ENDF/B Progress Report

32nd WPEC Meeting

11-15 May 2020, NEA Headquarters, Boulogne-Billancourt, France
(at least virtually)

D. A. Brown

for the Cross Section Evaluation Working Group

National Nuclear Data Center

Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

ENDF/B-VIII.0 was released on 2 Feb. 2018 by the Cross Section Evaluation Working Group (CSEWG)

ENDF B-VIII.0

Happy 50th Anniversary!*

ENDF/B-VIII.0
was released
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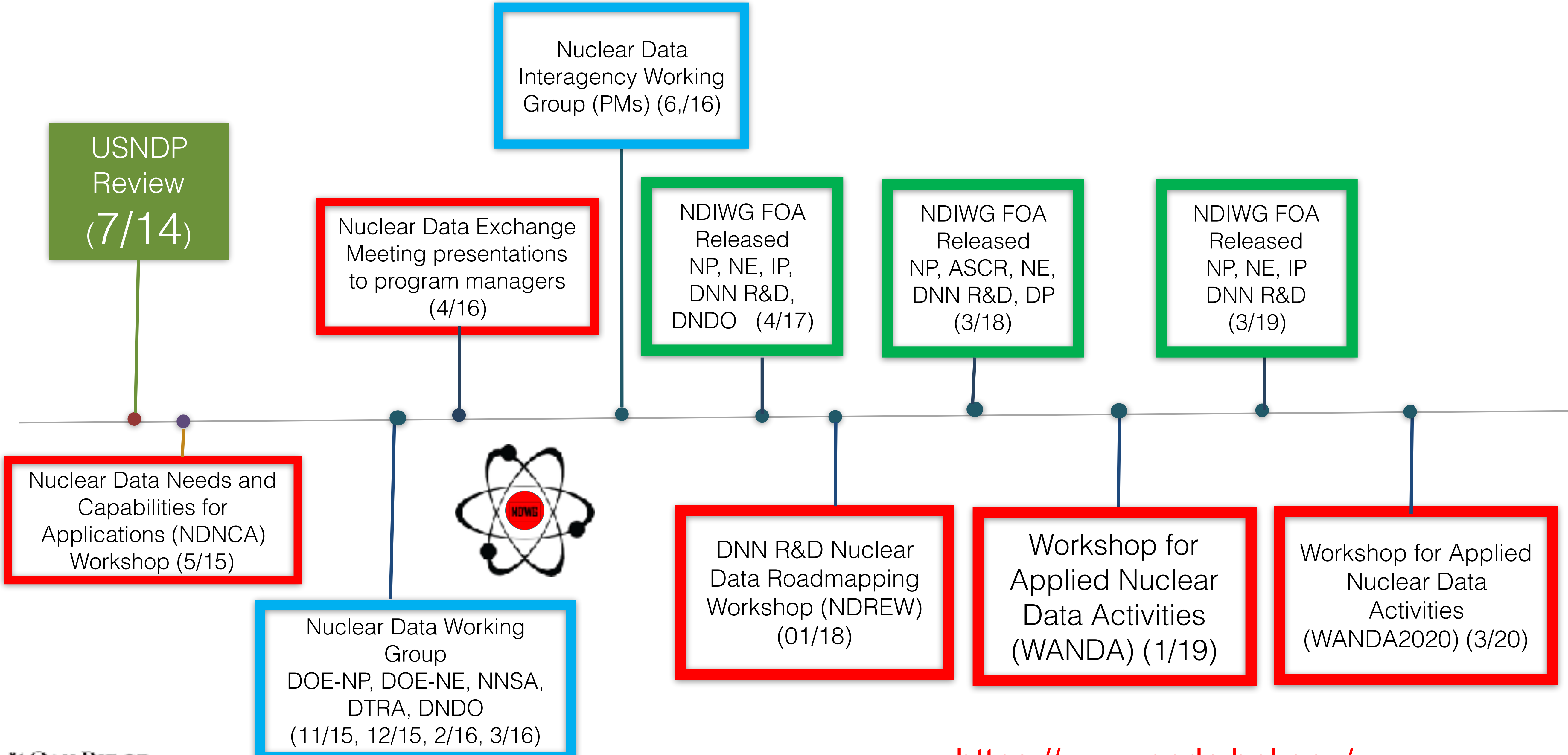
CSEWG's focus for 2019 & 2020 CSEWG is measurements and tool building

Evaluation work is ramping up

appy
0th
Anniversary!*

New planning & funding process

Recent Events in Nuclear Data



https://www.nndc.bnl.gov/

Slide from Cathy Romano (WANDA 2020)

The Nuclear Data Working group (NDWG)

- In FY19 we formalized the collaboration with a new charter

MISSION STATEMENT

- The goal of the Nuclear Data Working Group (NDWG) is to facilitate communication, collaboration, coordination and prioritization of nuclear data efforts across multiple program offices, the national laboratories, universities, and industry.

MEMBERSHIP

- Members shall be experts in their respective fields and be nominated to serve on the committee by program managers or national laboratories.
  - Up to 2 members can be nominated per program manager
  - Up to 2 members can be nominated per national laboratory

Please contact me romanoce@ornl.gov for information on participation

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The NDWG/WANDA process is a valuable addition to CSEWG planning and brought several new user communities to CSEWG

Please contact me romanoce@ornl.gov for information on participation

OAK RIDGE National Laboratory

Slide from Cathy Romano (WANDA 2020)

Welcome to Workshop for Applied Nuclear Data Activities 2020

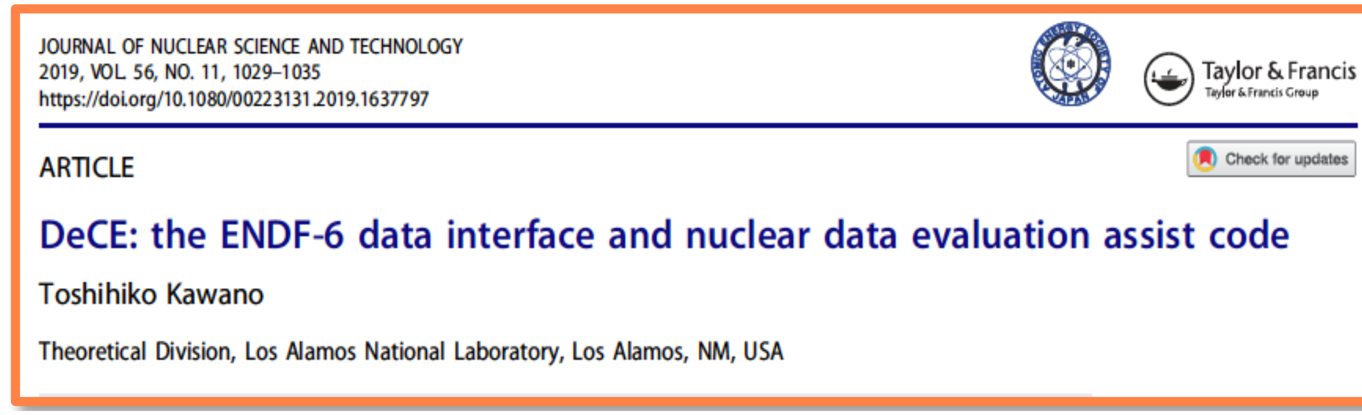
- Sponsored by the Nuclear Data Interagency Working Group
- Roadmapping Sessions:
  - Artificial Intelligence/Machine Learning for Nuclear Data
  - Detector Models, Atomic Data and Stopping Powers
  - Covariance/Sensitivity/Uncertainty/Validation and its impact on applications
  - Nuclear Data for Isotope Production and Target Fabrication
  - Neutron Induced Gamma Production and Gamma Decay
  - Scattering Transport and Shielding

OAK RIDGE National Laboratory

Slide from Cathy Romano (WANDA 2020)

New tools

Many open source tools


JOURNAL OF NUCLEAR SCIENCE AND TECHNOLOGY
2019, VOL. 56, NO. 11, 1029–1035
https://doi.org/10.1080/00223131.2019.1637797

Taylor & Francis
Taylor & Francis Group

Check for updates

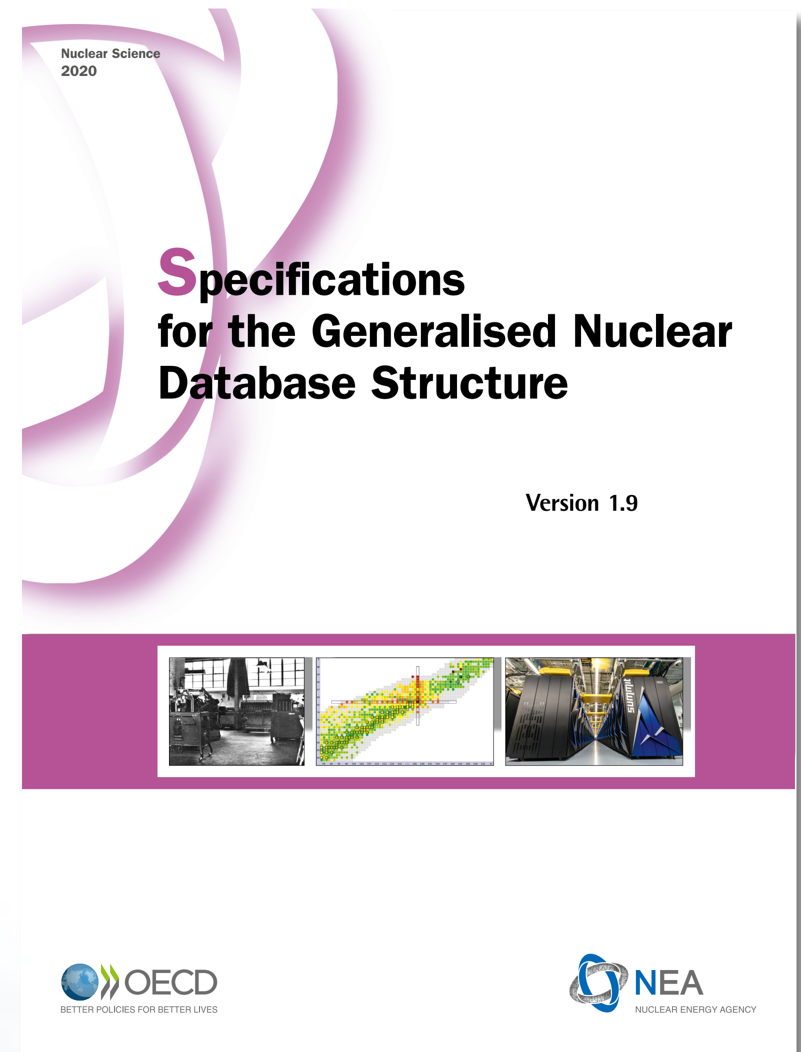
ARTICLE

DeCE: the ENDF-6 data interface and nuclear data evaluation assist code

Toshihiko Kawano

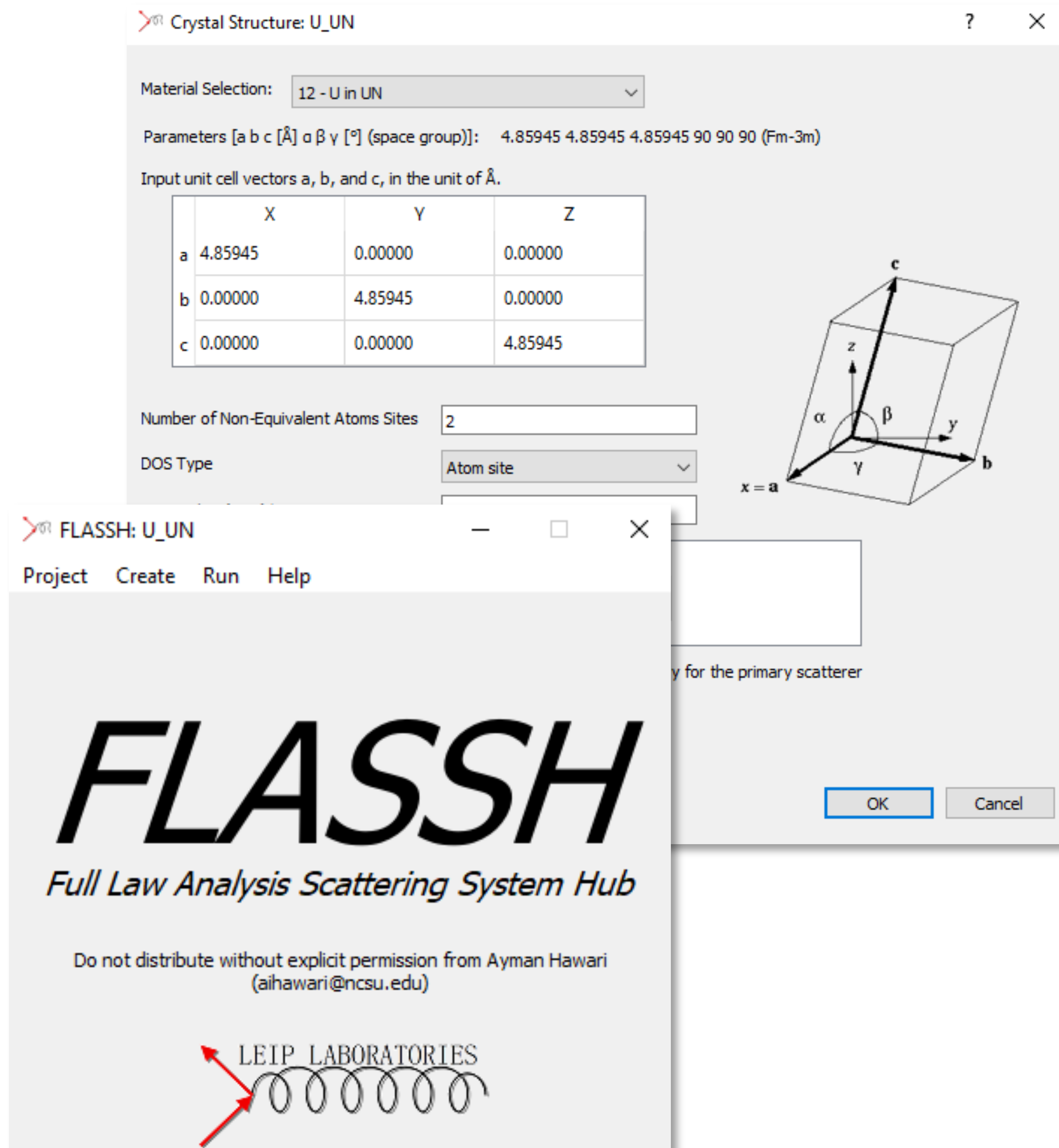
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA

- DeCE: the ENDF-6 data interface and nuclear data evaluation assist code, Kawano, J. Nucl. Sci. Technol. 56, 1029 (2019)
- AMPX open sourced
- SAMMY open sourced
- NJOY open sourced
- FUDGE, GIDI open sourced, new releases this FY
- And of course, GNDS



FLASSH Code

- *FLASSH* Code
  - Relaxed major approximations (incoherent, cubic, ect.)
  - Improved liquid physics
  - Improved output formatting
  - Warning Messages for the User
- *FLASSH* GUI
  - Error Checks
  - Crystal Structure Window/ Inputs
  - ENDF Header Formatting

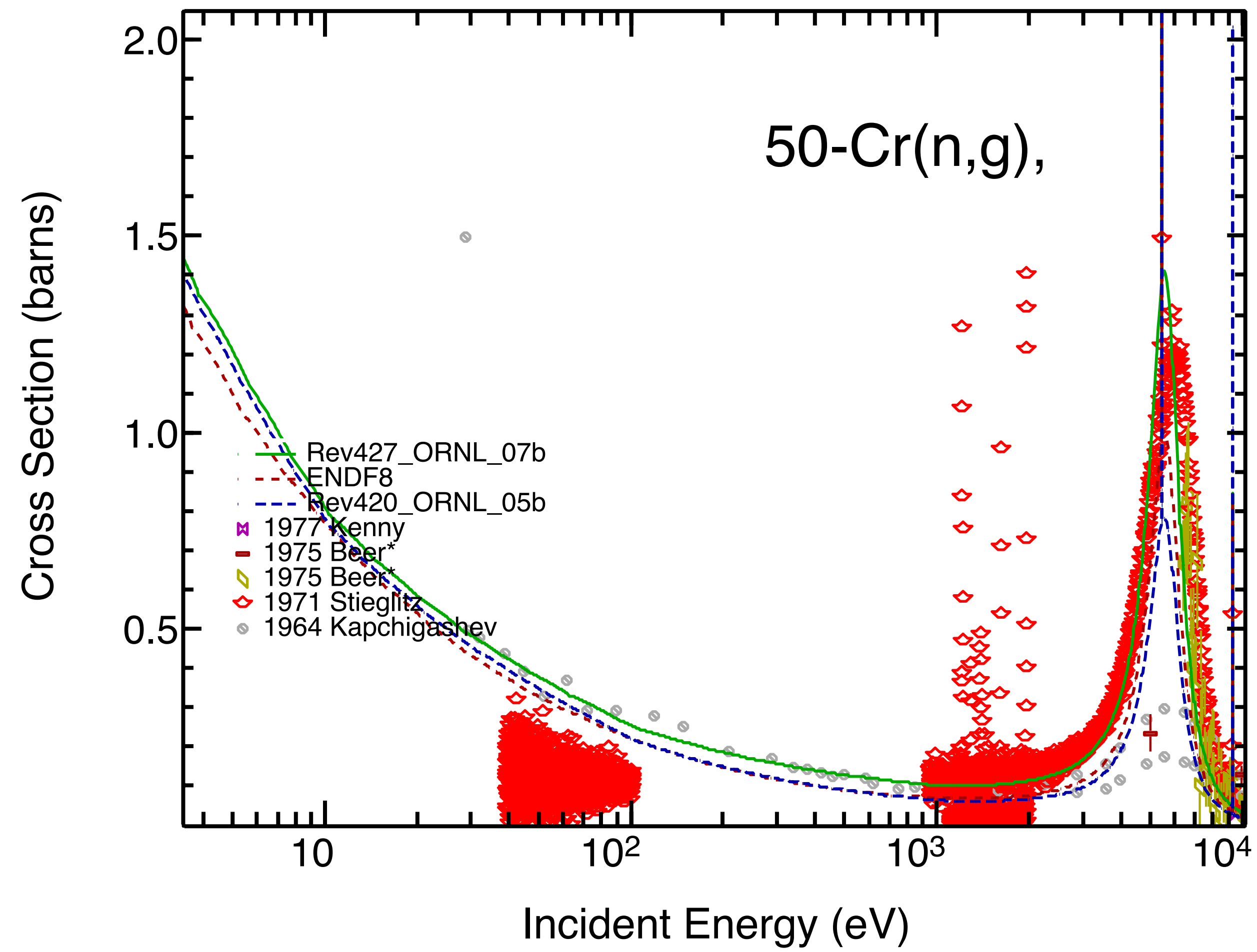


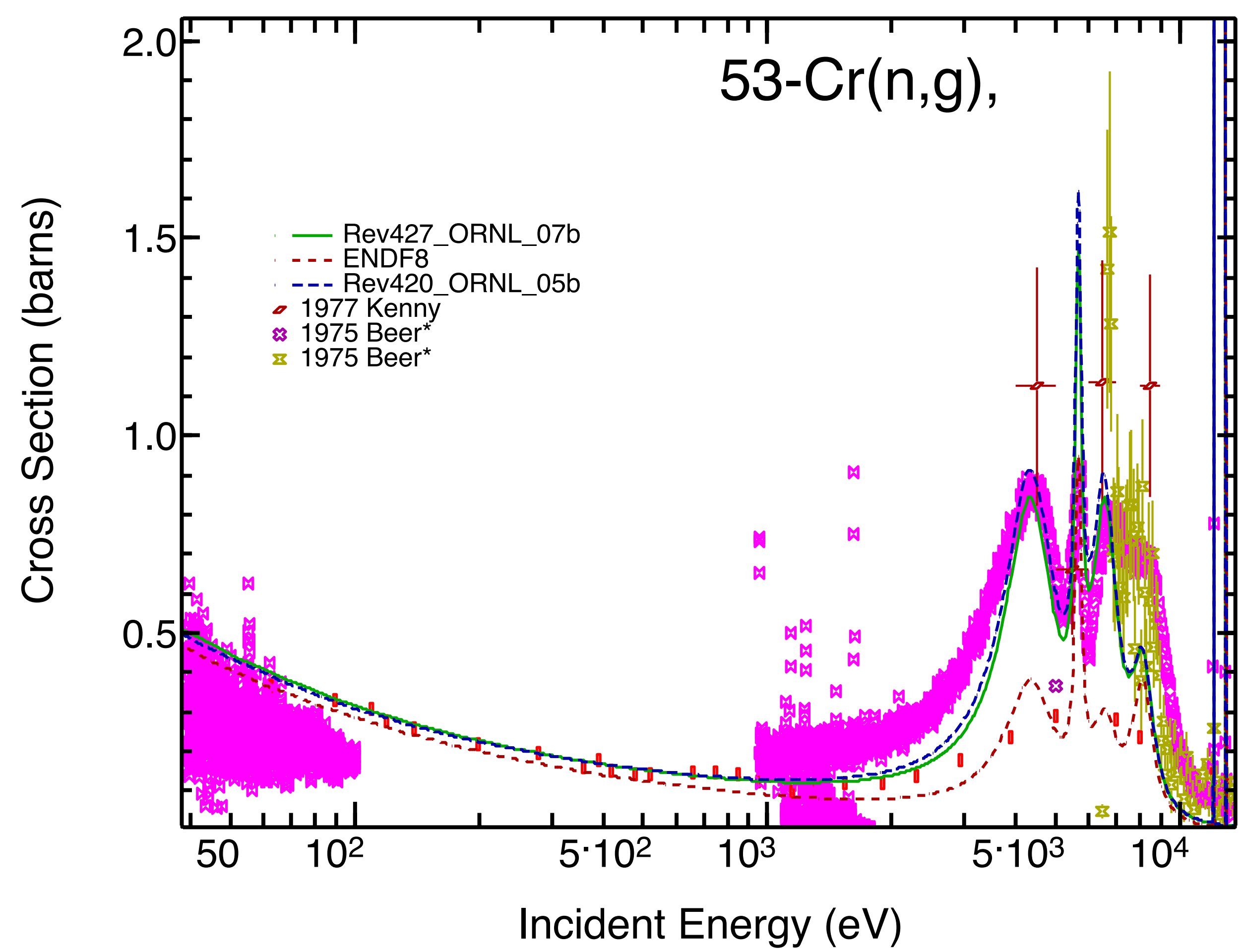
Slide from A. Hawari (SG-48 Talk)

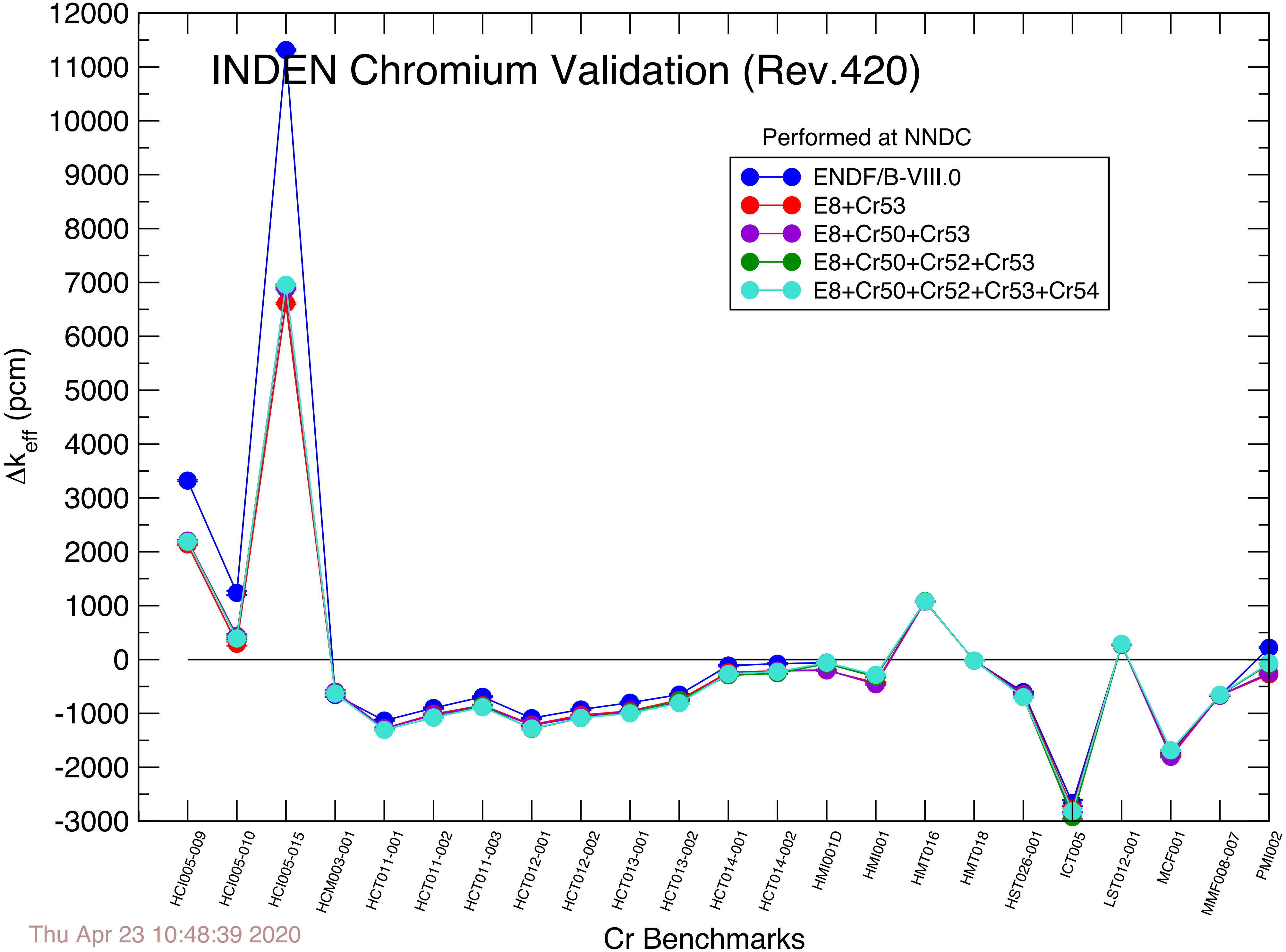
New evaluations

^{nat}Cr evaluations performance driven by similar cluster of resonances in ^{50}Cr & ^{53}Cr

- Evaluating multiple scattering corrections in legacy (Steiglitz et al.) and modern (Guber et al.) experiments (A. Cuadro)
- Added Direct+Semi-Direct from CUPIDO
- Working with M. Pigni (ORNL), R. Capote (IAEA), A. Trkov (JSI) to finalize



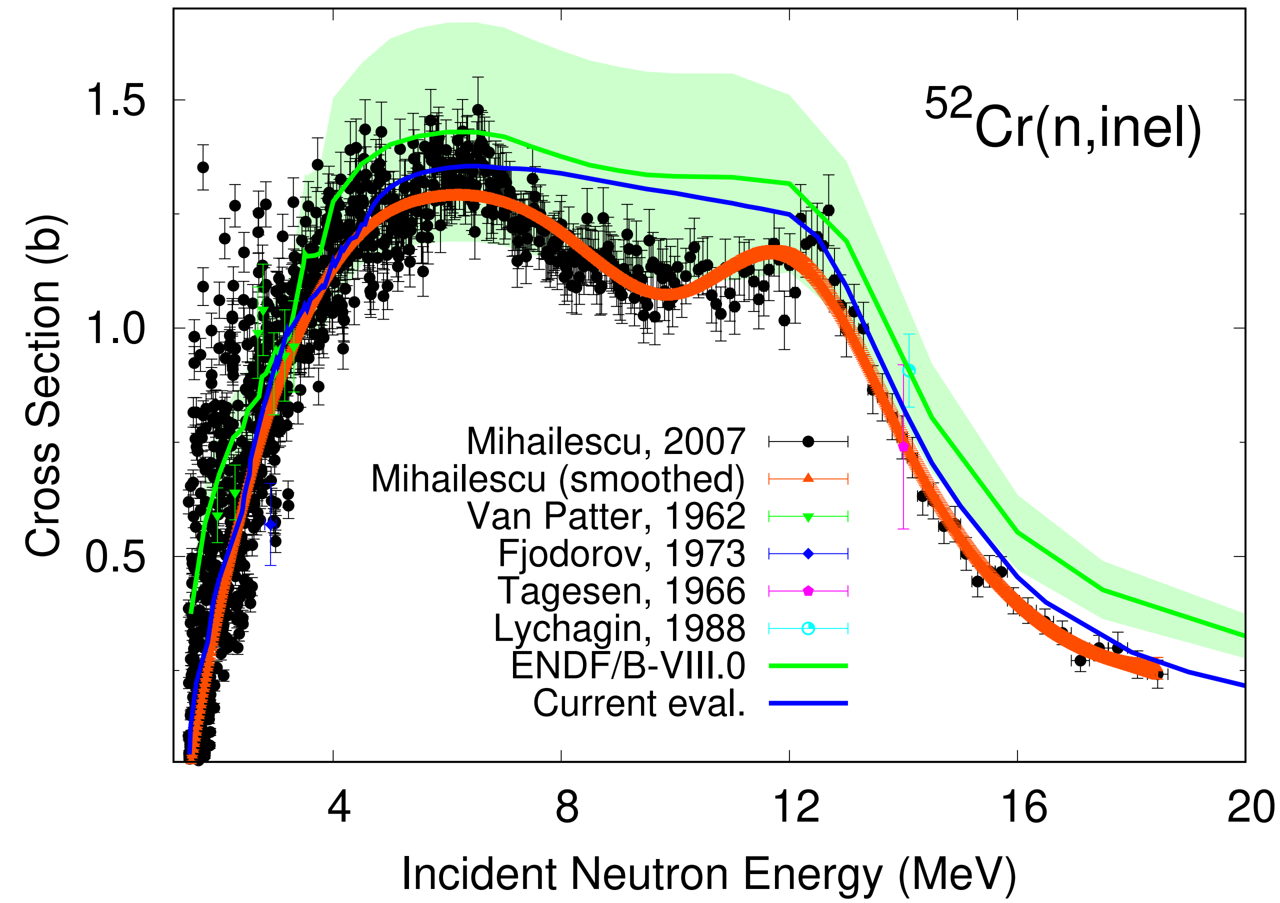


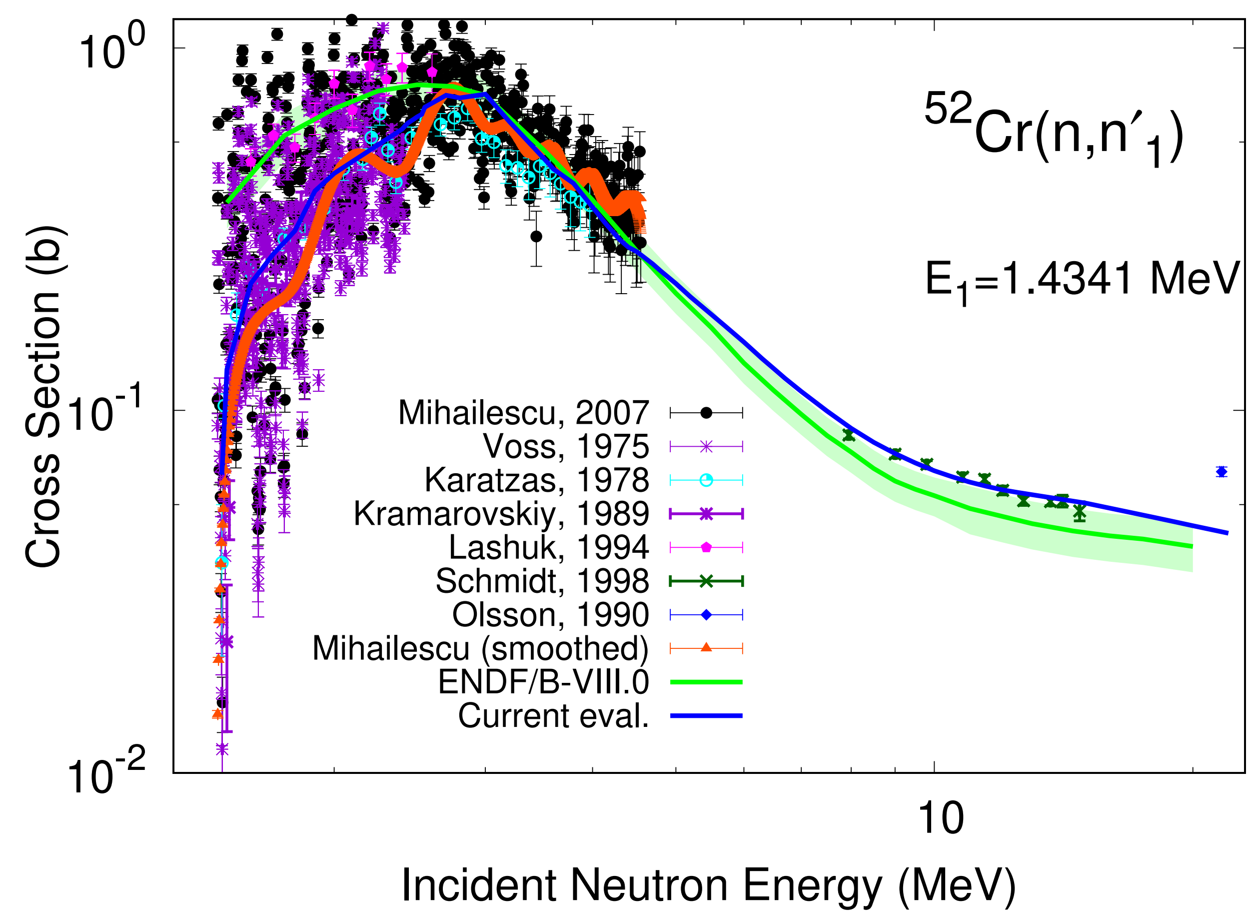


INDEN Chromium Validation (Rev.420)
Performed at NNDC
ENDF/B-VIII.0
E8+Cr53
E8+Cr50+Cr53
E8+Cr50+Cr52+Cr53
E8+Cr50+Cr52+Cr53+Cr54
Δk_{eff} (pcm)
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
HCI005-009
HCI005-010
HCI005-015
HCM003-001
HCT011-001
HCT011-002
HCT011-003
HCT012-001
HCT012-002
HCT013-001
HCT013-002
HCT014-001
HCT014-002
HMI001D
HMI001
HMT016
HMT018
HST026-001
ICT005
LST012-001
MCF001
MMF008-007
PMI002
Cr Benchmarks
Thu Apr 23 10:48:39 2020

High energy evaluations under better control

- Good (n,tot) & OMP
- Good reproduction of (n,n'g) data of Mihailescu et al.
- Match IRDFF cross sections
- Working on merging reconstructed & calculated angular distributions
- Working on correcting capture for missing resonances at RRR-Fast interface





New evaluations

LANL Light Element Evaluations

	H1	H2	H3	He3	He4	Li6	Li7
n	VIII.0	VII.1	VII.1	VII.1	VII.1	VIII.0	VII.1
p	VII.1	VII.1	VII.1	VII.1	**2020***	VII.1	2001**
d		VII.1	VII.1, 2018	VII.1	**2020**	VII.1	2003**
t			VII.1	VII.1	2011*	VII.1	--*
^{3}He				2001	2011*	VII.1	--
α					**2020***	--	--

- **Roman numerals refer to ENDF versions**
- **2011: not in ENDF/B-VIII.0**
- **2020: recent submissions “ENDF/B-VIII.b1”**

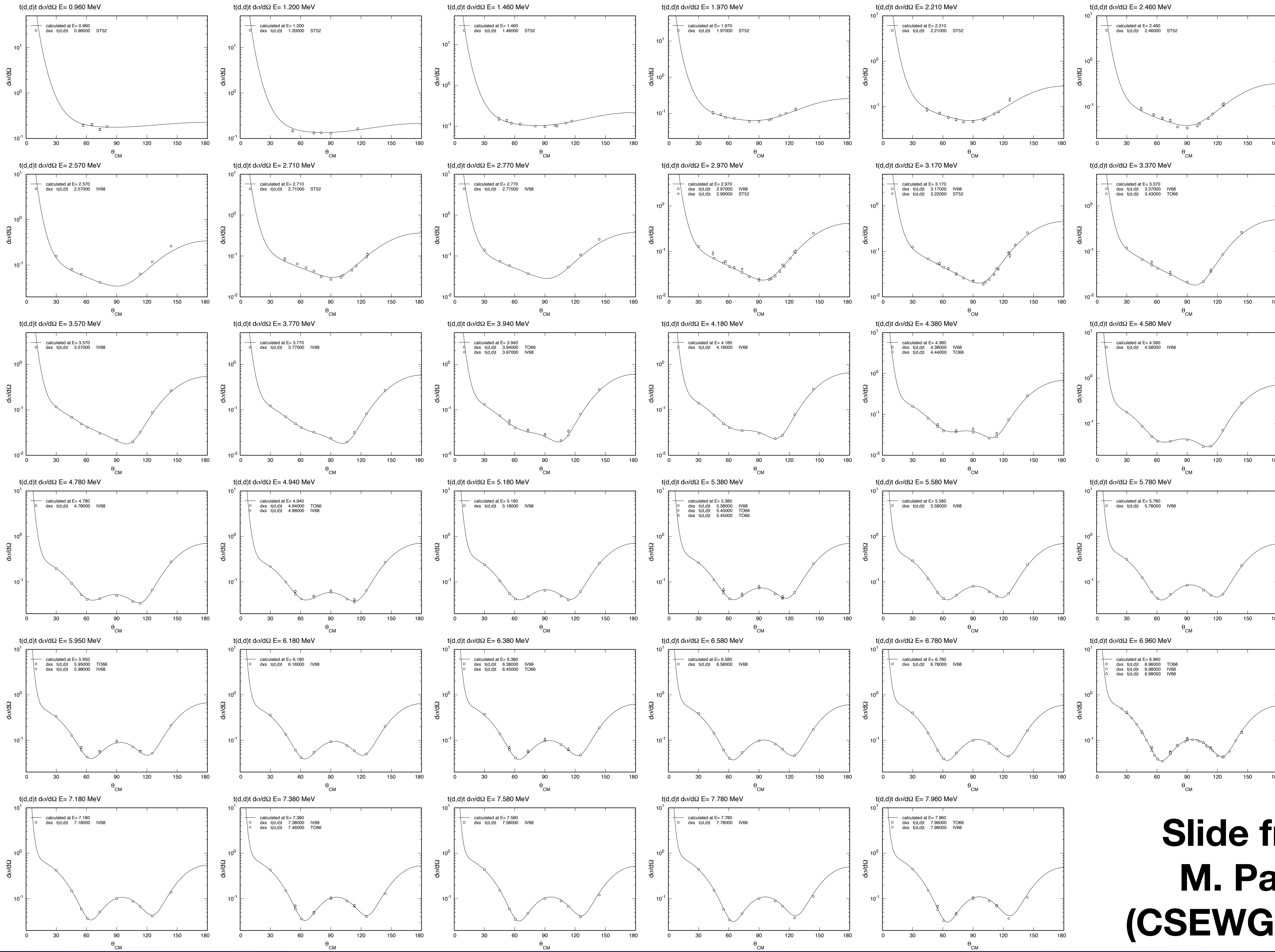
* Nuclei for which LLNL evaluations have been put into ENDF/B-VIII.0

**Nuclei for which LLNL evaluations replaced existing LANL evaluations in VIII.0

Slide from M. Paris (CSEWG 2019)

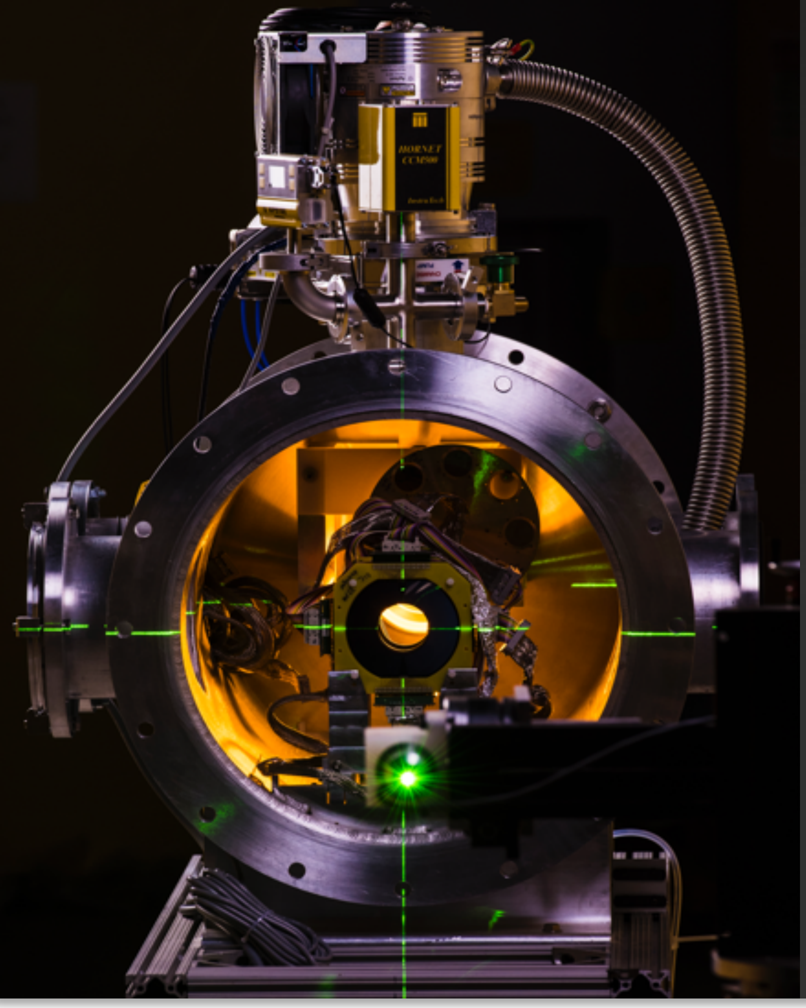
^{7}Li compound system evaluation

Angular distributions ^{4}He(t,el)



Slide from M. Paris (CSEWG 2019)

LA-UR-19-XXXXX



New Evaluation on Angular Distributions and Energy Spectra for Neutron-induced Charged particle Measurements

Korea Atomic Energy Research Institute: H.I. Kim
Theory Division (T-2): T. Kawano, M. Herman

Physics Division (P-27): H.Y. Lee, L. Zavorka, S. Kuvin, A. Georgiadou

postdocs , guest scientists

Slide from H. Y. Lee (CSEWG 2019)

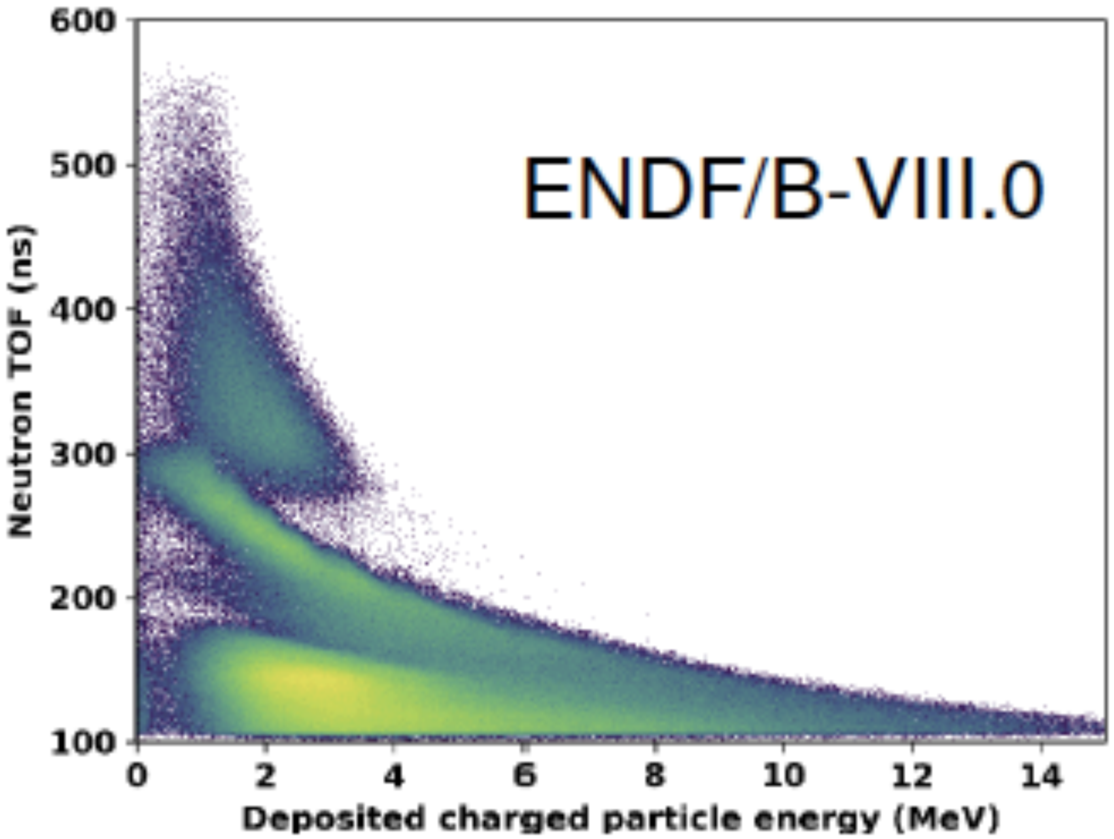
Newly updated Nuclei

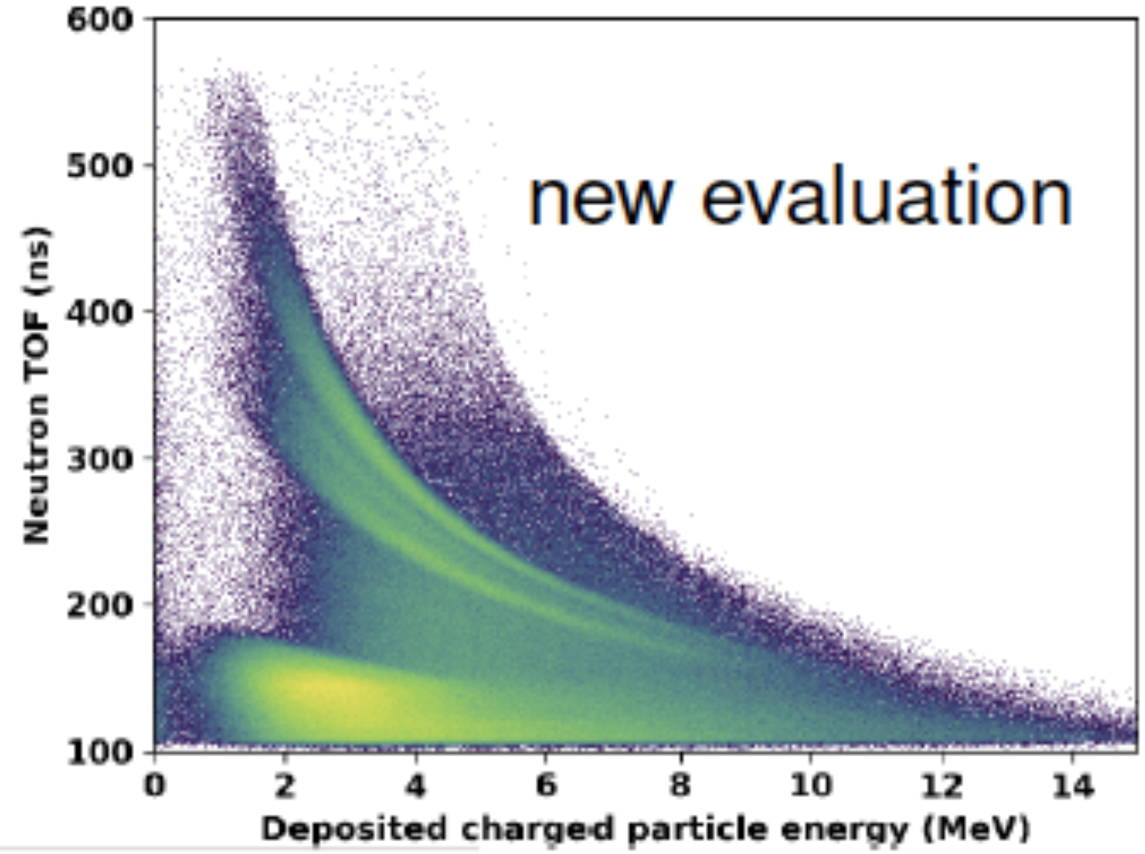
Numbers of discrete levels in the residual nuclei included to calculate (n,p) and (n,α) reaction cross sections. The numbers in parenthesis present the number of discrete levels given in ENDF/B-VIII.0, where '0' stands for no partical cross section given in the evaluation.

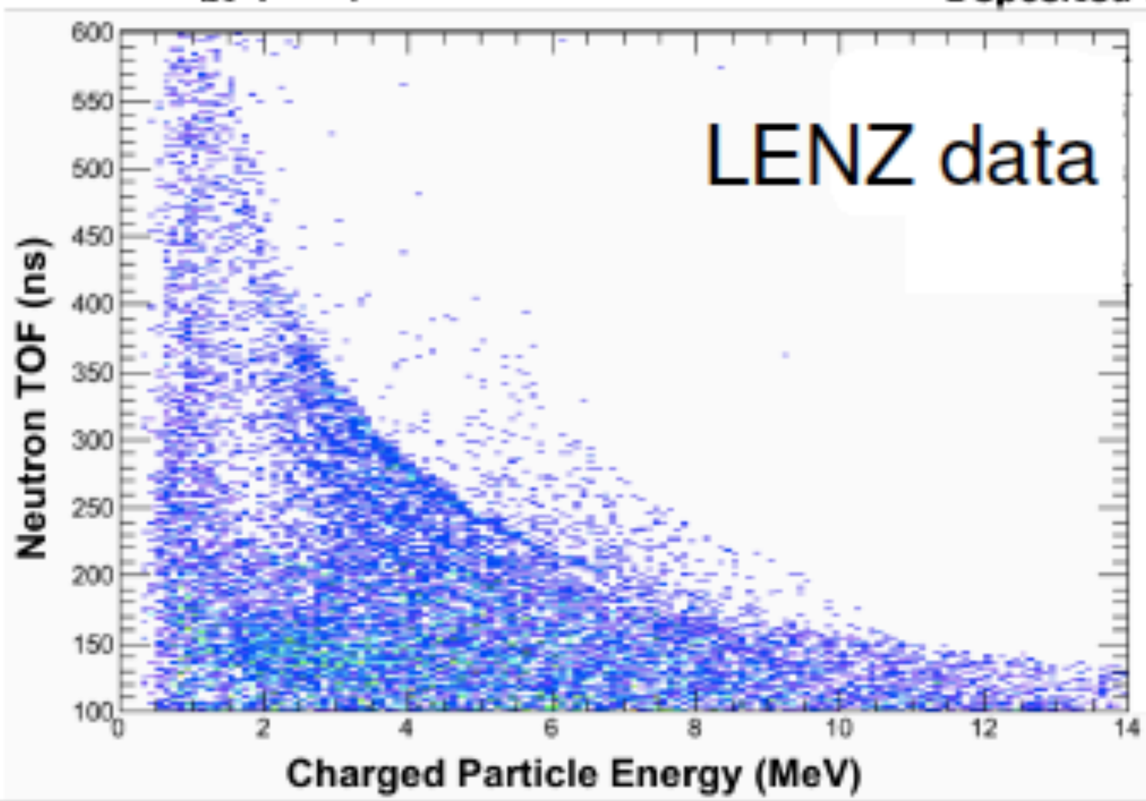
Target	p	α	Target	p	α	Target	p	α
^{27}Al	20 (20)	20 (20)	^{50}Cr	10 (0)	10 (0)	^{64}Zn	10 (0)	10 (0)
^{28}Si	14 (14)	16 (16)	^{51}Cr	10 (0)	10 (0)	^{65}Zn	10 (0)	10 (0)
^{29}Si	16 (16)	20 (20)	^{52}Cr	10 (0)	10 (0)	^{66}Zn	10 (0)	10 (0)
^{30}Si	6 (6)	12 (12)	^{53}Cr	10 (0)	10 (0)	^{67}Zn	10 (0)	10 (0)
^{31}Si	1 (1)	15 (15)	^{54}Cr	10 (0)	10 (0)	^{68}Zn	8 (0)	10 (0)
^{32}Si	1 (1)	1 (1)	^{54}Fe	34 (34)	24 (24)	^{69}Zn	17 (17)	18 (18)
^{35}Cl	30 (30)	21 (21)	^{56}Fe	10 (10)	19 (19)	^{70}Zn	1 (0)	1 (0)
^{36}Cl	16 (16)	32 (32)	^{57}Fe	18 (18)	39 (39)	^{73}As	10 (0)	10 (0)
^{37}Cl	10 (0)	6 (6)	^{58}Fe	17 (17)	10 (10)	^{74}As	10 (0)	10 (0)
^{39}K	10 (0)	10 (0)	^{58}Ni	10 (0)	10 (0)	^{90}Zr	12 (12)	9 (9)
^{40}K	10 (0)	10 (0)	^{59}Ni	10 (0)	10 (0)	^{91}Zr	6 (6)	40 (40)
^{41}K	10 (0)	10 (0)	^{60}Ni	10 (0)	10 (0)	^{92}Zr	1 (1)	40 (40)
^{46}Ti	10 (0)	10 (0)	^{61}Ni	10 (0)	10 (0)	^{93}Zr	17 (17)	27 (27)
^{47}Ti	10 (0)	10 (0)	^{62}Ni	10 (0)	10 (0)	^{94}Zr	10 (10)	40 (40)
^{48}Ti	10 (0)	10 (0)	^{63}Ni	26 (26)	28 (28)	^{95}Zr	16 (16)	9 (9)
^{49}Ti	10 (0)	10 (0)	^{64}Ni	10 (0)	1 (0)	^{96}Zr	3 (3)	10 (10)
^{50}Ti	9 (0)	10 (0)	^{58}Co	40 (40)	40 (40)	^{107}Ag	10 (0)	10 (0)
^{49}V	40 (40)	40 (40)	^{59}Co	10 (0)	10 (0)	^{109}Ag	31 (31)	2 (2)
^{50}V	10 (0)	10 (0)	^{63}Cu	10 (0)	10 (0)	^{180}Ta	10 (0)	10 (0)
^{51}V	10 (0)	10 (0)	^{64}Cu	40 (40)	40 (40)	^{181}Ta	10 (0)	10 (0)
			^{65}Cu	10 (0)	10 (0)	^{197}Au	10 (0)	10 (0)

Slide from H. Y. Lee (CSEWG 2019)

Comparison with experimental data (Brass target: 65 % ^{nat}Cu + 35 % ^{nat}Zn)

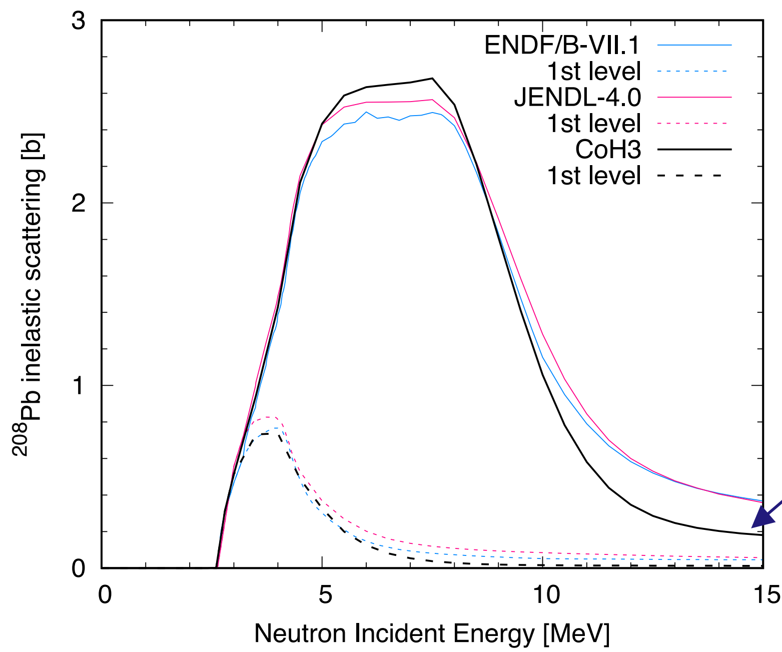






Slide from H. Y. Lee (CSEWG 2019)

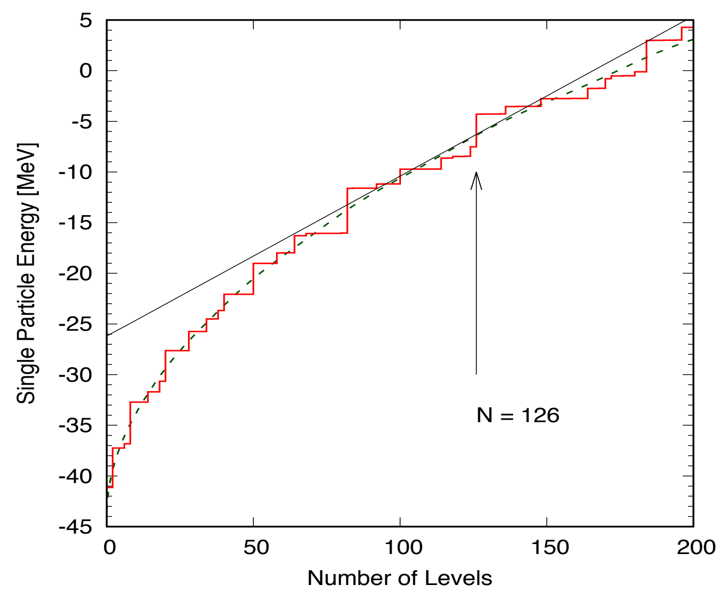
CoH_3 New Evaluation of ^{208}Pb, (n,n'), (n,2n), and (n,3n)

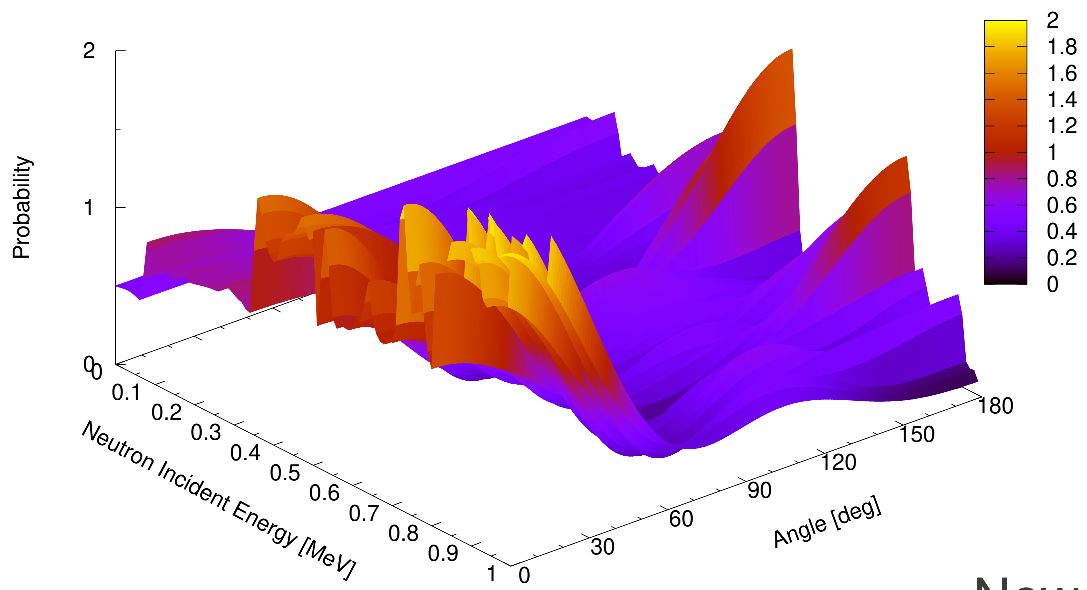


Pre-equilibrium estimated by the single-particle model based on FRDM

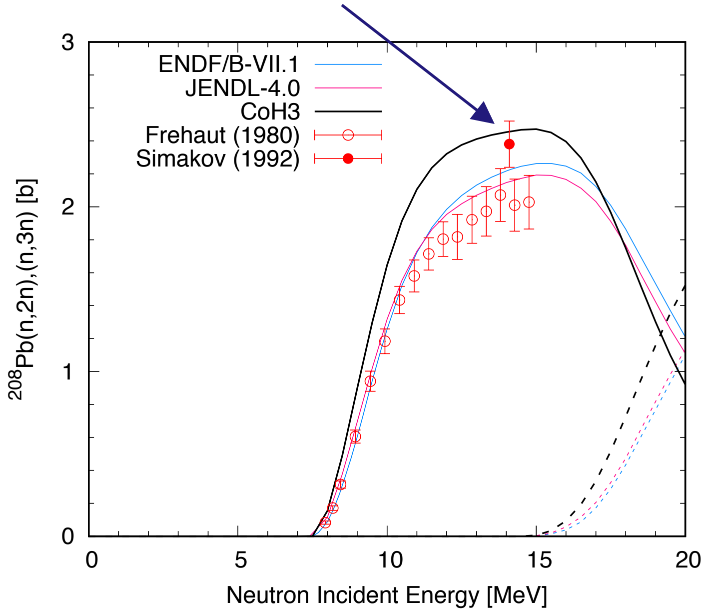
Strutinsky shell correction predicts lower single-particle level density

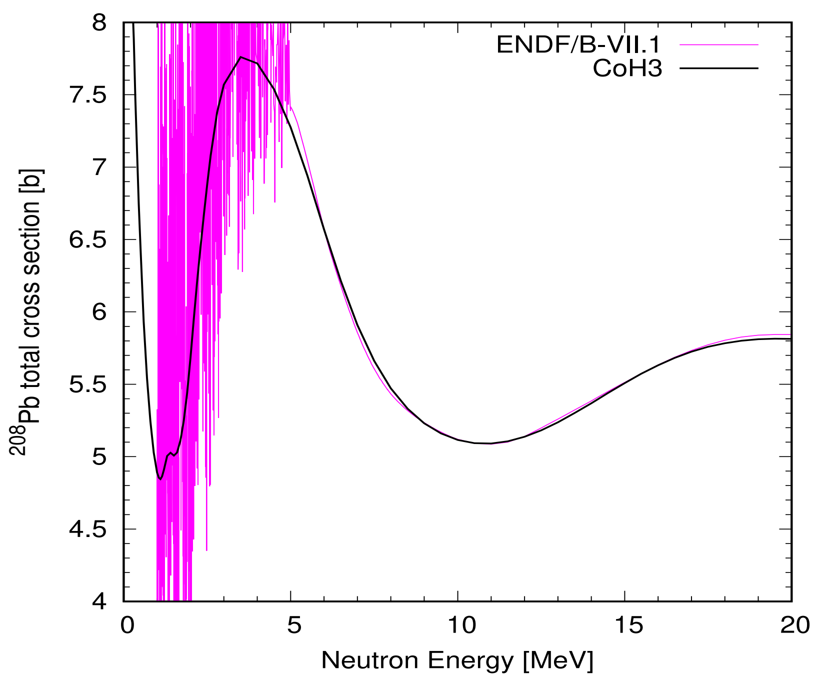
- lowers the pre-equilibrium emission
- increase (n,2n)





Angular distributions





- New evaluation better agrees Simakov data
- Need to re-investigate if Frehaut data should be renormalized

Slide from I. Stetcu (CSEWG 2019)

New evaluations

NAVAL NUCLEAR LABORATORY

Naval Nuclear Laboratory
Special Purpose O-17, O-18, Be-9 (α,n) Evaluations

Jesse Holmes
Andrew Pavlou
Jason Thompson
Mike Zerkle

Cross Section Evaluation Working Group

Brookhaven National Laboratory

November 5-7, 2018

The Naval Nuclear Laboratory is operated for the U.S. Department of Energy by
Fluor Marine Propulsion (FMP), LLC, a wholly owned subsidiary of Fluor Corporation.

NAVAL NUCLEAR LABORATORY

Problems with Kalbach-Mann Systematics

- O-17 and O-18 use Kalbach-Mann systematics for File 6 coupled energy/angle distributions for MT=4 (production of one neutron in the exit channel).

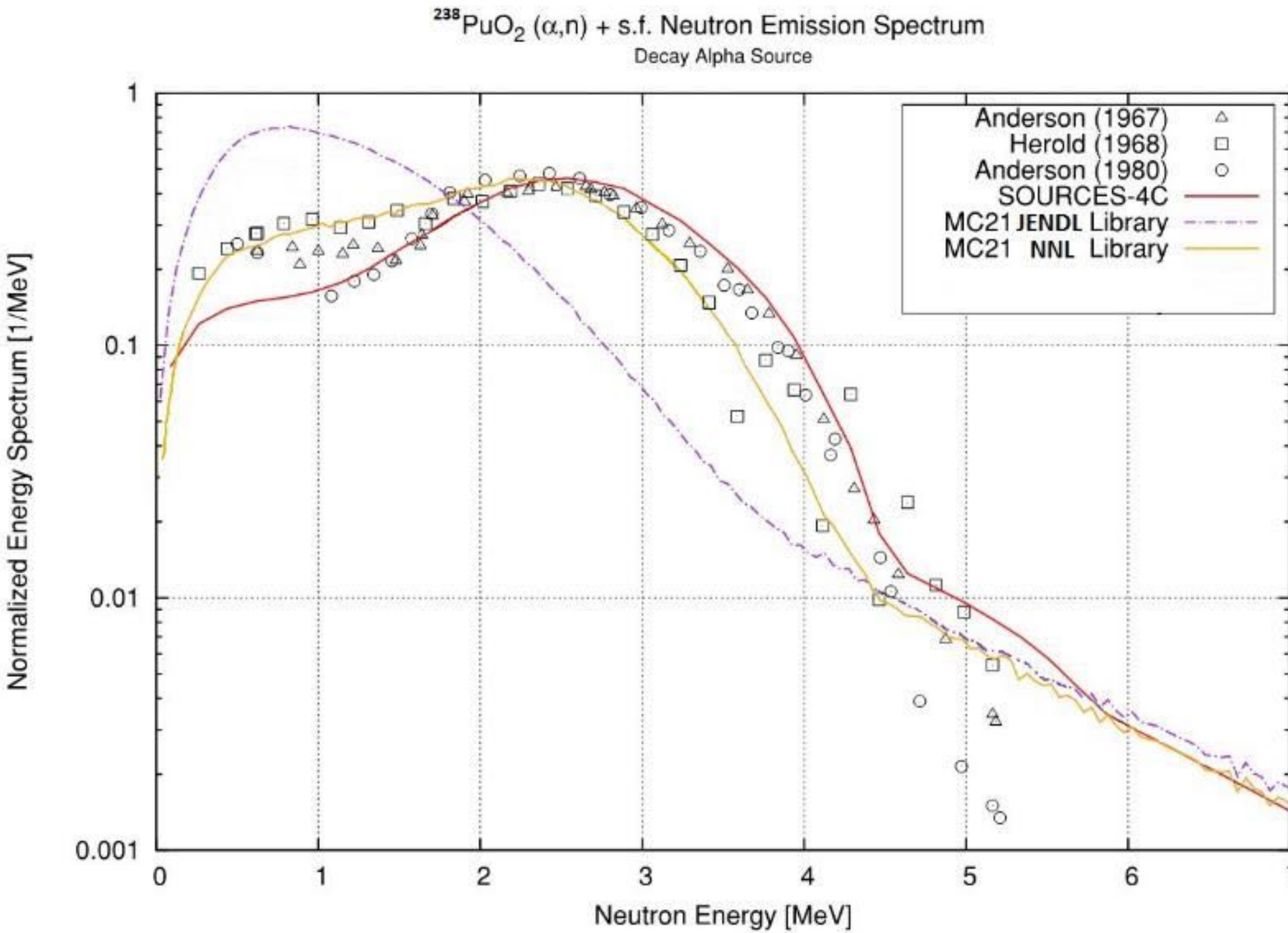
- Energy/angle distributions based on Kalbach-Mann systematics are decoupled from the partial cross sections for reactions leaving the residual in the ground state or particular low-level excited states.

- The Q-values of low-level n^{th} excited-state reactions (including the 0^{th} ground-state) are widely separated and strongly impact the emitted neutron energy spectrum for reactions induced by low-energy α particles.

- Kalbach-Mann theory for (α,n) neutron energy/angle distributions is appropriate for very-high-energy incident α particles (tens to hundreds of MeV), where high-level residual excited states (or a continuum excited state) dominate.
  - Not appropriate for low-energy α particles emitted by actinide decay (approx. 4-7 MeV), which will then undergo slowing down in materials of interest.

NAVAL NUCLEAR LABORATORY

Slide from J. Holmes (CSEWG 2018)



Slide from J. Holmes (CSEWG 2018)

NAVAL NUCLEAR LABORATORY

Summary

- NNL-modified special-purpose (α,n) evaluations for O-17, O-18, and Be-9 are being submitted for inclusion in ENDF/B-VIII.1.

- These evaluations are based on the original JENDL/AN-2005 evaluations with specific modifications by NNL to address physics deficiencies affecting neutron energy spectra. The NNL versions have been validated against experimental measurements.

- Other JENDL/AN-2005 (α,n) evaluations were tested by NNL. These are not being submitted by NNL as no modifications were made.

- For O-17, MF=3 cross sections are unchanged. MF=6 / MT=4 (using Kalbach-Mann) is removed and replaced with MF=6 / MT=50-53 (using isotropic two-body kinematics) and MF=6 / MT=91 (using original MF=6 / MT=4 Kalbach-Mann distribution). MF=6 / MT=22 is unchanged.

- For O-18, MF=3 cross sections are unchanged. MF=6 / MT=4 (using Kalbach-Mann) is removed and replaced with MF=6 / MT=50-54 (using isotropic two-body kinematics) and MF=6 / MT=91 (using original MF=6 / MT=4 Kalbach-Mann distribution). MF=6 / MT=16,22 are unchanged.

- For Be-9, MF=3 / MT=4,22 are modified to give ratios consistent with Geiger (1975). MF=3 / MT=201 is unchanged. MF=3 / MT=50-52,91 ratios are unchanged, but values are rescaled to be consistent with modifications to MF=3 / MT=4. MF=6 distributions are unchanged.

NAVAL NUCLEAR LABORATORY

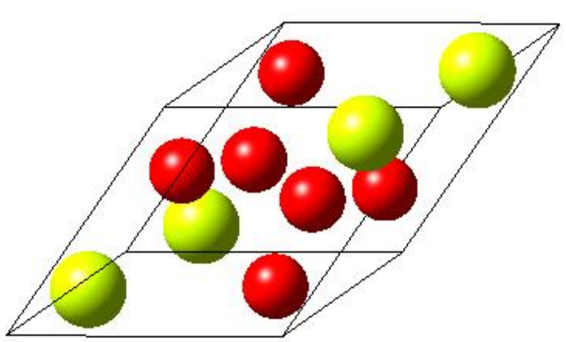
Slide from J. Holmes (CSEWG 2018)

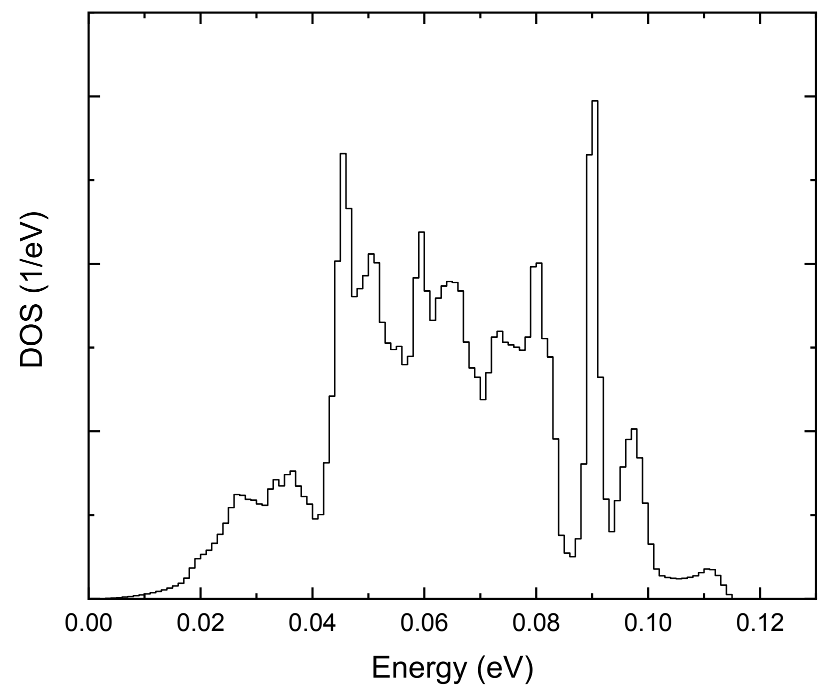
New evaluations

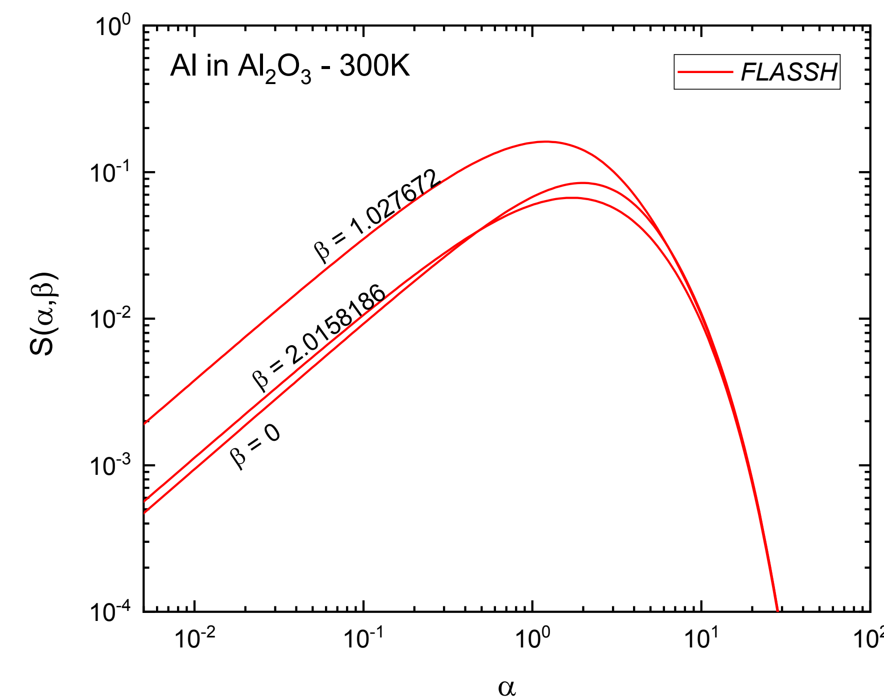
New to NNDC

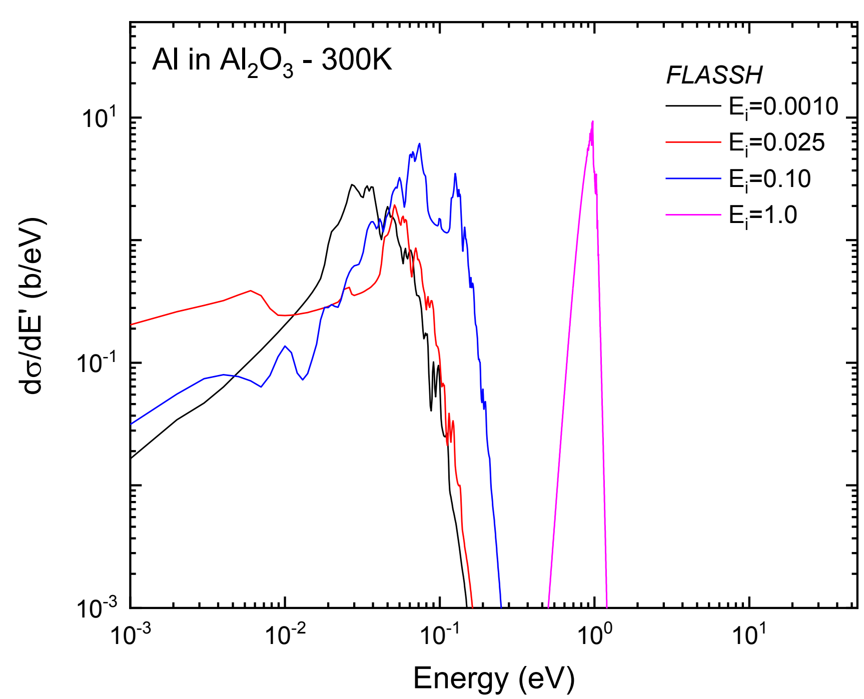
Single Crystal Sapphire TSL Data

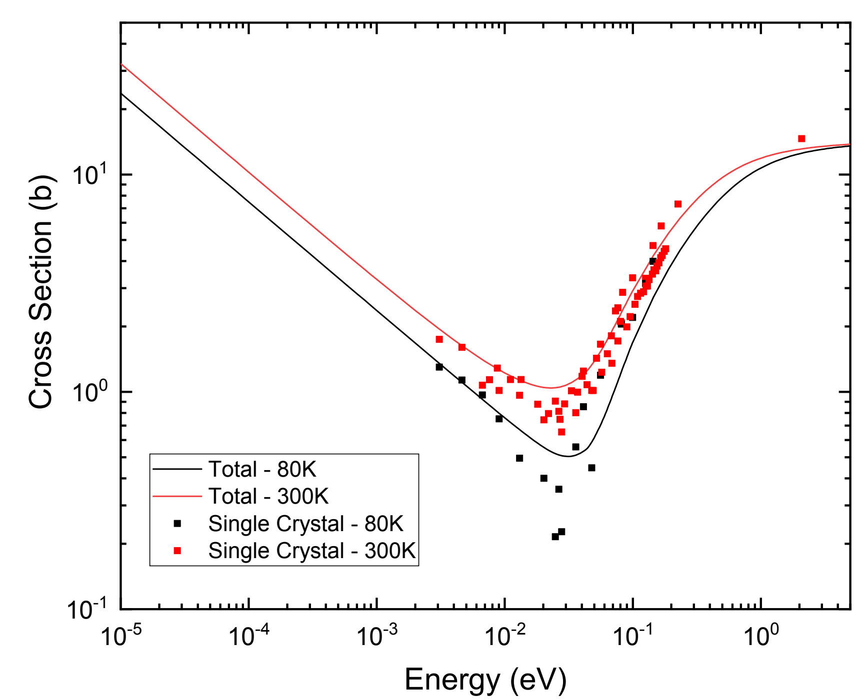
- *Ab initio* lattice dynamics
  - Predictive density of states (DOS)
  - Rhombohdral structure
  - 2x2x2 supercell
  - GGA-PBE







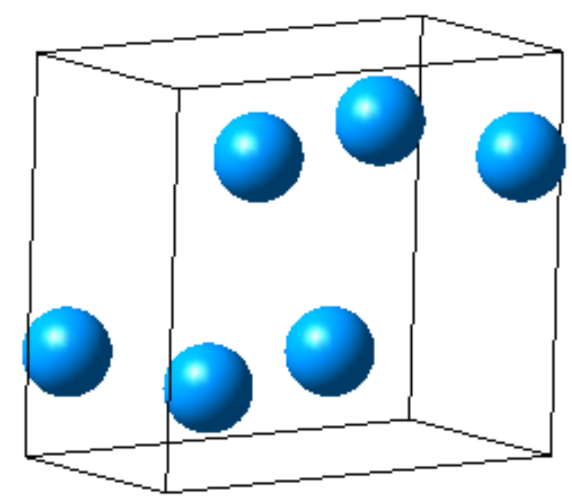




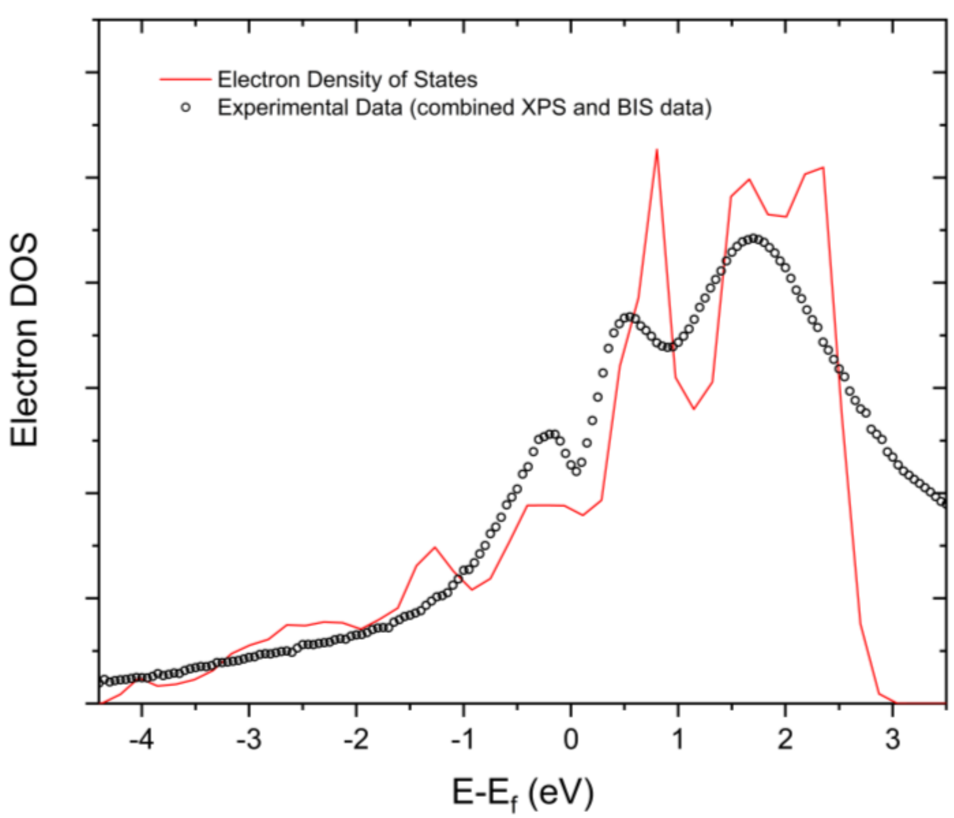
Slide from A. Hawari (SG-48 Talk)

Uranium Metal

- α-Uranium Metal
  - Stable up to 668ºC
- *Ab initio* lattice dynamics
  - DFT – GGA-PBE plus an effective Coulomb term (+U) of 1eV for the *5f* electrons plus spin-orbit coupling



- Orthorhombic structure
- 550 eV plane wave cutoff
- 12x12x7 k-mesh



	Experiment (4.2 K)	Calculated	Diff. (%)
a (Å)	2.8444	2.8565	0.42
b (Å)	5.8689	5.8706	0.03
c (Å)	4.9316	4.9834	1.05

Slide from A. Hawari (SG-48 Talk)

Other evaluations

- FLiBe (reported WPEC 30)
- Heavy Paraffinic Oil (reported WPEC 30)
- Hydrofluoric Acid (pending)

New evaluations

Oak Ridge National Laboratory

TSL Covariance - Overview

- Goal was to develop a procedure to generate covariance matrix for $S(\alpha, \beta)$ data that incorporated both computational simulations and experimental data
- Experimental data and computer simulation fit is achieved using the Unified Monte Carlo (UMC) method [1]
- Framework is material & simulation method independent
- Demonstrated using light water

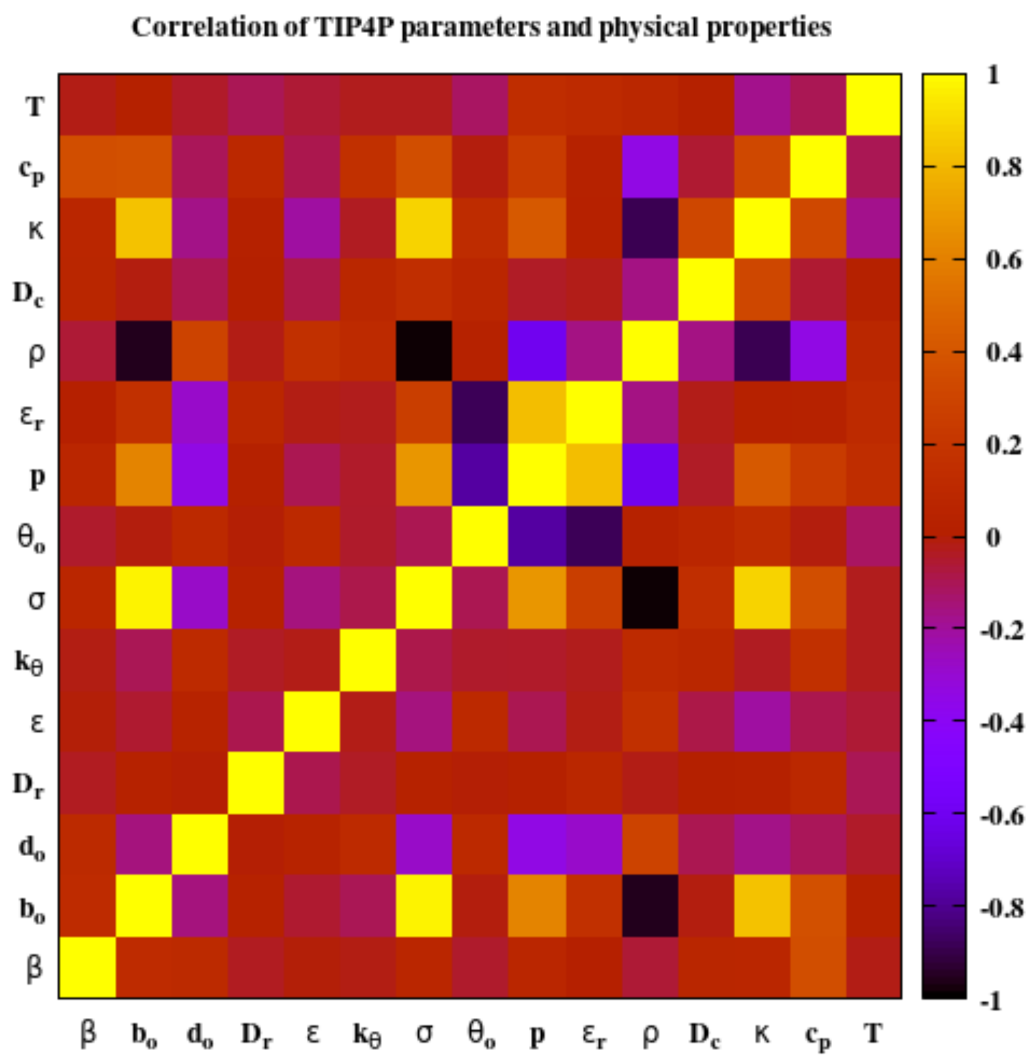
Slide from C. Chapman (CSEWG 2019)

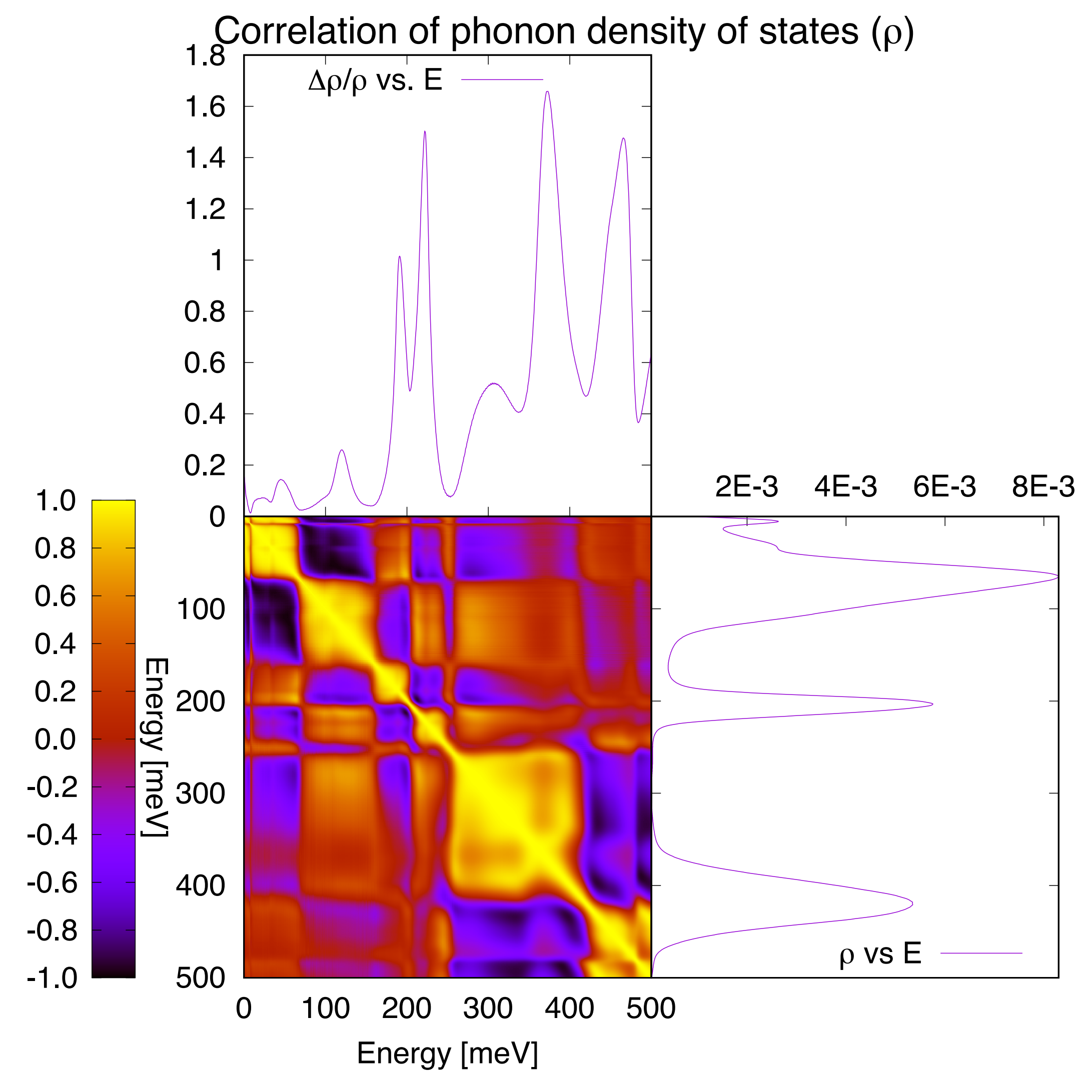
TSL Covariance - UMC

- UMC weights then used to calculate mean values and covariance matrices of:
  - TIP4P/2005f parameters
  - Thermophysical properties
  - pDOS
  - Double differential & total scattering cross section
- Mean values and variance of thermal scattering law $S(\alpha, \beta)$ also generated
  - Methods of storing $S(\alpha, \beta)$ covariance matrix not studied here

Slide from C. Chapman (CSEWG 2019)

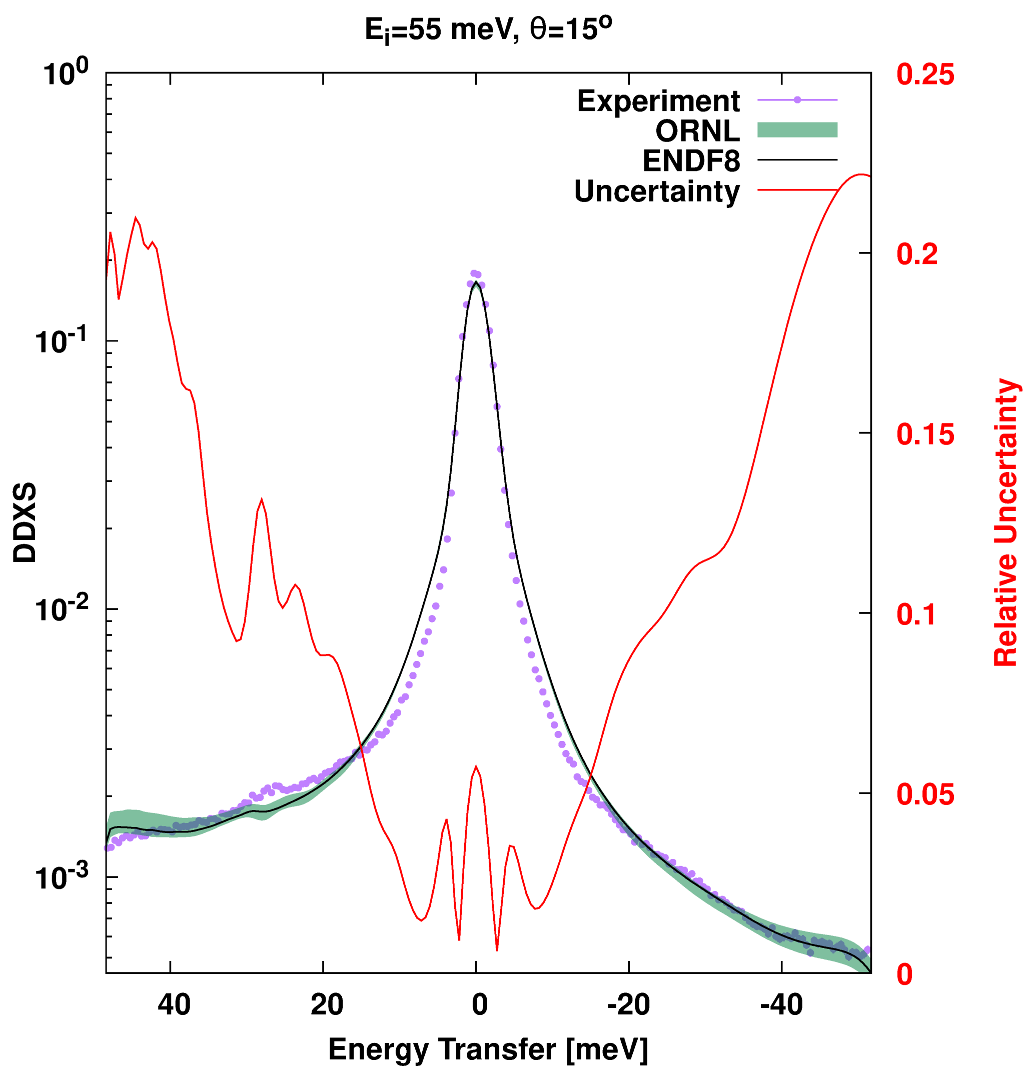
TSL Covariance - Correlation Matrices

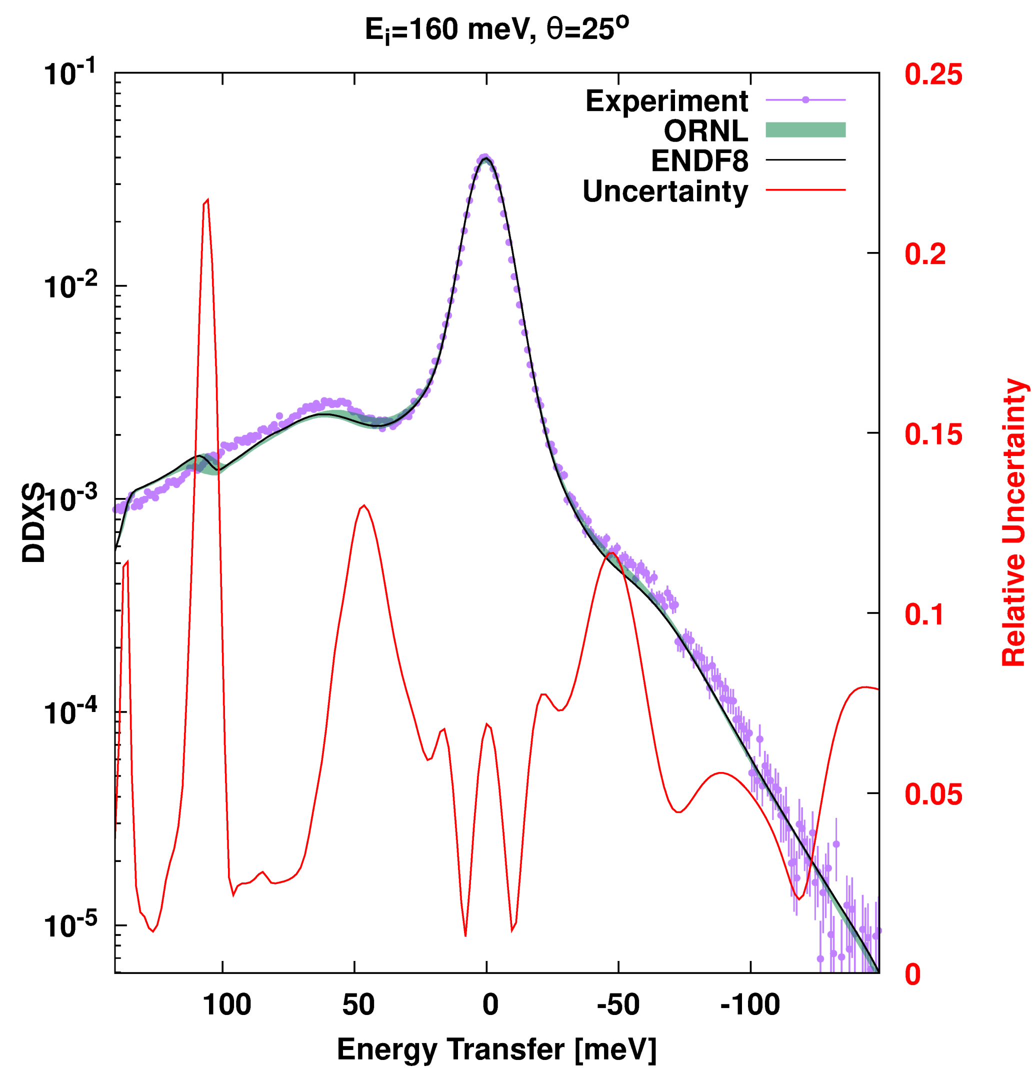




Slide from C. Chapman (CSEWG 2019)

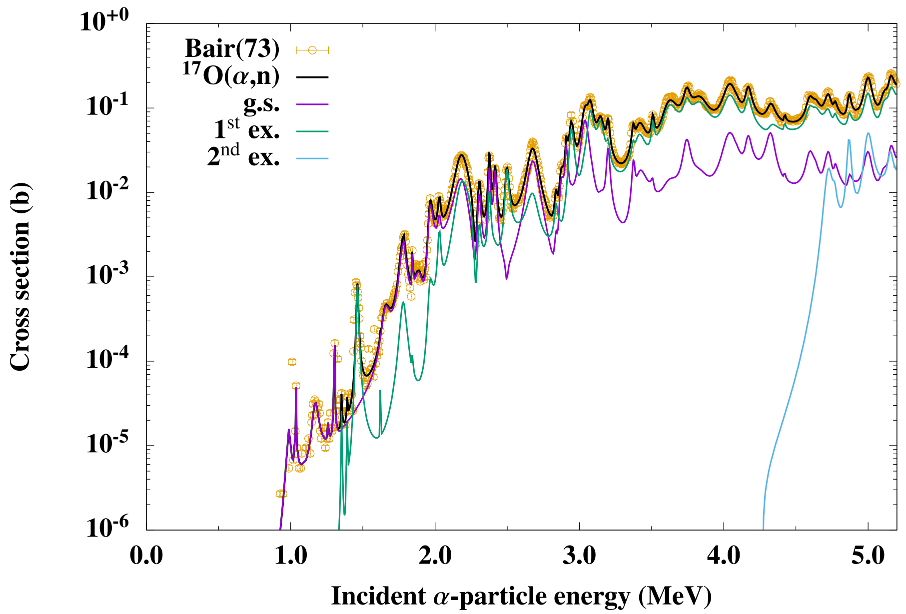
TSL Covariance - DDXS

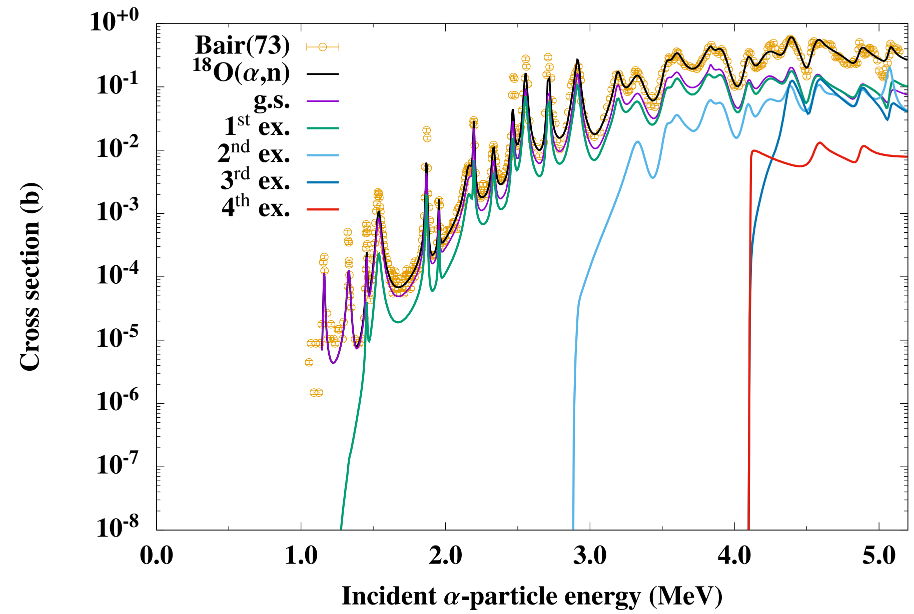


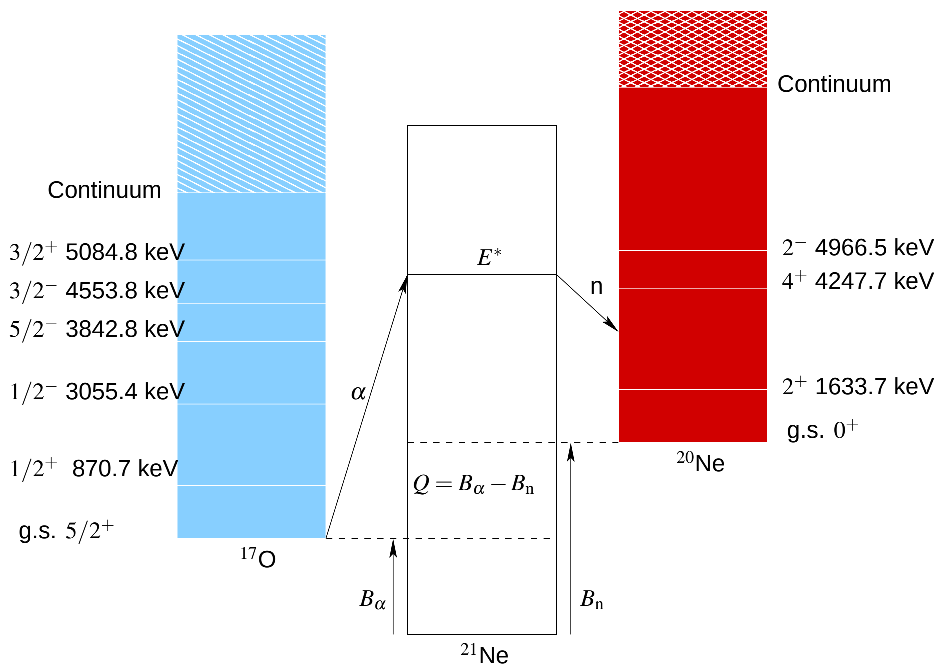


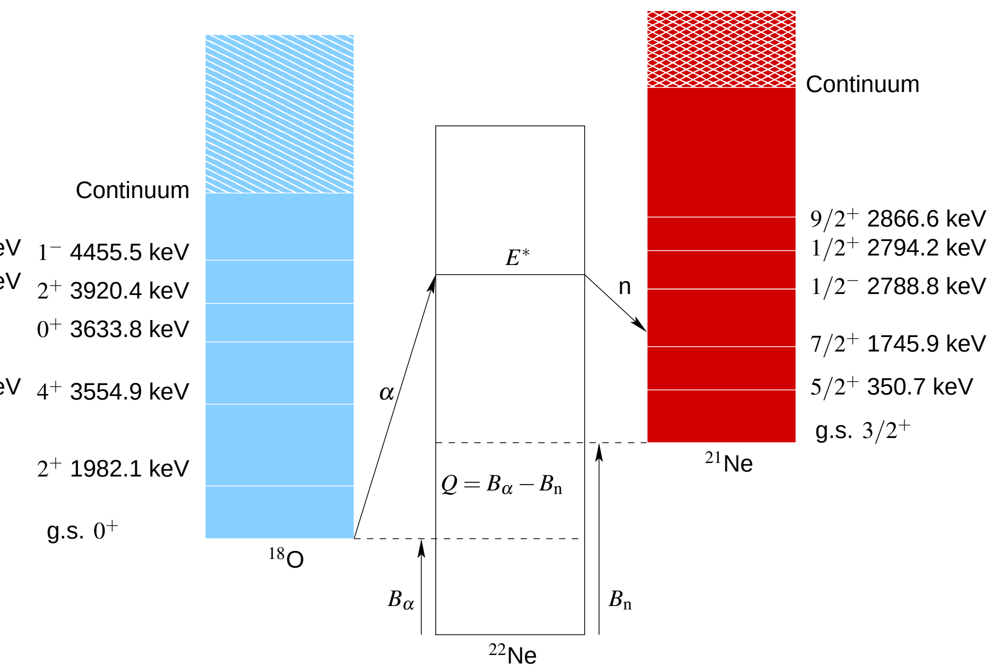
Slide from C. Chapman (CSEWG 2019)

α+^{17,18}O Partial Cross Sections









Slide from Marco Pigni (CSEWG 2019)

New evaluations

Rensselaer

Polyethylene, Lucite, Ice 1h by K. Remic using results from VISION, ARCS, and SEQUOIA @SNS

Annals of Nuclear Energy 120 (2018) 778–787

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Thermal scattering law of $(C_2H_4)_n$: Integrating experimental data with DFT calculations

Kemal Ramić [a,*], Carl Wendorff [a], Yongqiang Cheng [b], Alexander I. Kolesnikov [b], Doug L. Abernathy [b], Luke Daemen [b], Goran Arbanas [b], Luiz Leal [c], Yaron Danon [a], Li (Emily) Liu [a]

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ABSTRACT

Improvements in determination of the thermal scattering law of moderator materials (measuring, calculating and validating) are important for accurate prediction of neutron thermalization in nuclear systems. In this work a methodology for producing thermal scattering libraries from the experimental data for polyethylene $(C_2H_4)_n$ is discussed. Double differential scattering cross section (DDSCS) experiments were performed at the Spallation Neutron Source of Oak Ridge National Laboratory (SNS ORNL). New scattering kernel evaluations, based on phonon spectrum for $(C_2H_4)_n$, are created using the NJOY2016 code. Two different methods were used: direct and indirect geometry neutron scattering at ARCS and SEQUOIA, and VISION instruments, respectively, where the phonon spectrum was derived from the dynamical structure factor $S(Q,\omega)$ obtained from the measured DDSCS. In order to compare and validate the newly created library, the experimental setup was simulated using MCNP6.1. Compared with the current ENDF/B-VII.1, the resulting RPI $(C_2H_4)_n$ libraries improved both double differential scattering and total scattering cross sections. A set of criticality benchmarks containing $(C_2H_4)_n$ from HEU-MET-THERM resulted in an overall improved calculation of K_{eff}, although the libraries should be tested against benchmarks more sensitive to $(C_2H_4)_n$. The DFT + oClimax method is used and is shown to be most comprehensive method for analysis of moderator materials. The importance of DFT + oClimax method lies in the fact that it can be validated against all data measured at VISION, ARCS and SEQUOIA, and experimental total scattering cross section measurements.

1. Introduction

As the accuracy of simulations advances in many areas of nuclear science, code packages such as the Monte Carlo N-Particle code (MCNP), Goorley et al. (2016), are highly dependent on the accuracy of current Evaluated Nuclear Data Files (for example ENDF/B-VII.1), Chadwick et al. (2996). These evaluated libraries contain different nuclear reaction data, and most relevant for this work, these libraries contain thermal neutron scattering cross sec-

For most moderators, the current ENDF/B-VII.1 libraries were created using a theoretical phonon spectrum (or density of states). The ENDF/B-VII.1 library for polyethylene was created by Koppel, Houston and Sprevak in 1969 and was converted to ENDF 6 format in 1989 at Los Alamos National Lab. In 2016 new polyethylene library, using molecular dynamics to calculate the phonon spectrum, created by North Carolina State University Nuclear Reactor Program has been added to ENDF as ENDF/B-VIII.b5 library. These libraries were created to correctly reproduce the energy dependent

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Toward a better thermal scattering law of $(C_5O_2H_8)_n$: Inelastic neutron scattering and oClimax + NJOY2016

Kemal Ramić [a,*], Carl Wendorff [a], Yongqiang Cheng [b], Alexander I. Kolesnikov [b], Doug L. Abernathy [b], Luke Daemen [b], Goran Arbanas [b], Luiz Leal [c], Yaron Danon [a], Li (Emily) Liu [a]

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Lucite
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Density function theory
oClimax
VISION spectrometer
ARCS spectrometer
Specific heat capacity
Thermal conductivity

ABSTRACT

With the advancements in technology (both experimental and computational) the determination of the"true" experimental phonon spectrum became more accessible. In this work a methodology for producing thermal scattering libraries from the experimental data (namely the DFT + oClimax method) for lucite $(C_5O_2H_8)_n$ is discussed. Double differential scattering cross section (DDSCS) experiments were performed at the Spallation Neutron Source of Oak Ridge National Laboratory (SNS ORNL). New scattering kernel evaluations, based on the phonon spectrum for $(C_5O_2H_8)_n$,were created using oClimax and NJOY2016 codes. In order to compare and asses the performance of the newly created library, the experimental setup was simulated using MCNP6.1. Compared to the current ENDF/B-VIII.0, the resulting RPI $(C_5O_2H_8)_n$ library improved the calculation of both double differential scattering and total scattering cross sections. A set of criticality benchmarks containing $(C_5O_2H_8)_n$ from HEU-MET-THERM resulted in an overall improved calculation of K_{eff}. The DFT + oClimax method is shown to be the most comprehensive method for analysis of moderator materials, due to the fact that it can be verified against all data measured at VISION, ARCS and SEQUOIA neutron spectrometers at SNS ORNL, and experimental total scattering cross section measurements. This method also provides a new technique for calculating any phonon spectrum-related quantities such as scattering law kernel, specific heat capacity, thermal conductivity, etc. for any solid state material.

1. Introduction

Historically the thermal scattering law (TSL) libraries, as part of Evaluated Nuclear Data Files (for example ENDF/B-VII.1) Chadwick et al. (2011), have been generated either from theoretically com-

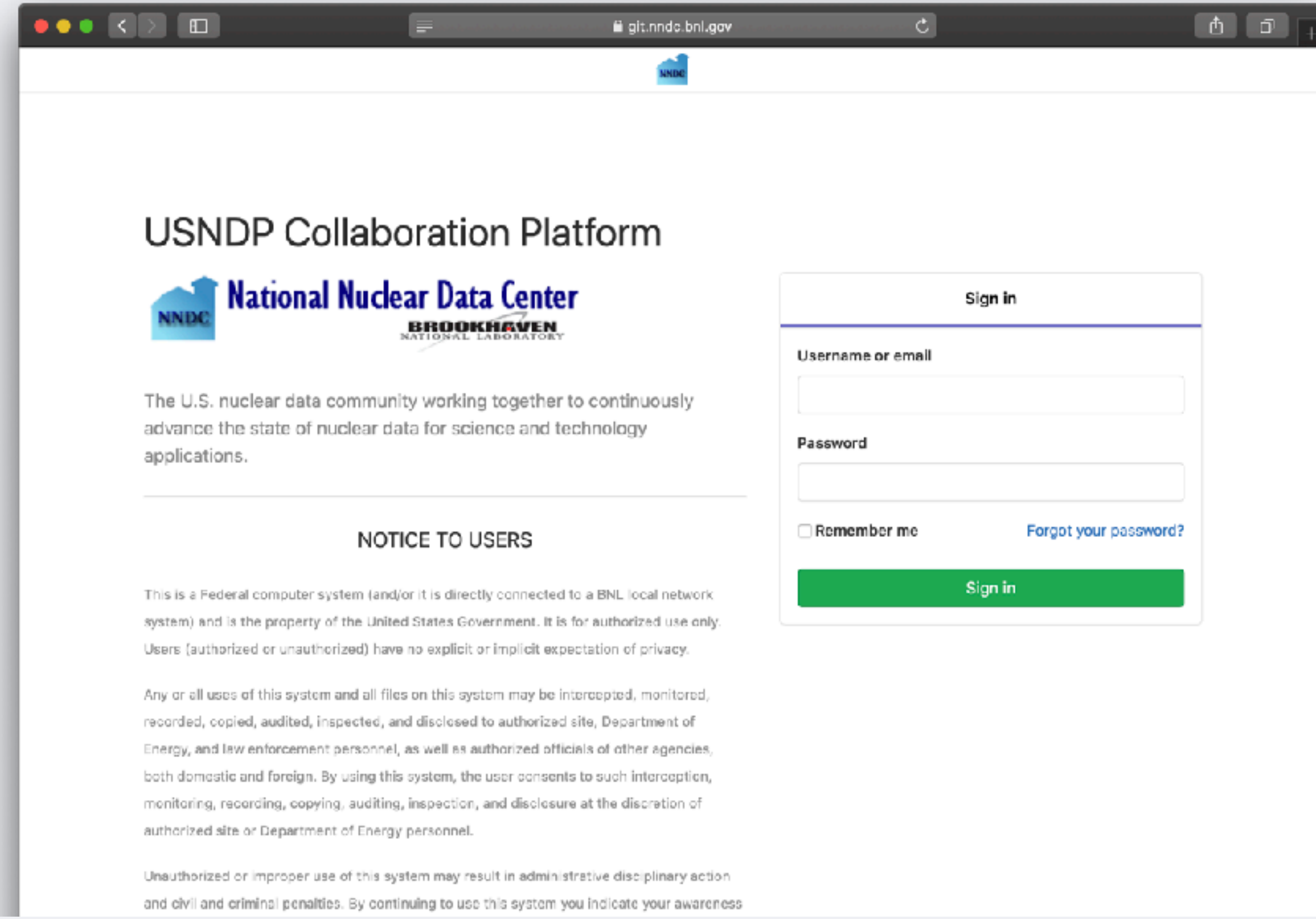
North Caroline State University (NSCU) group, have been added to ENDF as ENDF/B-VIII.0 libraries. Furthermore, our Nuclear Data Group at Rensselaer Polytechnic Institute (RPI), has developed a new methodology for creation of TSL libraries Ramić et al. (2018). The newly developed method integrates experimentally

So much more…

- ^{239}Pu intermediate structure (M. Pigni, ORNL)
- ^{238}U(n,n’) (M. Vorabbi, BNL)
- ^{234,236}U(n,f) (LANL)
- ^{9}Be(g,n) (J. Thompson, NNL)
- Pb isotopes (P. Brain, RPI)
- FPY (LANL, BNL)
- 135 decay datasets revised (R. Lorek, BNL)
- Revised atomic libraries (D.E. Cullen, retired)
- Minor actinide nubars (R.Q. Wright, retired)
- Review/steal IAEA Photonuclear Library
- Review/steal JEFF-3.3 TNSL evaluations

New workflow

We are transitioning from GForge to gitlab.nndc.bnl.gov



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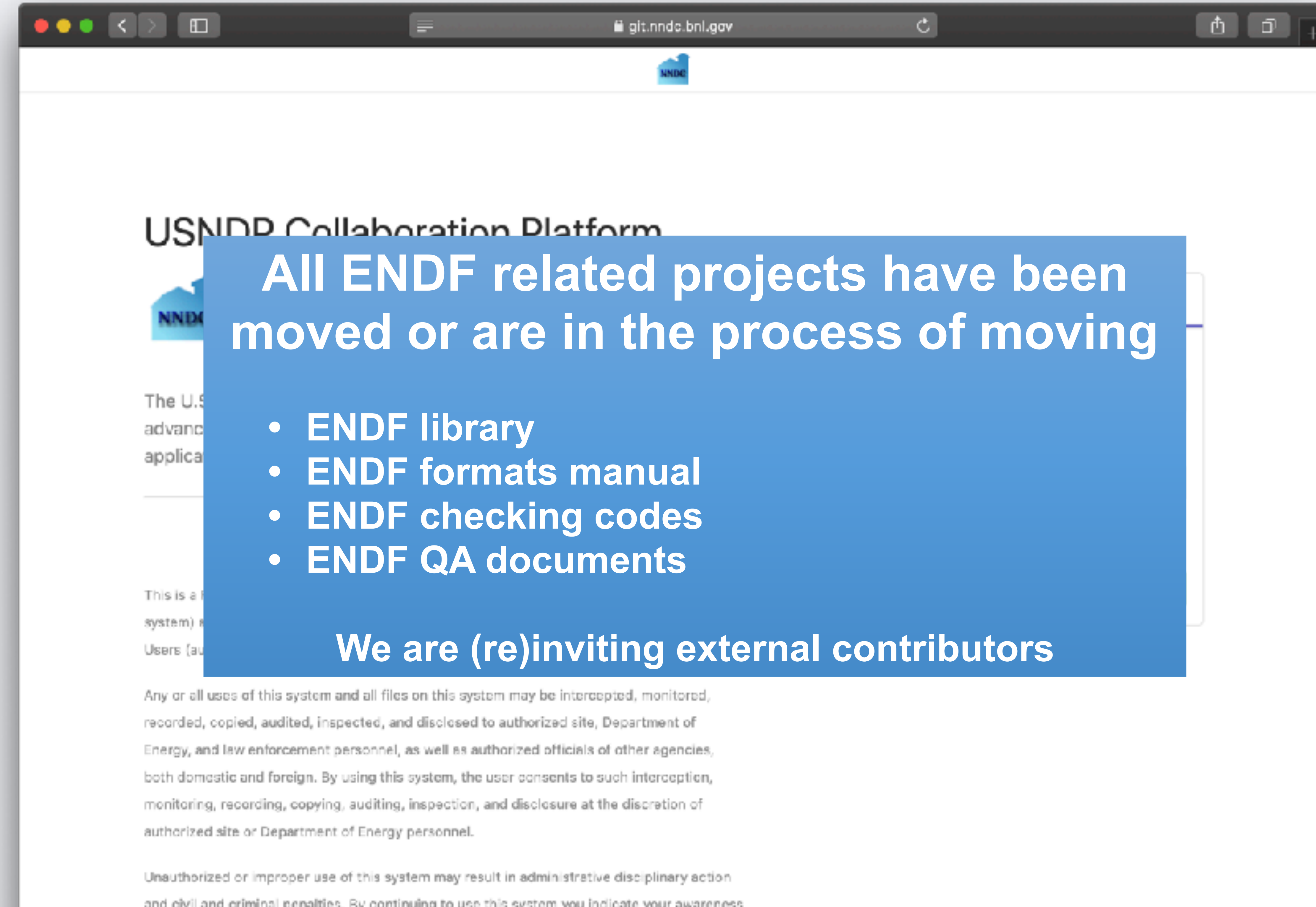
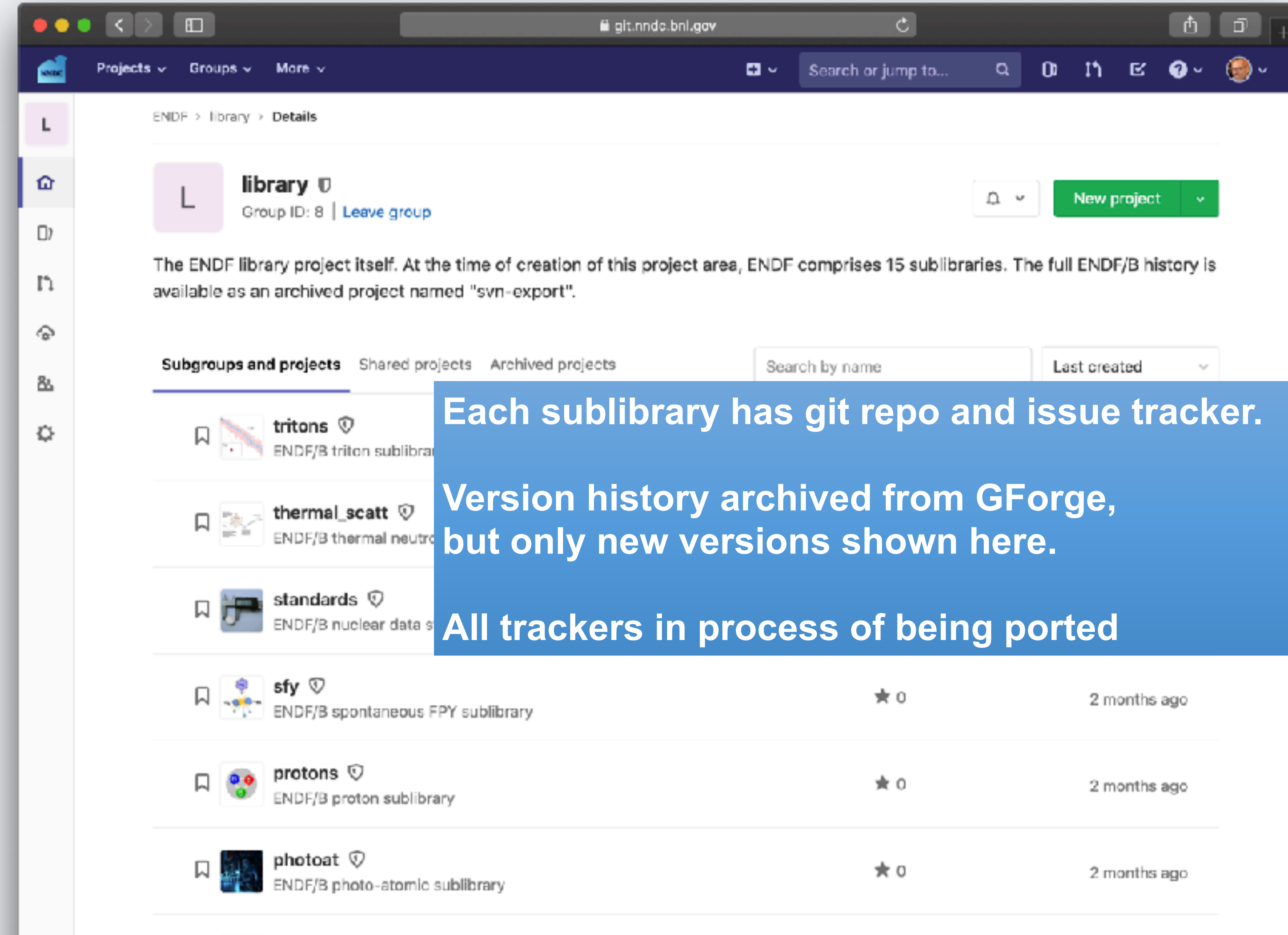


All ENDF related projects have been moved or are in the process of moving

- ENDF library
- ENDF formats manual
- ENDF checking codes
- ENDF QA documents

We are (re)inviting external contributors

We are transitioning from GForge to gitlab.nndc.bnl.gov

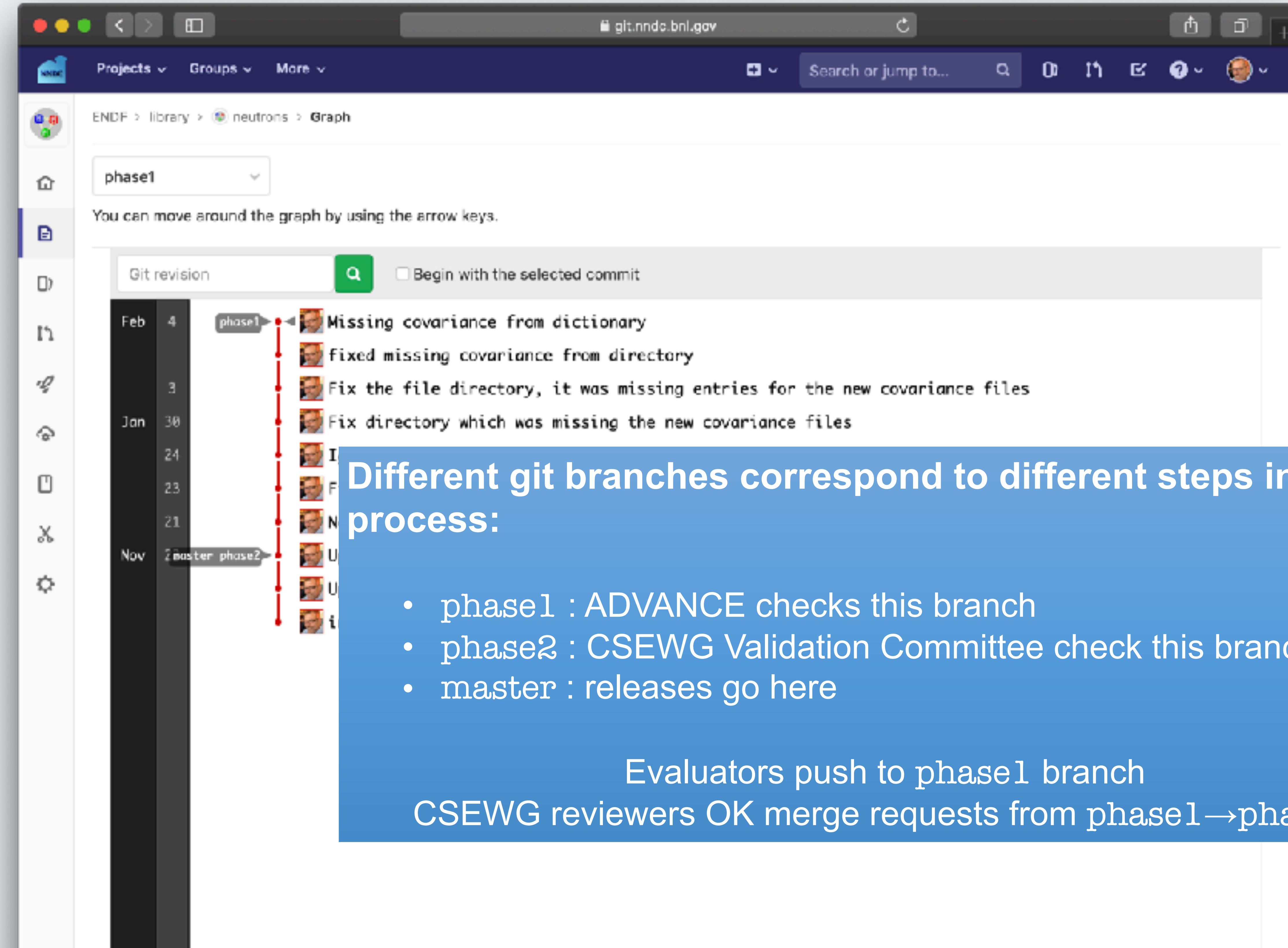


Each sublibrary has git repo and issue tracker.

Version history archived from GForge, but only new versions shown here.

All trackers in process of being ported

We are transitioning from GForge to gitlab.nndc.bnl.gov

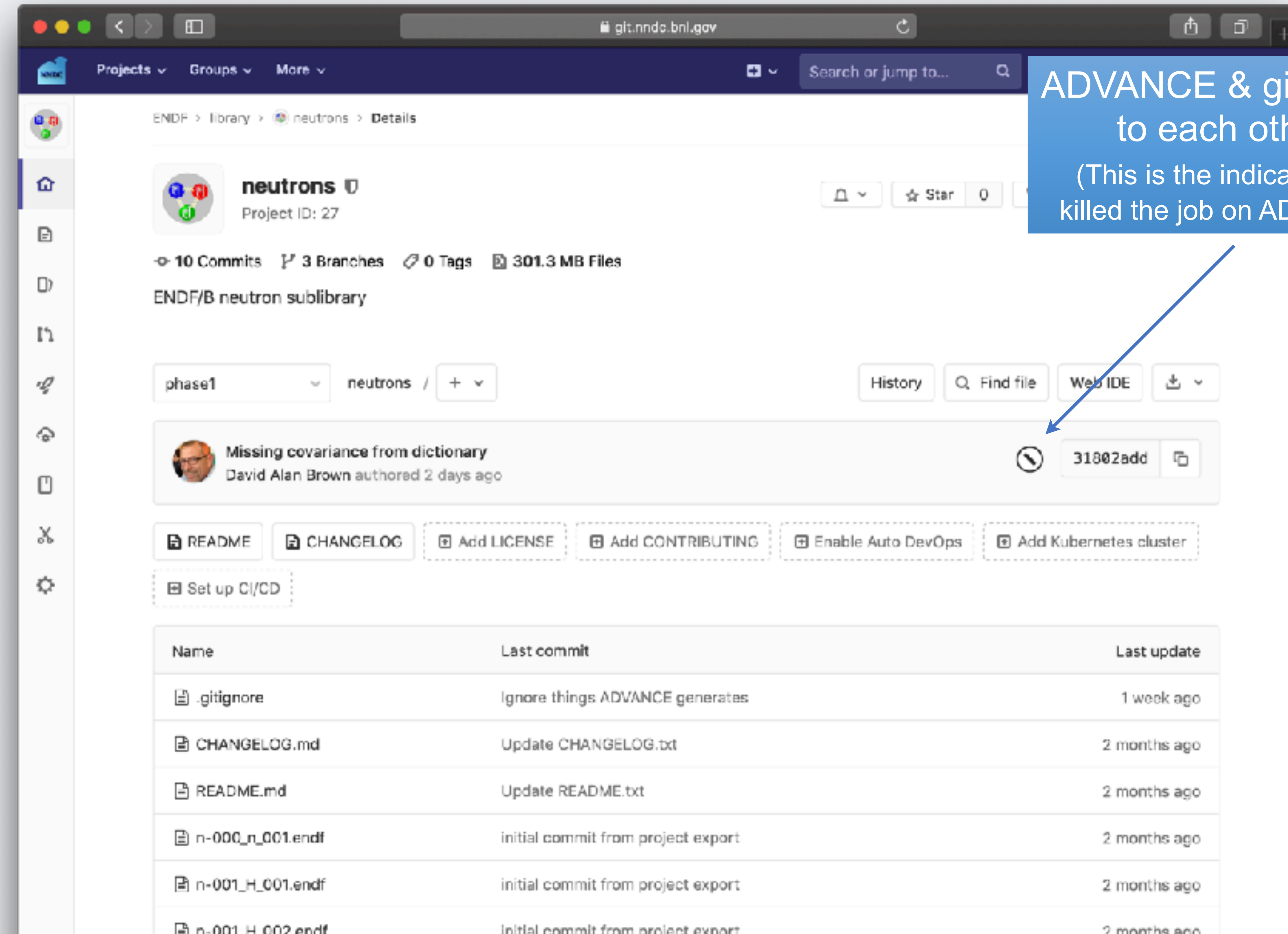


Different git branches correspond to different steps in QA process:

- `phase1` : ADVANCE checks this branch
- `phase2` : CSEWG Validation Committee check this branch
- `master` : releases go here

Evaluators push to `phase1` branch
CSEWG reviewers OK merge requests from `phase1`→`phase2`

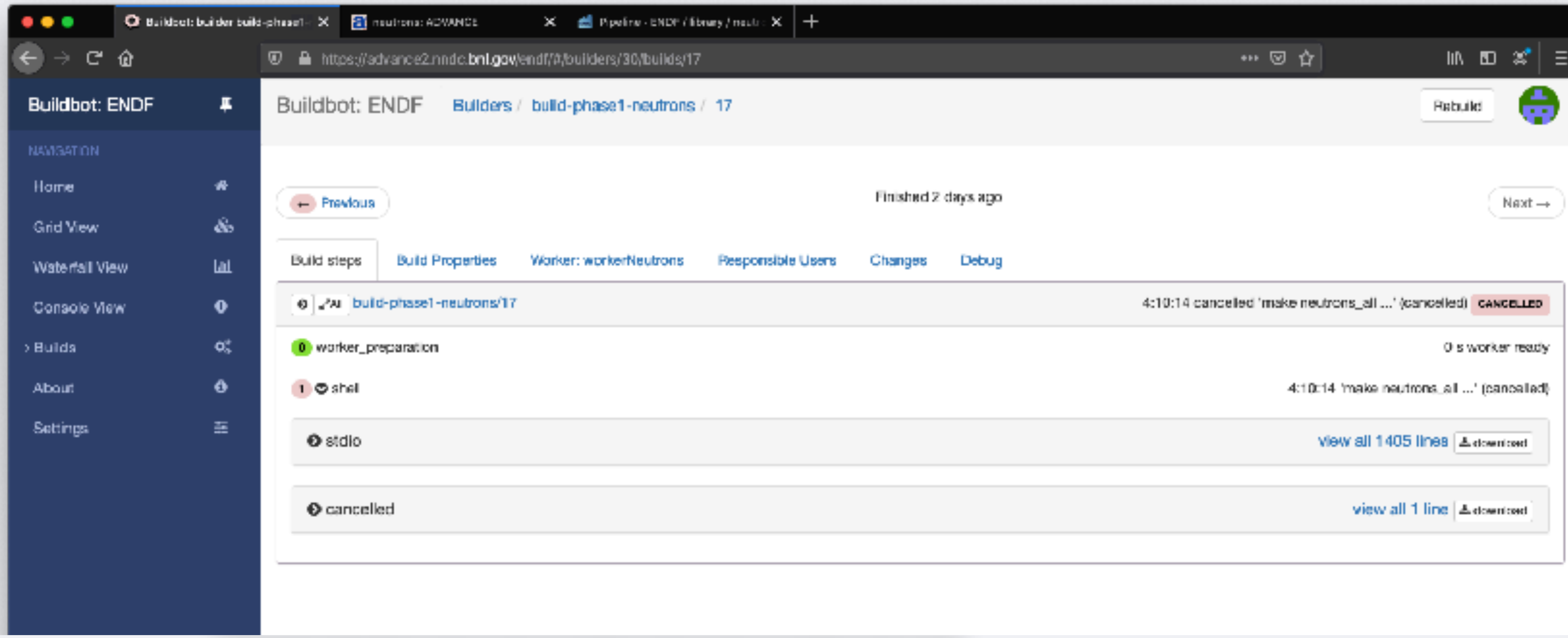
We are transitioning from GForge to gitlab.nndc.bnl.gov



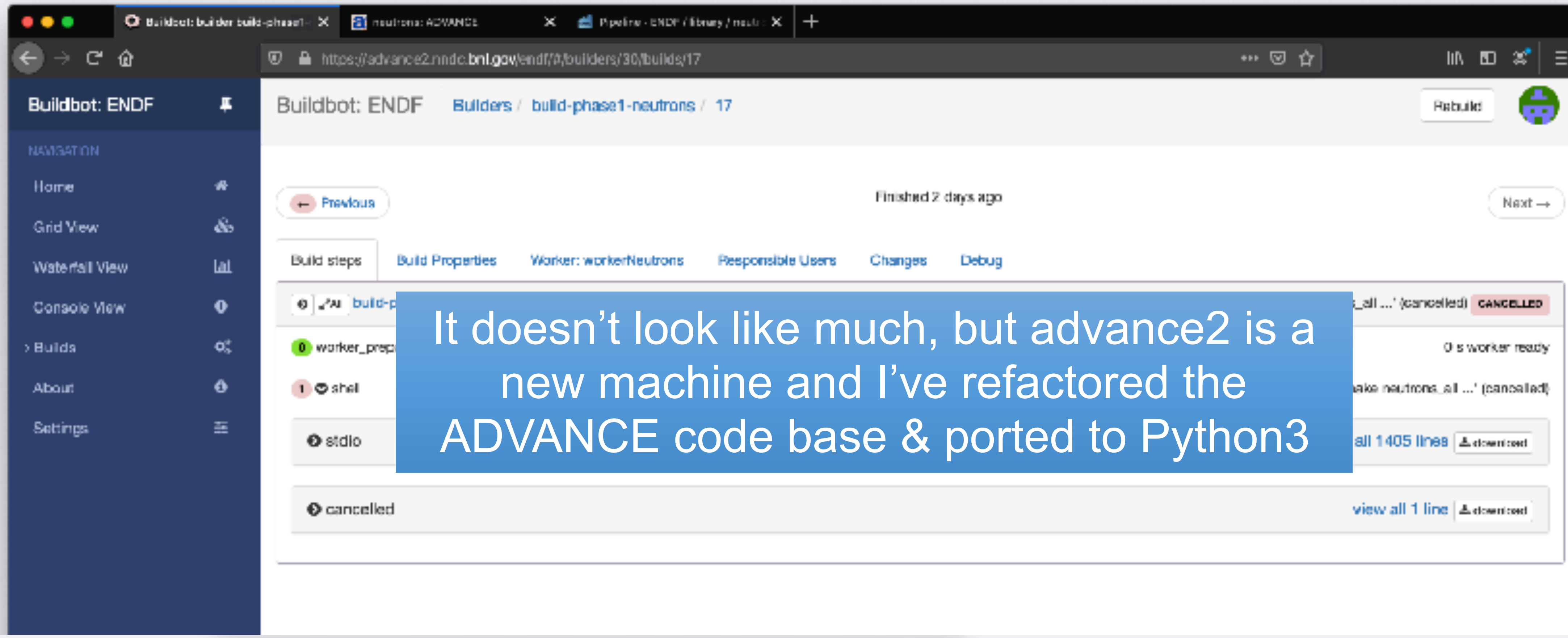
ADVANCE & gitlab talk to each other!

(This is the indicator that I killed the job on ADVANCE)

ADVANCE job dashboard

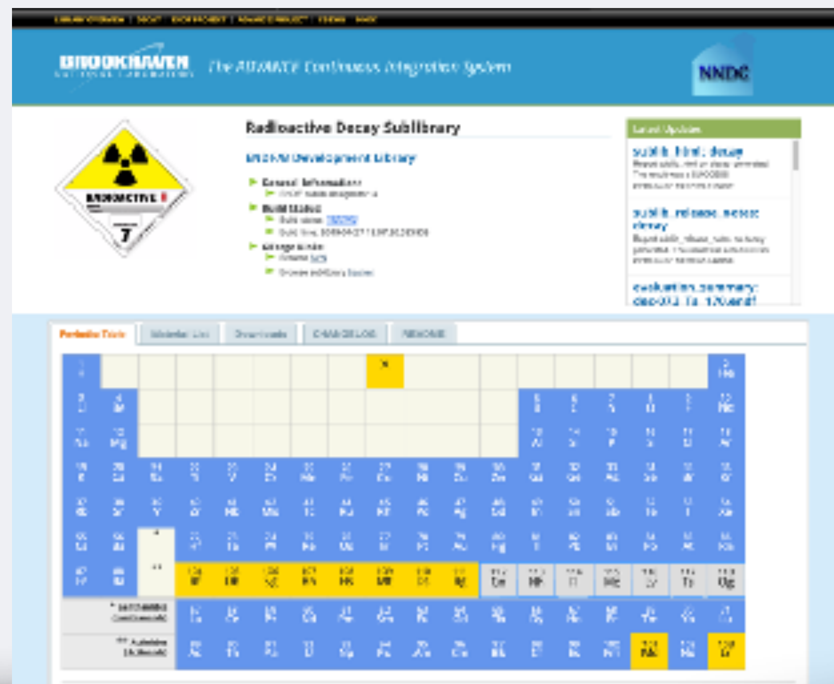


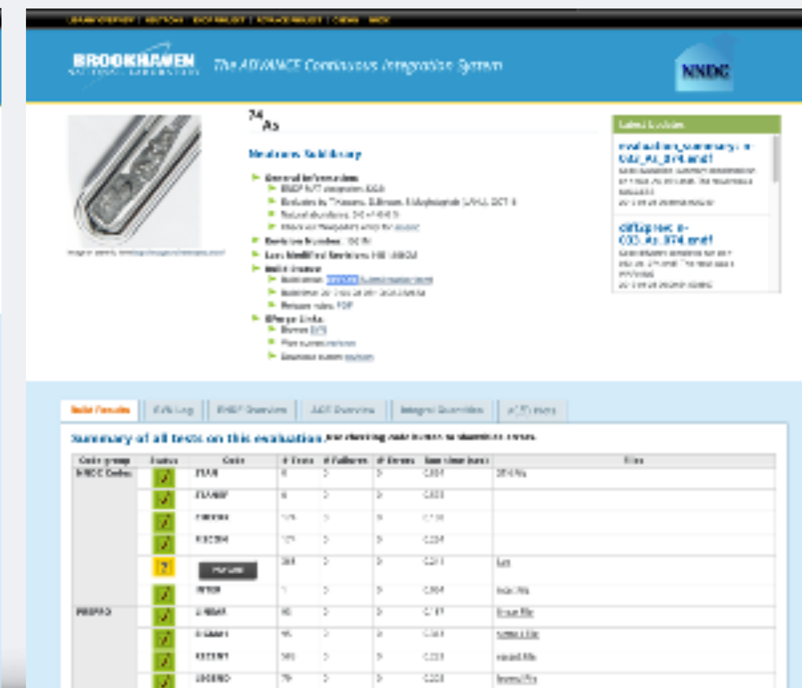
ADVANCE job dashboard



It doesn't look like much, but advance2 is a new machine and I've refactored the ADVANCE code base & ported to Python3

Build reports published to *https://www.nndc.bnl.gov/endf/b7.dev/qa*





Next ENDF?

- CSEWG has not made a decision on either a timeline or a version number
- We already have enough content to warrant tagging the first beta release
- COVID-19 and the new ENDF workflow are slowing development