IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Consultancy Meeting on Model Code Output & Application nuclear Data Form Structure White paper

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Background

- Nuclear observables and data forms are at the foundations of most nuclear programs
- IAEA's member countries traditional efforts in research, development and technologies have been in support of each member's needs; they differs
- Those efforts have concentrated on answering the needs of a few major applications one at a time: energy, reactor, accelerator physics, medical, etc.
- However the scenarios are shifting in support of:
  - new experiment analysis, old experiment re-analysis
  - materials, earth and life sciences
  - extended incident & outgoing particles energy range
  - cross-country, -continent collaboration on new technologies
- Although the field is considered as established, not every corner or stone of the nuclear landscape is been properly or even entirely mapped or turned

Purposes

The purpose of the event is to assess:

- the actual capabilities, successfully deployed methods,

tools and protocols

- future needs in terms of model code output and application nuclear data form structure

in the different members' state

with the aim of testing/prototyping/developing and deploying and sharing cutting-edge nuclear data form structure to support high-fidelity Multiphysics simulation efforts

A partnership between fundamental sciences and applications,

Along the lines of PREPRO, CRECTJ6, FUDGE, TAGNDS, TARES, DeCE, TEFAL, GIDI, MCGIDI,…

Aims

- The nuclear data exists so it must be good enough for all applications !!
- Cross-section only is not enough, other observables are sometime even more important
- This compellingly depends on the applications: criticality, transport-shielding, experiment analysis, time inventory, materials, earth and life sciences, ..

- For selected range of targets, particles and incident energy
- Every prompt outgoing particles: n, α, p , γ
  - with their spectra and angular distribution
- All daughter residuals and decay emissions
  - state and energy; Z, A
- Capable of answering the atomic, molecular matter state
  - solid, liquid, gas, plasma, bounds

Intentions

- Gouge the lesser actinides, the materials
- Probe the short lived
- go deeper than the neutron map only
- Improve/extend missing angular distribution and energy spectra
- Scouts the nuclear landscape for gems
- Extends the incident particles and their energy ranges
- Populates the missing quantities

Theoretical-practical sciences to support application needs

Partnership between fundamental sciences and applications needs in quick steps

Motivations

- The nuclear data file format impact the interpreted forms through formalisms
- The format choice impact the simulation granularity
  - s30: explicit channels description
  - s0: implicit description mf3-mt5*mf6
- Not every format are suitable everywhere
  - There is evidence that the Kalbach-Mann physics, formalism does not represent well the energy spectra tails of outgoings
    - (α,n), (p,n), (γ,n), (d,n),..
- Charge particles emission, mainly α and p that leaves the residual in an excited states shows symmetric distributions of the outgoing charge particles. The anisotropy need to be taken into account in MC simulations
- Direct component(s) do not have the same outgoing distribution as compound one(s), even for (n,n')..ENDF-6 does not allow to differentiate !!

Motivations

- There is a need to simplify, streamline, shorten the "processing" steps
- Nuclear data modeller and MC code developer must communicates more efficiently
- Model codes outputs need to interact better, more directly with simulation code requirements:
  - why having to tabulate, organise in equiprobable bins, b/sr when this can be done, is done at the modelling stage ?
  - data sampling need to be made easier and more robust
    - independent sampling
    - correlated sampling: cross-section and angle
    - equiprobable bins
    - equiprobable angles
    - Probability Distribution Function and Cumulative Distribution Function
    - uniform angular distribution across a channel partials at least
    - …

Motivations

- Overdone data forms:
  - 64 Legendre coefficients !! when 3-5 at most are used in unison across all channels and targets
  - numerous outgoing partials that do not allow the sum-up rule(s) to be obeyed: cross-section, outgoing energies and angles
  - open explicit channels in the MF-2 range not handled by formalism, or worse open implicit mt-5
  - implicit mt-5 accounting for part of an explicit channel particle emission
  - ..

- Underdone data forms:
  - outgoing energy spectra cut-off in the low KeV region or high MeV
  - isotropic when anisotropic
  - step, glitch at region's boundary
  - LAD = 1, Blatt and Biedenharn general expression for angular distribution
  - ..

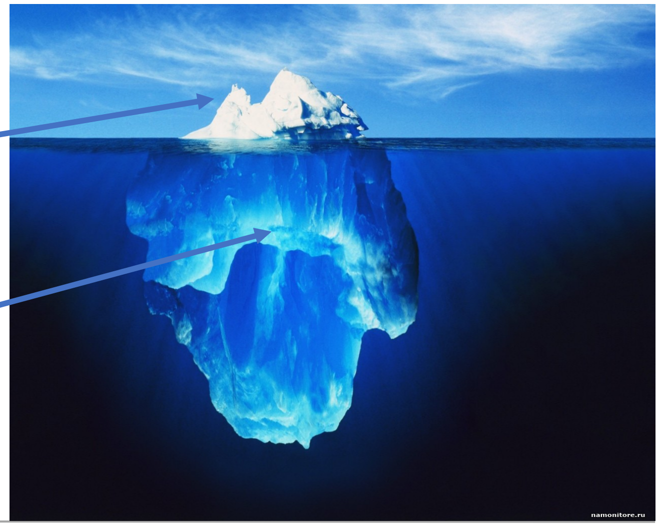
Motivations

- The tables, output streams of the model codes and/or nuclear data assembler need to be more palatable to the style and form of the nuclear data library needed by modern application code
- Why always having to pre or process nuclear data forms when at least partial direct access is entirely possible ?
- Why evaluator article plot do not correspond exactly to the pendf (unionised, linearised) used by a MC code ?
- Why angular distribution are not tabulated? they will be or worse represented by polynome that will be shortened !!
- Why emitted spectra do not extend, cover there full incident particle range?
- Why only the tip of the iceberg:

cross-section?

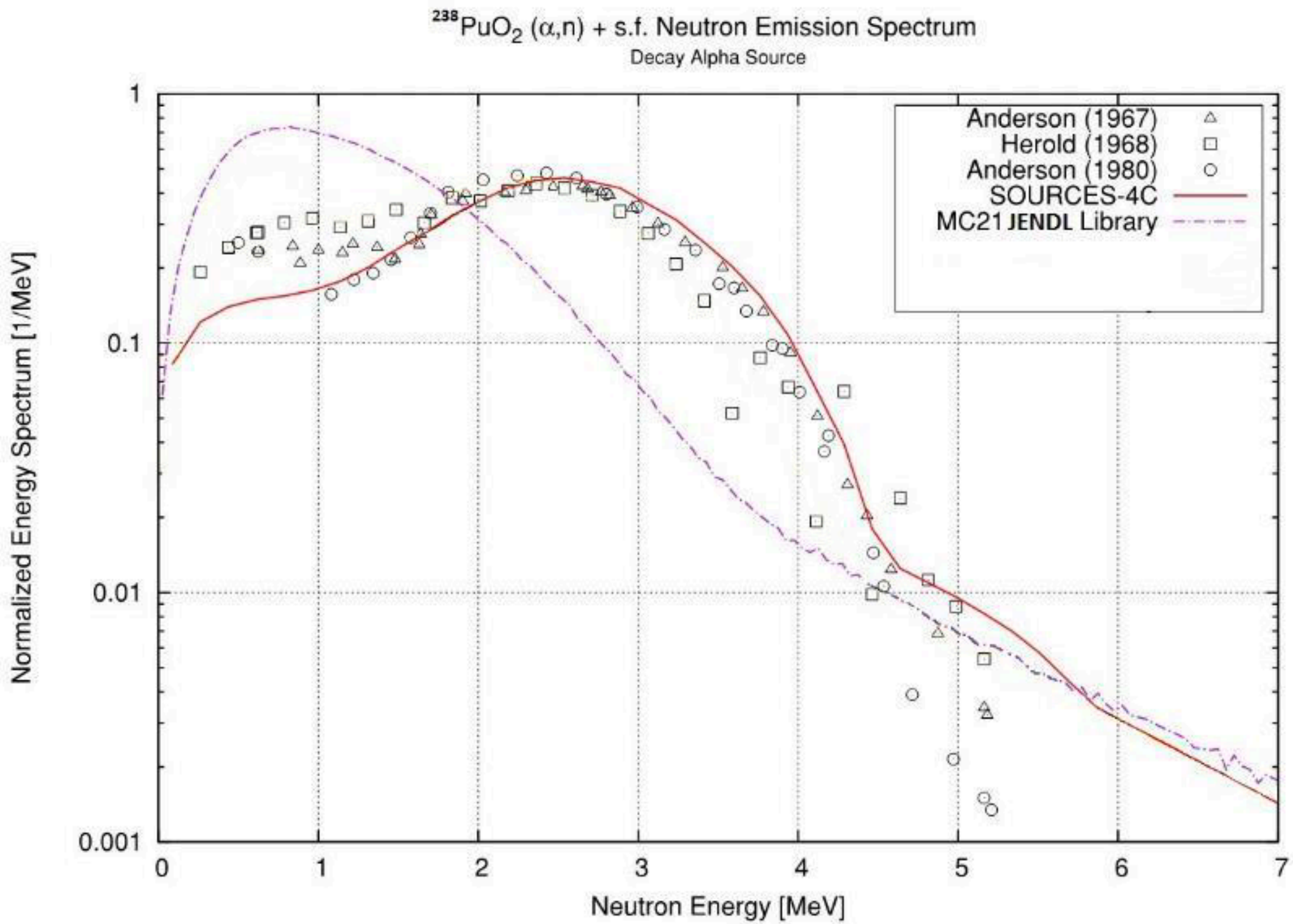
when there is also secondaries

angular, spectral distributions



JENDL/AN-2005 (α,n) testing in MC21

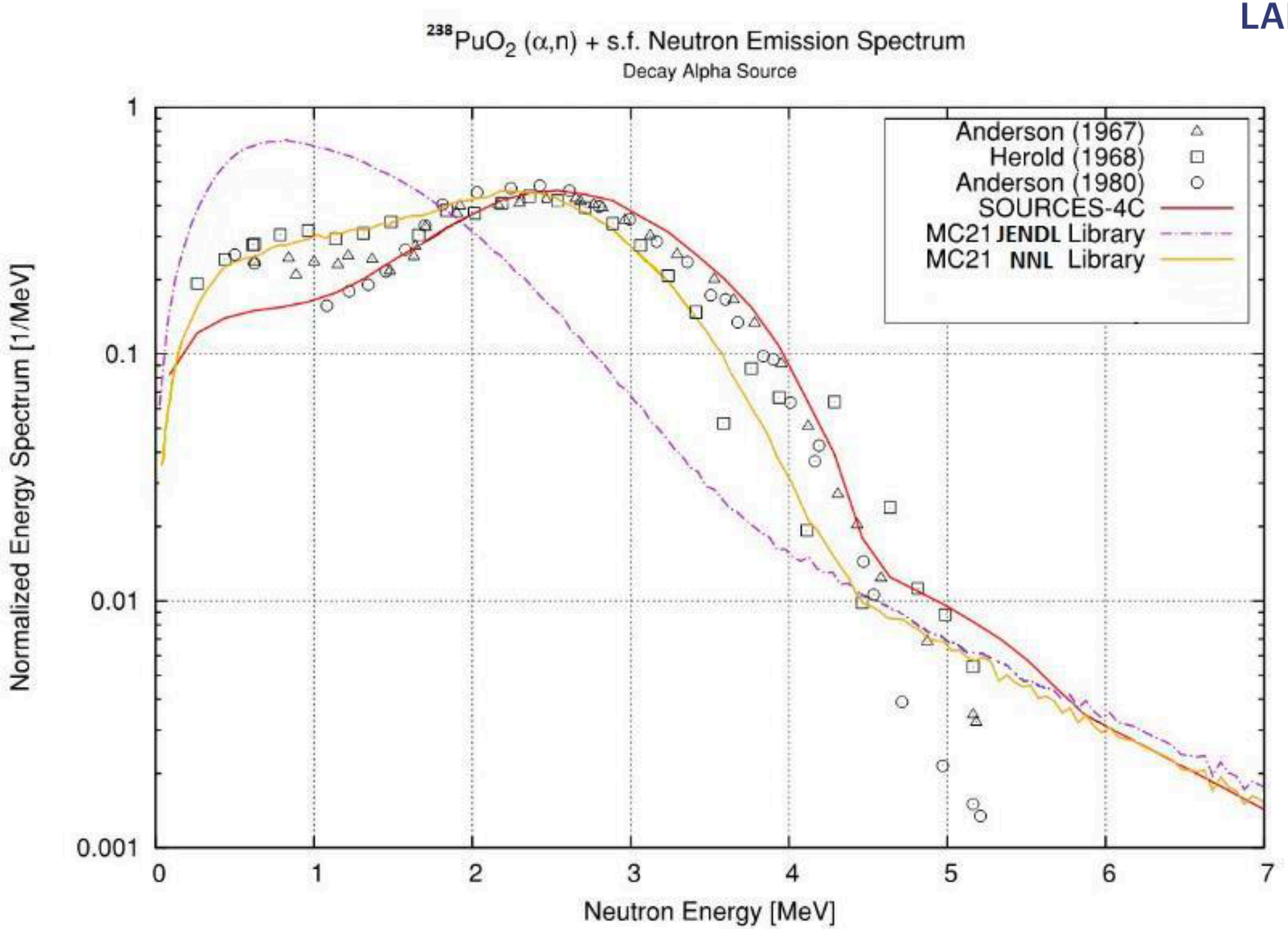
- CSWEG 2018, special purpose evaluation and testing



Jesse Holmes et al., CSEWG (2018)

NNL $O^{17,18}$ (α,n) testing in MC21

- File 6 Neutron Energy/Angle Modifications for O^{17},O^{18} (File 3 cross sections are unchanged)



Jesse Holmes et al., CSEWG (2018)

JENDL/AN-2005 (α,n) NNL modifications

NAVAL NUCLEAR LABORATORY

MT	Reaction	Description
4	(α,n)	Production of one neutron in the exit channel. Sum of MT=50-91.
16	(α,2n)	Production of two neutrons and a residual.
22	(α,nα')	Production of a neutron and an α particle, plus a residual.
28	(α,np)	Production of a neutron and a proton, plus a residual.
50-90	$(\alpha,n_{0\text{-}40})$	Production of a neutron, with the residual in the 0^{th}-40^{th} excited state.
91	(α,n_c)	Production of a neutron in the continuum not included in the above discrete representation.
201	(α,Xn)	Total neutron production.

Nuclide	Cross Section MF3 MTs	JENDL version MF6 MTs	NNL version MF6 MTs
O17	4 22 50-53 91 201	4 22	22 50-53 91
O18	4 16 22 50-54 91 201	4 16 22	16 22 50-54 91

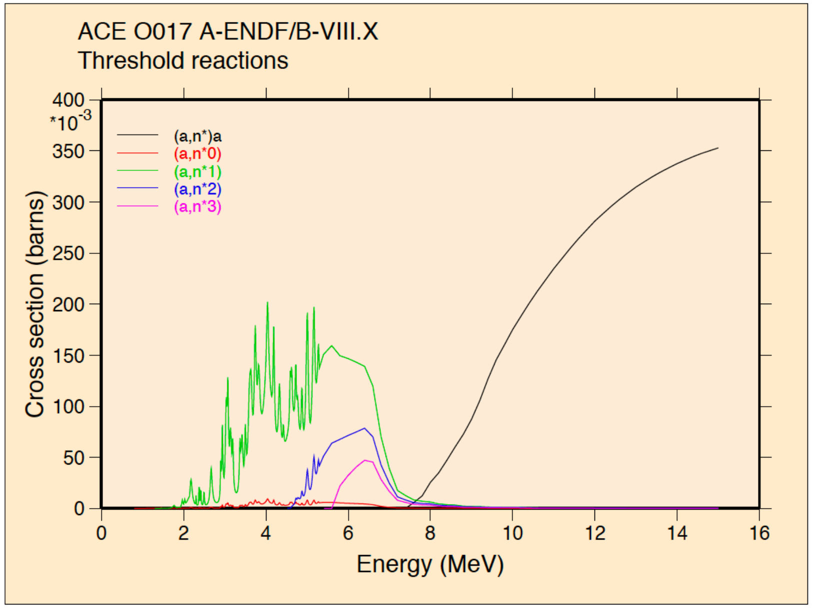
Color-coded MT values indicate neutron energy/angle distribution treatment

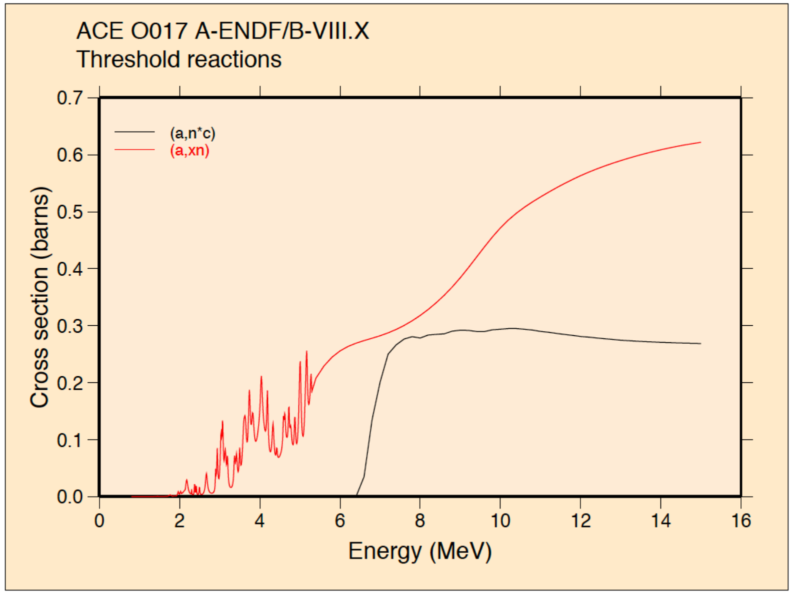
Green: Kalbach-Mann coupled energy/angle distribution
Red: Isotropic two-body kinematics

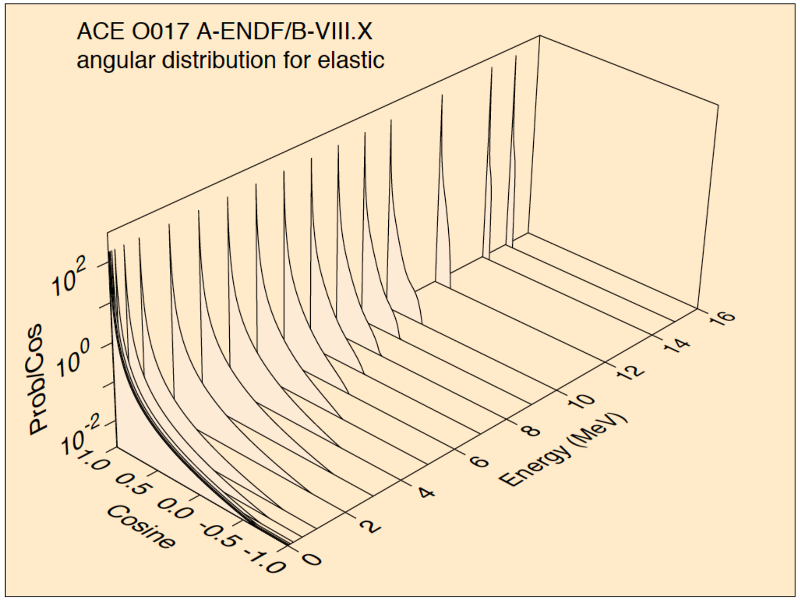
Jesse Holmes et al., CSEWG (2018)

JENDL/AN-2005 (α,n) IAEA extension

- Add MF-3,6 MT=2 Elastic scattering cross section: nuclear + interference terms







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Enhancements deployable to all 17 targets of JENDL/AN-2005

and

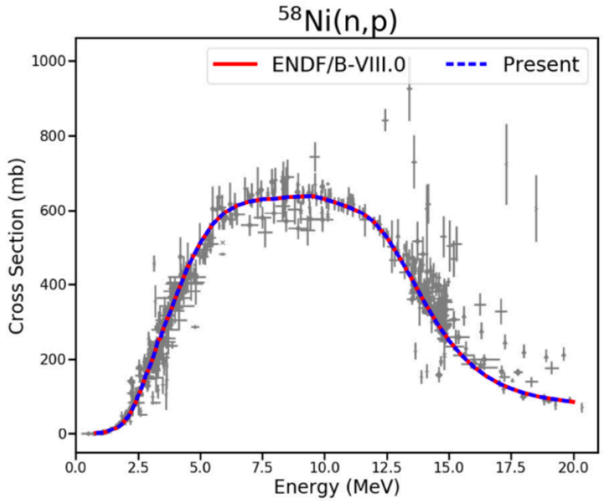
de-facto all other charged particle libraries that would follow this form structure

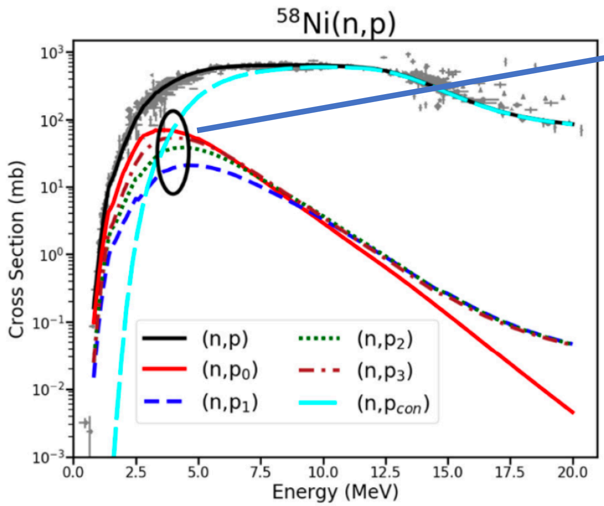
ENDF/B-VIII.x LANL extensions

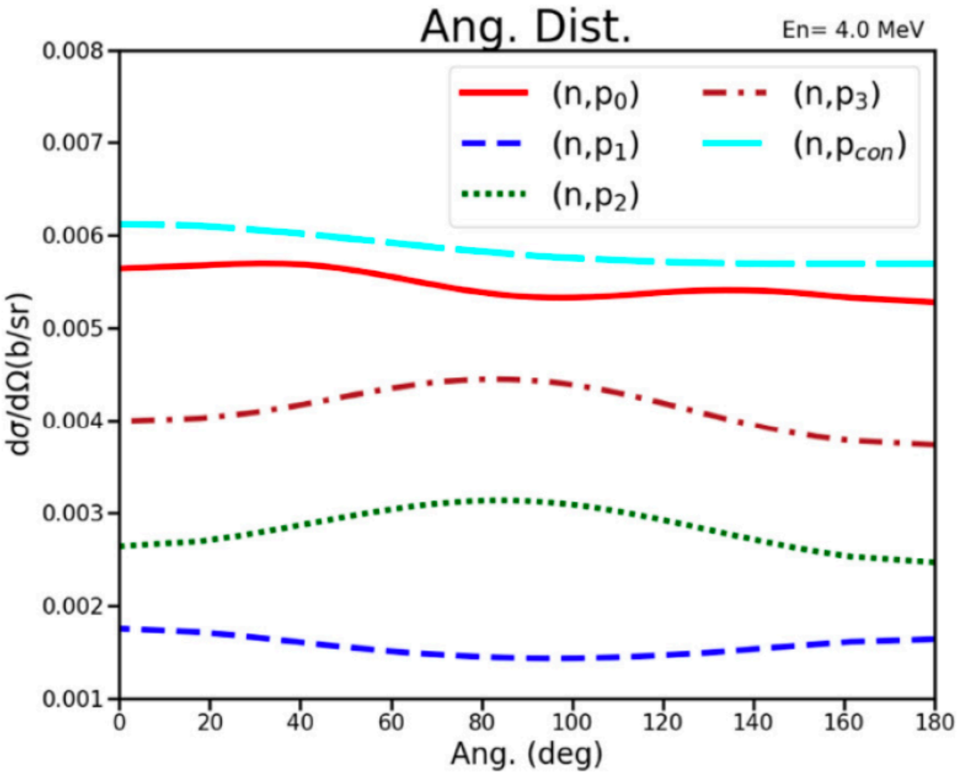
New evaluation on angular distributions and energy spectra for neutron-induced charged-particle measurements

H.I. Kim, H.Y. Lee, T. Kawano, A. Georgiadou, S.A. Kuvin, L. Zavorka, M.W. Herman

https://doi.org/10.1016/j.nima.2020.163699



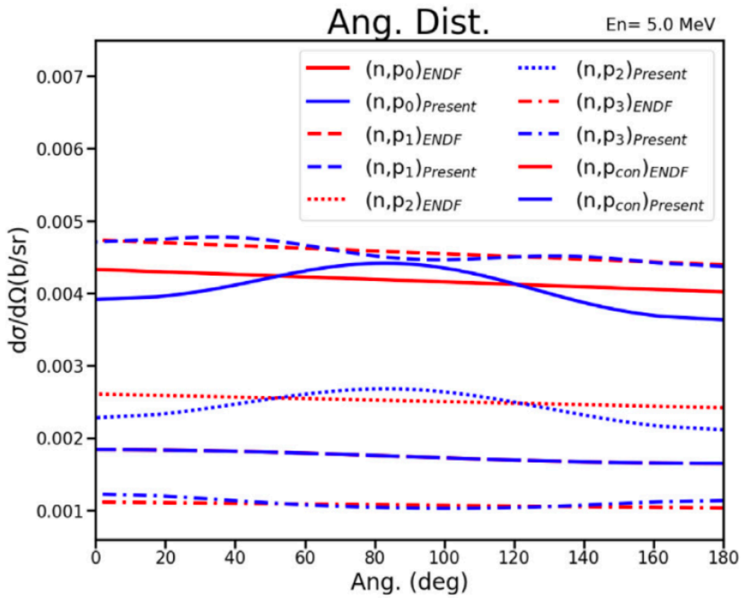


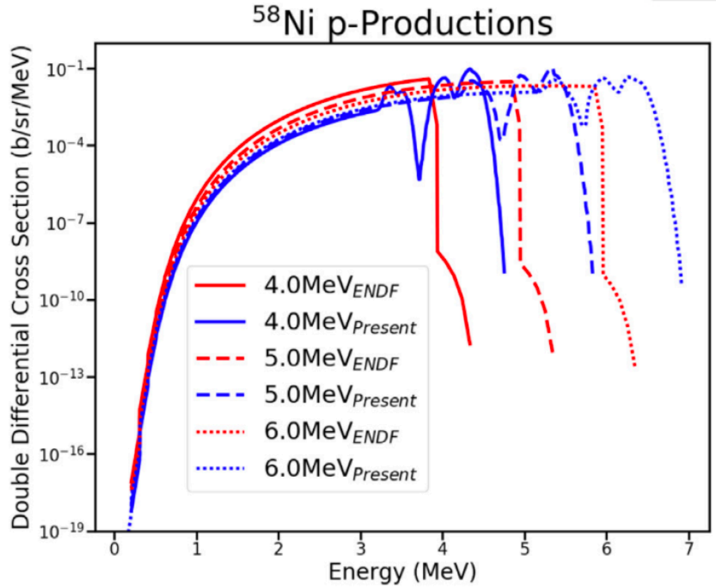


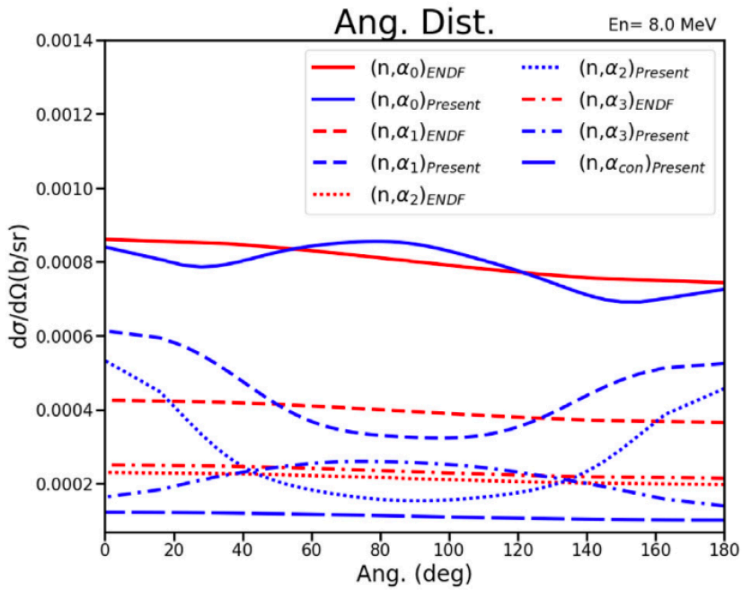
ENDF/B-VIII.x LANL extensions

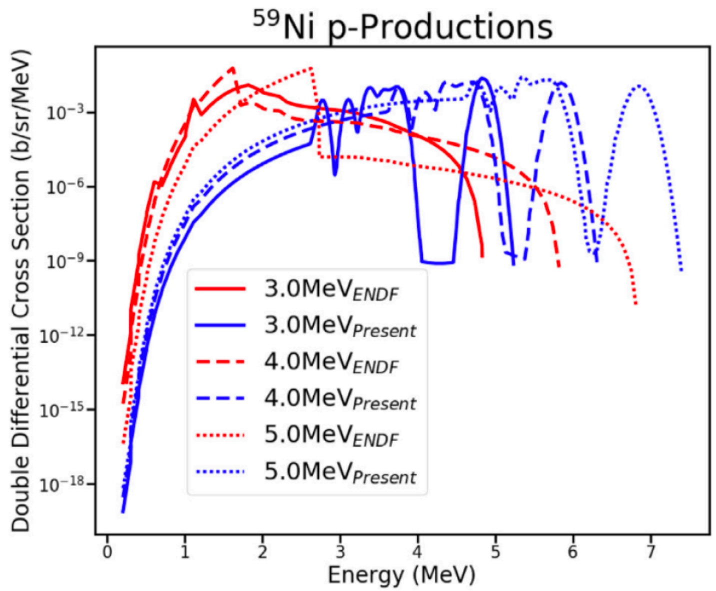
- ^{54}Fe angular distributions for discrete level of (n,p) and (n,α)
- $^{58-59}Ni$ p production

Los Alamos NATIONAL LABORATORY EST.1943



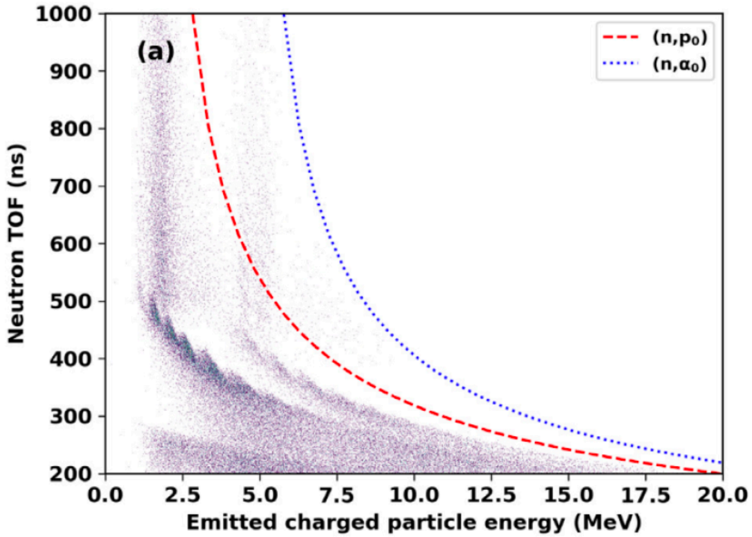


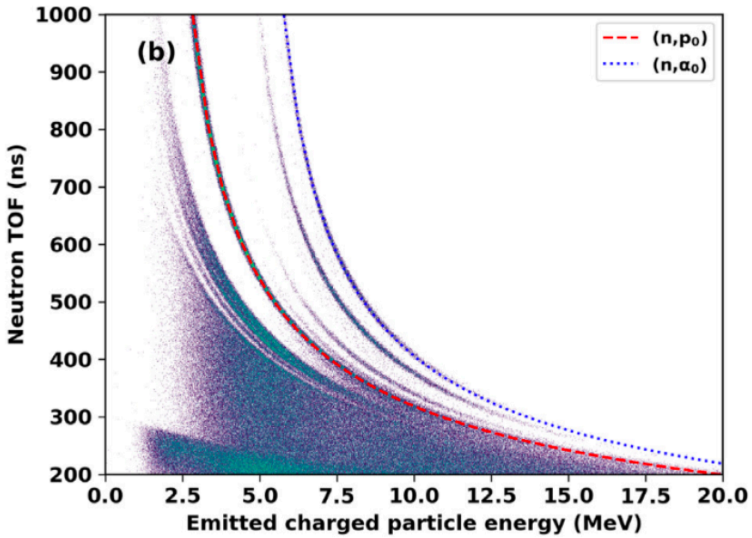




ENDF/B-VIII.x LANL extensions

- Enhanced nuclear data forms that enable, empower the simulations tools





Courtesy H.I. Kim (KAERI)

MCNP6 simulations using double-sided silicon strip detectors for detecting emitted charged particles induced by neutrons on ^{59}Ni.

a) using ENDF/B-VIII.0
b) using the new evaluation

c) dash and doted curves are the kinematic curve for the ground state of (n,p) and (n,α) reactions

Strategy

- Build from the existent when possible
- Enhances the data forms, makes them worthwhile
- Complete, finish the library

- Complement, constrain with theory when needed

- Test/prototype/develop and deploy/share cutting-edge nuclear data form structure
- Support high-fidelity Multiphysics simulation efforts

A partnership between fundamental sciences and applications

Thank you for your attention!

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