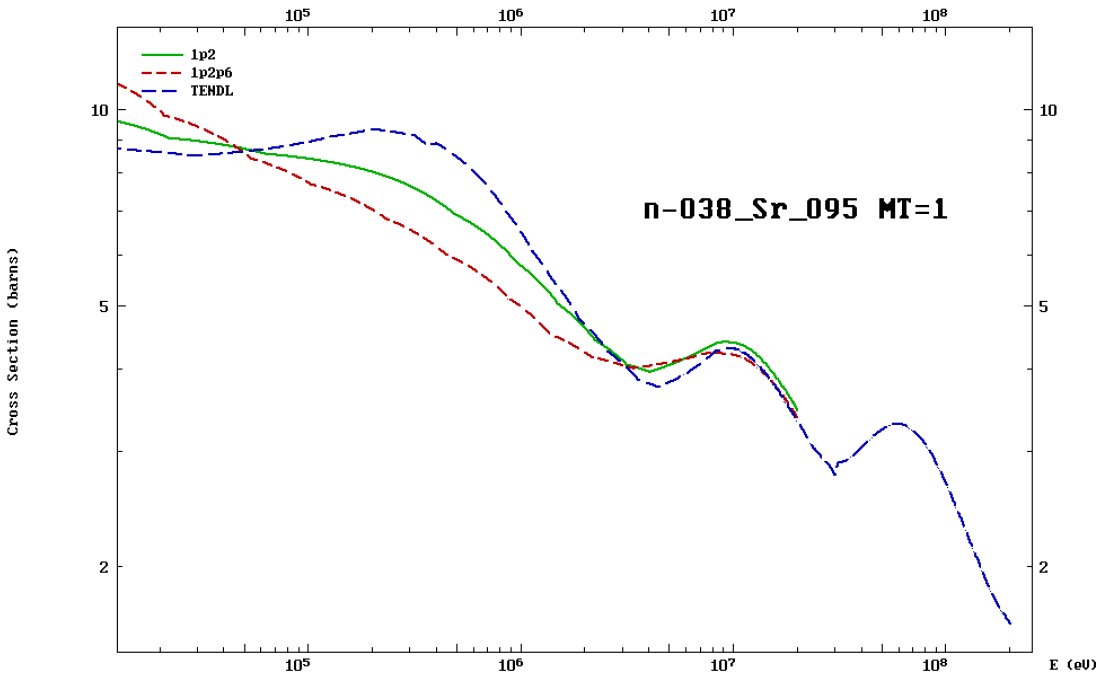
Interesting band structure but not GS…

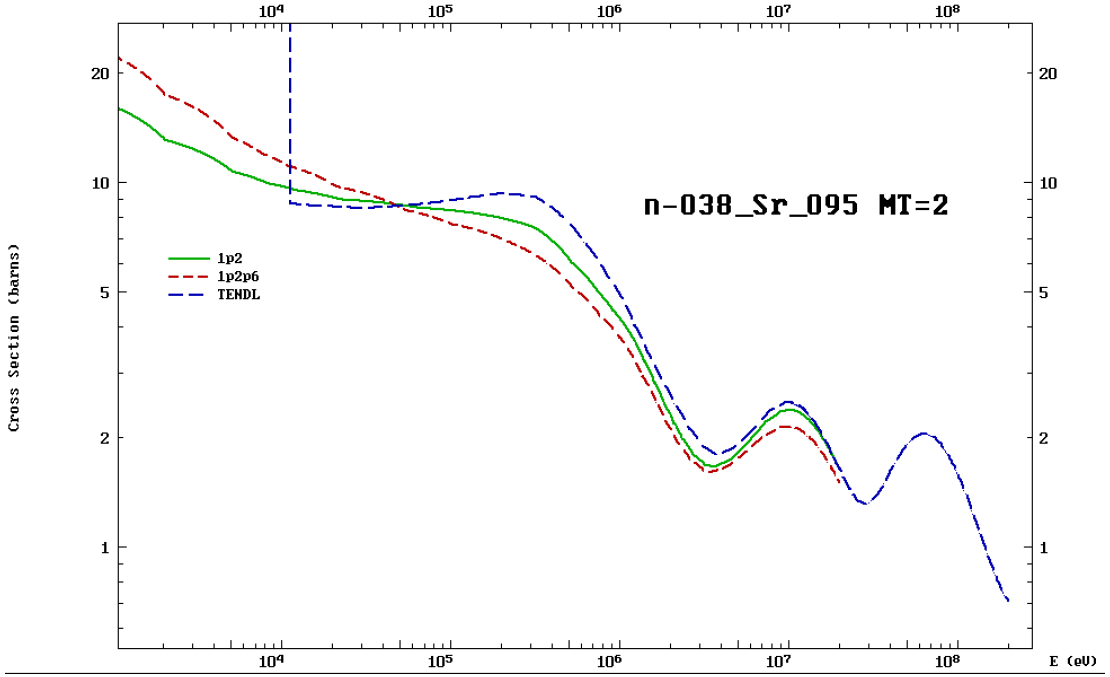


Preliminary results!

Could 7/2+ be 5/2+?

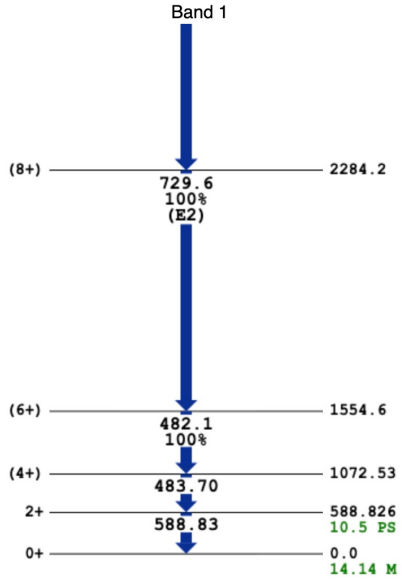
- ENSDF favors 7/2+ from conversion coefficients : mainly E2.
- If 5/2+, a 556-keV E2 decay to the GS should be seen.
- No 556-keV γ ray observed -> argues against 5/2+.
- ^{95}Sr is deformed, so a separate GS rotational band could be expected.
- We did $1/2^+_{GS} \rightarrow 3/2^+ \rightarrow 5/2^+$ for the GS band.



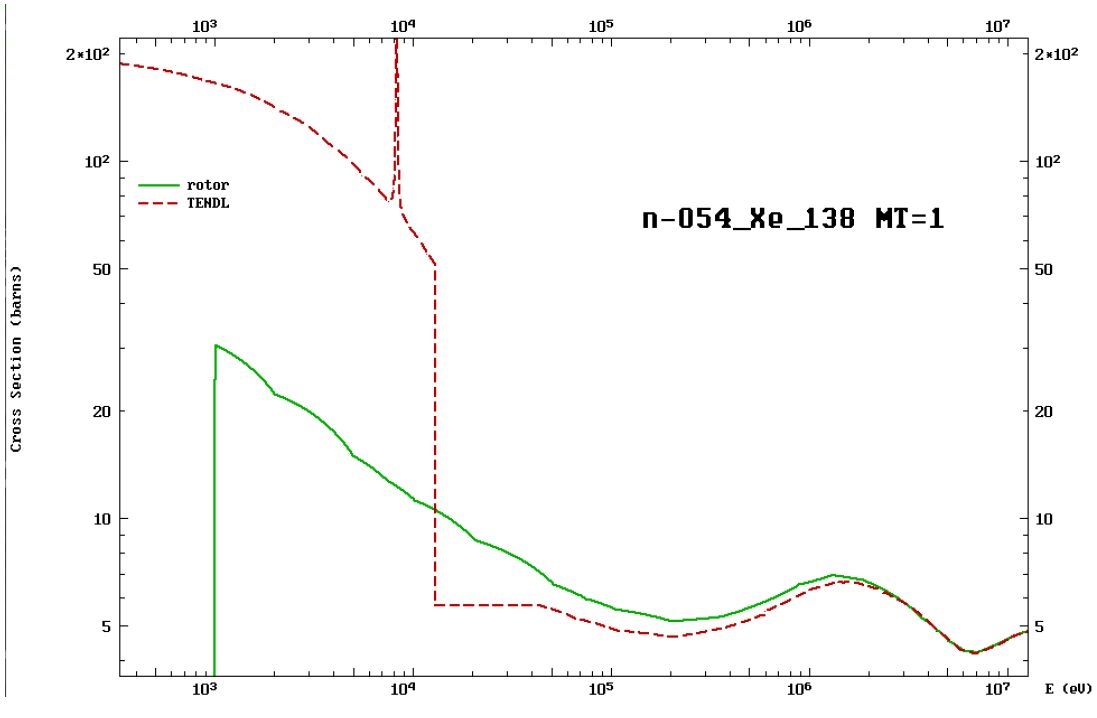


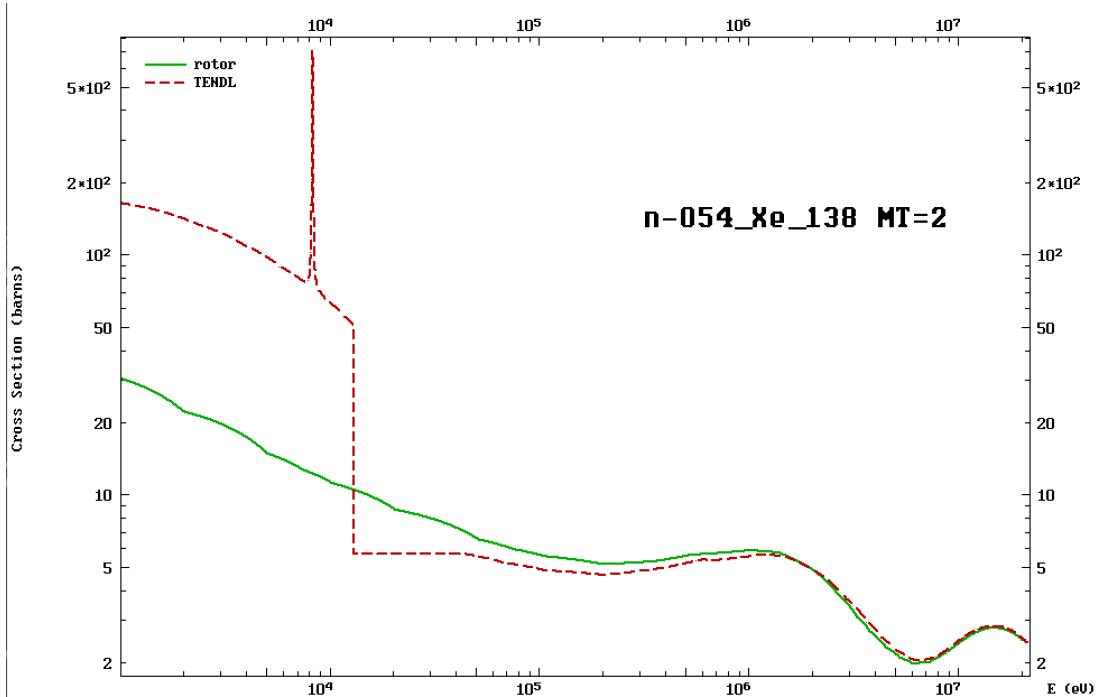
^{138}Xe (Z=54)

Preliminary results!



Nice rotor!





Resonance Region

Describing unknown resonances as a “big” Unresolved Resonance Region

RREFPOS's resonance region

Model for capture:

$$\sigma_\gamma(E) = \sigma_{\gamma 0}\sqrt{\frac{E_0}{E}} + (\text{single resonance}) + (\text{URR})$$

Single resonance is a FUDGE requirement.

Need:

- Prescription to determine thermal c.s.
- Single S-wave resonance
- EMPIRE output converted to URR parameters

- D_0, LD from RIPL systematics, currently use D_0, eventually take J=0 LD
- Γ_γ from RIPL
- Γ_n reverse engineered from $T_c = 2\pi\ \Gamma_n / D_0$, but SPRT form is better

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EAF-2009 prescription (used by TENDL)

Systematics based on guessing a functional form. Landed on this:

$$\sigma_{n\gamma} = C_1 (aU)^{C_2} \text{ with } C_1 = 1.10 \text{ x } 10^{-5},\ C_2 = 3.12$$

a and U are Gilbert Cameron LD parameters

Fit is not inspiring => factor of 100x uncertainty

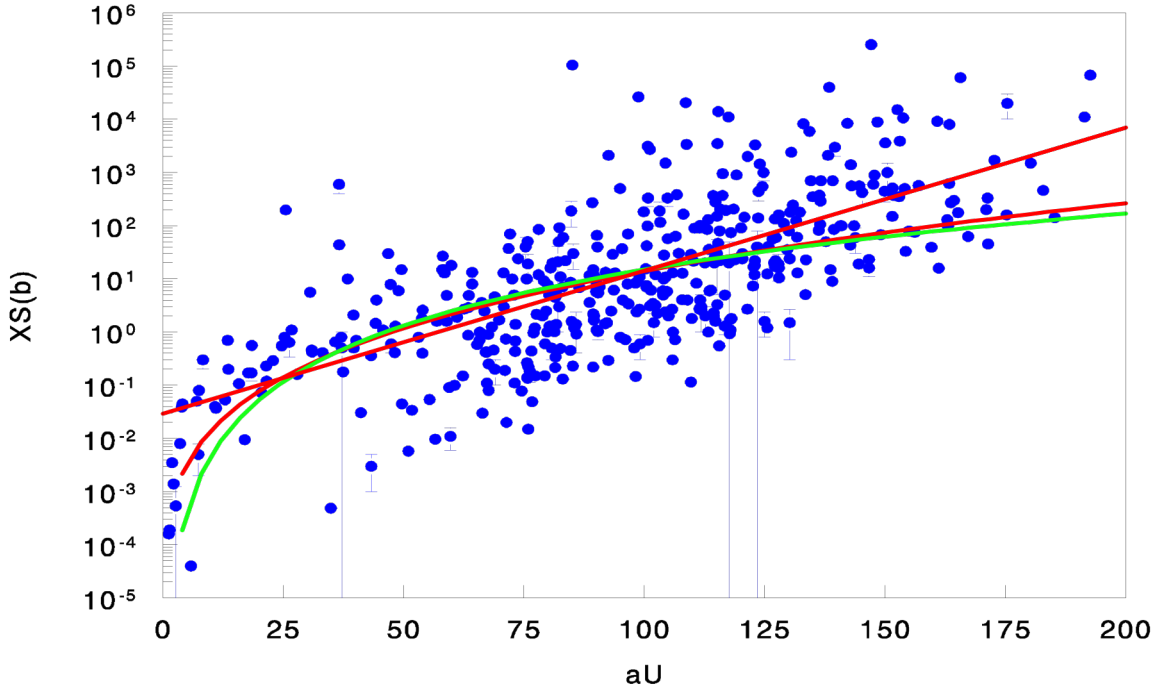
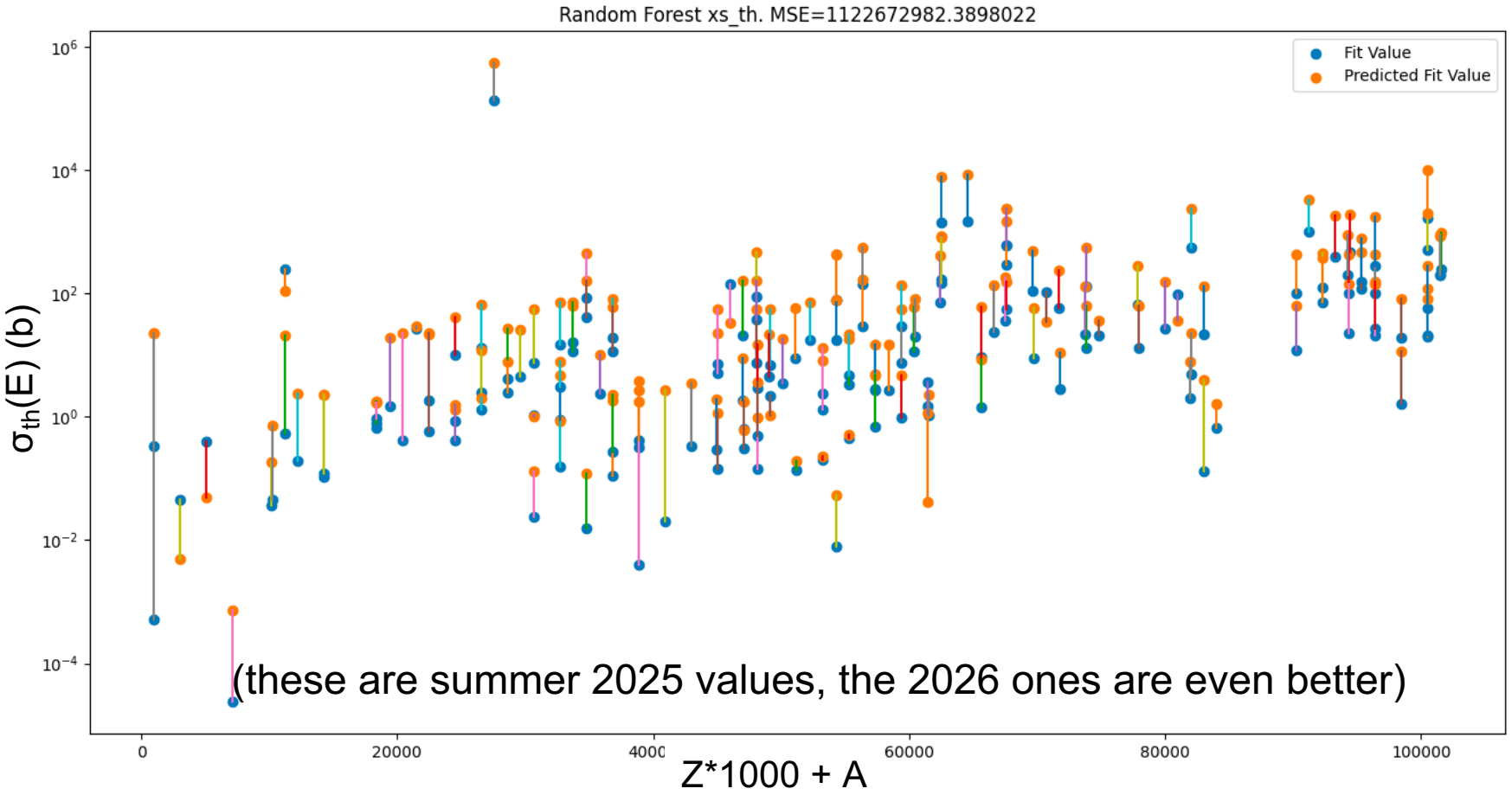


Figure 5. Thermal capture cross sections (recent data taken from [29] plotted against aU). The old systematic of equation (2) is shown as the green curve. The newly fitted curves, both linear and power fits, are shown in red.

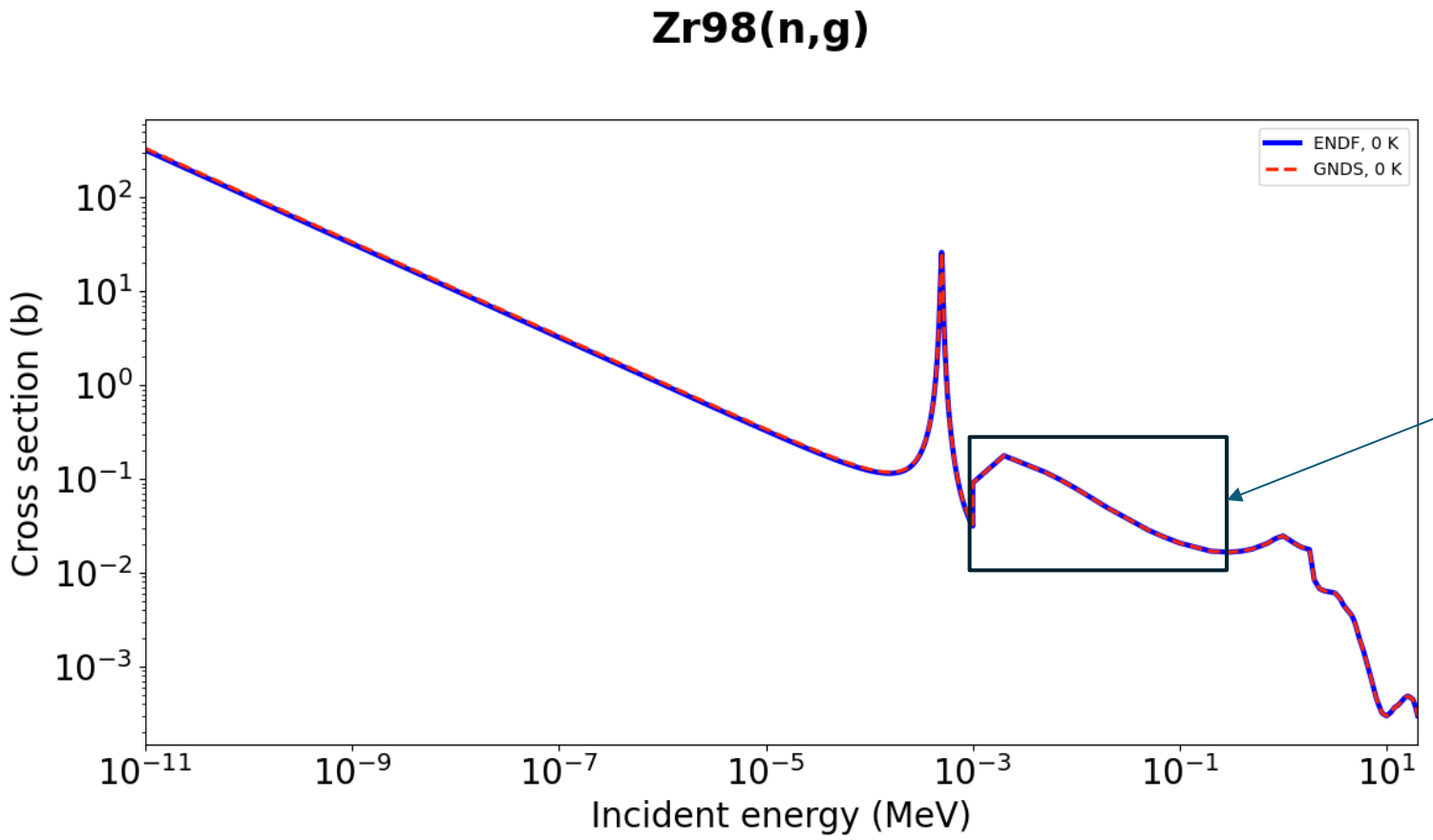
As a side effect of an Intentional Forensics Venture, developed an ML approach that outperform EAF-2009 by 10x



Also provides alternative estimates of average spacing and average capture area

We have a functioning EMPIRE→ENDF (and GNDS) resonance pathway. It needs refinement.

Preliminary results!



URR is here, but now we need a way to use it

https://git.nndc.bnl.gov/dbrown/urr-formatter

1st complete file

Summary and Outlook

- We completed fast region calculations for *almost* **all** nuclei in our primary goal list
- Approach to resonance seems to be working: First preliminary complete file produced
- Did not have time here to address other components of the project
  - Level density measurements
  - ML-based extrapolated cross sections and UQ
  - More details: BNL-229070-2025-INRE, arXiv:2606.03720, BNL-230279-2026-FORE
- Next steps:
  - Produce complete files for all nuclei in primary goal list
  - Submit to ENDF library
  - Collect feedback from potential user community
- Project outcome should be a better starting point for inventory library for those specific nuclei

Acknowledgements

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