Nuclear Reactors, Evaluations, Library Development

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École Joliot-Curie, 28 Sep. - 03 Oct. 2014

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5’

- 1995: “Magistere” in Physics, M.S., University of Orsay, France
- 1995-98: PhD Theoretical Nuclear Physics, University of Bordeaux
  - Multi-dimensional quantum tunneling
  - Proton emission from deformed nuclei
  - *(some extended stays at Berkeley, Seattle, Los Alamos)*
- 1998-2000: postdoc, Theoretical Division, Los Alamos National Laboratory (LANL), USA
  - Quantum mechanics
  - Nuclear Fission
- 2001-present: staff scientist, LANL, Theoretical Division, Nuclear Physics Group
  - Nuclear reaction theories (Chadwick, Kawano)
  - Nuclear fission (Möller, Sierk, Madland, Lynn)
  - Nuclear data evaluations (Chadwick, Young, Kawano)

Thanks to many collaborators

- Theory: T.Kawano, D.Neudecker, A.C.Kahler, I. Stetcu, M.Paris, G.M.Hale, P.Möller, A.J.Sierk, D.G.Madland, J.E.Lynn
- X-Computational Physics: M.B.Chadwick, M.White, J.P.Lestone
- LANSCE: R.C.Haight, F.Tovesson
- C-NR: M.Jandel, A.Couture, S.Mosby
- BNL, LLNL, ORNL, INL, U. New Mexico, U. Michigan, …
- IAEA, NEA, CEA, …

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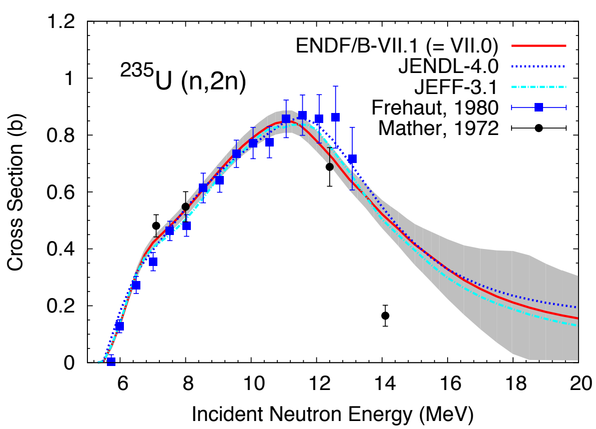
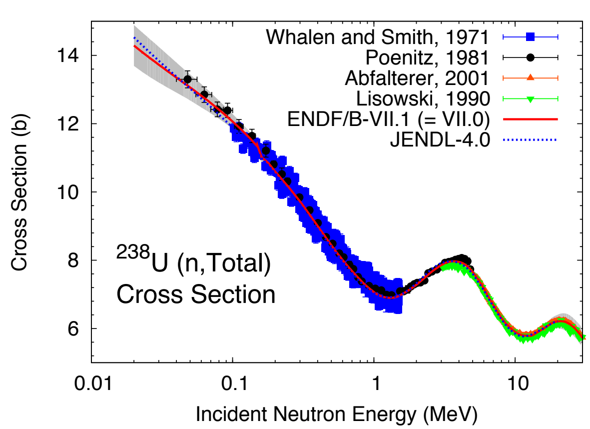
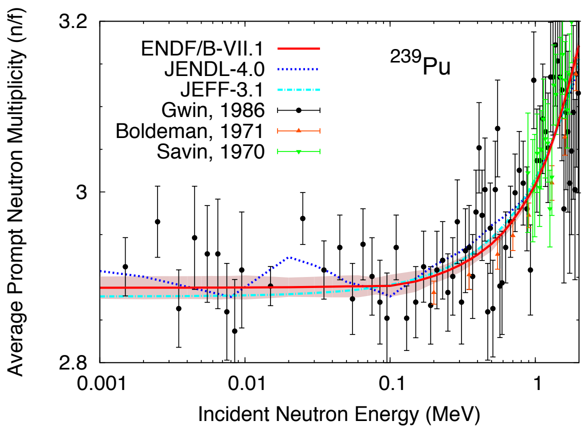
- What is a nuclear data evaluation?
- The need for evaluations
- In practice
- How to perform an evaluation?
  - Retrieving and analyzing experimental data
  - Uncertainties & errors
  - Theories, Models & Codes
  - Putting it together
- Integral data testing
- International efforts & CIELO

What is a Nuclear Data Evaluation?

- An attempt to represent the true values of nuclear reaction data, e.g., cross sections, angular distributions of secondary ejectiles, etc.







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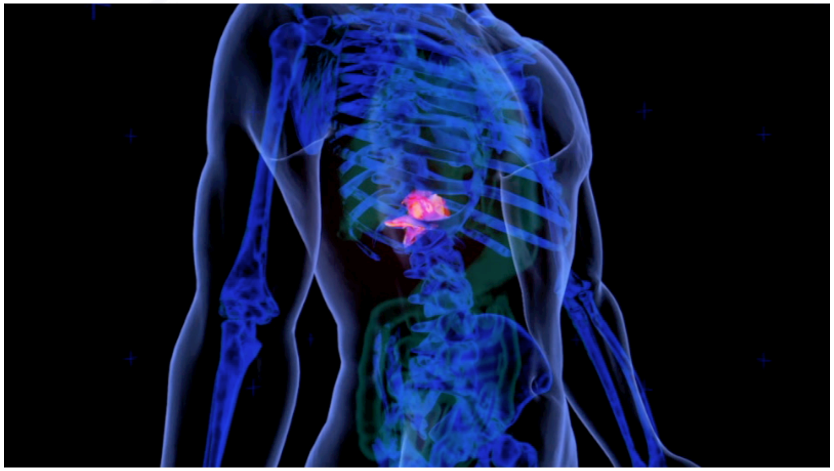
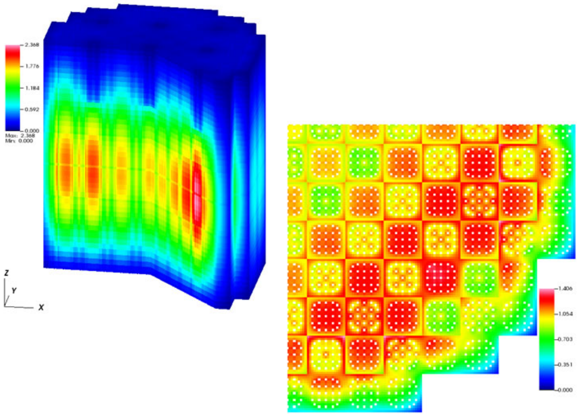
Nuclear Applications and the Need for Nuclear Data

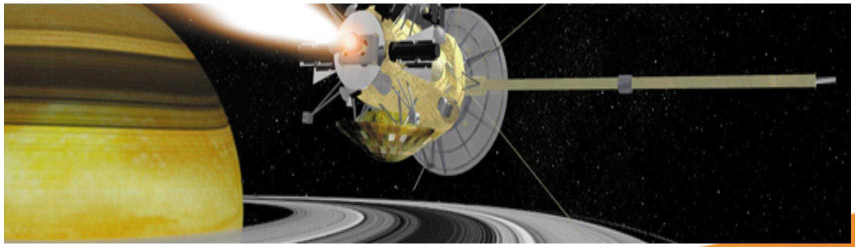


Very small amounts of radioactive material injected in the body will emit gamma rays that can be detected and "imaged".

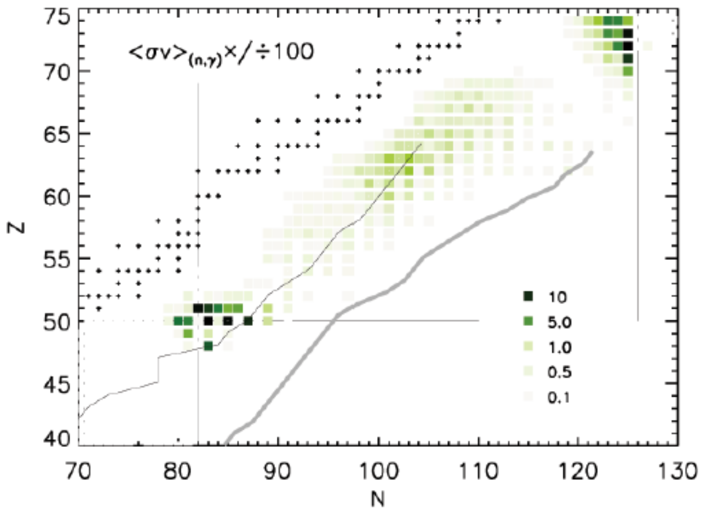


MPACT simulations of the fission rate distribution in the fuel rods for the initial criticality of the reactor at zero power. (from CASL, www.casl.gov)

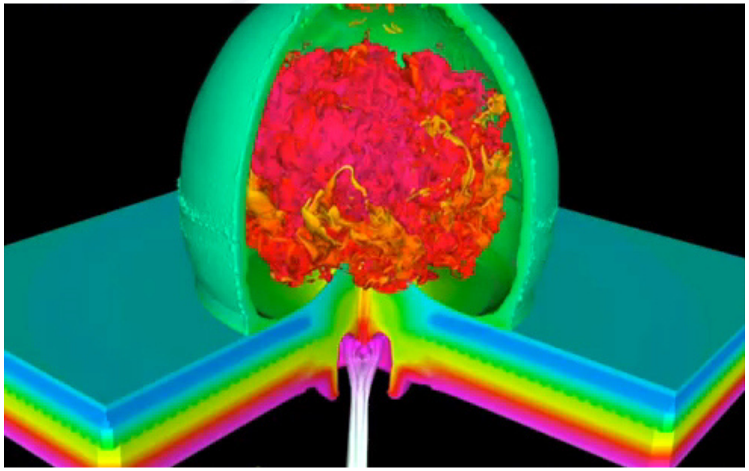
Radioisotope thermoelectric generators (RTGs) are used to power unmanned spacecraft, using the heat from plutonium to generate electricity.



Applications



Nucleosynthesis in astrophysics (plot by M.Mumpower)



A Los Alamos computer model helps scientists understand the hydrodynamics of how solids mix and flow as a result of a high-velocity projectile striking a metal surface

Passive and active neutron and gamma interrogation.

But… why do we need them?

- Don’t we know everything already?
- New applications require new data
  - Isotopes
  - Energies
  - Quantities, e.g., $d^2\sigma/dEd\Omega$
  - …
- Current data are not accurate enough
  - Discrepancies in C/E
  - Better simulations require better data
  - Extrapolation to new regions of nuclear chart
  - …

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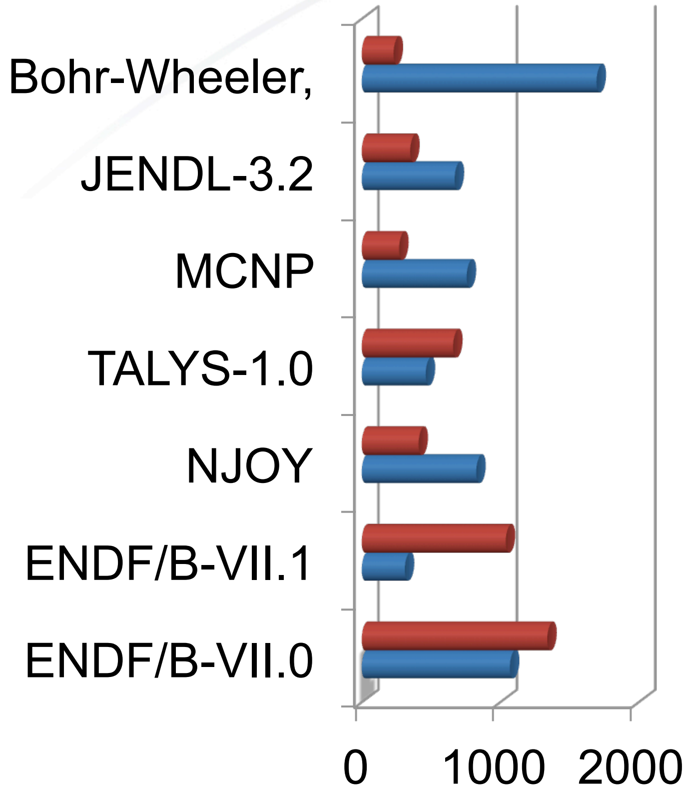
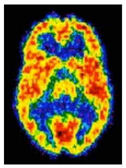
How to estimate the impact of nuclear data evaluations?



to compare with Kim Kardashian's wedding…
~150 (million) Google hits

- Nuclear Energy 
  - "As of May 2014, 30 countries worldwide are operating 435 nuclear reactors for electricity generation and 72 new nuclear plants are under construction in 15 countries," Nuclear Energy Institute (2014).
- Nuclear Medicine 
  - More than 25 million nuclear medicine procedures performed each year in the USA, J.Nucl.Med. 52, 24S (2011).
- …

In practice…

A nuclear data evaluation consists of a computer ASCII file in a specific format

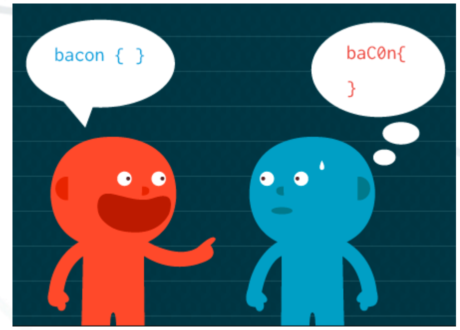
- General information (authors, comments on the evaluation process for different sections, etc)
- Resonance region parameters
- Cross sections for all open channels on a given incident energy grid (σ(E))
- Differential spectra (dσ/dE; dσ/dΩ) or/and double-differential spectra ($d^2\sigma/dEd\Omega$)
- Average fission neutron multiplicities, ν
- Average prompt fission neutron spectra, χ
- etc.
- Uncertainties (covariance matrices)

An evaluated library is a (consistent?) collection of such files

```
 3.908900+4 8.814210+1          0          0          0          03925 3 16    1
-1.147600+7-1.147600+7          0          0          1          193925 3 16    2
         19          2                                            3925 3 16    3
 1.160670+7 0.000000+0 1.200000+7 7.250379-2 1.250000+7 2.733047-13925 3 16    4
 1.300000+7 4.878440-1 1.350000+7 6.701030-1 1.400000+7 8.235300-13925 3 16    5
 1.410000+7 8.500000-1 1.450000+7 9.561400-1 1.500000+7 1.070000+03925 3 16    6
 1.550000+7 1.145000+0 1.600000+7 1.180000+0 1.650000+7 1.210000+03925 3 16    7
 1.700000+7 1.230000+0 1.750000+7 1.235000+0 1.800000+7 1.240000+03925 3 16    8
 1.850000+7 1.240000+0 1.900000+7 1.240000+0 1.950000+7 1.235000+03925 3 16    9
 2.000000+7 1.230000+0                                            3925 3 16   10
 0.000000+0 0.000000+0          0          0          0          03925 3  099999
```

Sample of the ENDF/B-VII.1 file for n+^{89}Y
[MF=3, MT=16, (n,2n) cross section]

OECD/WPEC Subgroup 38



- "Beyond the ENDF format:
  A modern nuclear database structure"
- GND: "Generalized Nuclear Data" format
- Leadership from LLNL/BNL
- Some of the goals: (from D.P.McNabb, May 2012)
  - Next generation more comfortable with and interested in modern concepts (XML, HDF5,MySQL, Python, Java)
  - Leverage vast, well-tested infrastructure
  - Remove artificial limits imposed by legacy formats
  - Link disparate databases to each other
- Significant efforts needed to move from ENDF to GND
  (even the name is controversial!)

Evaluated Nuclear Data Format (ENDF)

- A strict format to encapsulate nuclear reaction information
- Important identifiers: MAT for material, MF for reaction type, MT for reaction channel

- MAT=9546 for Am-242
- MF=3 for cross sections
- MT=1,2 for total, elastic
- …

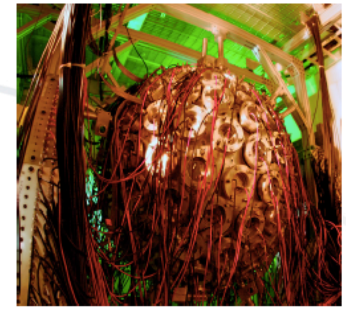
```
 9.524200+4 2.399801+2          1          1          0          19546 1451    1
 0.000000+0 0.000000+0          0          0          0          69546 1451    2
 1.000000+0 2.000000+7          0          0         10          79546 1451    3
 0.000000+0 0.000000+0          0          0        123         869546 1451    4
 95-Am-242 LANL       EVAL-DEC04 Talou,Young,Kawano                9546 1451    5
                      DIST-DEC06                                   9546 1451    6
----ENDF/B-VII        MATERIAL 9546                                9546 1451    7
-----INCIDENT NEUTRON DATA                                         9546 1451    8
------ENDF-6 FORMAT                                                9546 1451    9
                                                                   9546 1451   10
```

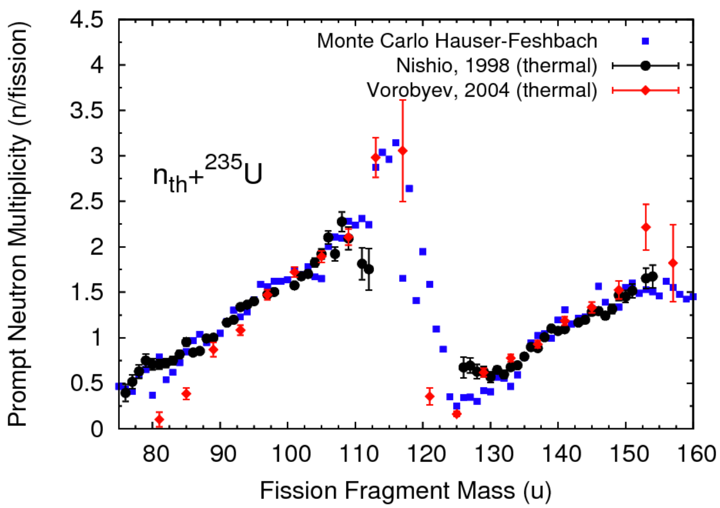
n+Am-242 ENDF/B-VII.1 File Header

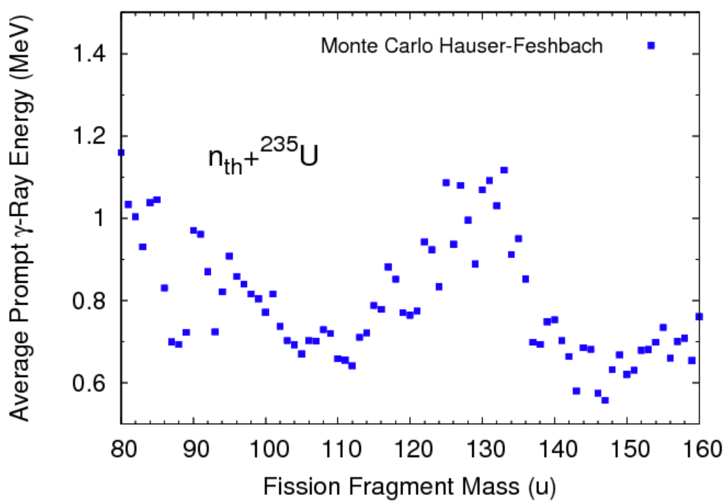
ENDF-6 Formats Manual
CSEWG Document ENDF-102, Report BNL-90365-2009 Rev.2
http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

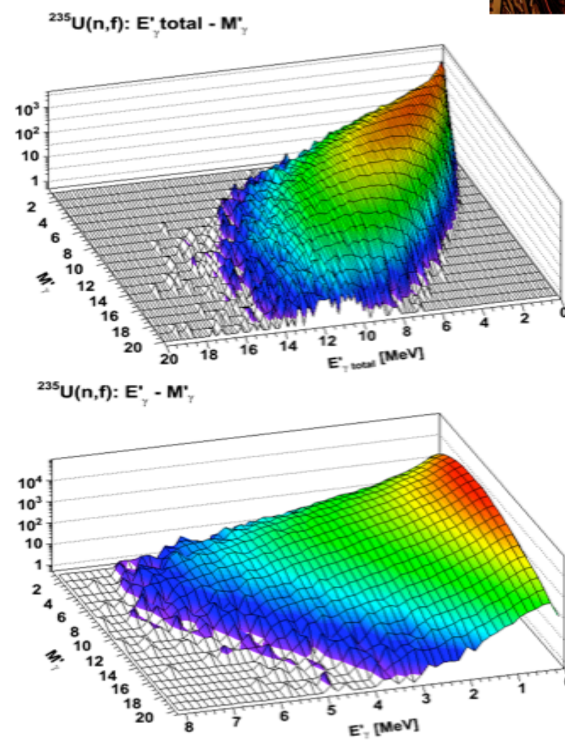
Can we store everything in data tables?

- Example: correlated data



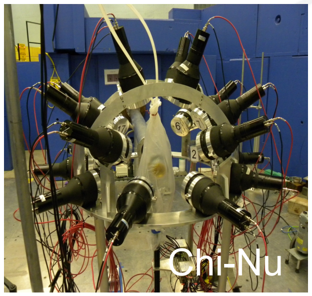






DANCE (Los Alamos) measurement of prompt fission γ-ray energy and multiplicity, M.Jandel et al.

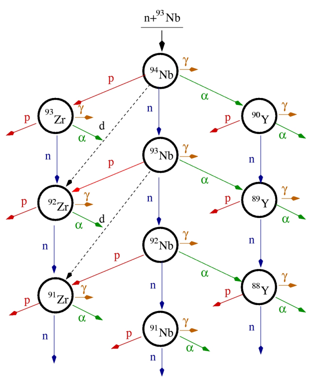
How to perform an evaluation?



(differential) Experimental Data

Comparisons

Theory/Modeling

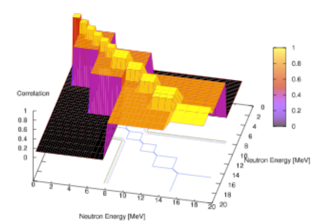


Model Input Parameters

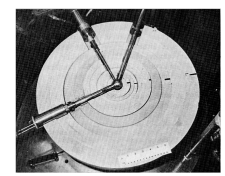
ENSDF
RIPL-3
…

"Least-Square Fits"

Uncertainty Quantification



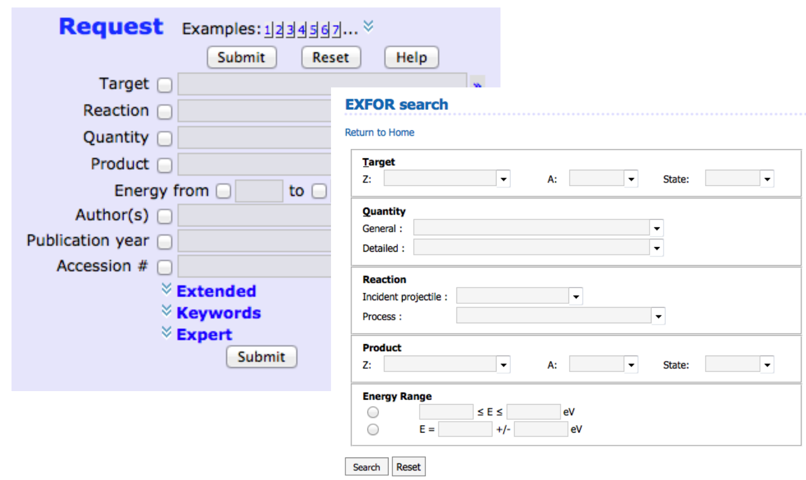
Comparisons with integral benchmarks

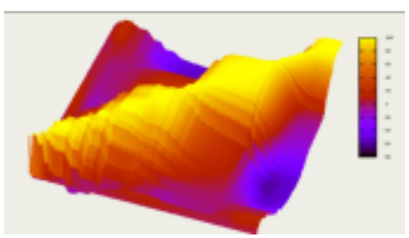


Feedback

Analyzing experimental data

- Online databases of experimental data (EXFOR)
- Retrieval & Visualization Tools
- Dealing with discrepant data sets
- Quantifying experimental uncertainties





http://www.nndc.bnl.gov/exfor/exfor.htm
http://www.oecd-nea.org/janisweb/search/exfor

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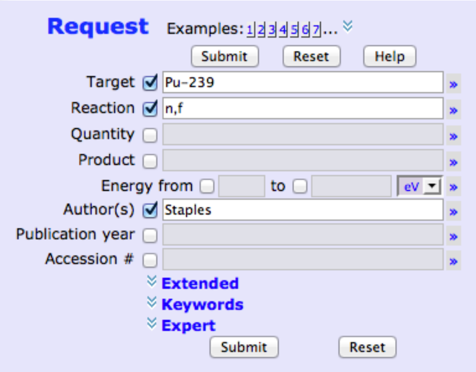
Retrieving experimental data

Searching for Prompt Fission Neutron Spectrum (PFNS) experimental from Parrish Staples, 1995



- Through a Nuclear Data Center (the EXFOR online database)

n	Display	Year	Author-1	Energy range,eV		Points	Reference	Subentry#P	NSR-Key	
1)	94-PU-239(N,F),,NU/DE,,REL C4: MF5 MT18									
Quantity: [MFQ] Diff. fiss. neutron multiplicity d/dE(n)										
1	Info X4+ X4± T4	1995	P.Staples+	5.00e5	3.50e6	275	+ J,NP/A,591,41,1995	13982003	1995ST22	E2=6e5:1.6e7

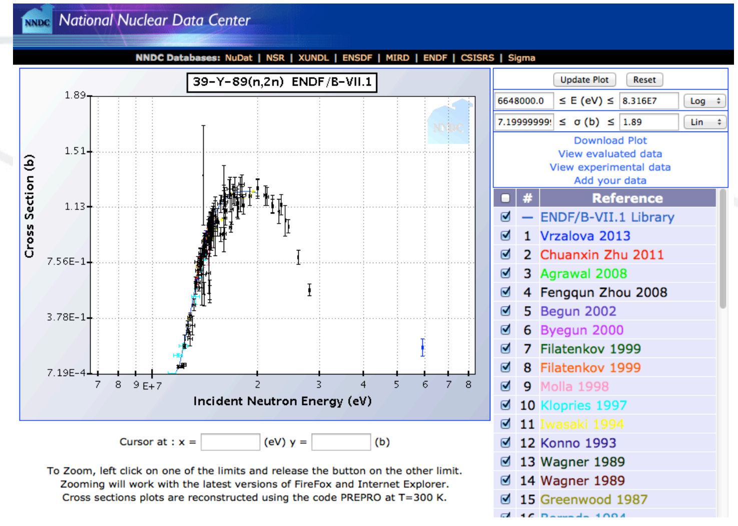
- Through literature search (Google works too!)

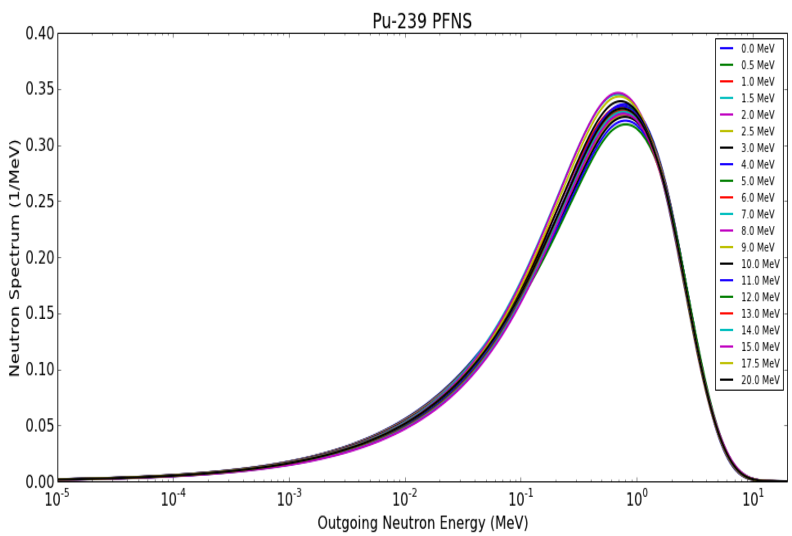
Prompt fission **neutron** energy **spectra** induced by fast... | INIS
inis.iaea.org/search/search.aspx?... International Atomic Energy Agency
by P Staples - 1995 - Cited by 41 - Related articles
Prompt fission **neutron** energy **spectra** for 235 U and 239 Pu have been measured for fission **neutron** energies ... by **Staples**, P. (Massachusetts Univ., Lowell, MA (United States). ... 591(1); ISSN 0375-9474; CODEN NUPABL; 14 Aug **1995**; p.

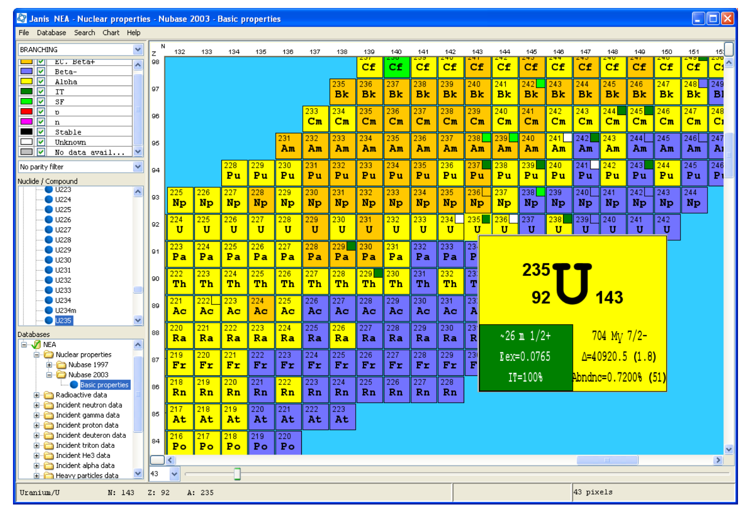
We will walk through some examples during the mini-workshop

Visualization Tools

- SIGMA (NNDC)
- JANIS (NEA)
- “Home-made” (gnuplot, matplotlib, …)







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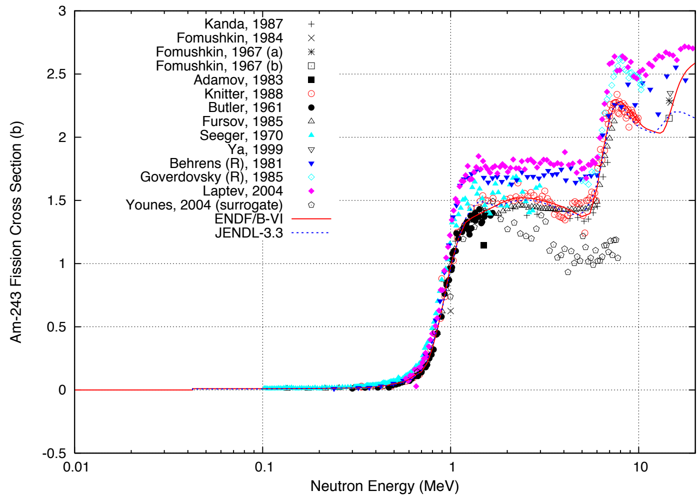
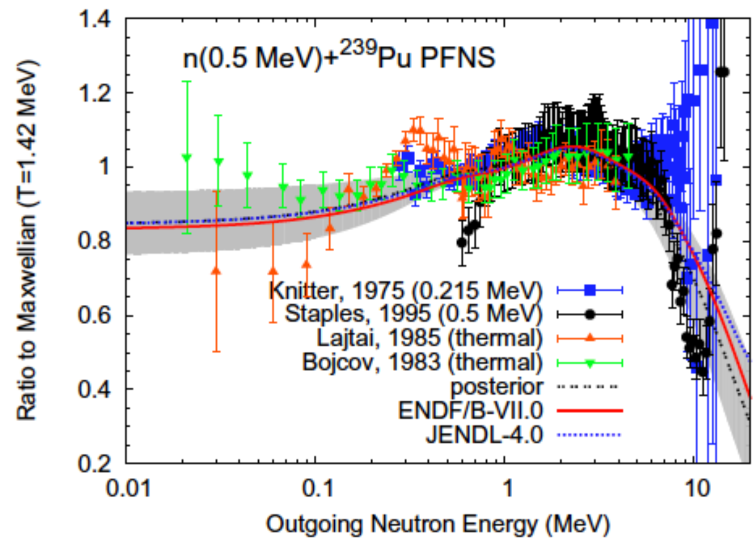
Dealing with discrepant data sets





Average cross sections calculated with the **ZEBRA (Zero Energy Breeder Reactor Assembly)** reactor spectrum favors low-energy group.

"The fission cross-section ratios for 240Pu and 243Am and the reference nucleus 235U obtained in the "shape" measurements have been normalized using the existing data of Staples *et al*. [7] and **Behrens *et al*. [8]** in the energy range about 1-2 MeV.", A.B.Laptev et al., Nucl. Phys. A734 (2004) E45-48

Quantifying Uncertainties & Correlations

- What is an uncertainty?
- Statistical vs. Systematic
- How to report them?
- Constructing a covariance matrix

"Experimental Nuclear Reaction Data Uncertainties: Basic Concepts and Documentation," D.L.Smith and N.Otuka, Nucl. Data Sheets **113**, 3006 (2012)

Probability, Uncertainty, … A (very) concise reminder

- Probability function
  $$f(x) = P(X = x)$$
  $$0 \leq f(x_i) \leq 1; \sum_i f(x_i) = 1$$
- Expected value (mean)
  $$\mu_X = E(X) = \int x f(x) dx$$
- Variance and standard deviation
  $$\sigma_X^2 = E\left[((X - E(X))^2\right]$$
  $$\text{std} = \sigma_X = \sqrt{\sigma_X^2}$$
- Covariance
  $$\text{cov}(X, Y) = E\left[(X - E(X)).(Y - E(Y))\right]$$
- Correlation
  $$\rho(X, Y) = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y}$$

Constructing a covariance matrix:

^{237}Np (n,f) Cross Section Measurement, F.Tovesson et al., LA-UR-06-7318

$$R_{ab}(E) = \frac{\sigma_a(E)}{\sigma_b(E)} = \frac{N_b}{N_a}\left[\frac{w_1^{-1}(E).C_1(E)-C_1^{Bg}(E)}{\epsilon_1(E).\Phi_1(E)} - \sum_{i\neq a} N_i^1\sigma_i(E)\right] / \left[\frac{w_2^{-1}(E).C_2(E)-C_2^{Bg}(E)}{\epsilon_2(E).\Phi_2(E)} - \sum_{j\neq b} N_j^2\sigma_j(E)\right]$$

- Fission Cross Section Ratio Measurement main sources of uncertainty:
  - Statistical
  - Number of atoms in the samples
  - Dead-time corrections
  - Background
  - Neutron flux
  - Cross sections for impurities
  - …

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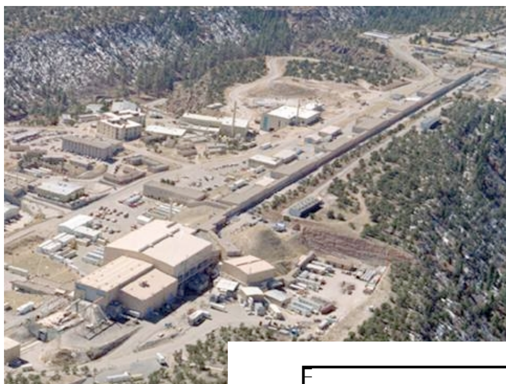
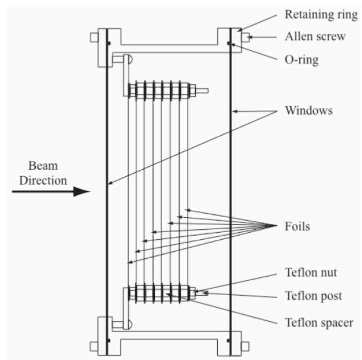
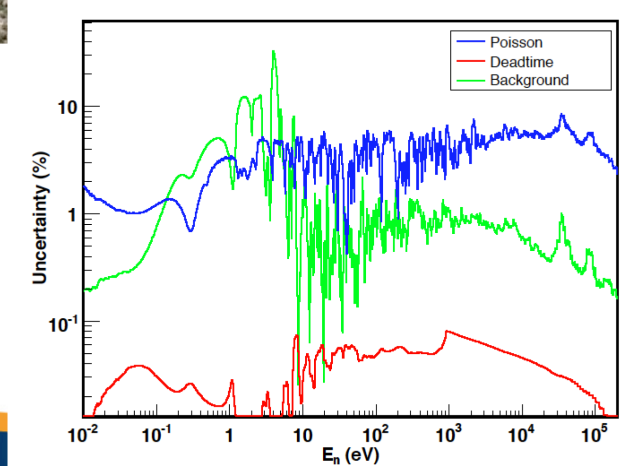
^{237}Np (n,f) Cross Section Experimental Covariance Matrix

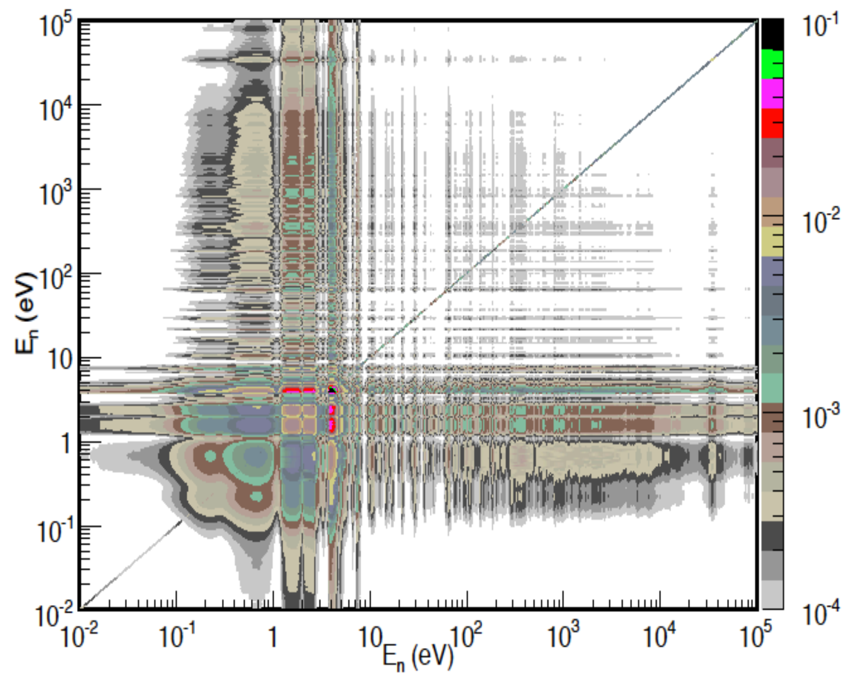
$$R_{ab}(E) = \frac{\sigma_a(E)}{\sigma_b(E)} = \frac{N_b}{N_a}\cdot\frac{\epsilon_2(E)}{\epsilon_1(E)}\cdot\frac{\Phi_2(E)}{\Phi_1(E)}\cdot\frac{w_1^{-1}(E).C_1(E)}{w_2^{-1}(E).C_2(E)-C_2^{Bg}(E)} - \frac{N_b.\epsilon_2(E).\Phi_2(E)}{w_2^{-1}(E).C_2(E)-C_2^{Bg}(E)}\cdot\left[\frac{N_c}{N_a}.\sigma_c(E) + \frac{N_d}{N_a}.\sigma_d(E)\right]$$

- This experiment:









We will produce a covariance matrix in the mini-workshop

Nuclear Reaction Theories & Modeling

- Why do we need them?
  - No (accurate!) experimental data available for all isotopes, energies, etc.
  - Extrapolations
  - Complete evaluated data (e.g., all open channels) for applications

- Different energy regimes, different mass ranges, different representations
  - Low-A nuclei: R-matrix fits
  - Medium to heavy nuclei:
    - Low energies (thermal to ~keV): resolved resonance parameters
    - Unresolved resonance region: probability tables
    - Fast range (up to ~200 MeV): statistical theories, e.g., Hauser-Feshbach
    - Higher energies: intra-nuclear cascades

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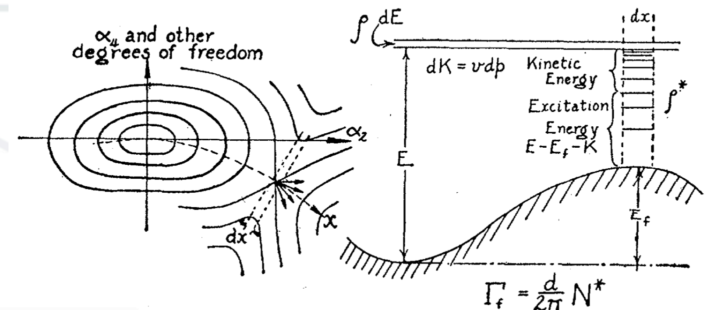
NNSA National Nuclear Security Administration

Los Alamos NATIONAL LABORATORY EST. 1943

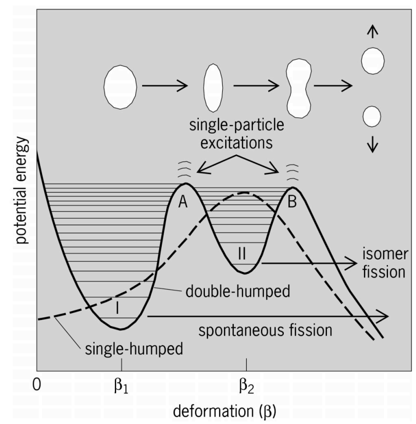
Nuclear Reaction Models

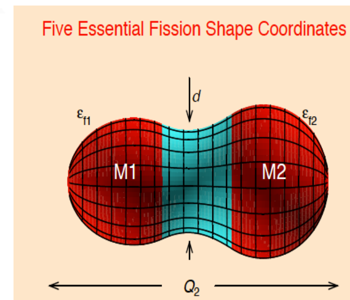
- Resolved-resonance and URR ranges
  (see F.Gunsing, this school)
- Fast neutron energy range:
  (see S.Hilaire, this school)
  - Optical model and coupled-channel calculations to obtain
    - Direct elastic and inelastic cross sections
    - Reaction and shape compound cross sections
    - Transmission coefficients for individual reaction channels
  - Pre-compound reactions
    - Exciton model, FKK, TUL, NWY
  - Hauser-Feshbach statistical theory
  - Fission cross section theory
  - Many phenomenological ingredients

Fission Cross Section Modeling

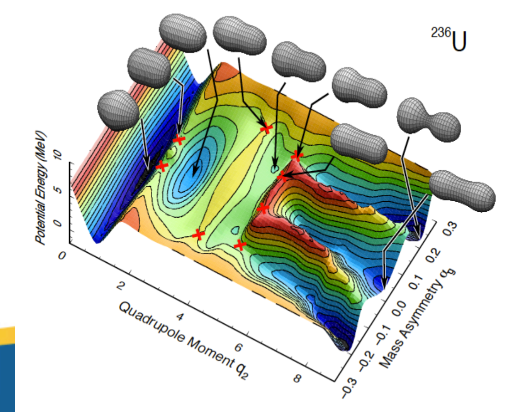


- A.Bohr's transition states
- Transmission coefficients calculated as barrier tunneling penetrability
- Liquid-drop model + shell-corrections → double-humped fission barriers
- Significant complications:
  - Double-humped structure
  - Transition states
  - Level density on top of barriers
  - Inertia tensor
  - Etc.
- Many adjustable parameters!



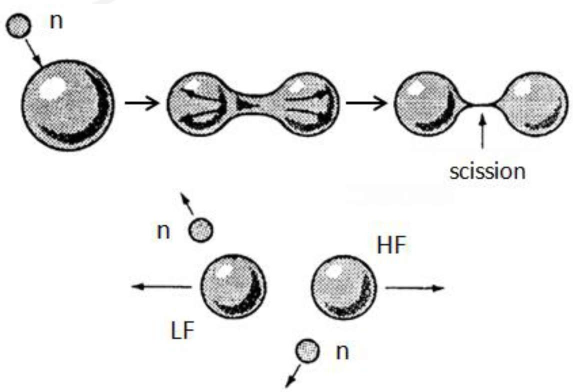


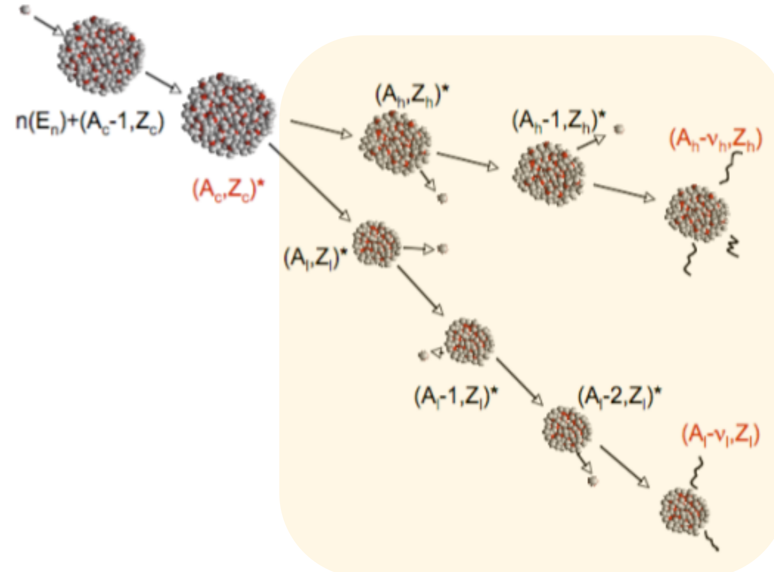
Finite-Range Liquid Drop Model
P.Möller (LANL)
5D ; more than 5 million point calculations



Prompt Fission Neutrons

(see F.Gönnenwein, this school & FIESTA2014)





- A fission event leads (most often) to the formation of two complementary and excited fission fragments.
- Prompt fission neutrons are emitted within 10^{-18}s to 10^{-14}s from the scission time.
- Prompt fission gammas are mostly emitted following the emission of neutrons.

Two basic questions:

- How many neutrons are emitted per fission?
- What is their energy distribution?

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PFNS Modeling

- Madland-Nix model, Nucl. Sci. Eng. **81**, 213 (1982)
  - Evaporation spectrum in c.m. of fragments
  - Kinetic boost in the laboratory
  - Triangular temperature distributions in light and heavy fragments
  - Average over spectra from both fragments
  - Average over many distributions
  - → computes average neutron spectrum and multiplicity

$$N(E) = \frac{1}{2\sqrt{E_f}T_m^2} \int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} d\epsilon \sigma_c(\epsilon)\sqrt{\epsilon} \times \int_0^{T_m} dT k(T) T \exp(-\epsilon/T)$$

- Monte Carlo Hauser-Feshbach modeling
  - Lemaire, Talou et al., Phys. Rev. C 72, 024601 (2005)
  - Vogt, Randrup et al., Phys. Rev. C 73, 014602 (2009)
  - Litaize and Serot, Phys. Rev. C 82, 054616 (2010)
  - Stetcu, Talou et al., Phys. Rev. C 90, 024617 (2014)
  - → computes detailed neutron and gamma distributions and correlations

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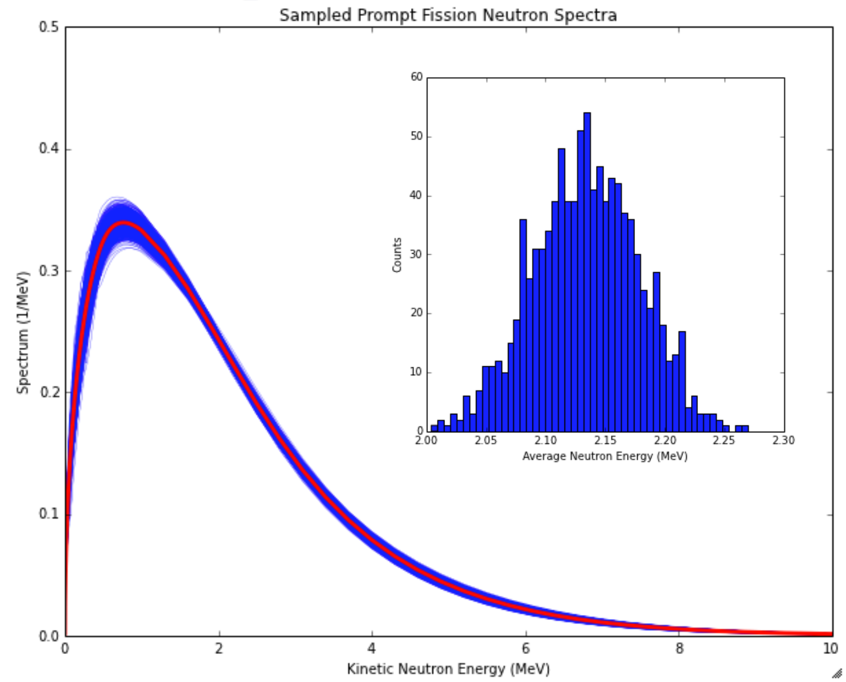
Constraining Model Parameters & UQ

- Sampling the model input parameter space
  - Brute force Monte Carlo
  - Principal component analysis
  - …
- Model-predicted uncertainties
- Limitations?
  - Only model-based variances
  - Only model-based correlations
  - The model is assumed to be *perfect*!



We will generate those PFNS samples in the mini-workshop

Putting it together:
Model predictions and Experimental Data

- Why experiments are not enough…
  - Do not cover all energies, isotopes, angles, correlations, etc, of interest
  - Sometimes discrepant
  - Uncertainties, errors, …
- Why models are not enough…
  - Not often based on first principles → phenomenology
  - Adjustable parameters constrained by experiments
  - Model limitations
- We have to work together ☺

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A learning process

- The Bayesian Inference Scheme
  - A natural learning process
- Applying Bayes to Nuclear Data Evaluations
  - An example of applying Bayes to parameter fitting
- Other techniques: Monte Carlo, GLS, etc.

- "The logic of scientific data evaluation," F.H.Fröhner
- "Programming a Robotic Car," UDACITY Free Course, https://www.udacity.com/course/cs373

Bayes Theorem

(derived from basic probability theory)

likelihood　　prior

$$P(A|BC) = \frac{P(B|AC) \times P(A|C)}{P(B|C)}$$

posterior

- The *posterior probability P(A|BC)* of an hypothesis A given that both B and C are true is given by the product of a *likelihood function, P(B|AC)*, and a *prior probability, P(A|C)*.
- If B represent some experimental data that have been measured, and A is a physics model that represents the same physical quantity, P(A|BC) represents the probability that the model A is correct, given the observed B, under circumstances C.

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The Kalman filter

- R.E.Kalman, Trans. of the ASME- Journal of Basic Engineering, 82 (Series D): 35-45 (1960).
- First used in the Apollo space program for tracking trajectories

State transition model   Control input model

$$x_k = F_k x_{k-1} + B_k u_k + w_k$$

True state at time *k*   Control vector   Noise $w_k \sim \mathcal{N}(0, Q_k)$

+ observation at time *k*: $z_k = H_k x_k + v_k$ ← Observation noise $v_k \sim \mathcal{N}(0, R_k)$

Observation model

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The Kalman filter (cont'd)

- Two distinct phases: Predict and Update

Predict

$$x_{k|k-1} = F_k x_{k-1} + B_k u_k$$

$$P_{k|k-1} = F_k P_{k-1} F_k^T + Q_k$$

Update

$$y_k = z_k - H_k x_{k|k-1}$$

$$S_k = H_k P_{k|k-1} H_k^T + R_k$$

Optimal Kalman gain →

$$K_k = P_{k|k-1} H_k^T S_k^{-1}$$

$$x_k = x_{k|k-1} + K_k y_k$$

$$P_k = (I - K_k H_k) P_{k|k-1}$$

} Updated state and covariance estimates

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Kalman filter and Nuclear Data Evaluations

- No dynamics: u_k, B_k, F_k disappear
- No prediction step: $x_{k|k-1}=x_{k-1}$; $P_{k|k-1}=P_{k-1}$

The Kalman filter is used as a recursive Bayesian estimation.

$$x_k = x_{k-1} + K_k(z_k - H_k x_{k-1})$$
$$P_k = (I - K_k H_k) P_{k-1}$$

with

$$H_k = \frac{\partial z_k}{\partial x_k}$$
$$K_k = P_{k-1} H_k^T (H_k P_{k-1} H_k^T + R_k)^{-1}$$

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Extended Kalman filter

- First-order Taylor series expansion around x_0

$$y = f(x) + e \simeq f(x_0) + C(x - x_0) + e$$

Sensitivity matrix

- Following the notations of T.Kawano, Nucl. Sci. Eng. 131, 107 (1999):

$$x_1 = x_0 + XC^T(CXC^T + V)^{-1}(y - f(x_0))$$
$$P = X - XC^T(CXC^T + V)^{-1}CX$$

posterior (P) prior (X)

We will code a Kalman filter in the mini-workshop

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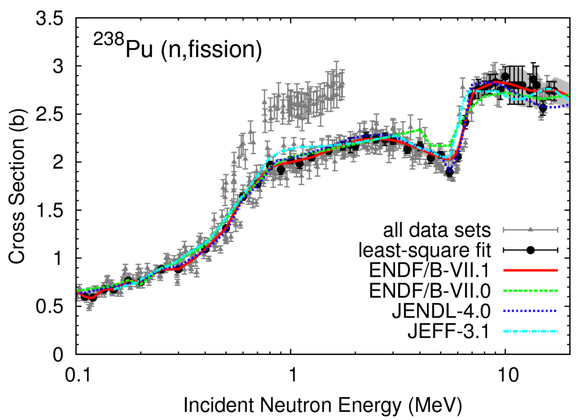
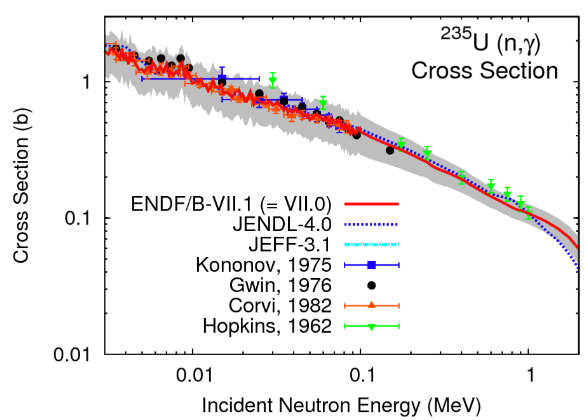
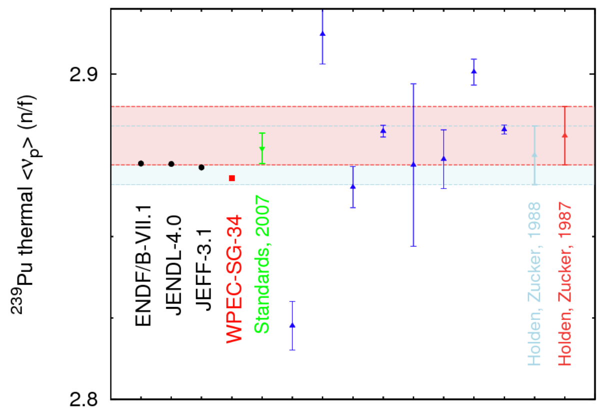
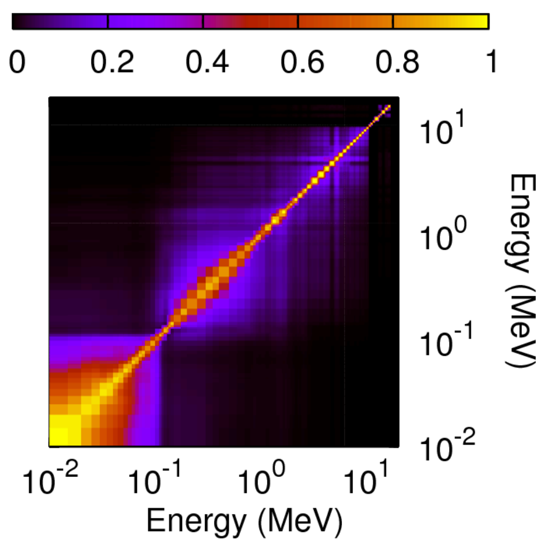
Final mean values and uncertainties

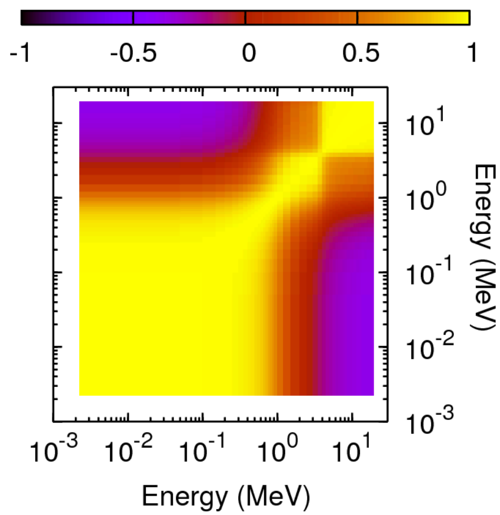
Some examples











More weight on the model tends to lead to stronger correlations.

Other techniques to estimate

Uncertainties on evaluated nuclear data

- "Filtered" Monte Carlo, A.Koning
- "Backward-forward Monte Carlo," E.Bauge
- "Unified Monte Carlo," D.L.Smith, R.Capote, M.Rising, P.Talou
- "Total Monte Carlo," A.Koning, D.Rochman

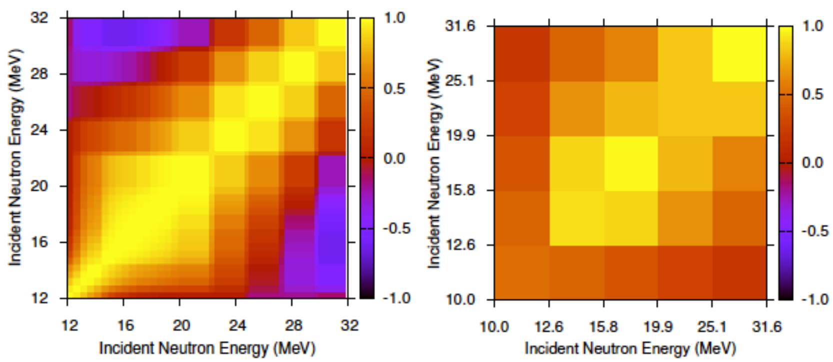
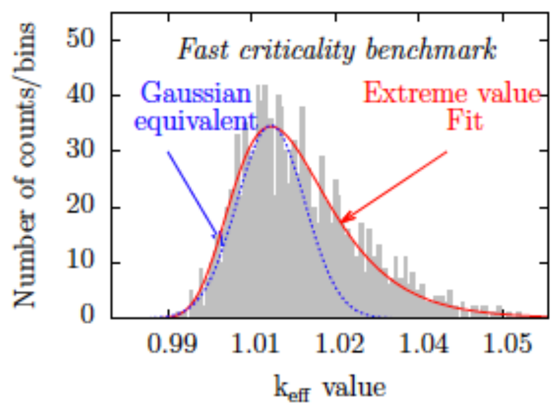


Figure 22: The correlation matrix for the ^{89}Y(n,2n) reaction obtained with KALMAN using full set of experimental data for all reaction channels (top). The same for MC method (bottom).

[OECD/NEA WPEC SG24 (2011)]



[A.Koning and D.Rochman, Ann. Nucl. Ene. 35, 2024 (2008)]

The “Standards”

A.D.Carlson et al., Nucl. Data Sheets 110, 3215 (2009)

- Used for calibration and ratio measurements
  → “eliminate the need for a direct measurement of the neutron fluence”
- Standard Reaction Cross Sections:
  H(n,n), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,$\alpha_1\gamma$), C(n,n), Au(n,γ), ^{235}U(n,f)
- Thermal constants
- Evaluations based on **experimental data only**!
- GMA least-square code
- Cross-isotope correlations included

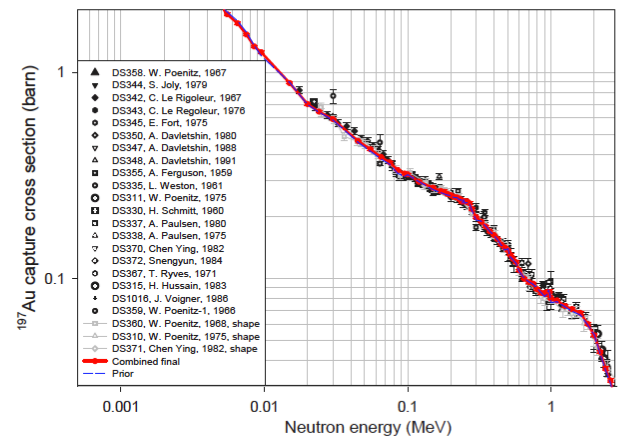
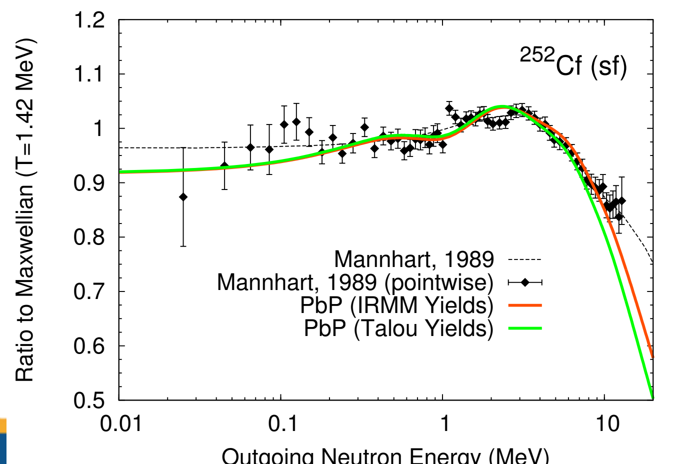


FIG. 7.29. Comparison of present and prior evaluations, together with experimental data for the Au(n,γ) reaction.

^{252}Cf (sf) standard Prompt Fission Neutron Spectrum



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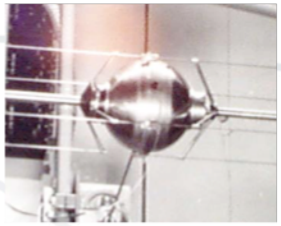
A Critical Look at Evaluated Uncertainties

Sir Winston Churchill: *"Statistics are like a drunk with a lampost: used more for support than illumination."*

- An uncertainty **IS NOT** a physical quantity!
- Is there only one right answer?
  - **No**, but do the evaluated uncertainties make sense?
- What if the models fail?
- Propagating Uncertainties in transport simulations (see later)

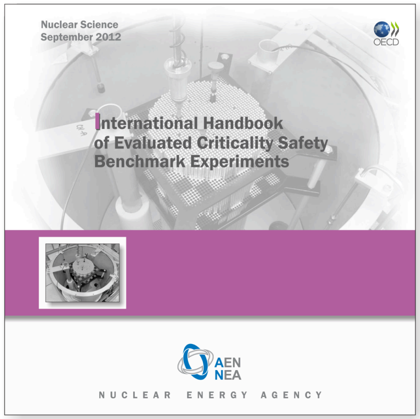
Integral Data Testing



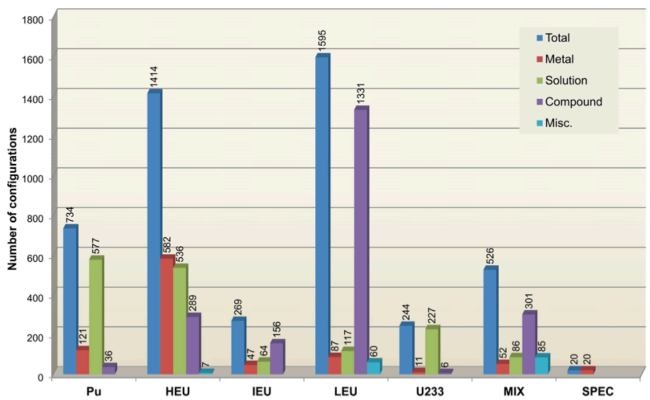
Jezebel ^{239}Pu critical assembly

Lady Godiva ^{235}U critical assembly

- Validating nuclear data evaluations
- Using radiation transport codes (e.g., MCNP) to simulate well-characterized experiments
- ICSBEP Handbook, "International Criticality Safety Benchmark Evaluation Project"



Handbook Contents



http://icsbep.inel.gov/handbook.shtml

Testing ENDF/B-VII.0

M.B.Chadwick et al, Nuclear Data Sheets **107**, 2931 (2006)

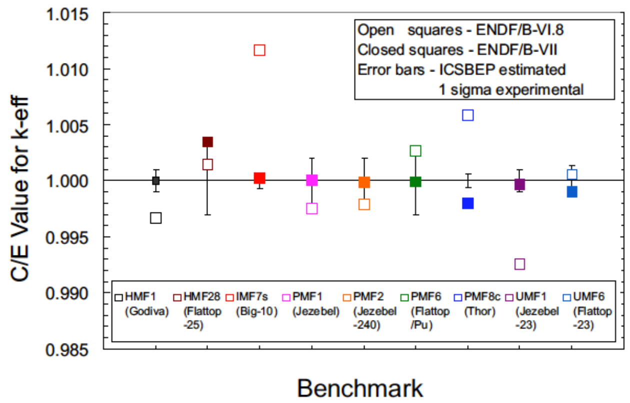


FIG. 86: LANL HEU, Pu and ^{233}U unmoderated benchmark C/E values for $k_{\rm eff}$ calculated with ENDF/B-VI.8 and ENDF/B-VII.0 cross section data.

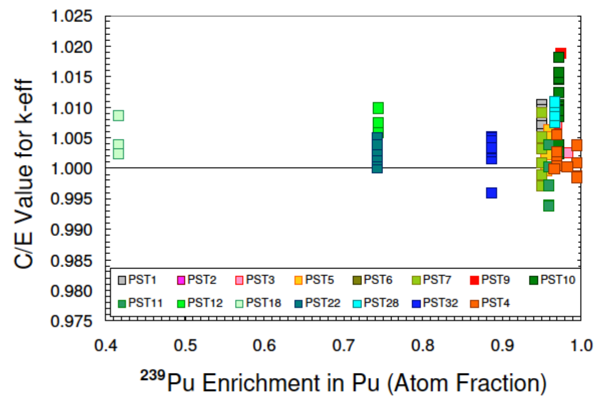
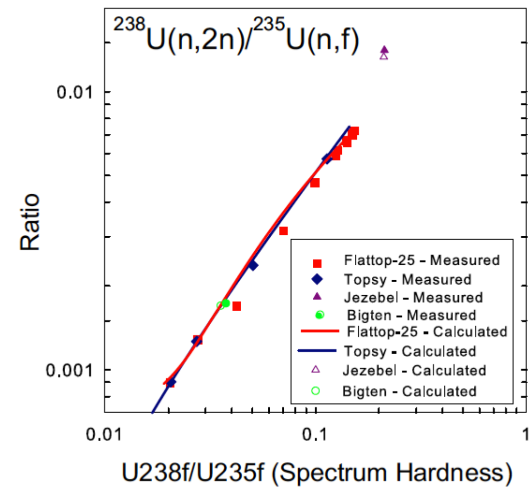


FIG. 101: PU-SOL-THERM benchmark C/E values for $k_{\rm eff}$ with ENDF/B-VII.0 cross sections as a function of the ^{239}Pu enrichment.



- Using the NJOY/MCNP code system
- Excellent agreement between MCNP5 and Tripoli-4.4.1 calculations

◆ Sometimes… we get the right result for the wrong reasons… Beware of compensating errors!

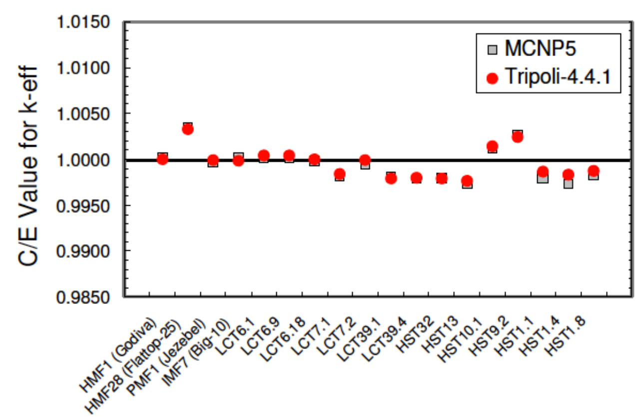


FIG. 103: C/E values for $k_{\rm eff}$ obtained with MCNP5 and Tripoli-4.4.1 codes using ENDF/B-VII.0. Excellent agreement is seen between these two independent calculations.

Propagation of PFNS Uncertainties in Transport Simulations

NUCLEAR SCIENCE AND ENGINEERING: **175**, 188–203 (2013)

Prompt Fission Neutron Spectrum Uncertainty Propagation Using Polynomial Chaos Expansion

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Received October 8, 2012
Accepted January 18, 2013

Principal Component Analysis (PCA)

→ PFNS realizations

$$\chi_m = \langle \chi \rangle + \sum_{k=1}^{K} \sqrt{\lambda_k} \vec{\varphi}_k \xi_{k,m}$$

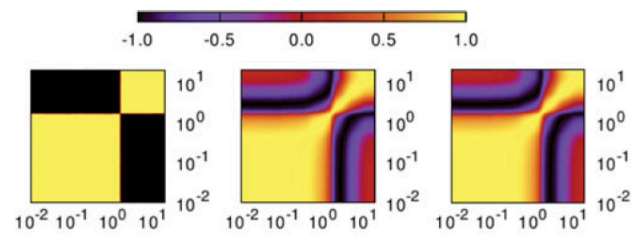


Fig. 3. The reconstructed correlation matrix of the $n + {}^{235}U$ PFNS depending on the PCA expansion order: (a) $K = 1$, (b) $K = 2$, and (c) ENDF/B-VII.1 library. Note that the axes on all plots are for the outgoing neutron energy in MeV.

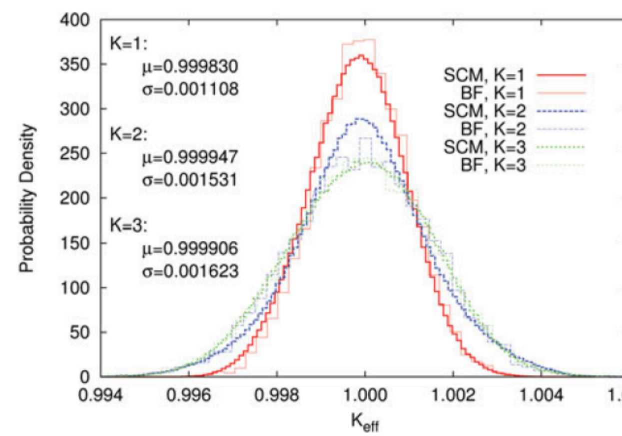
Polynomial Chaos Expansion (PCE)
Stochastic Collocation Method (SCM)

TABLE V

Jezebel Relative Uncertainties: k_{eff}, Total Leakage, and $\mathcal{I}^{(238f)}$, $\mathcal{I}^{(237f)}$, and $\mathcal{I}^{(239f)}$ Spectral Indices Assuming a Uniform Distribution for the Principal Components*

	Direct Sampling (10^4)				Stochastic Collocation Method (4^K)			
		Principal Components				Principal Components		
Integral Quantity	Monte Carlo Statistics[a] (%)	$K = 1$ (%)	$K = 2$ (%)	$K = 3$ (%)	Monte Carlo Statistics[a] (%)	$K = 1$ (%)	$K = 2$ (%)	$K = 3$ (%)
k_{eff}	0.0001	0.1069	0.1563	0.1621	0.0007	0.1041	0.1584	0.1611
Leakage	0.0001	0.0183	0.0199	0.0207	0.0006	0.0180	0.0189	0.0198
$\mathcal{I}^{(238f)}$	0.0026	1.1424	1.6902	1.6978	0.0145	1.1936	1.7023	1.7034
$\mathcal{I}^{(239f)}$	0.0018	0.1671	0.1678	0.1687	0.0101	0.1606	0.1707	0.1693
$\mathcal{I}^{(237f)}$	0.0021	0.7542	0.7827	0.7826	0.0114	0.7513	0.7922	0.7847

*Note that the number of transport solutions for each method are indicated in parentheses.
[a]Calculation based on $K = 3$ principal components.



"Total Monte Carlo"

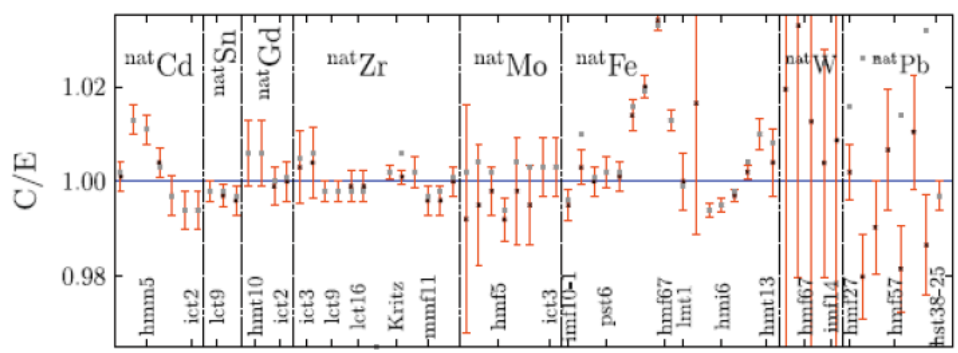
A new paradigm?

A.J.Koning and D.Rochman,
Nuclear Data Sheets **113**, 2841 (2012)

International Workshop on Nuclear Data Covariances, Santa Fe, NM, 2014

- **TALYS**: robust nuclear reaction model code
- Vary model input parameters within reasonable ranges
- TALYS-1.60 Evaluated Nuclear Data Library: TENDL-2014
(global default calculations + adjusted calculations for some isotopes/reactions)
- Complete covariance information

→ "Total Monte Carlo" by pursuing the evaluation process all the way through transport simulations, bypassing the need for covariances.



- Uncertainties on calculated benchmarks
- Non-normal distributions
- Adjustments
- Relies heavily on model calculations

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Library Development Efforts in the World

- ENDF/B-VII.1, USA, 2011 (B-VII.0, 2006)
- JEFF-3.2, Europe/OECD, 2014
- TENDL-2014, NRG, Petten, 2014
- JENDL-4.0, Japan, 2010
- ROSFOND, Russia, 2010
- CENDL-3.1, China, 2009

Who to trust?...

The CIELO Collaboration

OECD/WPEC Subgroup 40

- "Collaborative International Evaluated Library Organization Pilot Project"
- "A stronger and wider international collaboration is proposed to foster evaluated nuclear data advances and provide improved data for fission, fusion , and other nuclear applications," **M.B.Chadwick**, Project Proposal, 2013
- Initial focus on: ^{1}H, ^{16}O, ^{56}Fe, $^{235,238}U$, ^{239}Pu
- Some motivations:
  - Identify reasons for discrepancies between libraries
  - Produce higher-quality evaluations
  - Minimize missing out on key measured differential/integral data
  - Increased peer-review
  - Sharing work and responsibilities
- https://www.oecd-nea.org/science/wpec/sg40-cielo/

Concluding remarks

- Continued need for concerted efforts in theory, modeling and experiments
- Nuclear physics and nuclear data represent a "still modern" and vibrant field of fundamental as well as applied research

Noteworthy web links

- U.S. National Nuclear Data Center: http://www.nndc.bnl.gov
- OECD Nuclear Energy Agency Databank: https://www.oecd-nea.org/dbdata/
- IAEA Nuclear Data Services: https://www-nds.iaea.org/
- RIPL-3 database: https://www-nds.iaea.org/RIPL-3/
- ENDF-6 Manual: http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf
- MIT Open Courseware on Neutron Interactions and Applications: http://ocw.mak.ac.ug/courses/nuclear-engineering/22-106-neutron-interactions-and-applications-spring-2010/lecture-notes/
- CIELO: https://www.oecd-nea.org/science/wpec/sg40-cielo/