New paradigm for nuclear data evaluation

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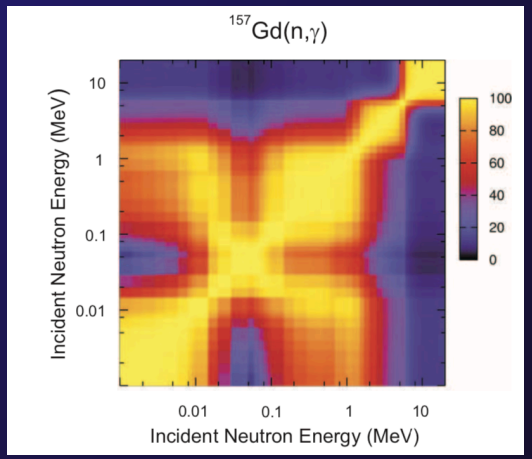
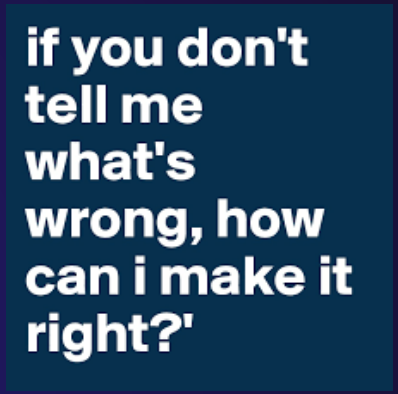
What are major issues with the current libraries?

- Integral experiments not fully included.
- General lack of cross-correlations
- Compensation of errors.
- Some evaluations are desperately old.
- Format is from the previous millennium (the new one waiting around the corner!).



What's wrong with our evaluation procedure?

- Only **partial updates** in each new release.
- **Clinch situation** - if evaluations for two materials contain compensating errors an evaluator reevaluating one of the materials can't remove a single error since library performance would suffer.
- **Full validation** performed after library released (or frozen).
- **Documentation** is not sufficient to reproduce the evaluation => we have to redo everything from scratch.



What is the New Paradigm (SARM3)?

Starting with the current library:

- **Store** all the details of evaluations in electronic form (inputs, codes, exp. data, assembly scripts) to allow automated adjustment and, if needed, re-evaluation of a file within days.
- **Adjust** the whole library to a representative and trustworthy set of integral experiments covering the whole field of applications, in response to each new or modified evaluation.
- **Review** each adjustment (help from automation needed).
  - if any **adjustment exceeds** an upper limit (e.g.1 sigma) it should be reviewed and, eventually, the material should be reevaluated.
- **Maintain 3** libraries (branches in version-control speak).
  - **A** - purely differential and model based.
  - B - A tuned to integral data (as existing ones).
  - **C** - fully adjusted (as discussed here).

What are the advantages of the new paradigm?

- **Preservation of the details** of evaluation procedure =>
  next evaluation can directly use the previous work
  (in some cases simple Bayesian update might be sufficient).

- **Cross-correlations** induced by the integral measurements
  (substantial ones point to possible **compensation of errors**.)

- Releasing evaluators from the **clinch situation** when they are unable to remove an error in an evaluation because it has been compensated by an error in another evaluation.

- Facilitated introduction of **new** experiments or model developments.

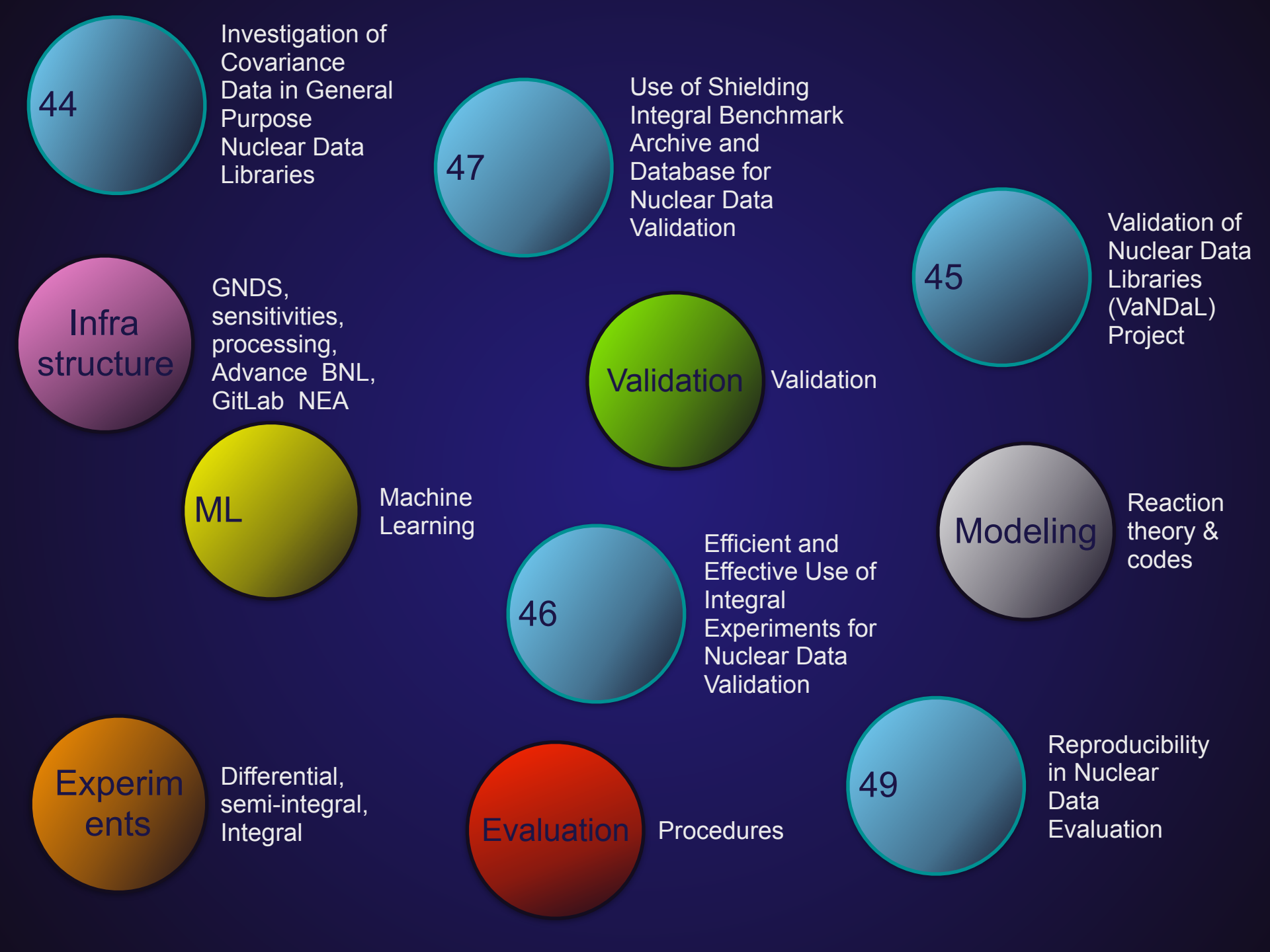
What else could be done?

- Storing **sensitivities to the model parameters** (useful for adjustment and reduced representation of covariances!)
- **Replacing tabulated** (formatted) data by direct use of the reaction model codes.
- Going **beyond linear** approximation (covariances).

What are specific needs of the new paradigm?
(in addition to: experiments, theory, codes, infrastructure …)

- Complete inputs for evaluations allowing to reproduce evaluation with a ‘click of a button’.
- Recommended set of trustworthy and representative benchmarks covering the whole field of applications along with sensitivities.
- Automated adjustment methodology(ies) (ML?).
- Automated review of the adjustment results (ML?).
- Repository for storing and versioning everything.

Actually, most of these are already under development!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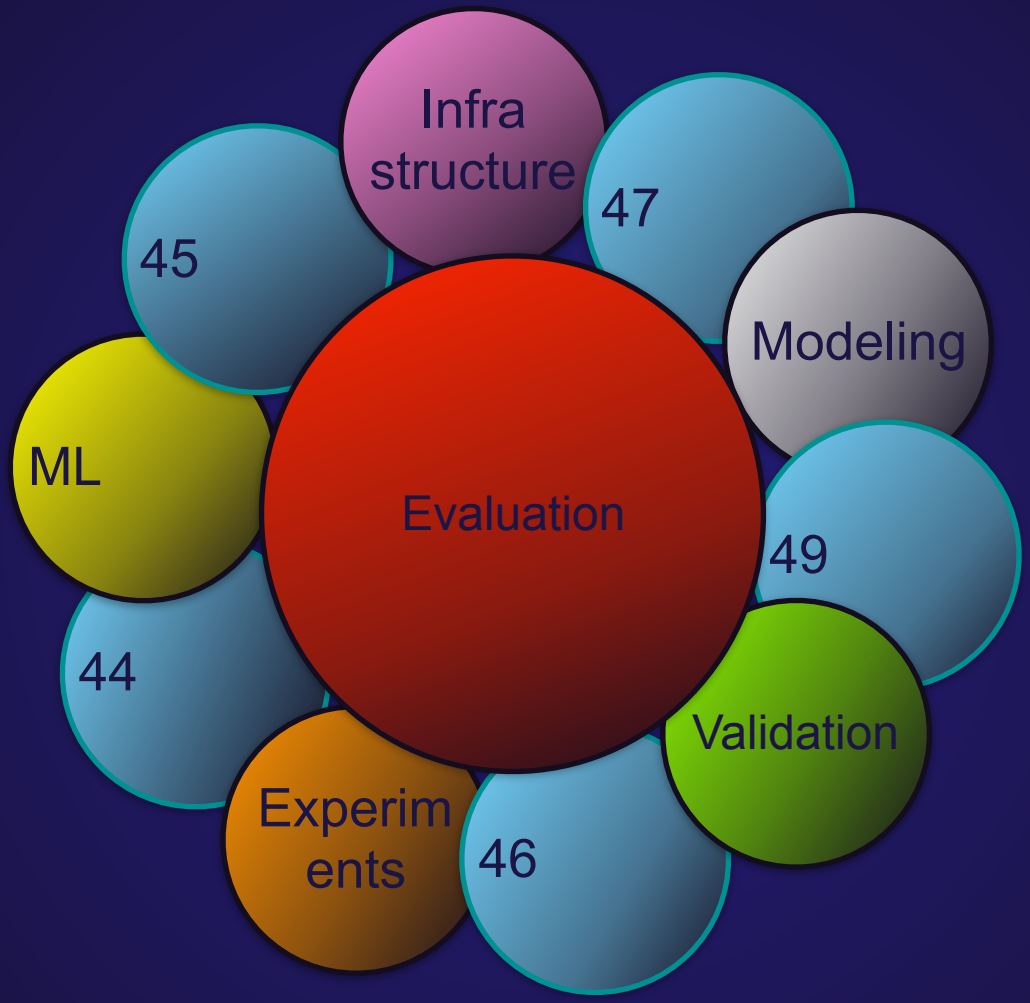
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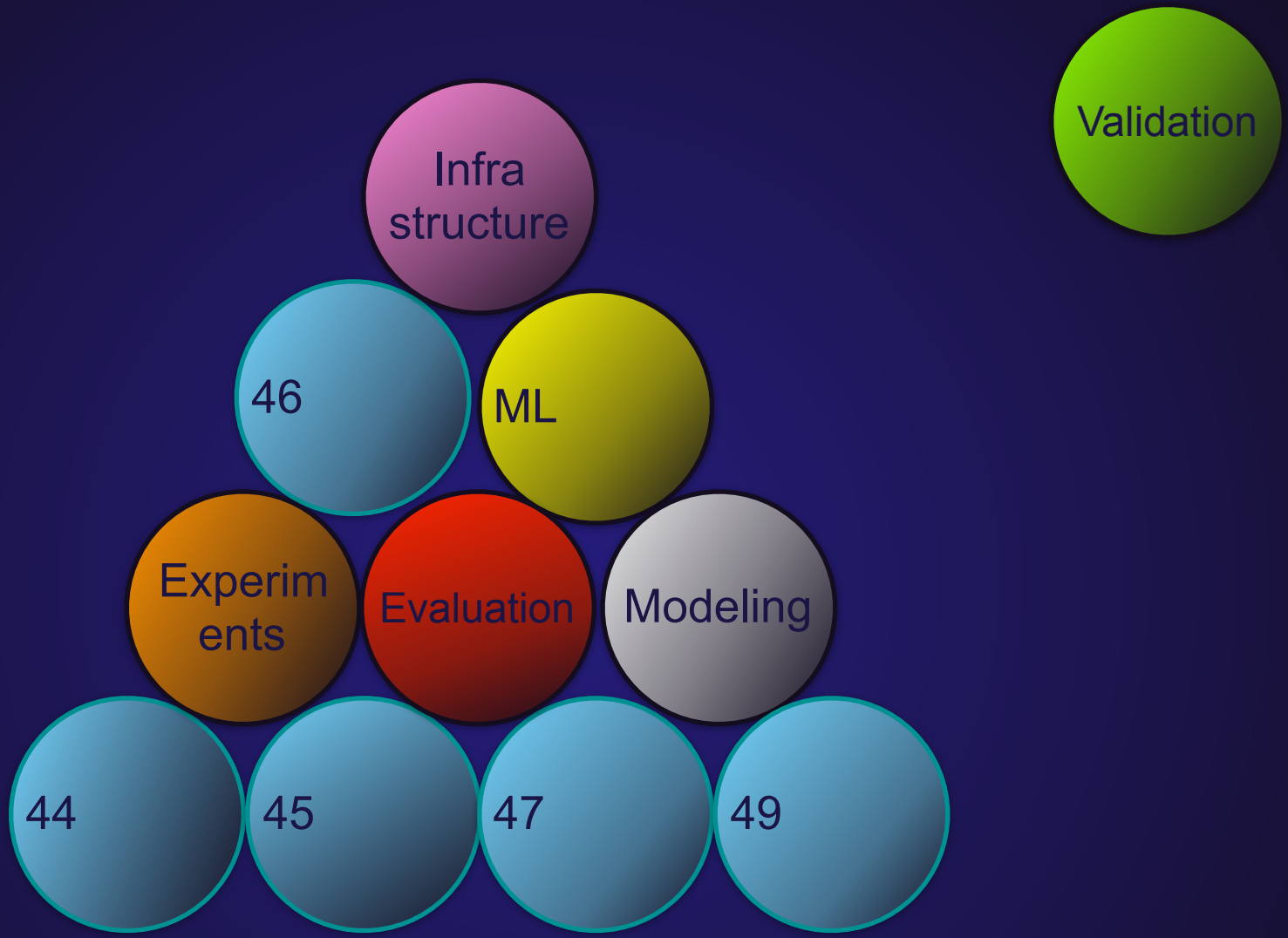
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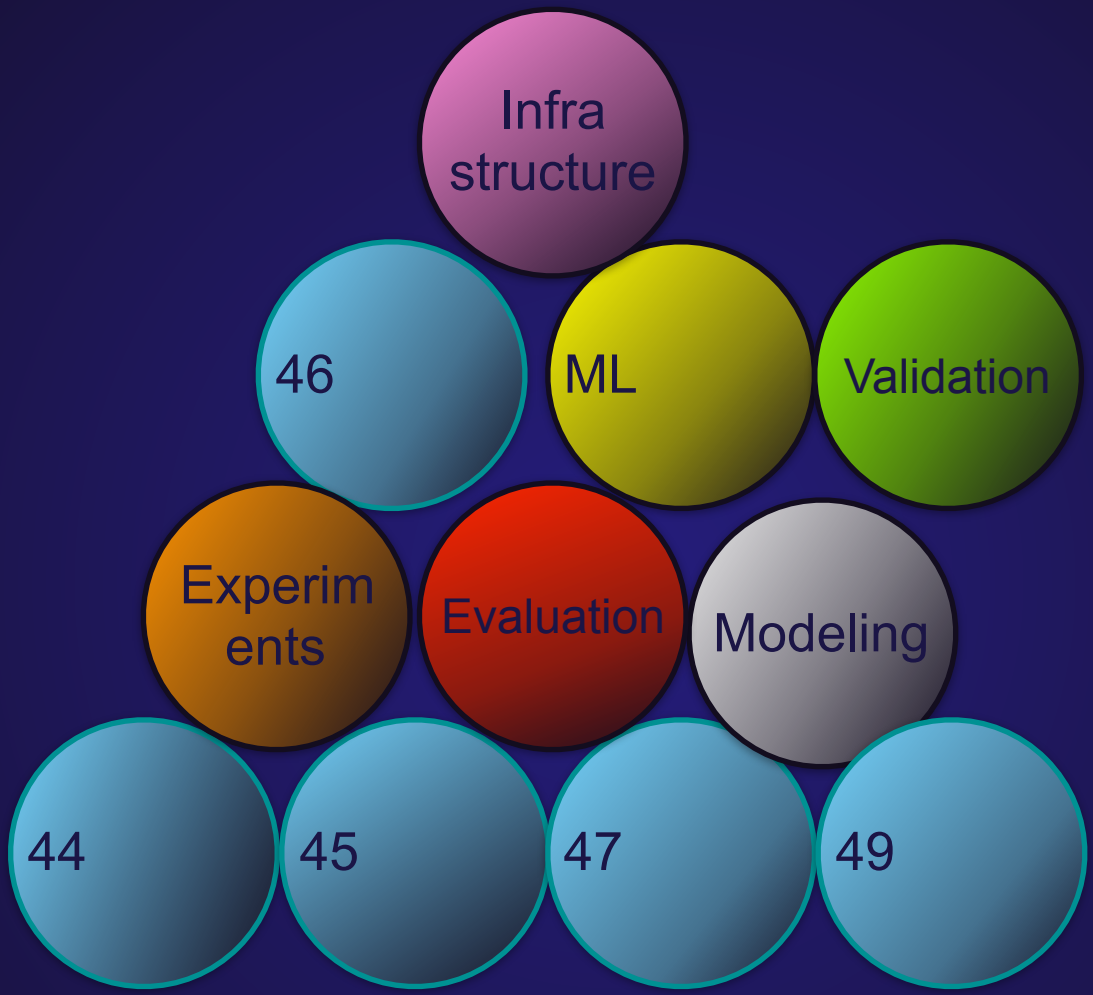
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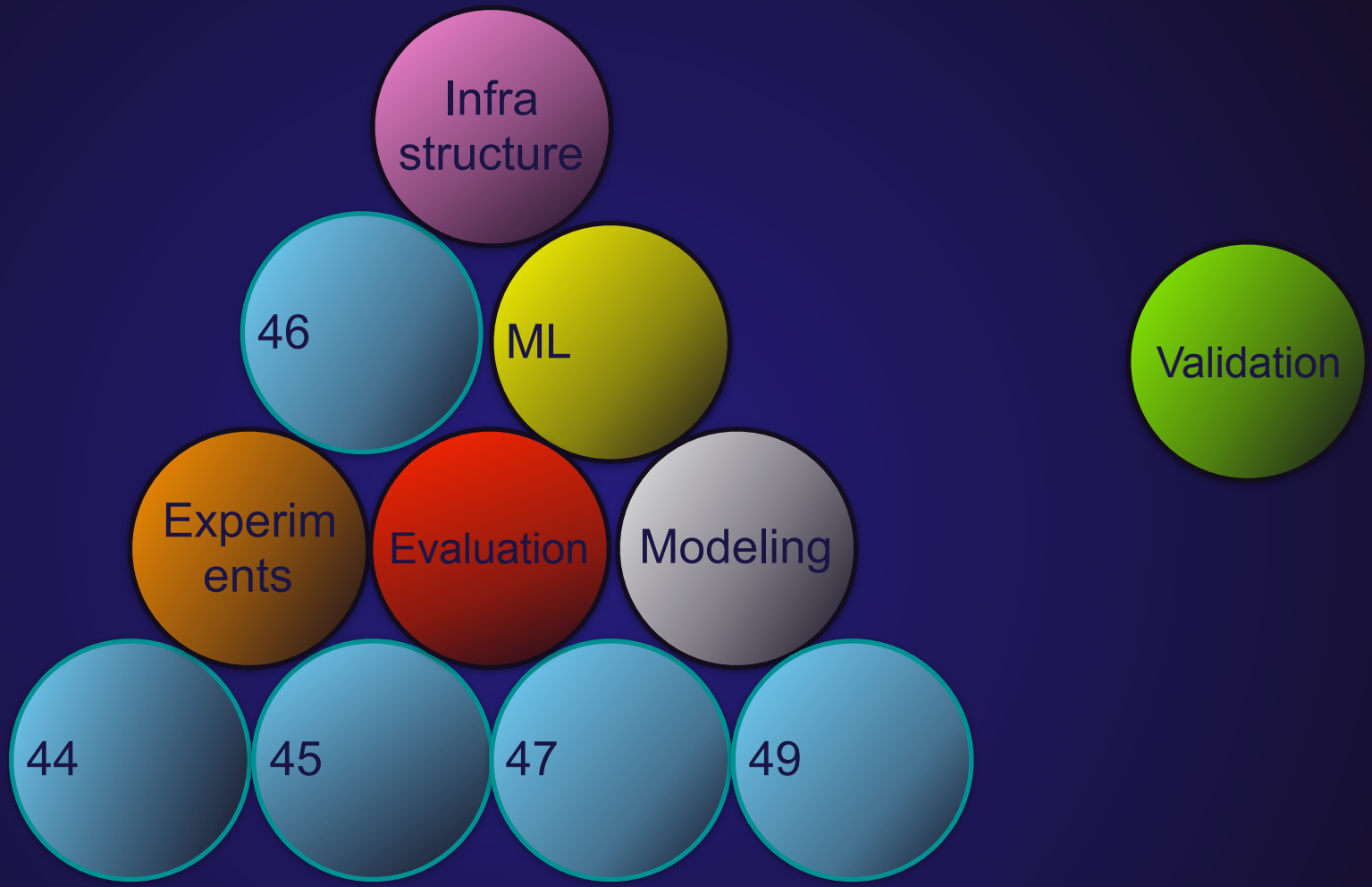
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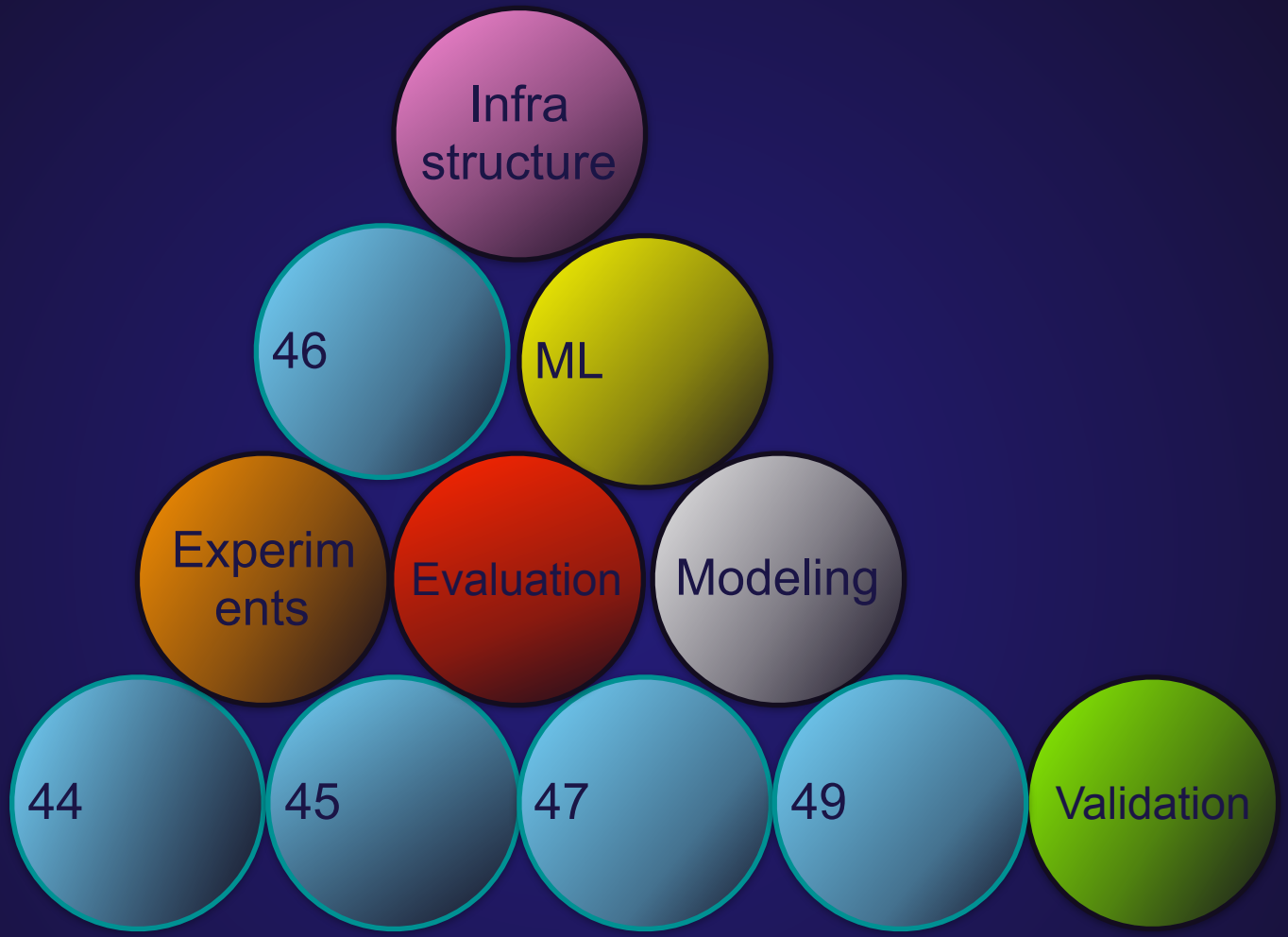
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Conclusions

The evaluation procedure remains very much **as it is, but**

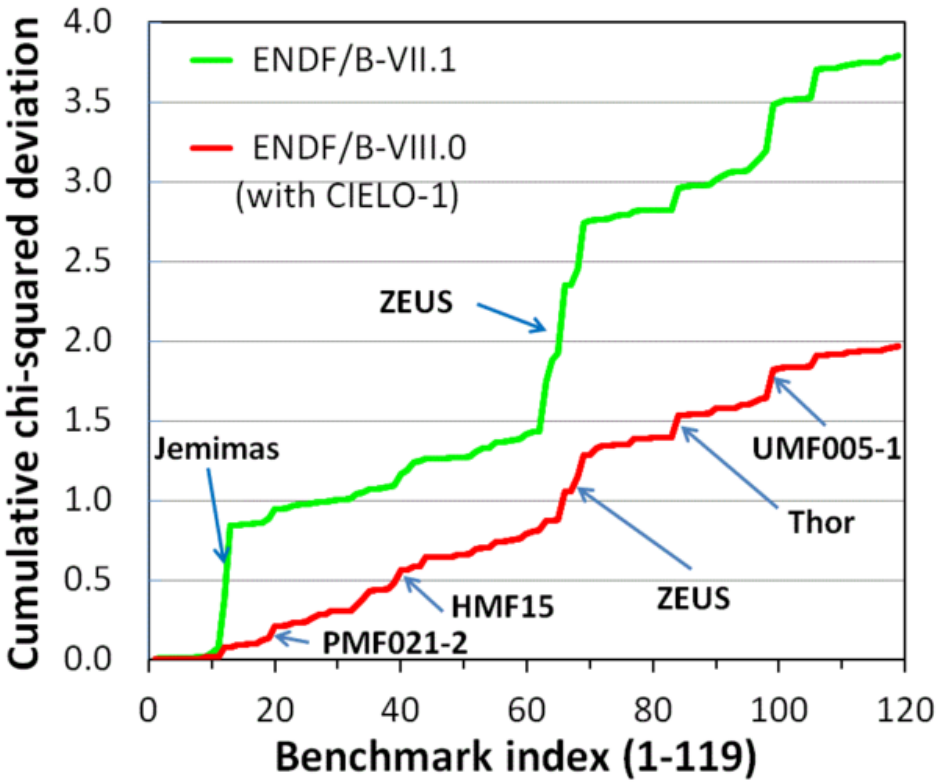
- Integral adjustment follows as part of the evaluation procedure.
- Explicit (digital) memory of the evaluation is preserved to allow for quick adjustment in the future.
- Relevant part of the library is readjusted with each new/updated evaluation (review is needed!)
- As a result of adjustment ‘compensation of errors’ is gradually reduced.
- Validation community gets involved as part of the evaluation team.
- Easy reevaluation facilitates quick usage of new experimental data, improvements in reaction modeling, and in adjustment methods (ML).

Ready to take questions:

1. Why it's time to make a change?
2. What is different today (from say 20 years ago)?
3. Will including integral experiments bias the library?
4. Are cross-correlation covariance matrix elements real?
5. What if different integral experiments produce different correlations?
6. Can we trust reaction models?
7. What if different adjustment methods produce different results?
8. What should be adjustment strategy?
9. Is assimilation feasible?
10. What are changes in assimilated model parameters?
11. What is a role of Machine Learning?

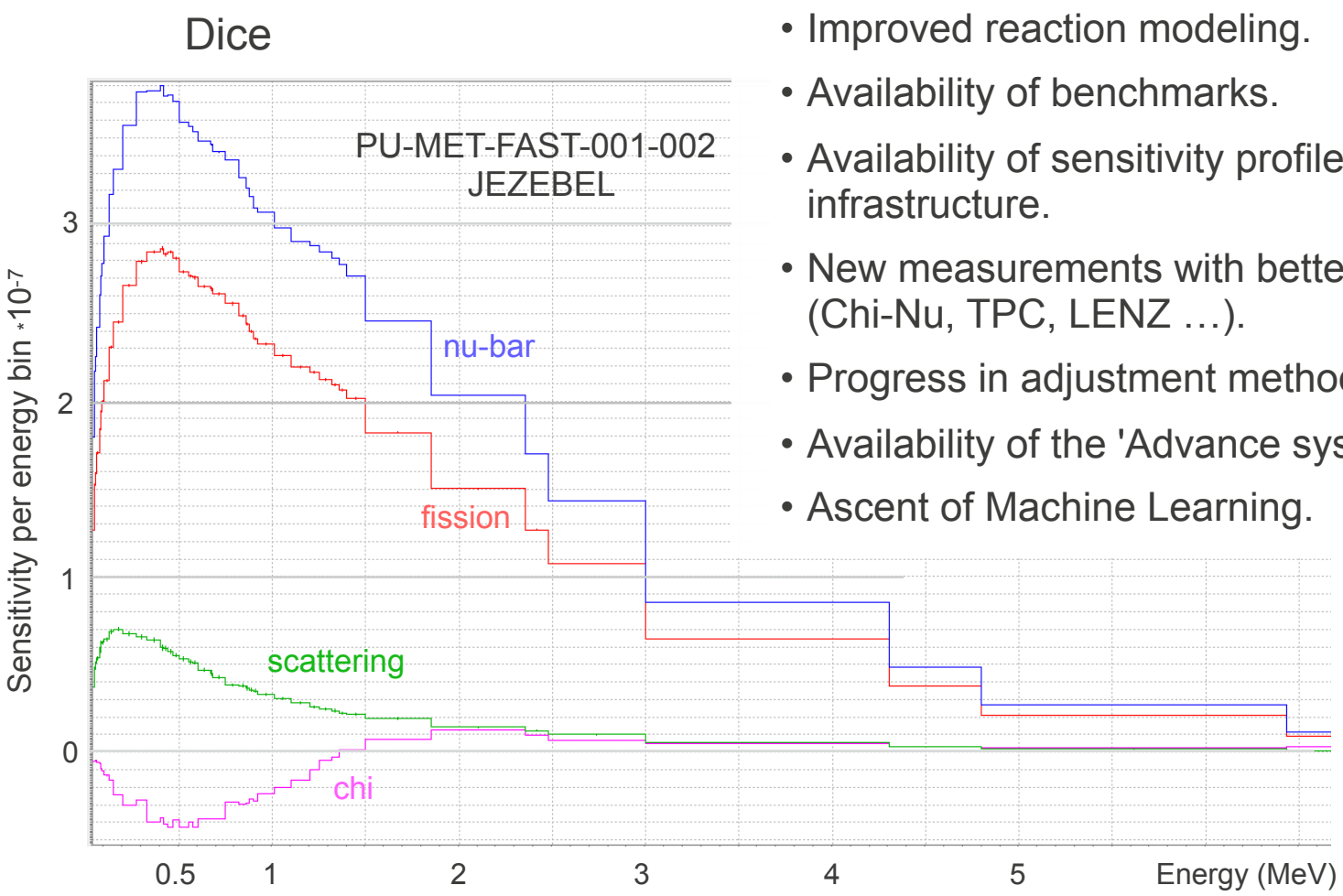
Why it's time to make a change?

- Libraries perform pretty well => we are probably quite close to the truth, therefore adjustment has good chance to work.
- Improving overall performance will be more and more difficult unless we upgrade our approach.



From NDS 148 (2018) 189

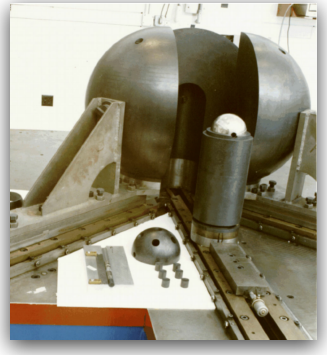
What is different today (from say 20 years ago)?



- Computing power.
- Improved reaction modeling.
- Availability of benchmarks.
- Availability of sensitivity profiles and related infrastructure.
- New measurements with better uncertainties (Chi-Nu, TPC, LENZ …).
- Progress in adjustment methods (WPEC SGs).
- Availability of the 'Advance system' at NNDC.
- Ascent of Machine Learning.

Will including integral experiments bias the library? (contentious topic - some authors filed ‘votum separatum’)

- Not really since we'll cover all available experiments in the 'representative' mode.
- We tune it anyway (and less 'scientifically').
- Adjusted library should be very close to the ‘tuned’ one.
- Different applications often mean different energy ranges and/or different materials.
- If different applications make contradictory calls we'll have to make a decision as we already do when facing discrepant data.



NEA-1517 SINBAD REACTOR--.

SINBAD REACTOR, Shielding Benchmark Experiments.

Are cross-correlation covariance matrix elements real?

- They are as real as the diagonal but none of them are as real as physical observables.

1 mb capture at ~14 MeV it's not just a good number, it's a law :)

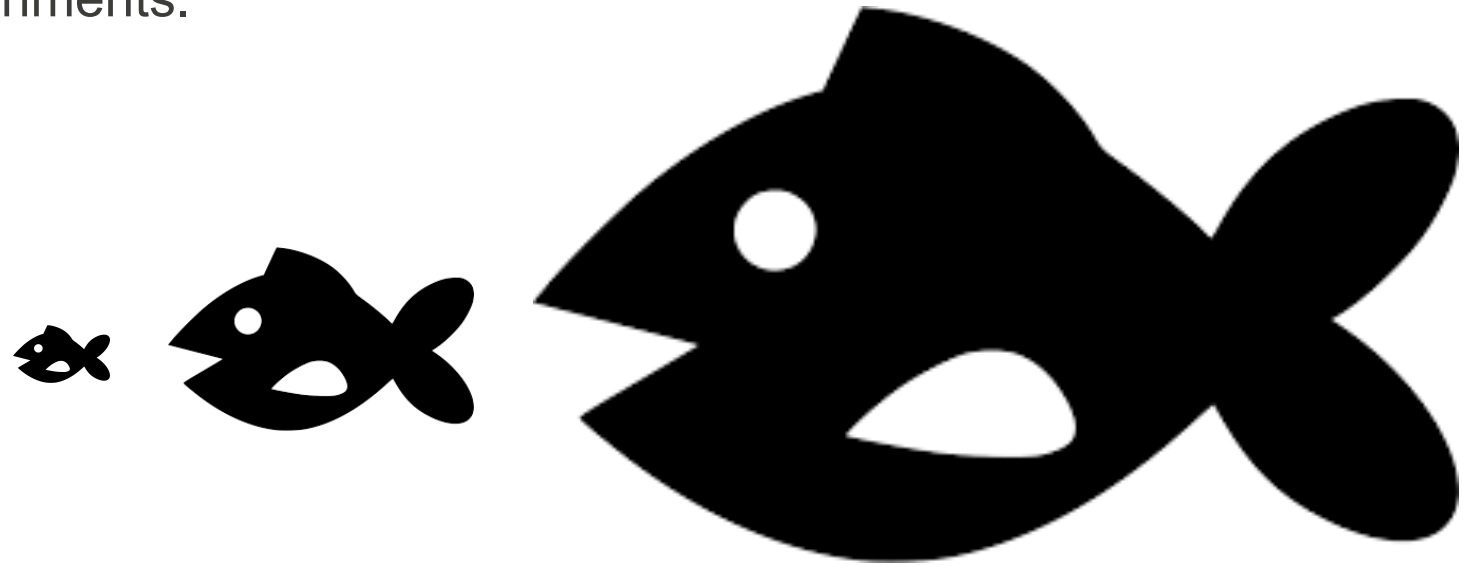
- Covariances represent degree of our knowledge (or ignorance) (glass half-full or half-empty).

- Cross-correlations are predominantly related to our firm determination to reproduce experimental results.

Experimental correlations are sort of accidental and, in principle, avoidable.

What if different integral experiments produce different correlations?

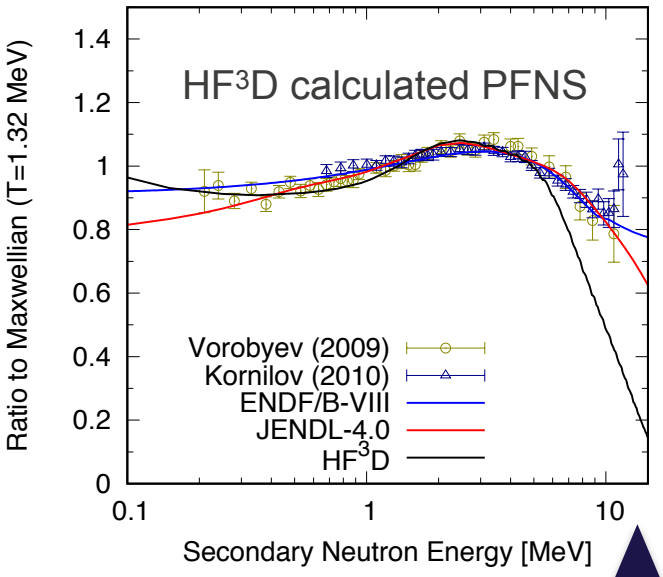
- Not a problem - stronger correlation wins over weaker one (as smaller uncertainty wins over bigger one). If a certain int. experiment (with **reasonable** uncertainty!) correlates two observables more than other experiments do the stronger correlation will not upset those other experiments.



Can we trust reaction models?

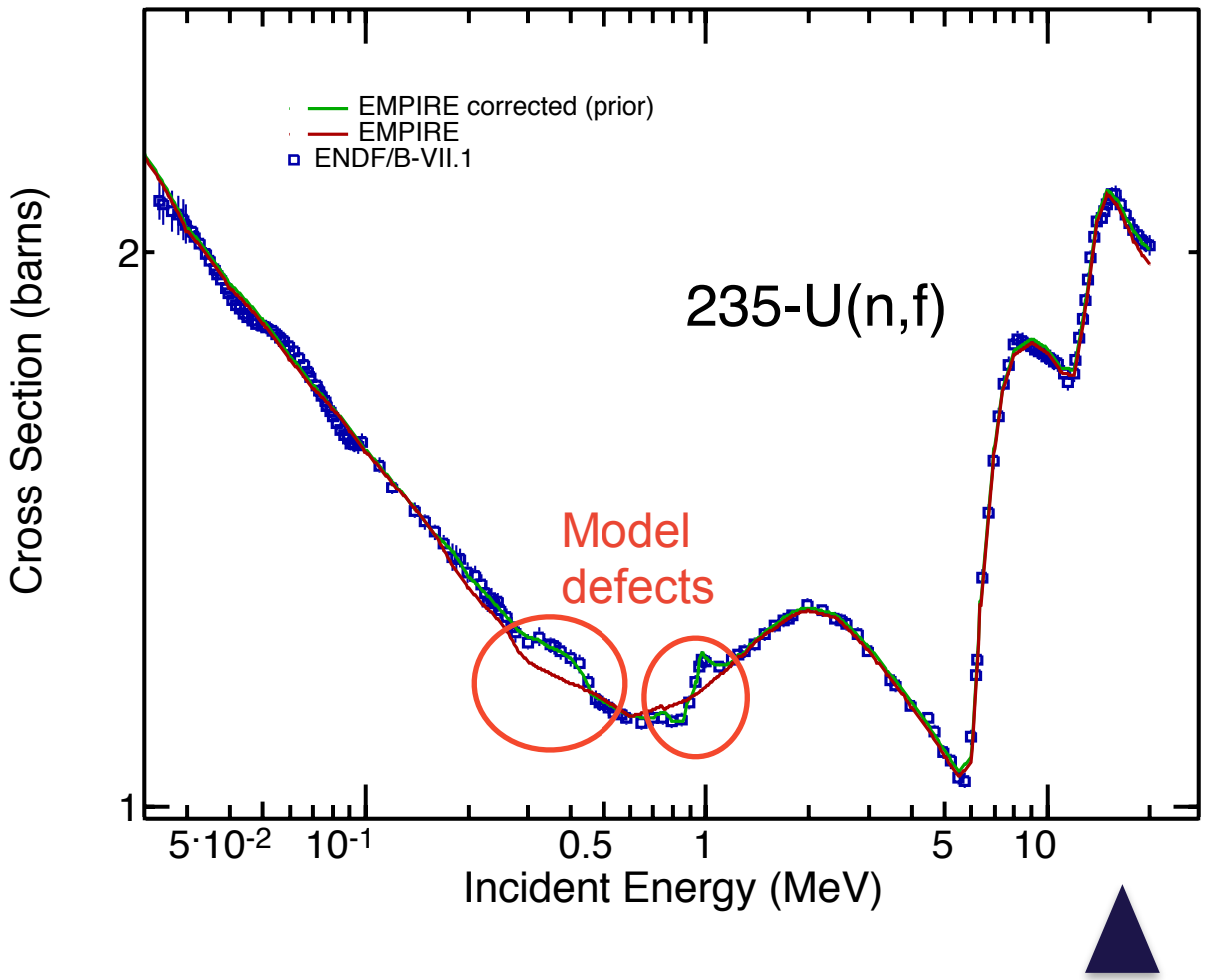
Reaction model can be anything between phenomenological up to first-principle microscopic one, i.e., the current best evaluation practice. Certainly different models/codes will have to be used.

- **Resonances** - Reich-Moore as a model driven by resonance parameters, no predictive power however**.**
- **Fast neutron** x-sections, spectra, ang. distr. and double differential x-sections can be generally reproduced within experimental uncertainties.
- **Modeling of nu-bar and PFNS** is getting better - soon we might be where our modeling of reaction x-sections and spectra is now.
- **Model defects** can be corrected with energy-dependent factors without violating physics constraints.



Can we trust reaction models (example)?

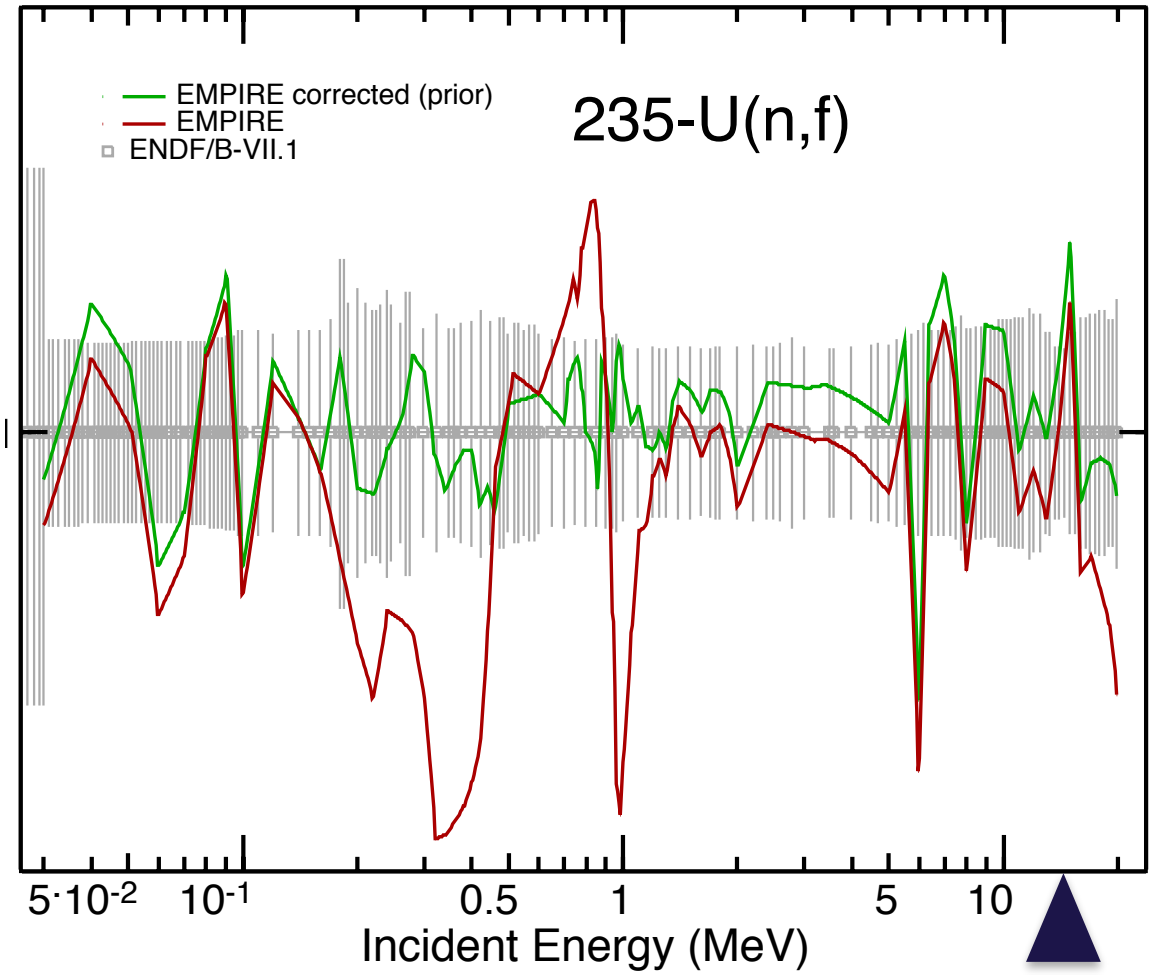
- Standard cross sections (VII.1 points) are pretty well described by pure EMPIRE calc. (red line)
- Model defects around 0.4 and 1 MeV can be fixed with energy dependent parameters



Can we trust reaction models (ratio to standard)?

Improvement obtained with energy dependent parameters (green line).

With more work or a simple script any precision of reproduction can be reached.

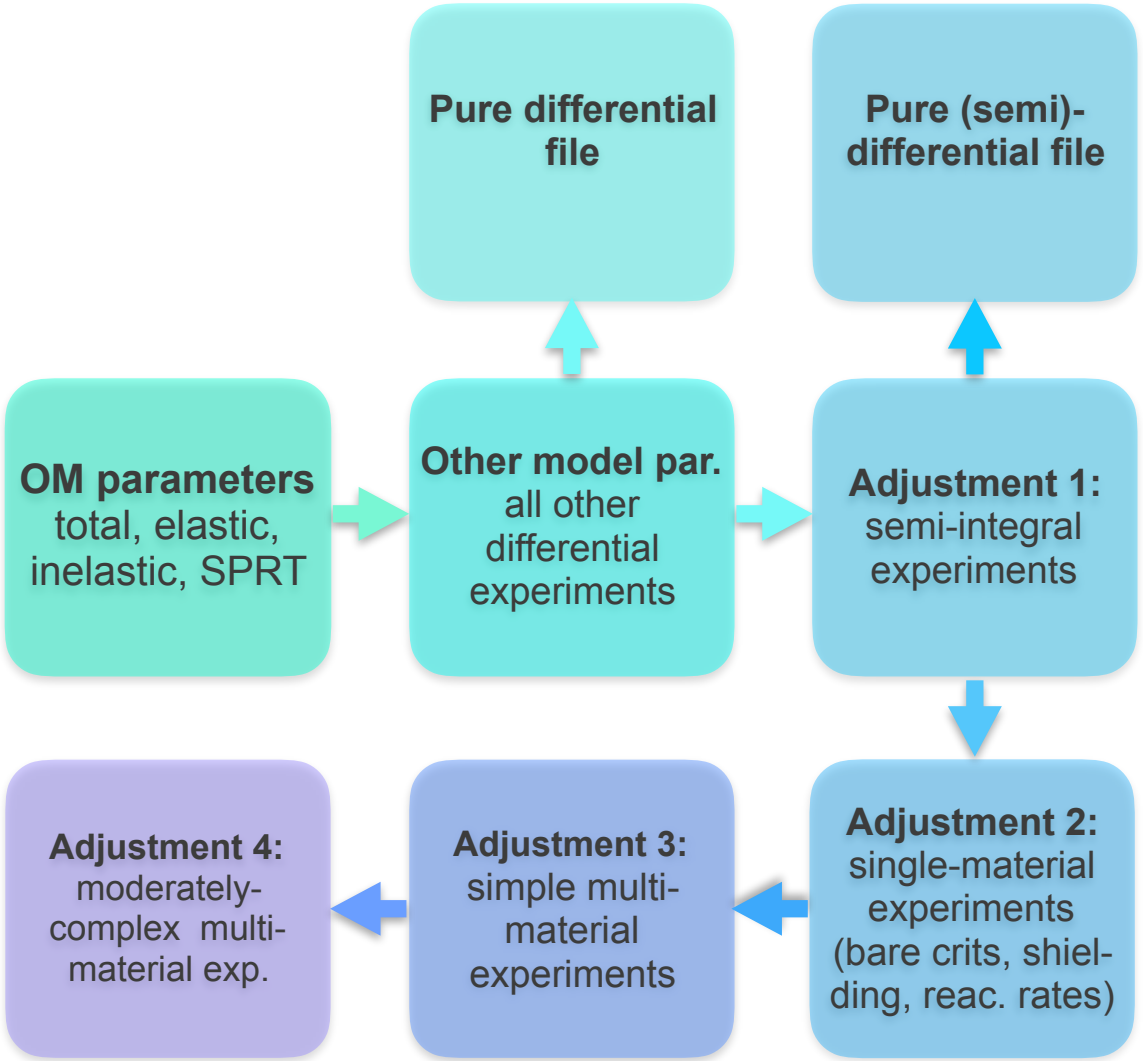


What if different adjustment methods produce different results?

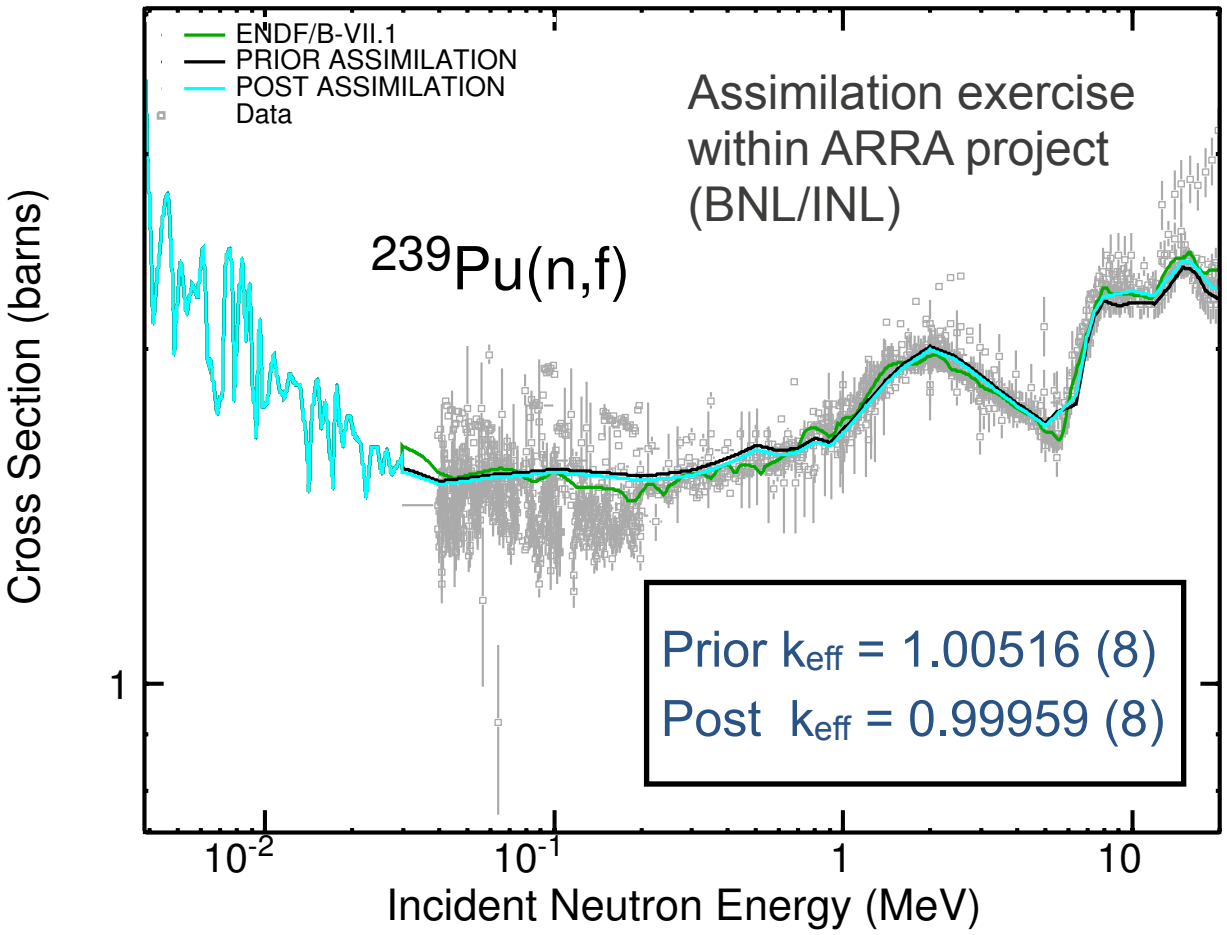
- It's too bad but that's nothing new! Experiments produce discrepant results, models calculate differently, even evaluators come up with disagreeing evaluations. We will have to cope with it as well.

What should be adjustment strategy?

- Subject of debate and personal preferences, however:
  - Don't drop everything into a **single pot**! I would advocate for a sequential approach, with covariances from every step.
  - I would also argue for consistent adjustment (**assimilation**) to impose reaction physics constraints.



Is assimilation feasible?



Assimilation is an adjustment in which adjustment is performed on model parameters and evaluation is produced by the model.

Experiment: JEZEBEL
Calculations: EMPIRE
Assimilation: KALMAN

What are changes in assimilated model parameters?

Parameter Name	pre-assimilation	post-assimilation
ATILNO-000	1.083	1.0851
ATILNO-001	0.907	0.9034
ATILNO-020	0.938	0.9380
ATILNO-030	0.988	0.9880
TUNEFI-010	0.833	0.8327
TUNE-000	2.228	2.2230
FUSRED-000	0.970	0.9700
RESNOR-000	1.320	1.3200
FISVF1-000	1.000	0.9995
FISVF1-010	1.000	1.0005
FISVF2-000	1.000	1.0042
FISVE1-000	1.000	0.9985
FISVE2-000	1.000	0.9995
FISHO1-000	1.000	0.9992
FISHO2-000	1.000	0.9992
FISAT1-000	0.917	0.9157
FISAT2-000	0.971	0.9717
FISAT2-010	0.981	0.9810
FISDL1-000	1.000	0.9999
FISDL2-000	1.000	0.9999
LDSHIF-000	1.100	1.0990
LDSHIF-010	1.063	1.0647
LDSHIF-020	0.917	0.9170
PFNALP-000	0.963	0.9613
PFNRAT-000	0.928	0.9279
PFNERE-000	0.999	1.0002
PFNTKE-000	0.984	0.9853

The change required for assimilation is very small in comparison to the uncertainties of the experimental cross sections.

Tiny changes in the parameters are well within the prior uncertainties of the parameters.

TAKE AWAY - since the current libraries are good priors and we'll use many more constraints the changes should be small.

What is a role of Machine Learning?

- We **don't know** yet! We've started it recently and first results are encouraging.
- At the lowest end of expectations, machine learning will automate and greatly speed up **analysis** of each adjustment that might be needed on a daily basis.
- Machine Learning may help to discover **hidden correlations**, identify **outliers**, point to possible **compensation of errors**, and eventually even perform the **adjustment**.