Nuclear Data's Hidden Dysfunctia: Applications Don't Actually Depend on Structure, Do They

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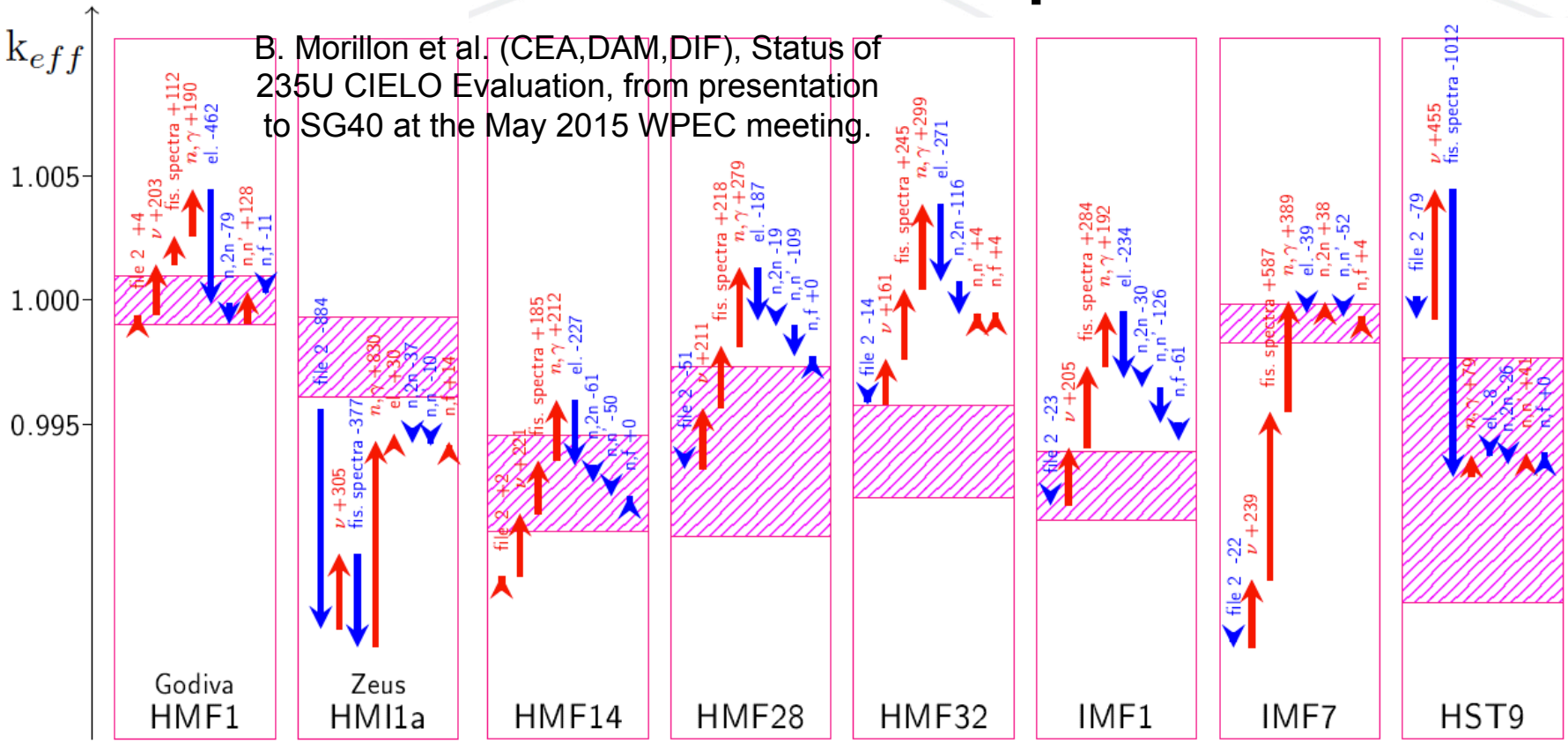
Workshop on Nuclear Data Needs and Capabilities for Applications, May 27-29, 2015

We are faced with compensating errors for which we have found non-unique solutions

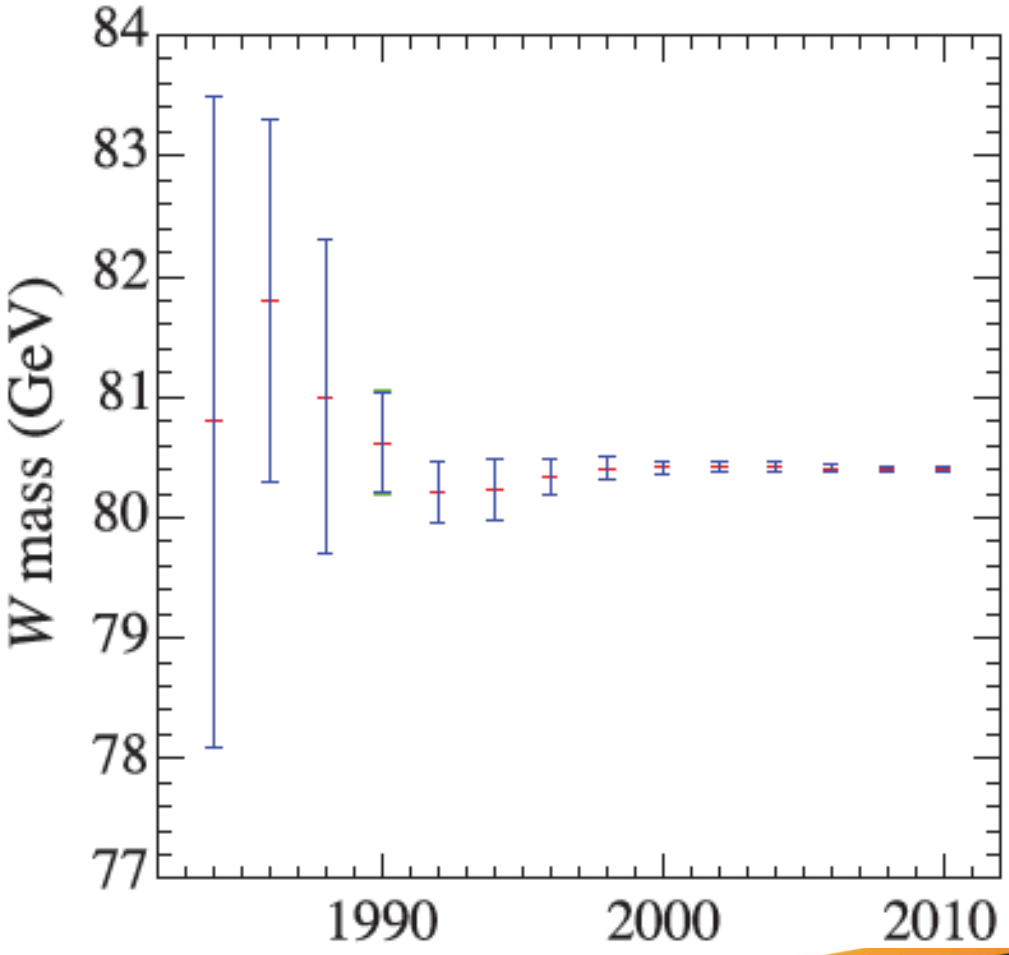


B. Morillon et al. (CEA,DAM,DIF), Status of 235U CIELO Evaluation, from presentation to SG40 at the May 2015 WPEC meeting.

This has launched us down a path to dig into the underlying issues; but from a reaction based perspective.
This talk will ask a different question.

Generally Idealized Vision Of the Evolution of Data Over Time

Error bars get smaller over time and mean value stays in general agreement with previous measurements

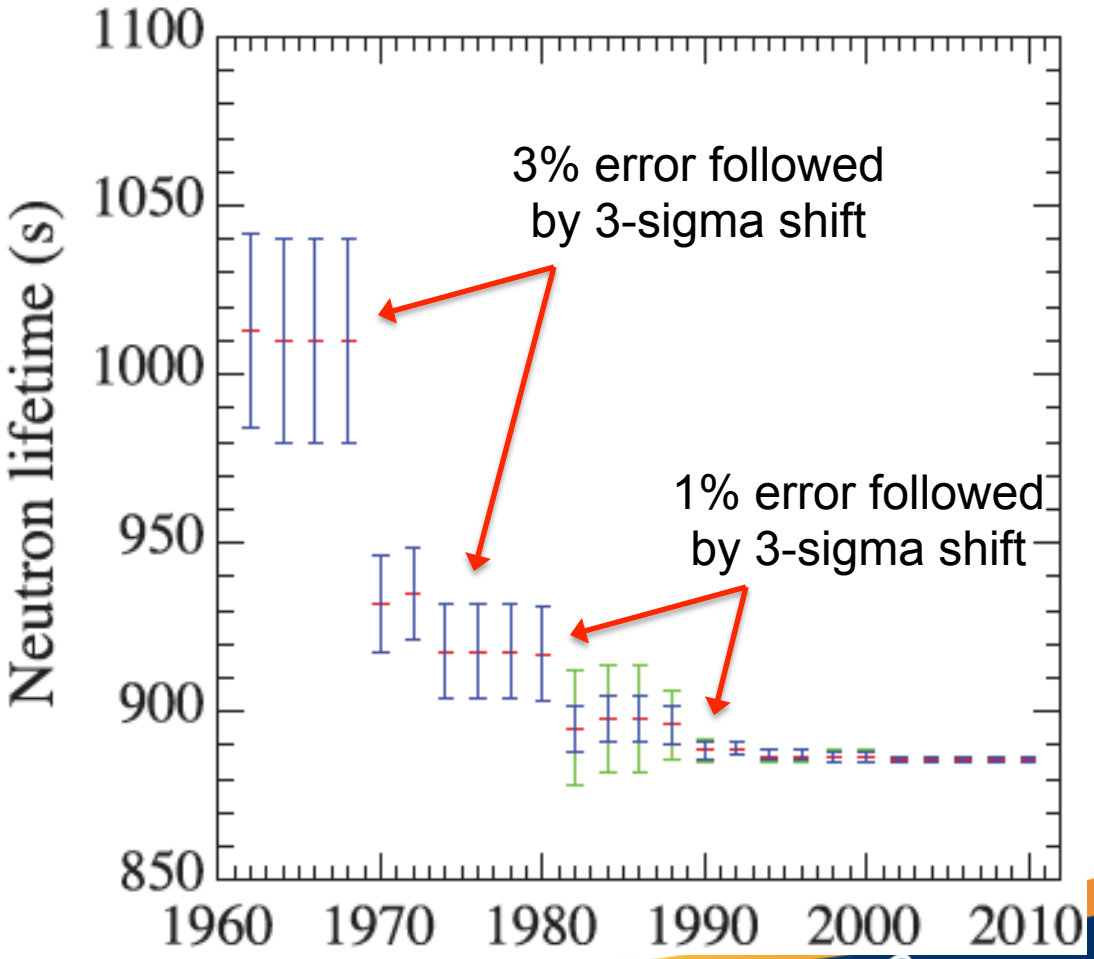


J. Beringer et al. (Particle Data Group), Review of Particle Physics, Physical Review D, Volume 86, Article 010001 (2012).

More Typically, Systematic Errors Shift Accepted Mean Values Over Time

We must be careful of over-estimating the 'independence' of experiments. *But* identifying and quantifying the corresponding systematic errors is difficult.

We have a wealth of reaction data that show shifts that are well beyond the 'quoted' uncertainties.

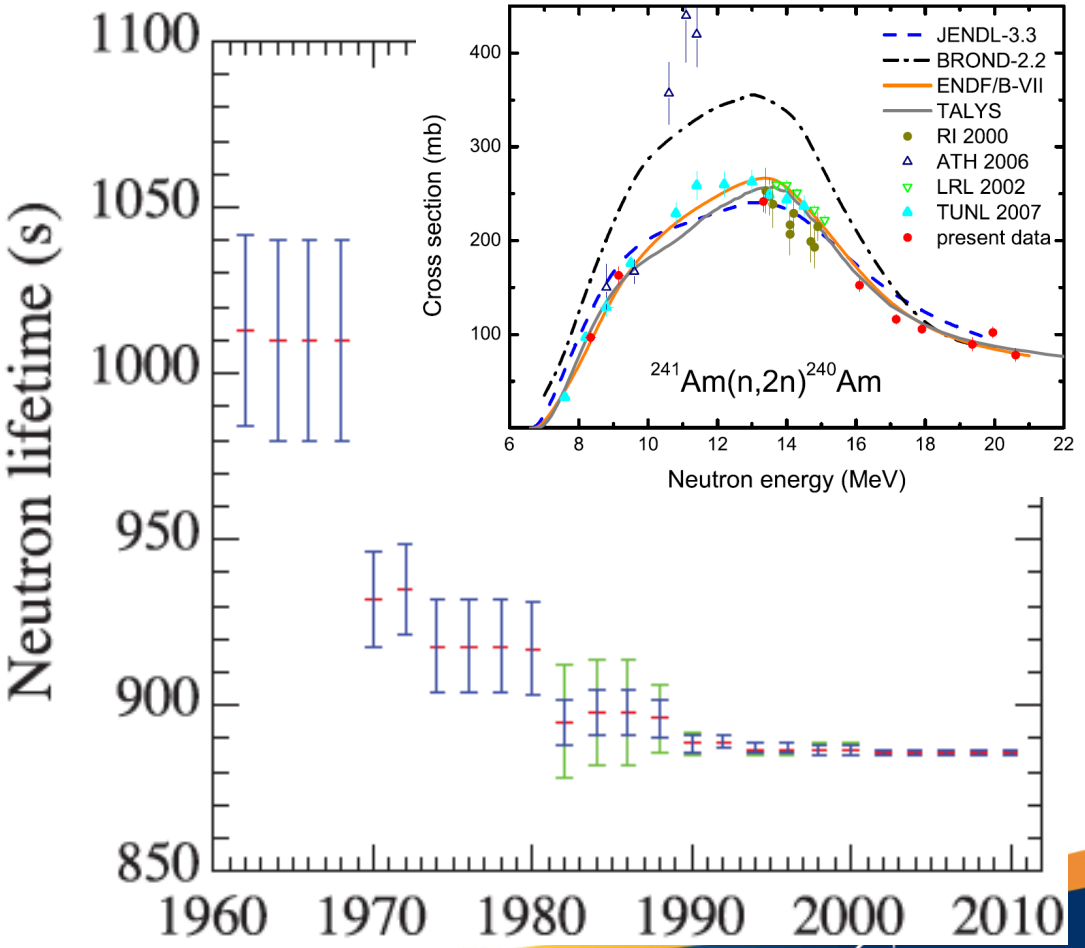


We must understand what is driving these shifts. In many cases, it is structure.

Unfortunately, the evidence of this that can be presented is more anecdotal than concrete.

Your help in examining this hypothesis is required.

This is going to require covariances for structure quantities, including things like discrete spin assignments.

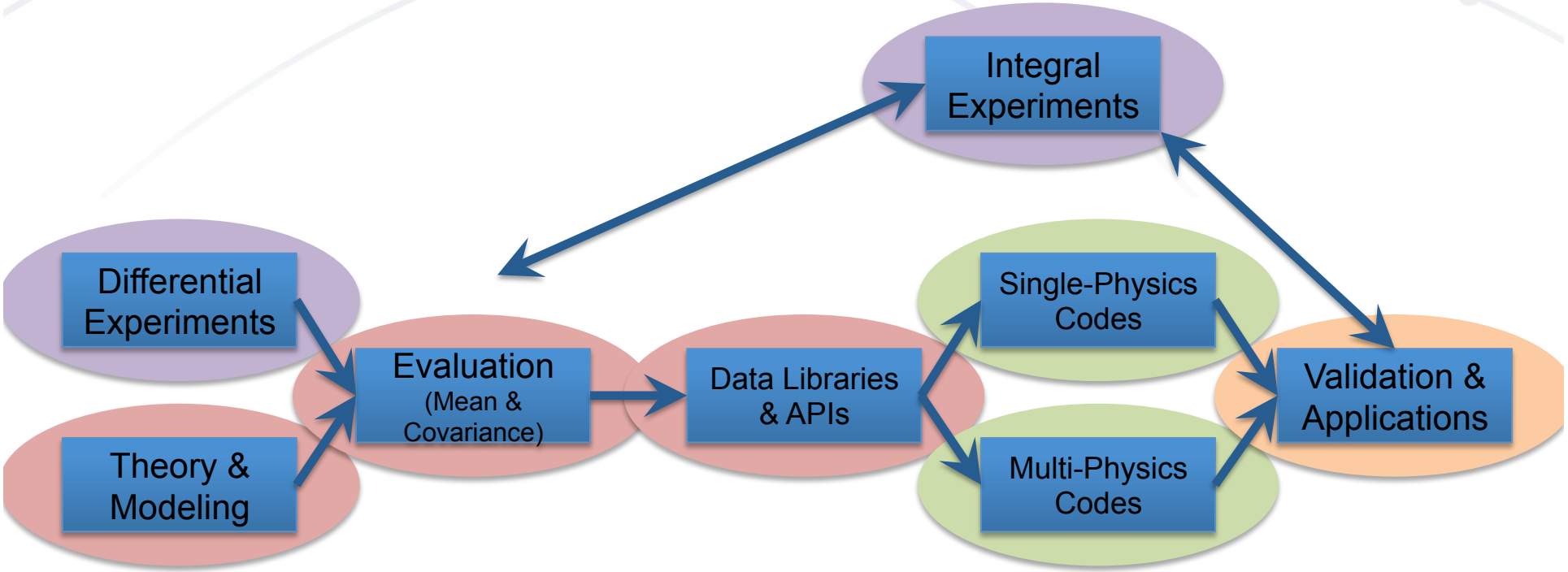


Parameter studies versus bounding estimates

- Many times we are asked to quantify the uncertainties associated with these data
  - Our answers tend to be of the “parameter” study kind that provide a narrow estimate around the mean value

- Is there some way we can provide a “bounding study” that accurately captures a “likely” potential jump in the mean value?

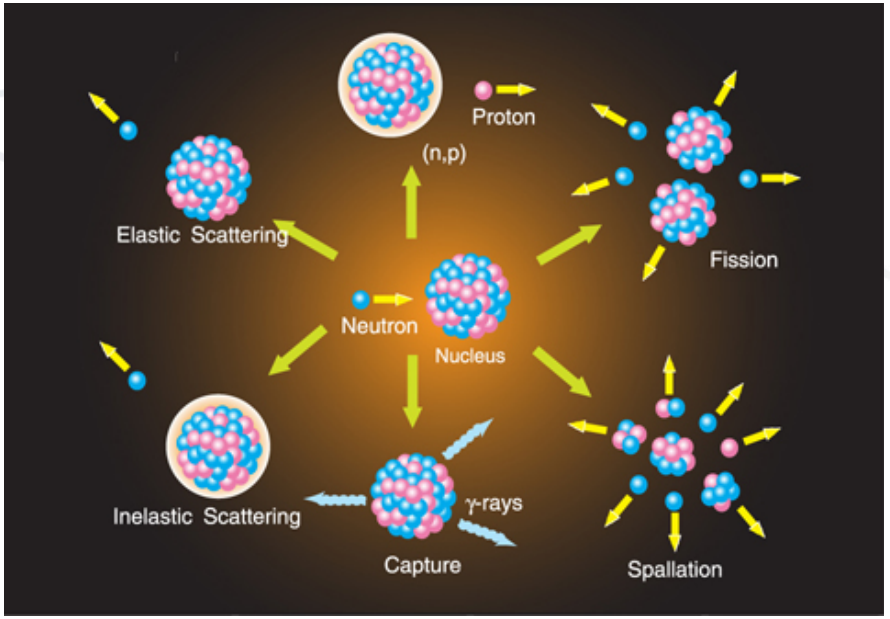
While theory and modeling are present nuclear structure is notably absent…



This is often the first slide I use to introduce our applied users to the nuclear data community. While the answer to the title question is obvious, it is not typically acknowledged. Our largest gap in understanding is between the structure community and the applied users.

I apologize up front for my own misperceptions and misunderstandings.

We need complete, self-consistent data – evaluations – that describe all interactions of all incident particles with all possible nuclei and accurately describe their outputs.



Nuclear theory* is essential to interpolate and extrapolate differential experimental data to provide evaluations.

***And nuclear theory is largely using the structure data as a black box.**

$$\frac{1}{v(E)}\frac{\partial\psi(\mathbf{r},E,\hat{\Omega},t)}{\partial t}+\hat{\Omega}\cdot\nabla\psi(\mathbf{r},E,\hat{\Omega},t)+\Sigma_t(\mathbf{r},E,t)\,\psi(\mathbf{r},E,\hat{\Omega},t)=$$
$$\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\nu_p(E')\,\Sigma_f(\mathbf{r},E',t)\,\phi(\mathbf{r},E',t)+\sum_{i=1}^{N}\frac{\chi_{di}(E)}{4\pi}\lambda_i C_i(\mathbf{r},t)+$$
$$\int_{4\pi}d\Omega'\int_0^\infty dE'\,\Sigma_s(\mathbf{r},E'\rightarrow E,\hat{\Omega}'\rightarrow\hat{\Omega},t)\psi(\mathbf{r},E',\hat{\Omega}',t)+s(\mathbf{r},E,\hat{\Omega},t)$$

Boltzmann transport equation

The US Nuclear Data Program is a key partner without whom the applied community would not be able to function

- The XUNDL and EXFOR compilation activities should be held up for emulation by other fields
- The ENSDF and ENDF evaluated data efforts supply the essential data required by applications
- We have strong bonds between the theory, modeling and evaluation communities and applications
- But the structure community is a great unknown

We need to build stronger relationships with the structure community.

Is this really how we do business?

Task: Create an upgraded Vanadium evaluation.

From Skip Kahler:
Unfortunately the newest evaluations appear to due worse in predicting keff. With the elemental V data the kcalc average is 1.00205 with a min-to-max range of 0.99811 to 1.00459. With the new isotopic V evaluations the average increases to 1.00404 with a min-to-max range of.0.99926 to 1.00701. Each of the 8 benchmark eigenvalues is larger with the new data, increasing by ~100 pcm to ~250 pcm. I haven't had time to look for a trend in this increase, but if you have any wiggle room to increase the capture/decrease scattering and/or make the high energy scattering angular distributions more forward-peaked so that the axial reflectors are not as effective, that might help.

Level	RIPL3	Tol
320.1	x	x
470	x	
928.7	x	x
1010	x	
1190	x	
1609	x	x
1813	x	x
1910	x	
2410	x	x

The "Fix" – TK: When I removed the ... levels, the over prediction problem was solved.

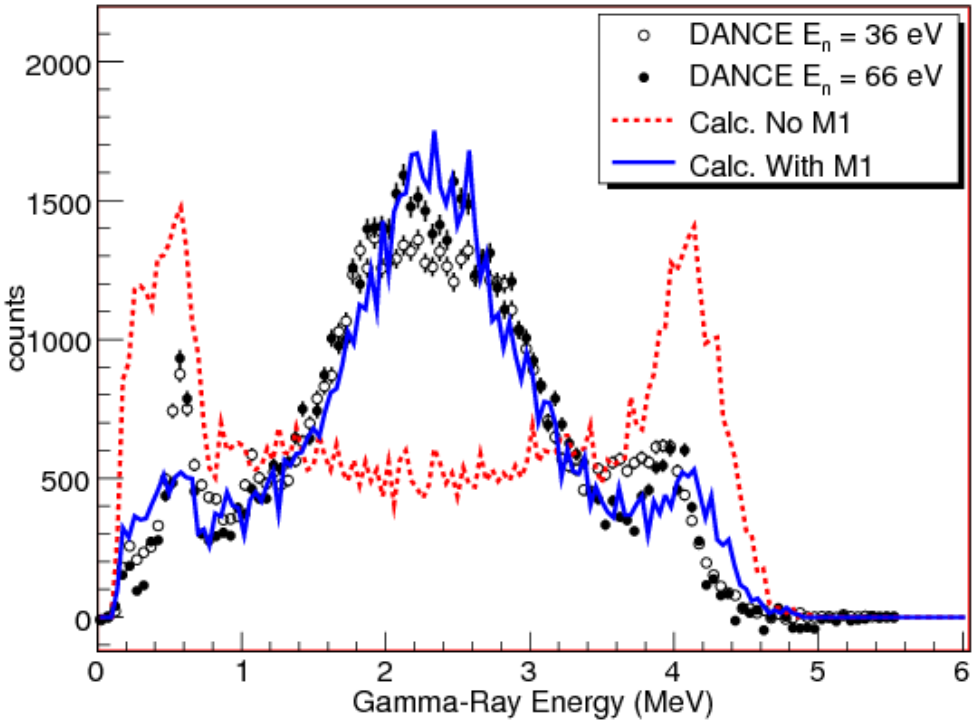
I pick on Kawano because I have only the greatest respect for him.

My worries are many.

- Blind adoption of RIPL-3.
- Blind abandonment of RIPL-3.
- Blind adoption of the ‘Table of Isotopes’.
  - No traceability for which ‘Table of Isotopes’.
- Blind assumption that actinide driver is ‘perfect’, hence we must ‘correct’ the vanadium data.
- We have lost the independence of these critical assemblies to validate the evaluation.
  - And yet we have not acknowledged this.

We can do better. We need to engage with the structure community to weigh-in on these issues.

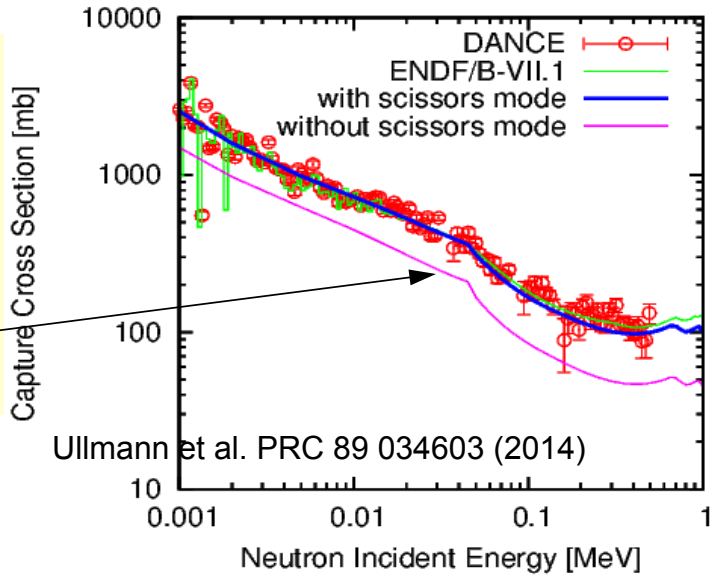
^{238}U(n,γ) Decay Spectrum



There are also many success stories…

- Original reaction model did not include 2.3 MeV “M1” enhancement
  - Model shown in **RED**
- Changes to M1 strength to include enhancement at 2.3 MeV were made to reproduced DANCE decay data
  - Model shown in **BLUE**
- These changes impacted the capture cross section and brought the agreement with measurement to within 30% (from 240%)

standard parameterization of photon strength functions under-estimate capture cross sections for actinides



Is “good” structure data enough to provide a “reasonable” reaction evaluation?

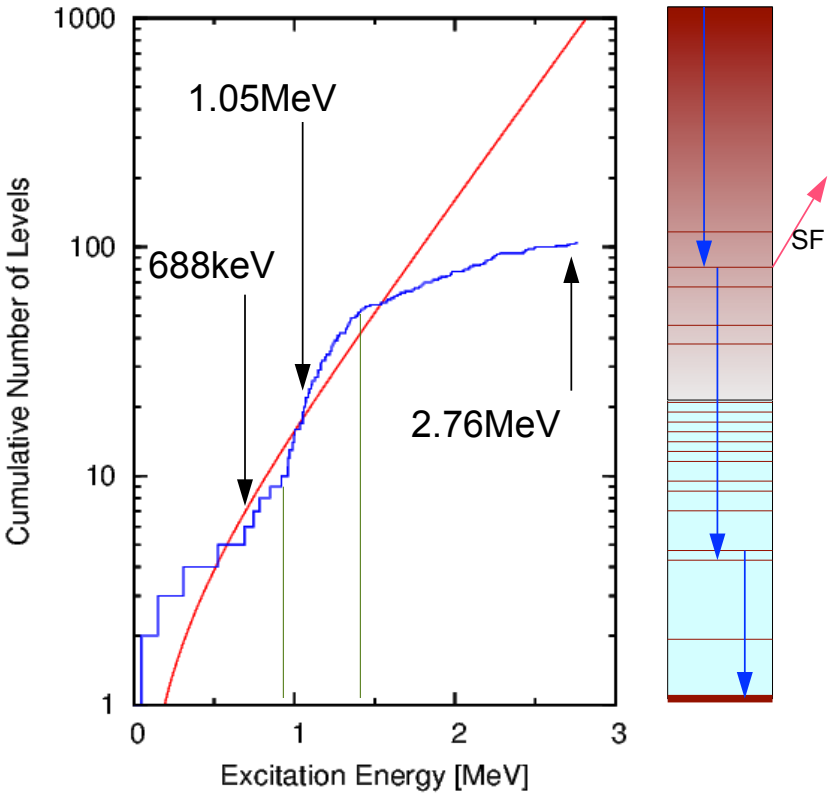
I am sure I lump into the term structure considerably more than the accepted definition.

- I believe this is what the “surrogate reaction measurement community” is trying to do
  - But they have asked the wrong question
    - Extract versus constrain
  - And thus they are reporting the wrong results

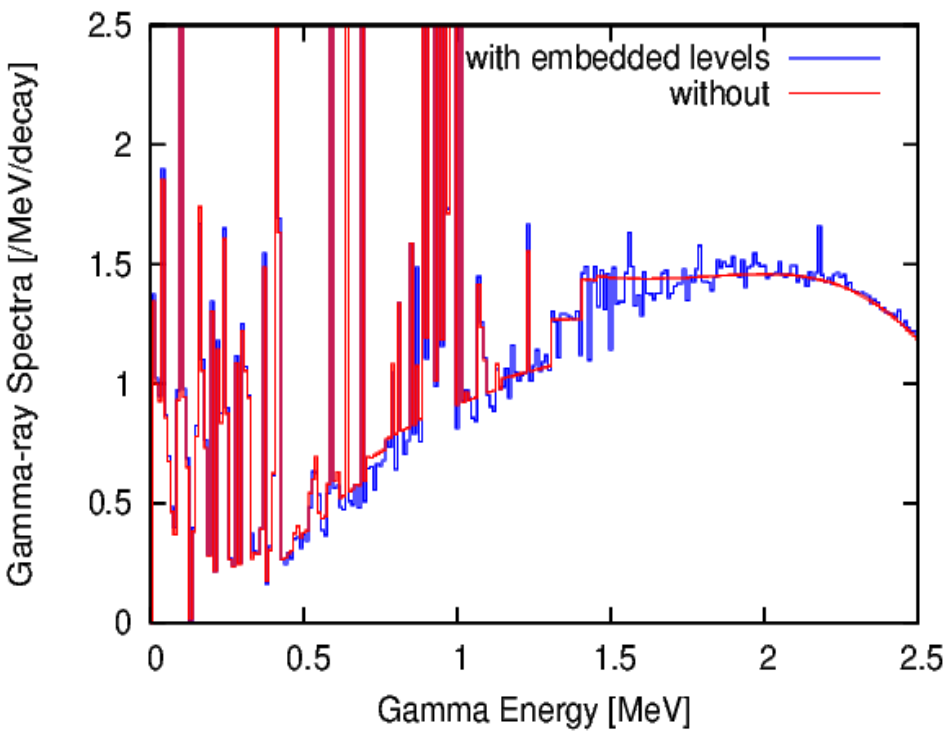
- Can we perform experiments that produce unstable nuclei (for which reaction measurements are difficult to impossible) and measure quantities which constrain our reaction models?

The next frontier, can we accurately predict all correlated emissions?

Overlapping discrete and continuum regions



More gamma lines can be observed



From Kawano: New embedded levels capabilities in CGM

The nuclear structure, reaction and application communities will have to work together to solve correlated emissions.

- Current evaluations are “average” emissions
- Data tables are feasible for a very limited range of correlated data; exponential growth of the tables will overwhelm data storage limitations
- Solution: embed models as sampling kernels
  - But these must be tuned in the same way as an equivalent evaluation

To be of highest value…

- Like the reaction data, the structure data must be “self-consistent and complete”
  - All energy, spin assignments, half-lives and decay modes must be given
  - Covariance data – ***quantified*** uncertainties
  - Where data are not measured, theory must “extrapolate” reasonable values
- And the resulting evaluations must be traceable, documented, verified and validated

It seems at times that we are arguing about the tiny details. Quite frankly, we are.

- It is a strongly held belief by many that if you worry about the details, the big picture will take care of itself.
- Sports is a wonderful analogy, showing us the importance of chasing that last hundredth of a second.
- In science, we are also often treading familiar ground in pursuit of making sure the ground is solid.

Details matter.

We worry about the details because we don't typically see the accident before it happens. That's why we plan for the worst.

- Planning for the worst comes in two parts. Do you know what to do in an emergency? Have you provided the resources to do it?
- In science, we are often ponderously slow. If there are aspects of a problem of critical importance, having a robust program in place is the only mitigation for the unknown.

We keep moving beyond the bounds of our predictions.

Backup Slides

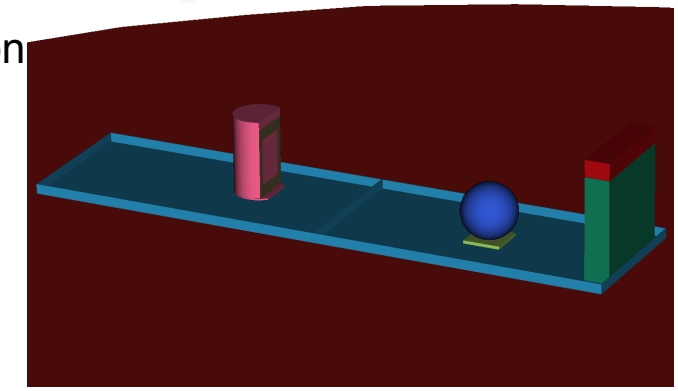
Abstract

- The applied nuclear data community focuses on

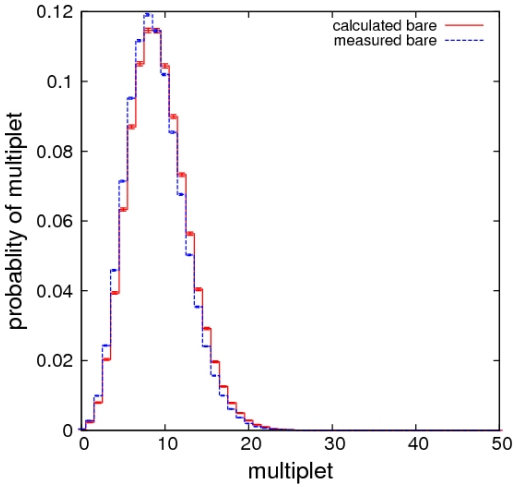
S. Bolding, C.J. Solomon

Pu Data Questions from Multiplication Inference Measurements

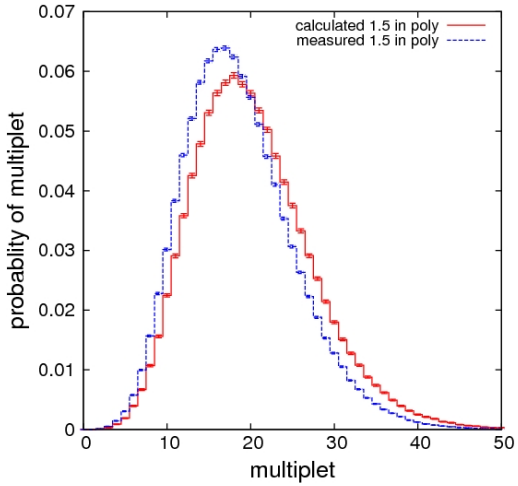
Multiplication inference (non-integral) measurements of the BeRP ball have been compared to MCNP multiplication patch and MCNP-Polimi simulations (geometry to the right).



Both independent modifications to the MCNP base code to calculate the multiplication distributions **over estimate the multiplicity** using ENDF/V-II.0 Pu data.



Bare BeRP Ball

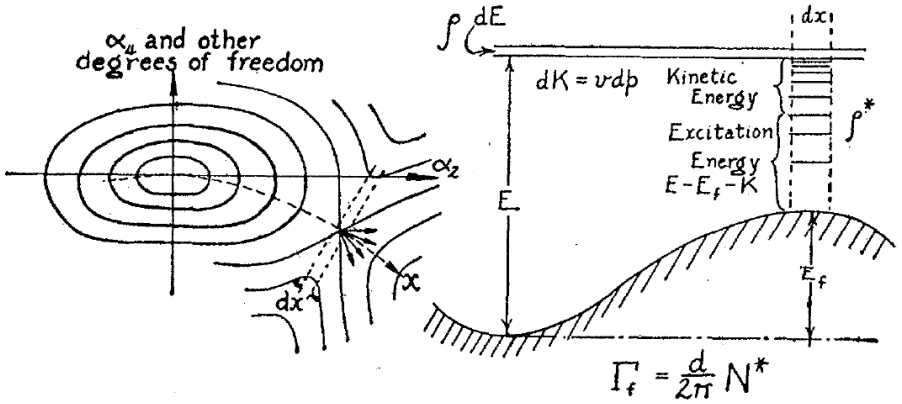


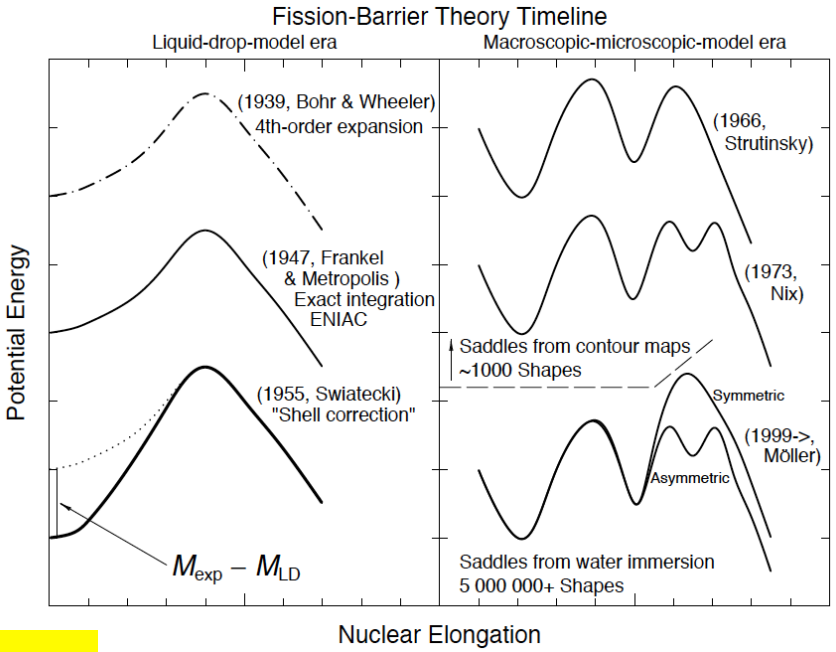
BeRP Ball w/ 3" poly. reflector

Systematic modeling errors have been investigated and cannot account for the discrepancies.

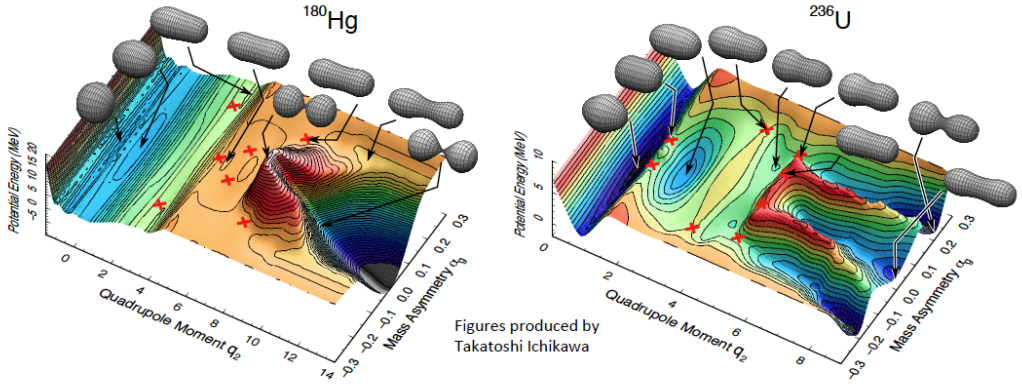
Might uncertainties in Pu data, e.g., **χ(v)**, χ(E), Σ_f, Σ_a, etc., be the source of the discrepancies?

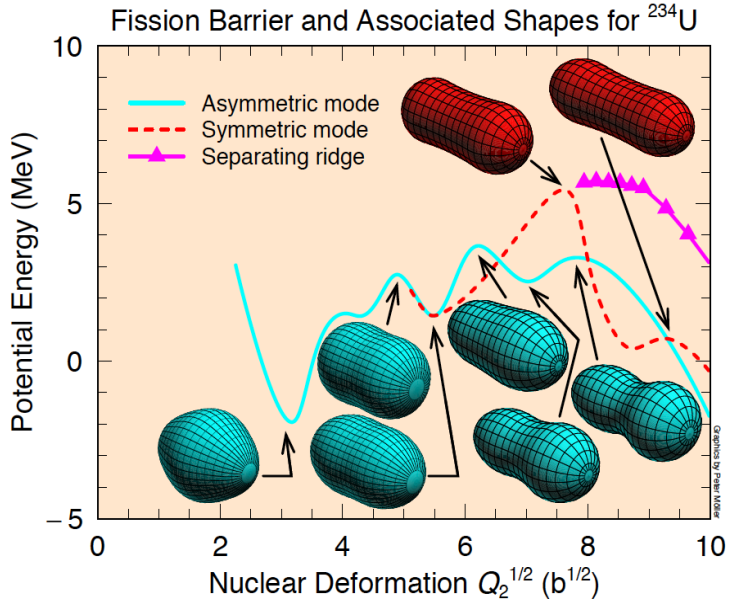
Fission Theory Then and Now



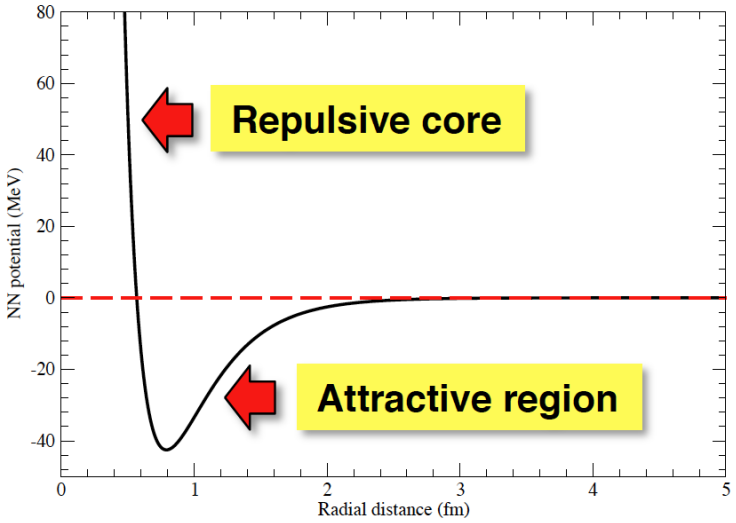


Modern macroscopic, microscopic theory traces back to formulation by N. Bohr and J. Wheeler, The Mechanism of Nuclear Fission, Phys. Rev. 56 (1939) 426.



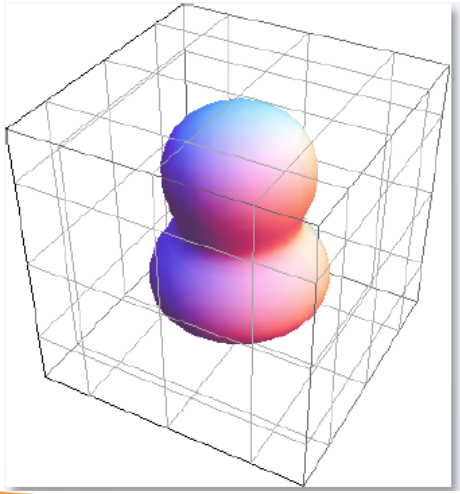


First Principles Fission Theory Remains a Grand Challenge



- We don't yet have a fundamental theory of the nucleon-nucleon interaction
- Fission is a difficult quantum problem that is too complicated to describe with full many-body wave function

We must be clever.
- Walid Younes, Fission Experiments and Theoretical Advances (FIESTA2014).



Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing ⇒ $20^3 \times 2 = 16000$ lattice points:

$$\binom{16000}{94} \times \binom{16000}{146} \approx 10^{608} \text{ configurations!!!}$$

The Data Dilemma

- If you have no data, you get to make it up
- If you have one data set, it must be correct
- If you have two data sets, they are both wrong
  - And everyone is just going to pick their favorite
- When you have many data sets, you get to make it up again

It is not enough to make the most accurate measurement. It will always be viewed within the broader historic context and we must understand *all* systematic errors.