



**IAEA**

International Atomic Energy Agency

*Atoms for Peace and Development*

# CoNDERC

## White paper & status

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Nuclear Data Section

NAPC, IAEA



# The CoNDERC project 2018 - 2024

- The purpose of the project entitled **C**ompilation of **N**uclear **D**ata **E**xperiments for **R**adiation **C**haracterisation is to provide and transfer into technology the experimental integral radiation information that can be used as part of the Validation and Verification processes of nuclear model and code systems, and to provide various schema to perform the V&V processes
- The aim is to provide all experimental methods, protocols, know how and calculational information in such computational ways that it can easily, seamlessly and rapidly be deployed in support of the many scientific systems that need them: model, inventory, transport, material sciences, Multiphysics code systems,...

# Key elements

- Identify and compile a set of radiation characterization benchmarks (both computational and experimental) that includes spectral indices, reaction rates, decay heat, resonance integral, particle emissions, radiations source terms
- Assess and review the data, including quantification of uncertainties, then compile the data into computer format for dissemination
- Perform simulations of each benchmark cases with a suitable code system and nuclear libraries and produce a database/repository of the necessary input files to repeat those simulations for other settings

# Lexical semantics: R&V&V

**Regression, Unit test:** with save outputs and results files, the current execution is compared to the above templates

**Verification:** analytical and semi-analytical solutions to an equation (Boltzmann, Bateman, Schrödinger, Dirac, etc.) may exist, to ensure that the simulation tool is solving the correct equation

**Validation:** combination of code, schema and processed nuclear data to produce results comparable to observables

# Lexical semantics: characterization metrics

Prompt, delayed, decay heat

Integral power, power density, power deposition,..

Reaction rates, emitted particles rates and spectra

Dose, particle fluence, dpa, activity, gas production, activation, depletion, breeding, radiation,..

Fission yields: cumulative and spontaneous, radionuclides yields

Fission products, residual nuclei, transmutation,..

# Benchmarks experiments

1. JAEA time dependent Fusion Neutron Source decay heat experiments (73 materials, 2/3 irradiation campaigns)
2. ~~UCB DT-source NIF concrete (gamma dose rate)~~
3. Li(p,n) (up to 150 MeV) angular neutron yields
4. Fission pulse decay heat experiments ☆
5. Fission delayed neutron experiments
6. Selected criticality experiment with reaction rates from ICSBEP, IRPhEP, REAL-IAEA, ... ☆
7. Experimental MACS from ASTRAL & KADoNiS ☆

black to be done

blue done, work in progress

☆ in this talk

# Benchmarks experiments

8. Spectrum-averaged xs in reference spectra (e.g. Cf-252,ACCR,LR-0, etc.)
9. Resonance integrals (based on the Atlas, other experiments, compilation)
10. Resonance integrals and thermal xs based on kayzero database for NAA
11. Time dependent gamma measurements from PNNL (fission) and UK (fusion)
12.  $(\gamma,n)$  experimental data (Laser-Compton scattering from TUNL and New Subaru)
13. Integro-differential benchmark (from EXFOR or otherwise)
14. Shielding and leakage benchmarks from SINBAD (including models) ☆
15. Reference spectra for computational analysis: 122 ☆

black to be done

blue done, work in progress

☆ in this talk

# Portal <https://www-nds.iaea.org/conderc/>

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## Compilation of Nuclear Data Experiments for Radiation Characterisation (CoNDERC)

The purpose of the CoNDERC project is to transfer into technology the experimental integral radiation information that can be used as part of the Validation and Verification processes of nuclear model and code systems, and to provide various schema to perform the V&V. Under the auspices of the IAEA Nuclear Data Section, individuals and institutions are assembling several of databases and code infrastructures based on their own V&V activities mainly associated with inventory, activation-transmutation, source term and radiation shielding R&D.

### Decay Heat

[Fusion Events](#)

[Fission Events](#)

### V&V Protocol

[Spectra](#)

[Photonuclear](#)

[Pencil Beam](#)

[NG-24M RR](#)

[Effective RR](#)

### Shielding

[Aspis](#)

[CIAE](#)

[FNS](#)

[NIST](#)

[Oktavian](#)

[Pulsed](#)

[Replica](#)

[Tiara](#)

### Beyond Keff

[MCNP](#)

[TRIPOLI](#)

[OpenMC](#)

### Experiments

[Thermal Resonance](#)

[Baghdad Atlas](#) ↗



















# CoNDERC contributors

- A handfull of experts and national laboratory generous contributions

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## Contributing individuals and institutions

- Y. Ding 
- Michael Fleming 
- Ian Gauld 
- Mark R. Gilbert 
- Aaron Hurst 
- Cedric Jouanne 
- Albert C. Kahler 
- Bor Kos 
- Ludmila Marian 
- Fujio Maekawa 
- Steven C. van der Marck 
- Paul Romano 
- Rene Reifarh 
- Shin Okumura 
- Jean-Christophe Sublet 
- Tadashi Yoshida 



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# Spectra

- The majority of neutron-application spectra stem from light-water assemblies, mock-ups, piles or reactors where the integral responses are strongly, if not solely, influenced by the energy ranges of the fission spectra, resonance range and thermal Maxwellian
- Fusion spectra that have been obtained from magnetic confinement (MCF) or inertial confinement fusion (ICF) simulation and present typical D-D 2.5 MeV, or D-T 14 MeV peaks sometimes accompanied by a higher-energy tail, but also showing rather different slowing-down profiles
- Accelerator-driven beam secondary spectra are important in their role in nuclear sciences, nuclear observables, materials research and medical applications

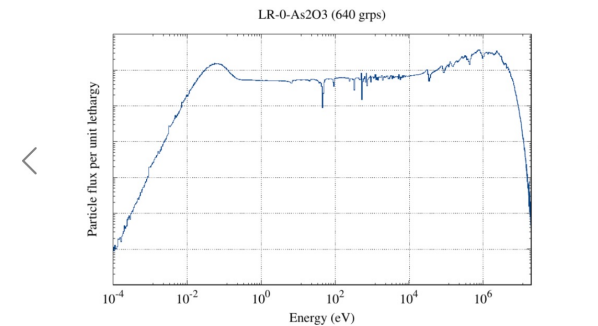
# Spectra

- 122 spectra from all over the World, all types, piles, NPPs, research reactor, spallation, FBRs, Maxwellian, Am-Be, at temperatures,
- one gamma from LMJ flash
- plots and numerical data



The collapsed cross-sections, reaction rates depend strongly on the nature of the projectile spectra, and so it is important to use the appropriate spectrum together with the appropriately-weighted cross-section data. With the advances of modern simulation software and high-resolution spectra the user is reminded of the importance of the tails, low or high-energy ones, on the reaction rates.

The majority of neutron-application spectra stem from light-water assemblies, mock-ups, piles or reactors where the integral responses are strongly, if not solely, influenced by the energy ranges of the fission spectra, resonance range and thermal Maxwellian. Fusion spectra that have been obtained from magnetic confinement (MCF) or inertial confinement fusion (ICF) present typical D-D 2.5 MeV, or D-T 14 MeV peaks sometimes accompanied by a higher-energy tail, but also showing rather different slowing-down profiles. Accelerator-driven beam spectra are important in their role in nuclear data acquisition and materials research, but also for medical therapeutic and diagnostic applications. [\[More..\]](#)



Download all data   
 [ 19.1 MB, 855 files ]

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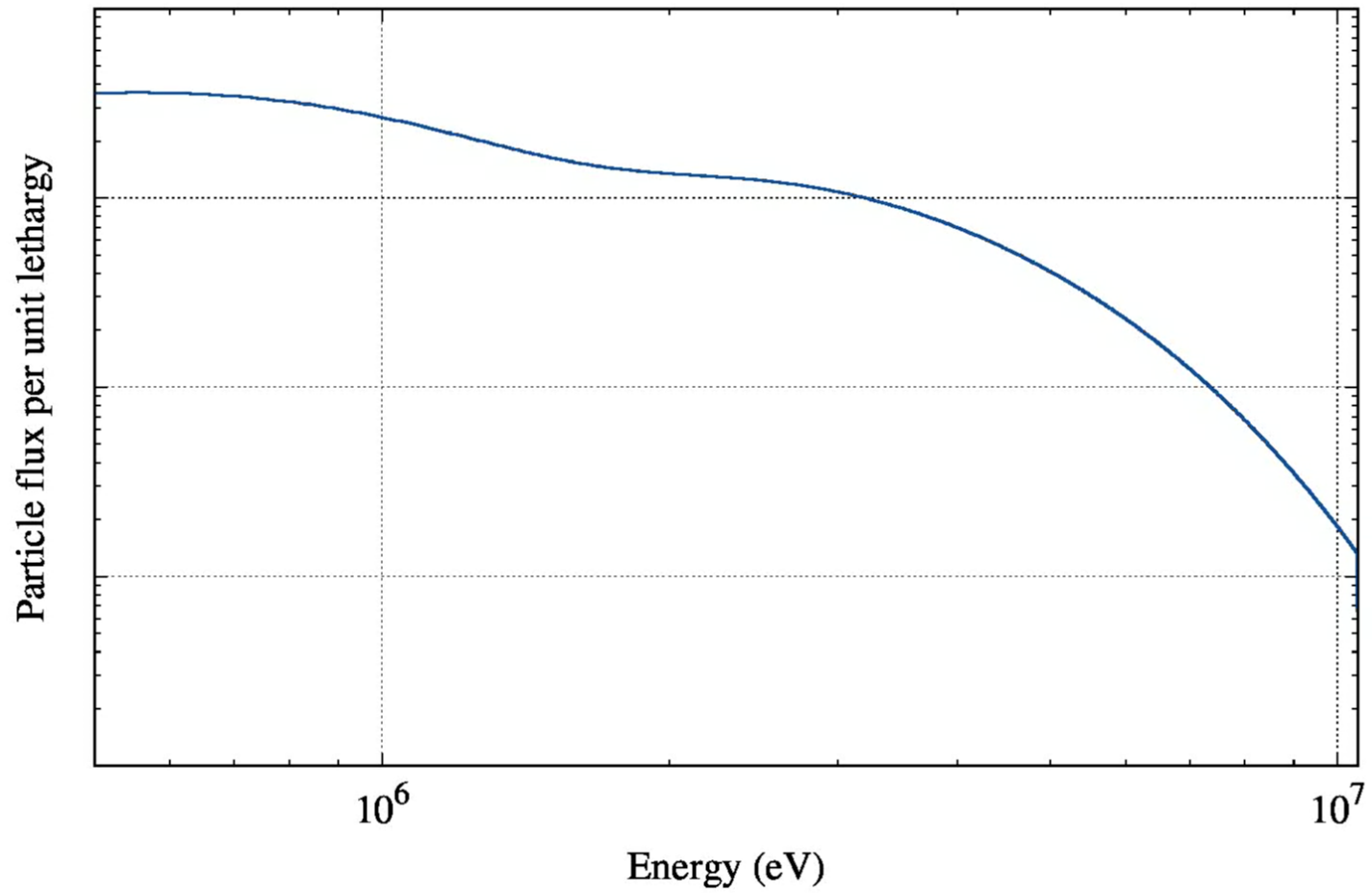
Show  entries

Search:

Order	Name	Group	Particle	arb_flux.txt	figure.png	Description
1	acrr-cdpoly-640	640	n	<a href="#">ACRR-CdPoly</a>	<a href="#">ACRR-CdPoly</a>	SNL MCNP
2	acrr-ff-cc-32cl-640	640	n	<a href="#">ACRR-FF-CC-32Cl</a>	<a href="#">ACRR-FF-CC-32Cl</a>	SNL MCNP
3	acrr-lb44-640	640	n	<a href="#">ACRR-LB44</a>	<a href="#">ACRR-LB44</a>	SNL MCNP
4	acrr-plg-640	640	n	<a href="#">ACRR-PLG</a>	<a href="#">ACRR-PLG</a>	SNL MCNP
5	fbr-6in-leakage-640	640	n	<a href="#">FBR-6in-leakage</a>	<a href="#">FBR-6in-leakage</a>	SNL MCNP
6	frec-ii-ff-640	640	n	<a href="#">FREC-II-FF</a>	<a href="#">FREC-II-FF</a>	SNL MCNP

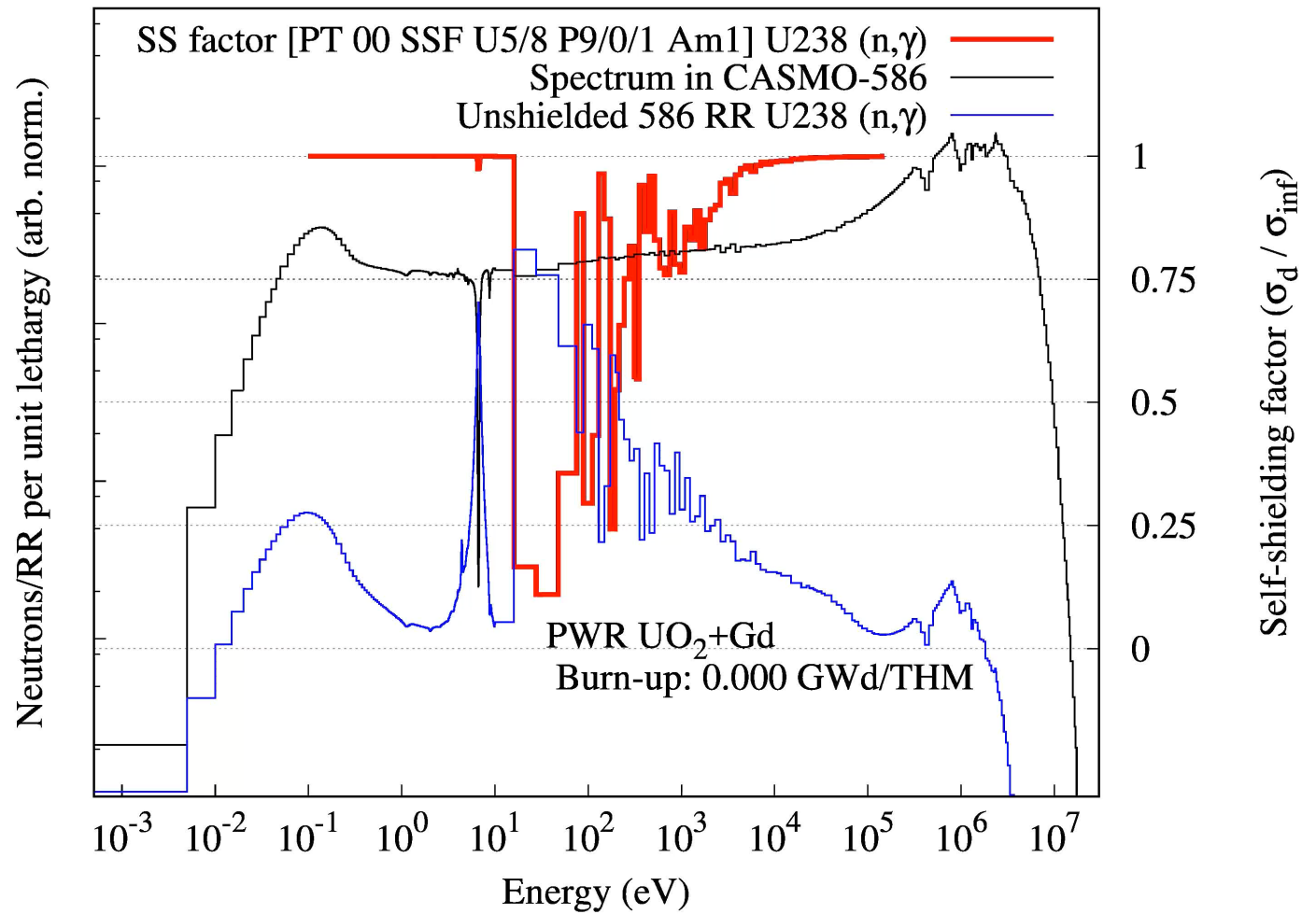
# Spectra shape shifting

IRT-M (1000 grps)



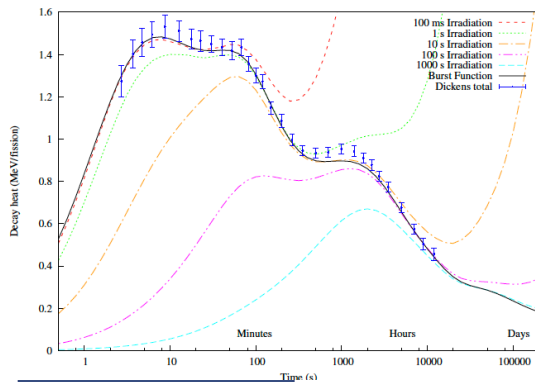
# Spectra shape shifting

Reaction Rates  
below the  
Unresolved and Resolved  
Resonance Range  
are strongly impacted !!



# Fission pulsed events

- 29 complete experimental datasets from the World over in one place
- Scobie 1971
- ...30 years
- Ohkawashi 2001



Author (first)	Institute	Year	Publication	Measured nuclide(s)
Gunst	Bettis Atomic Power Laboratory	1975	NSE 56 241	$^{233}\text{U}$ , $^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{232}\text{Th}$
Shure	Bettis Atomic Power Laboratory	1979	NSE 71 327	$^{235}\text{U}$ , $^{239}\text{Pu}$
Fiche	Atomic Energy Commission CEA	1976	NEACRP-L-212	$^{239}\text{Pu}$ , $^{233}\text{U}$
Lott	Atomic Energy Commission CEN	1973	J Nucl En 27	$^{235}\text{U}$
Friesenhahn	IRT Corporation (EPRI)	1976	EPRI NP-180	$^{235}\text{U}$
Friesenhahn	IRT Corporation (EPRI)	1979	EPRI NP-998	$^{235}\text{U}$ , $^{239}\text{Pu}$
Schrock	UC Berkeley (EPRI)	1978	EPRI NP-616	$^{235}\text{U}$
Baumung	Karlsruhe	1981	KfK 3262	$^{235}\text{U}$
Yarnell	Los Alamos National Laboratory	1978	LA-7452-MS	$^{239}\text{Pu}$ , $^{233}\text{U}$ , $^{235}\text{U}$
Yarnell	Los Alamos National Laboratory	1977	LA-NUREG-6713	$^{235}\text{U}$
Dickens	Oak Ridge National Laboratory	1978	ORNL/NUREG-39	$^{235}\text{U}$
Dickens	Oak Ridge National Laboratory	1978	ORNL/NUREG-34	$^{239}\text{Pu}$
Dickens	Oak Ridge National Laboratory	1978	ORNL/NUREG-47	$^{241}\text{Pu}$
Johansson	Uppsala University	1987	NEACRP-L-302	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{238}\text{U}$
Johnston	UK Atomic Weapons Res. Est.	1965	J Nucl En 19	$^{239}\text{Pu}$
Schier	University of Massachusetts Lowell	1993	DOE/ER/40723-1	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{238}\text{U}$
Schier	University of Massachusetts Lowell	1993	DOE/ER/40723-2	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{238}\text{U}$
Schier	University of Massachusetts Lowell	1994	DOE/ER/40723-3	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{238}\text{U}$
Schier	University of Massachusetts Lowell	1996	DOE/ER/40723-4	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{238}\text{U}$
Akiyama	University of Tokyo	1982	JAESJ 24 9 (in Japanese)	$^{235}\text{U}$ , $^{239}\text{Pu}$ , $^{233}\text{U}$
Akiyama	University of Tokyo	1988	JAERI-M 88-252	$^{232}\text{Th}$ , $^{233}\text{U}$ , $^{235}\text{U}$ , $^{238}\text{U}$ , $^{239}\text{Pu}$
Ohkawachi	Japan Nuclear Cycle Devel. Inst.	2001	J Nucl Sci Tech sup 2 2002	$^{235}\text{U}$ , $^{237}\text{Np}$
Fisher	Los Alamos National Laboratory	1964	Phys Rev B, 1959	$^{232}\text{Th}$ , $^{233}\text{U}$ , $^{235}\text{U}$ , $^{238}\text{U}$ , $^{239}\text{Pu}$
McNair	UK Atomic Weapons Res. Est.	1969	J Nucl En 23	$^{235}\text{U}$ , $^{239}\text{Pu}$
MacMahon	Scottish Research Centre	1970	J Nucl En 24	$^{235}\text{U}$
Jurney	Los Alamos National Laboratory	1979	LA-7620-MS	$^{239}\text{Pu}$ , $^{233}\text{U}$ , $^{235}\text{U}$
Murphy	UK Atomic Weapons Res. Est.	1979	AEW-R 1212	$^{235}\text{U}$ , $^{239}\text{Pu}$
Scobie	Scottish Research Centre	1971	J Nucl En 25	$^{235}\text{U}$

29

1

# Experimental MACS from ASTRAL # KADONIS

- Second stage of KADONIS upgrade, 78 traditional + 58 activations (136)
- *The  $^{197}\text{Au}(n, \gamma)$  standard!! @ $kT=30$  keV changed from  $582 \pm 9$  mb (Kadonis 0.3 and earlier) to  $612 \pm 6$  mb*

<https://exp-astro.de/astral/>

## ASTRAL

ASTrophysical Rate and rAw data Library

[Home](#)

[Internal](#)

View Maxwellian-Averaged Cross Section

Isotope

(Examples: Ba138, Ta180m, Se.)

173 isotopes found in database.

Download table of ASTRAL MACS (1 line per isotope)

Kind of reaction:   Release version:

KT  $\geq$   keV (leave open for full range)

KT  $\leq$   keV (leave open for full range)

ASTRAL Releases

Version:

[Experimentelle Astrophysik](#) | [Goethe Universität Frankfurt](#) | [IAP](#) | [Datenschutz](#) | [Impressum](#) | [Kontakt](#)



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### Thermal Resonance

Thermal cross section, Maxwellian average, Integral information up to the end of the resonance ranges in their numerical forms are underpinning many aspects of theoretical and experimental nuclear sciences. Since the dawn of the nuclear ages, books and charts have conveyed such information on printed papers out of the World's library.

The table below simply represents a 21<sup>st</sup> century collection of published nominal values in a simple computer readable format. Its specificity relies in its availability, upgradability and technological use, acknowledging the nuclear physicists from which it stems from:

#### Documentation

- EXFOR
- S.F. Mughabghab in [Atlas of Resonances \(6<sup>th</sup> Edition\)](#)
- N.E. Holden in [Handbook of Chemistry and Physics \(99<sup>th</sup> Edition\)](#)
- I. Dillmann, R. Plag, F. Kappeler and T. Rauscher in [KADoNIS v1.0, v0.3](#)
- J. Kopecky in [UKAEA-R\(15\)30](#)
- R. Reifarth in [Summary Report](#) and [ASTRAL](#)

Download all data

[ 173.4 KB, 2 files ]

or

[Access individual data sets](#)

thermal-res-table.txt

148.5 KB

*Last updated: 2020-09-15 14:06:29*

# Shielding

- Upon specific request of member states, beyond Keff and radiation shielding benchmark are now also considered in CoNDERC
- Building from the existent: IAEA consultancy achievements, generous contributors and moving forward ensemble
- MCNP6®, TRIPOLI-4® and OpenMC input decks have been developed for:

Shielding		
Aspis	CIAE	FNS
NIST	Oktavian	Pulsed
Replica	Tiara	



# Shielding: e.g. Oktavian

- Computational

- experimental data
- expert crafted Monte Carlo input decks
- validation Monte Carlo outputs
- for different libraries

- Documentation

- open literature
- open declassified report
- figures

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### Documentation

- B. Kos and I. A. Kodeli, "MCNP modelling of the TIARA SINBAD shielding benchmark" ([INDC\(NDS\)-0785](#))
- B. Kos and I. A. Kodeli, "MCNP modelling of the ASPIS Iron88 SINBAD shielding benchmark" ([INDC\(NDS\)-0771](#))
- S.C. van der Marck, "Shielding Benchmark calculations with MCNP-4C3 using JEFF-3.1 Nuclear Data" ([21616/05.69455/P](#))
- [More references..](#)

Download all data   
[ 2.0 MB, 161 files ]

or

[Access individual data sets](#)

```
oktavian_exp
├── oktavian_Co_tal21.exp
├── oktavian_Cr_tal41.exp
├── oktavian_W_tal41.exp
├── oktavian_Pb_tal41.exp
├── oktavian_LiF_tal21.exp
├── oktavian_Mn_tal21.exp
├── oktavian_LiF_tal41.exp
├── oktavian_Si_tal21.exp
├── oktavian_Si_tal41.exp
├── oktavian_Co_tal41.exp
├── oktavian_Cu_tal41.exp
├── oktavian_Mn_tal41.exp
├── oktavian_Al_tal41.exp
├── oktavian_Mo_tal21.exp
├── oktavian_Ti_tal21.exp
├── oktavian_Cr_tal21.exp
├── oktavian_Zr_tal21.exp
├── oktavian_Cu_tal21.exp
├── oktavian_Mo_tal41.exp
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├── oktavian_W_tal21.exp
└── oktavian_Ti_tal41.exp
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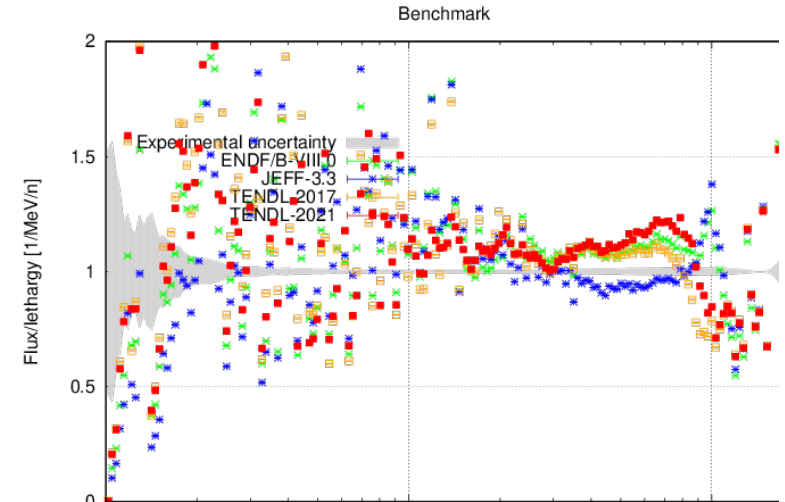
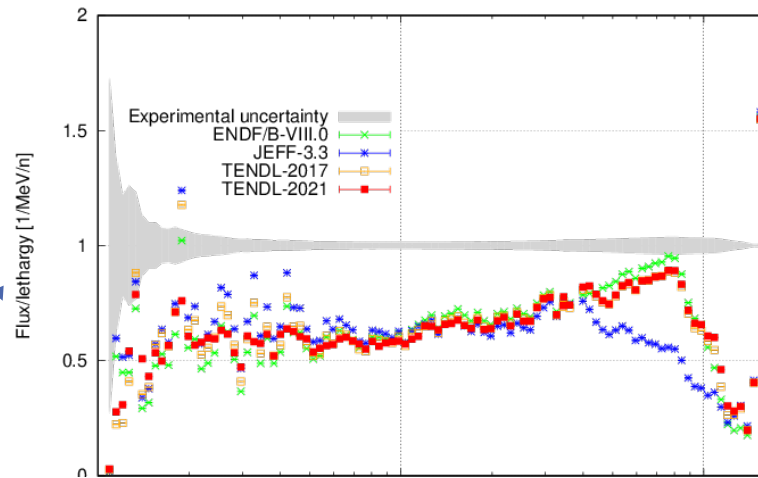
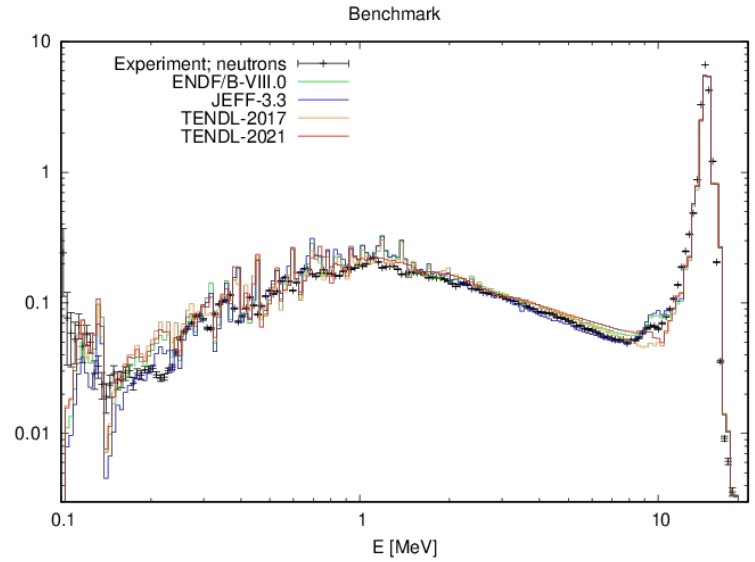
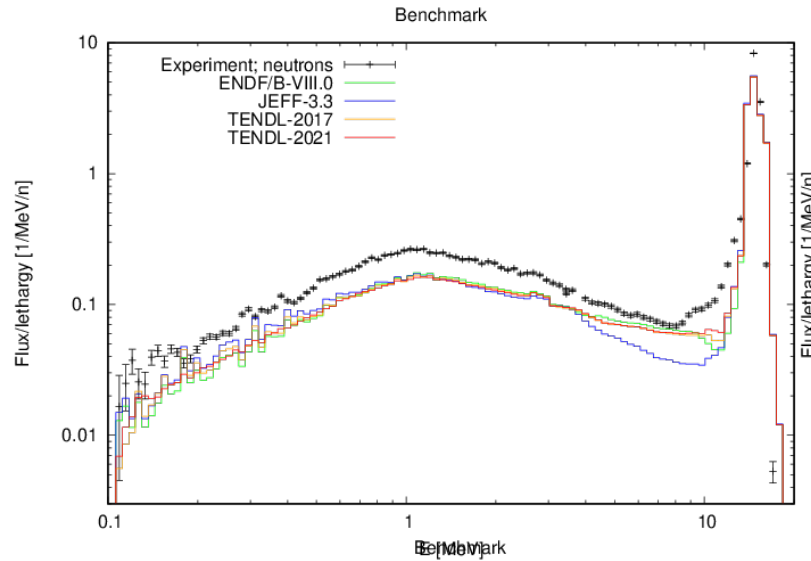
```
MCNP
```

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MCNP
├── oktavian_exp
├── outp_tendl17
├── outp_jeff33
├── Inputs
│   ├── inp_oktavian_Mo
│   ├── inp_oktavian_Cr
│   ├── inp_oktavian_Mn
│   ├── inp_oktavian_Al
│   ├── inp_oktavian_Ti
│   ├── inp_oktavian_Si
│   ├── inp_oktavian_W
│   ├── inp_oktavian_Zr
│   ├── inp_oktavian_Co
│   ├── inp_oktavian_LiF
│   └── inp_oktavian_Cu
├── outp_endfb80
└── outp_jendl40
```

# Shielding

- Oktavian  
Co X  
Zr ~
- Log-Log  
could be  
deceptive

- 10 to 50% !!

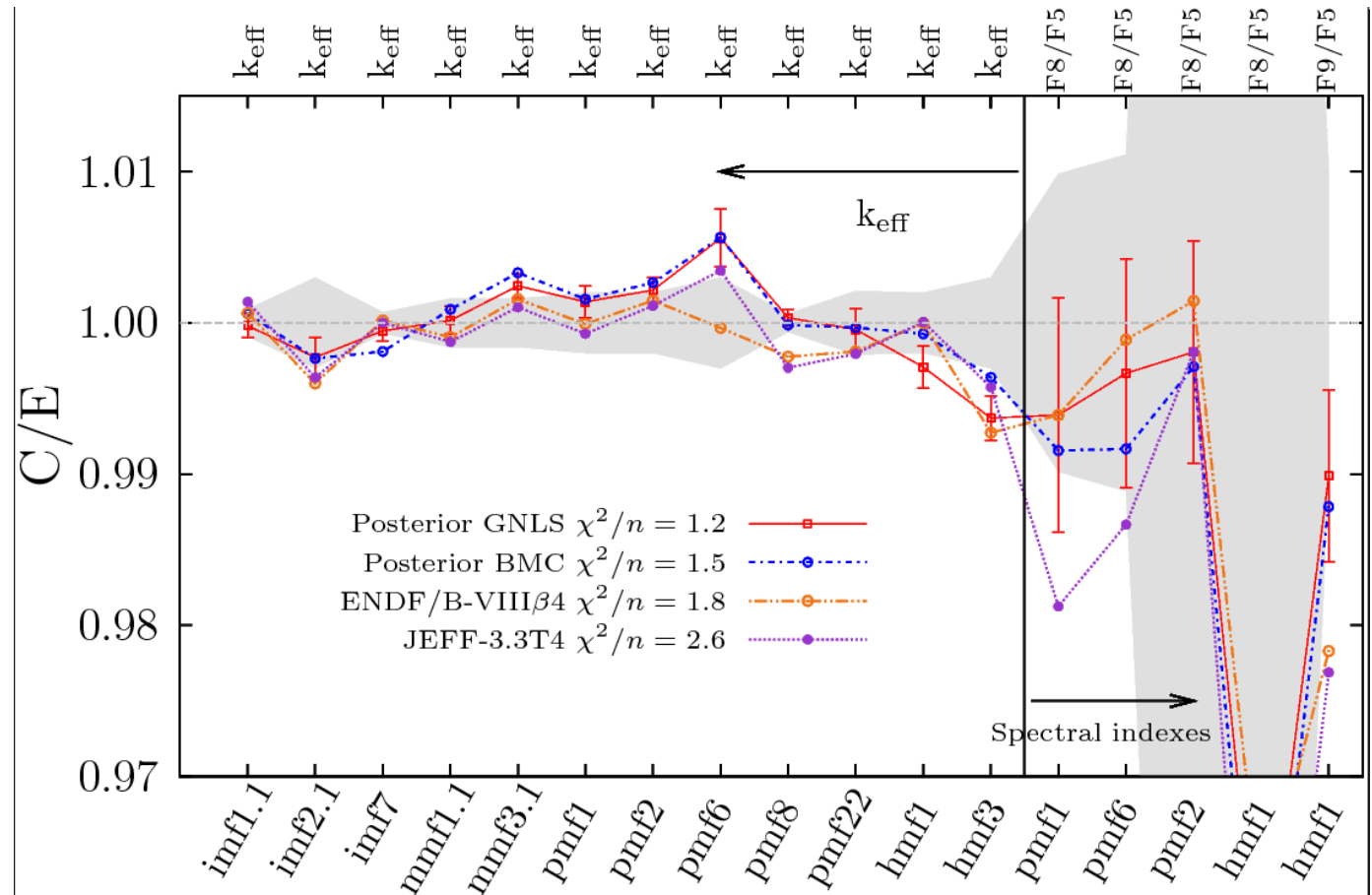


# ICSBEP & reaction rates: beyond $K_{\text{eff}}$

- International Criticality Safety Benchmark Evaluation Project (ICSBEP)
- International Reactor Physics Experiment Evaluation Project (IRPhEP)
- Compile critical and subcritical benchmark experiment data into a standardized format to validate simulation tools and cross-section libraries
- In addition to criticality some benchmark evaluations also contain spectral indices and measured reaction rate data
- Another class of experimental data that can provide additional qualification of the underlying nuclear data and simulation tools

# ICSBEP & reaction rates: beyond $K_{eff}$

- Good  $K_{eff}$  C/E with small uncertainty
- More troubled spectral indices C/E
- Right for the wrong reasons?



Courtesy D. Rochman (PSI)

# ICSBEP and IRPhEP Handbooks

- MCNP6® , TRIPOLI-4® and OpenMC input decks with reaction rate (spectral index) or pin power data

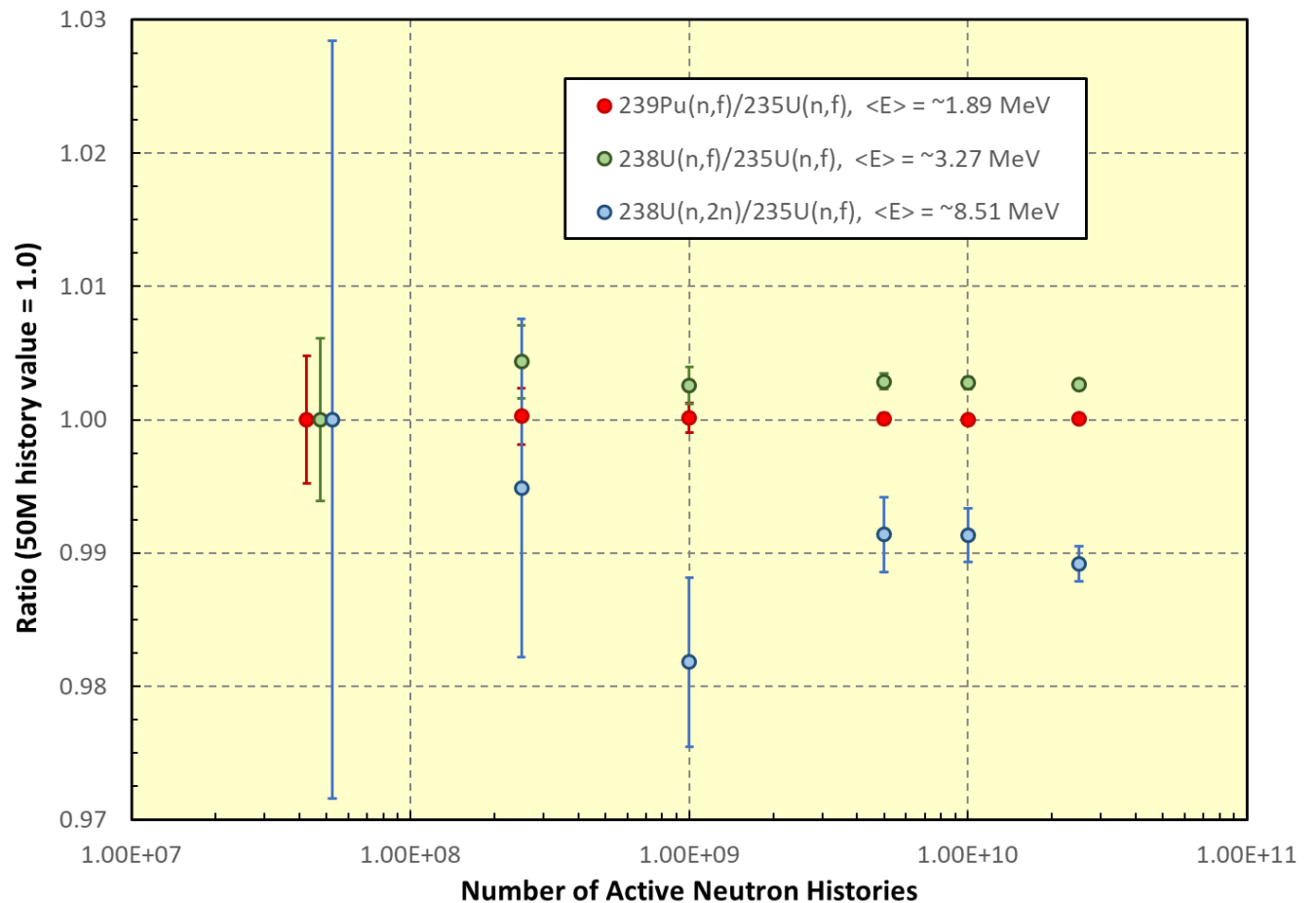
Legacy Assembly Name	ICSBEP Benchmark Identifier
Godiva	HEU-MET-FAST-001
Flatop-25	HEU-MET-FAST-028
Jezebel	Pu-MET-FAST-001
Flatop-Pu	Pu-MET-FAST-006
Thor	Pu-MET-FAST-008
'dirty' Jezebel	Pu-MET-FAST-002
Big-10	IEU-MET-FAST-007
Babcock & Wilcox 15x15	LEU-COMP-THERM-008
Dimple-LWR	LEU-COMP-THERM-055
Jezebel-23	U233-MET-FAST-001
Flatop-23	U233-MET-FAST-006
Pu BR-1 core	FUND-IPPE-FR-MULT-RRR-001

# Running strategy

- up to six MCNP6® “kcode”
- 50 million (50M) and 250 million (250M) active neutron histories
  - 5100 cycles (100 warmup cycles and 5000 active cycles) with either 10,000 or 50,000 neutrons per cycle
  - remaining jobs were run with 50 warmup cycles and 2,500,000 neutrons per cycle
- These jobs were stopped/continued after 450, 2050, 4050 and 10050 cycles, for a total of 1 billion (1B), 5 billion (5B), 10 billion (10B) and 25 billion (25B) active histories, respectively
- For a given f4 tally we also specify an identical \*f4 tally. Division of the \*f4 tally result by the f4 tally result yields the average energy for that reaction  $\langle E \rangle$

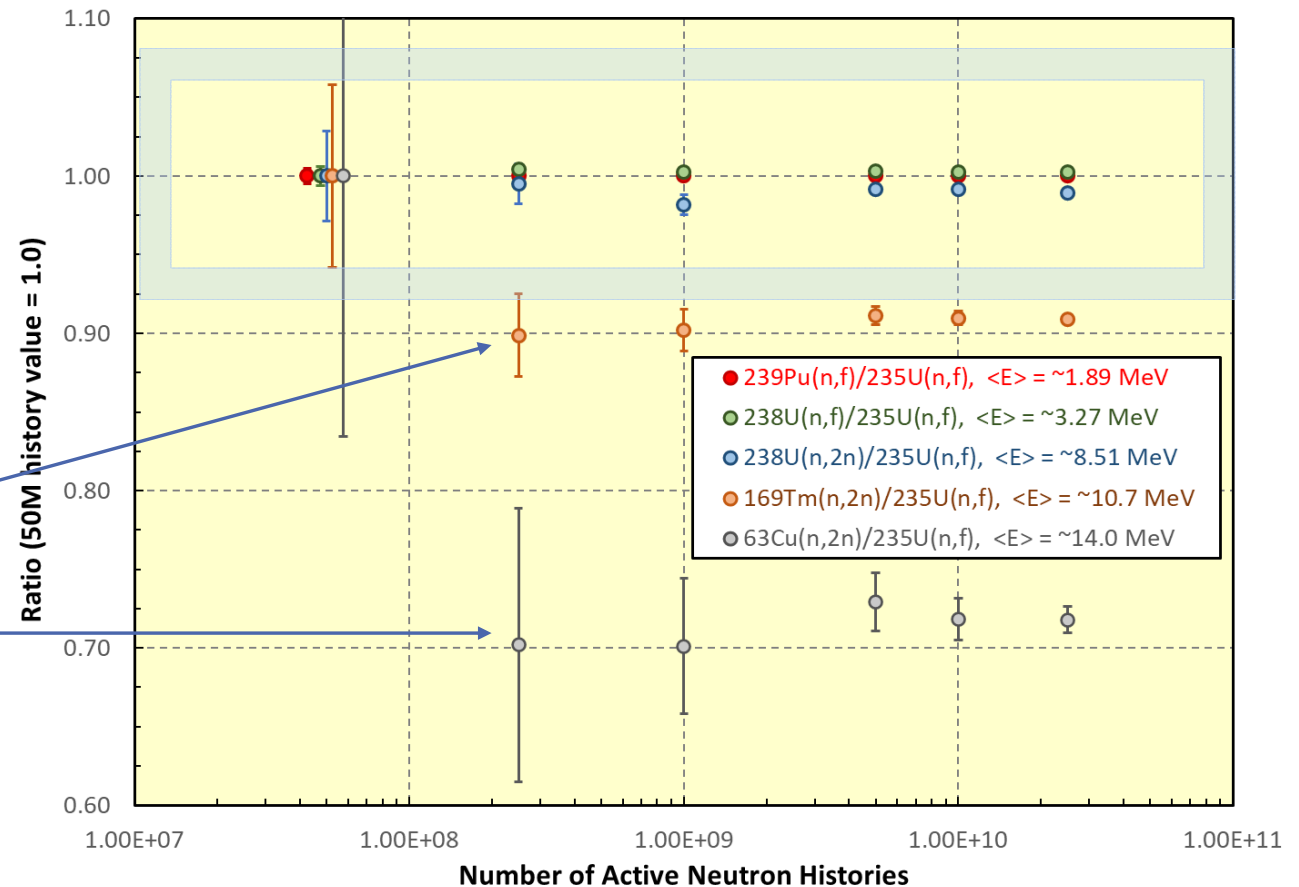
# PMF1 (Jezebel Rev 4) - MCNP6® & ENDF/B-VIII.0

- Spectral index variation with increasing neutron histories
- 50 million to 25 billion,  $25 \times 10^9$
- $\langle E \rangle$  8,5 MeV – 2% deemed acceptable



# PMF1 (Jezebel) - MCNP6® & ENDF/B-VIII.0

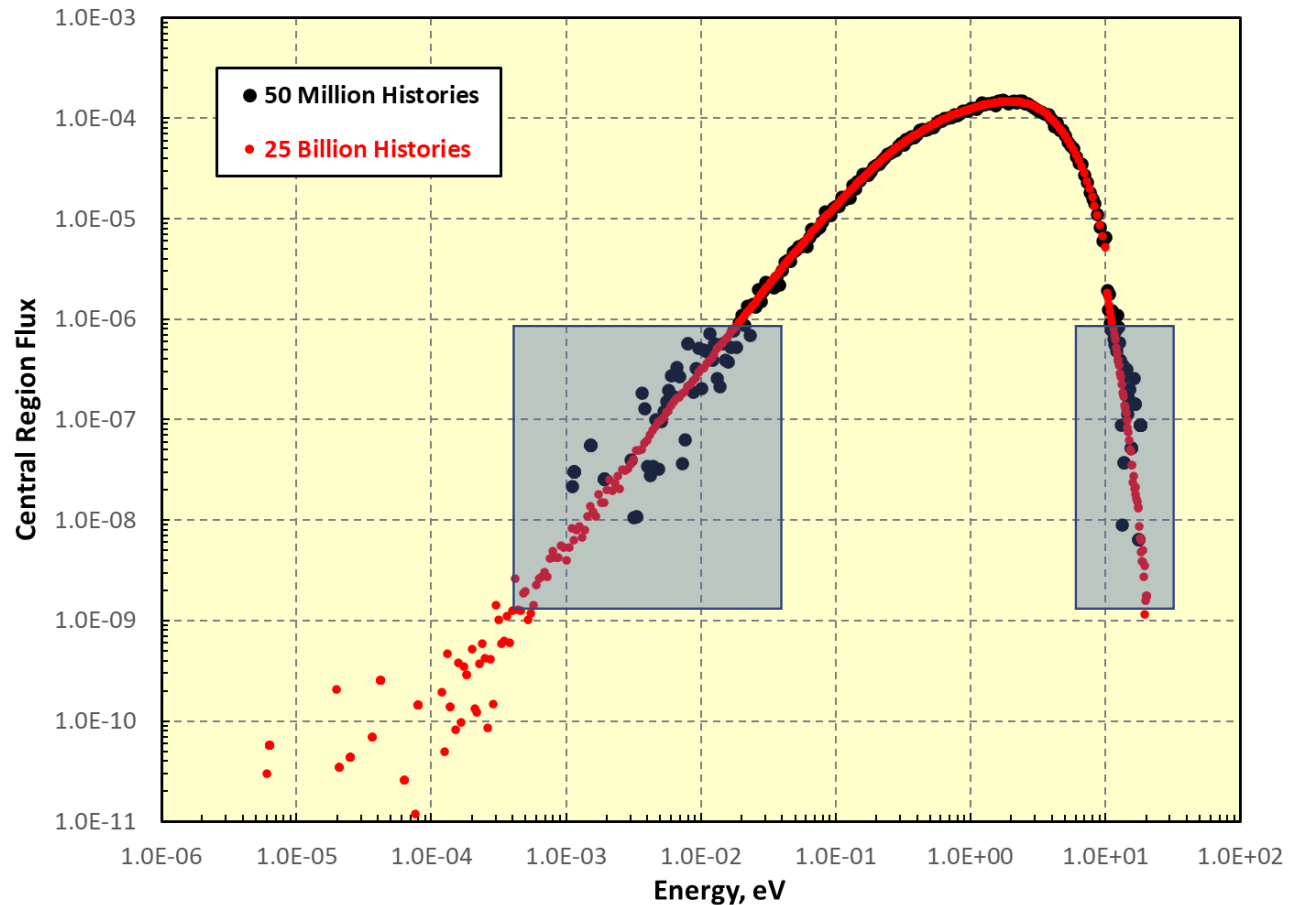
- Zoom out
- 50 million to 25 billion  $25 \times 10^9$
- $\langle E \rangle$  8.5 MeV – 2%
- $\langle E \rangle$  10.7 MeV - 10%
- $\langle E \rangle$  14 MeV - 30%





# Jezebel PMF1 central region flux

- Histories x 500
- High tail – sharp decrease
- Low tail – more scattered but has the potential to notably impact capture, fission
- Span 5 decades



# Spectral Indices: Jezebel PMF1

- Shaded area
- Good C/C +/-2%
- C/E divergence -5% to 25% increase with energy

Central Region Spectral Index	Measured value	MCNP6® Calculated Average Energy, MeV	MCNP6®	TRIPOLI-4®	C/C	C/E
PMF1 (Jezebel)						
$^{238}\text{U}(n,\gamma) / ^{235}\text{U}(n,f)$	0.0677	0.87	0.0644	0.0644	1.01	<b>0.95</b>
$^{238}\text{U}(n,f) / ^{235}\text{U}(n,f)$	0.2133(23)	3.3	0.2120	0.2122	0.99	0.99
$^{238}\text{U}(n,2n) / ^{235}\text{U}(n,f)$	0.0106	8.5	0.0132	0.0131	0.98	<b>1.25</b>
$^{237}\text{Np}(n,f) / ^{235}\text{U}(n,f)$	0.9835(140)	2.3	0.9769	0.9776	0.99	0.99
$^{239}\text{Pu}(n,f) / ^{235}\text{U}(n,f)$	1.4609(13)	1.9	1.4273	1.4275	1.00	0.98
$^{55}\text{Mn}(n,\gamma) / ^{235}\text{U}(n,f)$	0.00235(3)	0.83	0.00282	0.00283	1.02	1.20
$^{63}\text{Cu}(n,\gamma) / ^{235}\text{U}(n,f)$	0.00989(6)	0.91	0.0101	0.0101	1.01	1.02
$^{169}\text{Tm}(n,\gamma) / ^{235}\text{U}(n,f)$	0.0931	0.69	0.1061	0.1059	1.02	1.14
$^{169}\text{Tm}(n,2n) / ^{235}\text{U}(n,f)$	0.00313	10.7	0.00371	0.00375	0.98	1.19

# Conclusions

- Live web portal, explicit with graphics, tables, datasets
- Deployable data streams, full download
- V&V codes inputs & outputs
- Experimental information in computer forms
- Safe repository
- Partly accessible through GitHub

- Priority next ?



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# CoNDERC White paper & status

Thank you for your attention!

