WPEC SG44 Subgroup Report
Investigation of Covariance Data in General Purpose Nuclear Data Libraries

Vladimir Sobes

US National Nuclear Data Week
Brookhaven National Laboratory
November 4-6, 2019
Upton, NY, USA

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ACKNOWLEDGEMENTS
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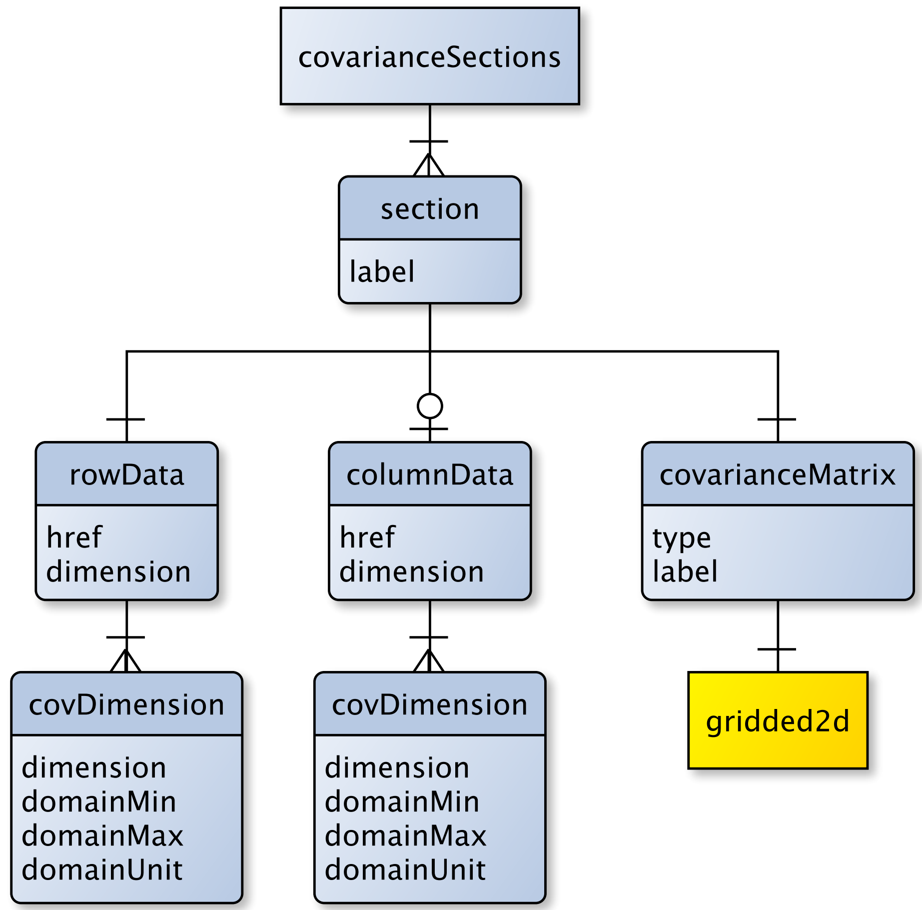
Progress on the Development of Thermal Scattering Covariance Formats

Aaron G. Tumulak, Brian Kiedrowski, Won Sik Yang, Hansol Park, Vladimir Sobes

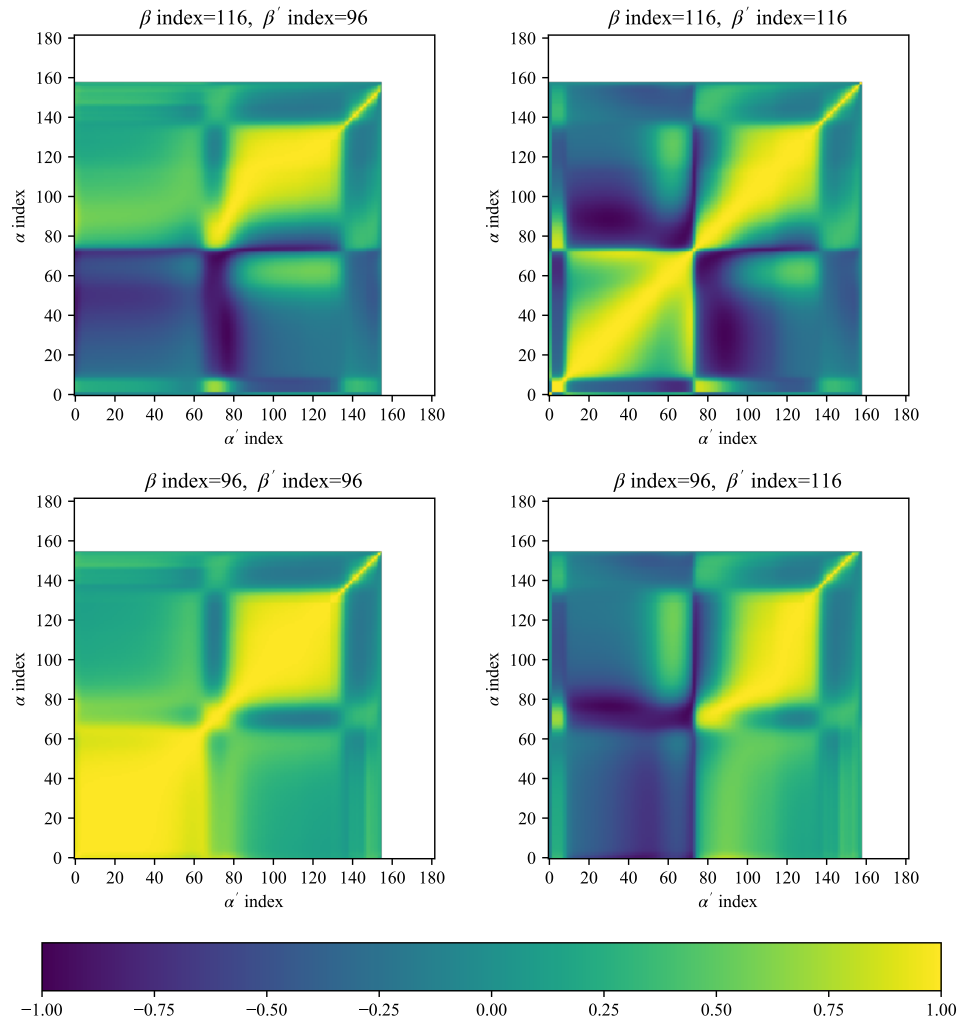
Format Proposal

- As of ENDF-6, there is no format for expressing covariances across two $S(\alpha, \beta)$ values.
- The full covariance matrix is divided into 2D sections.
- rowData (one required): specifies corresponding value for each row of covarianceMatrix
- covDimension (one or many): specifies fixed parameters in covarianceMatrix
- columnData (zero or one): used for cross-covariance sections



Demonstration

- 1000 random realizations of H in H2O were obtained from WPEC SG38 website.
- Same 182 α points and 259 β points from each realization.
- Covariance data was obtained using standard sample statistics.
- Full covariance matrix occupies about 17.78 GB in HDF5 format (double precision)
- Same data in XML will certainly be larger
- The proposed format allows for a coarser grid over covariance through rowData and columnData.



New paradigm for nuclear data evaluation

M. Herman[1],
D. Brown[2], R. Capote[3], M.B. Chadwick[1], W. Haeck[1],
T. Kawano[1], D. Neudecker[1], P. Talou[1], A. Trkov[3], M. White[1]

1) Los Alamos National Laboratory
2) Brookhaven National Laboratory
3) International Atomic Energy Agency

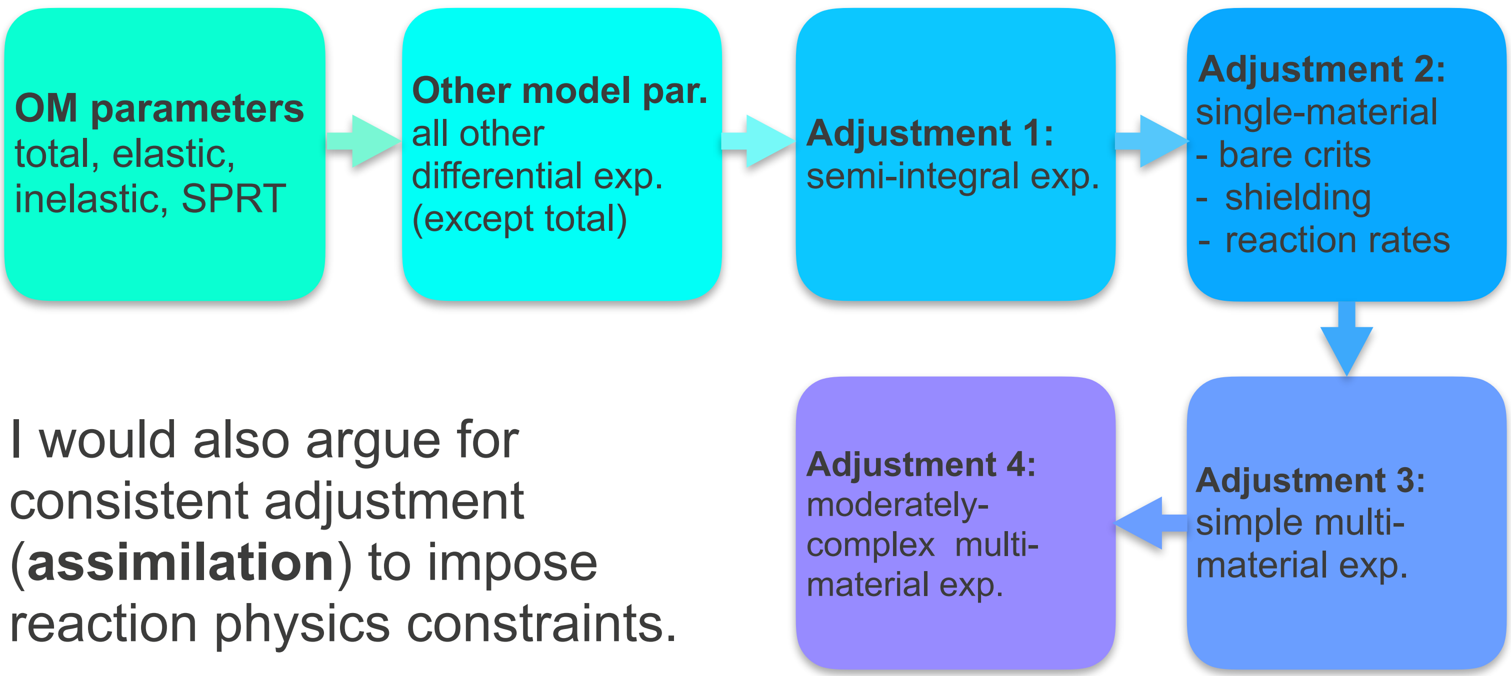
LA-UR-19-24625

What is the New Paradigm?

- Store **all** the details of evaluations in electronic form (inputs, codes, exp. data, assembly scripts) to make it possible to readjust evaluations in a matter of days.
- Adjust the whole library to a **representative** and **trustworthy** set of integral experiments covering the **whole available field**.
- Readjust the **whole library** 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 should be adjustment strategy?

- Subject of debate and personal preferences. I do not want to get into this now, however:
  - Don’t drop everything into a **single pot**! I would advocate for a sequential approach, with covariances from every step e.g.:



  - I would also argue for consistent adjustment (**assimilation**) to impose reaction physics constraints.

The role of fission yield correlations to obtain realistic uncertainty values in the summation method

A.A. Sonzogni, E.A. McCutchan

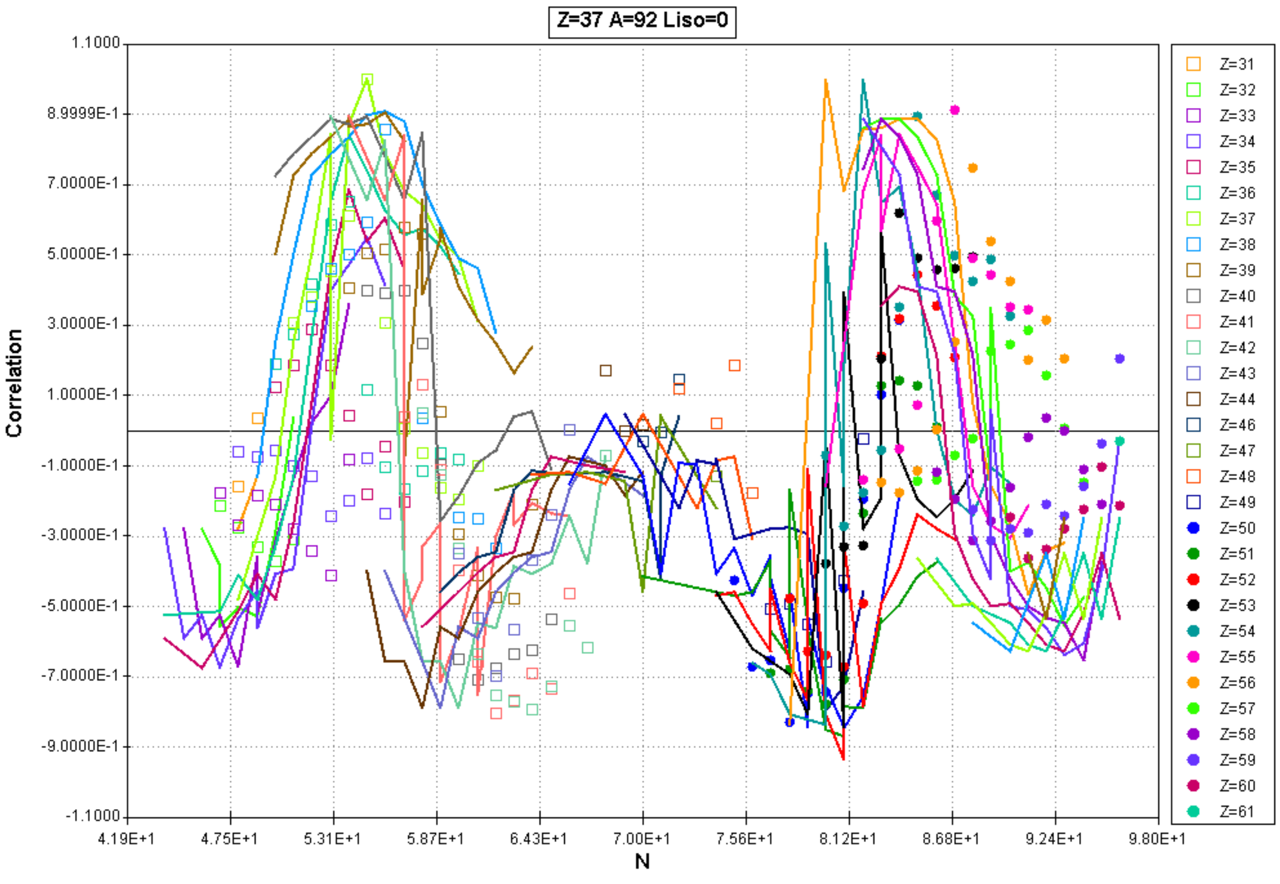
National Nuclear Data Center

Summation Method

Using ENDF/B-VIII.0 decay data, we can calculate cumulative yield correlations:

$C_i = I_i + \Sigma\, b_{ik}\, I_k$, where b_{ik} are decay probabilities and I_k are independent yields.

For instance, $C(^{92}Rb) = I(^{92}Rb)+I(^{92}Kr)+0.0195 \times I(^{93}Kr)+0.67 \times I(^{92}Br) + 0.68 \times I(^{93}Br)$



^{92}Rb Cumulative (lines) and independent (symbols) fission yield correlations for ^{235}U(n,f).

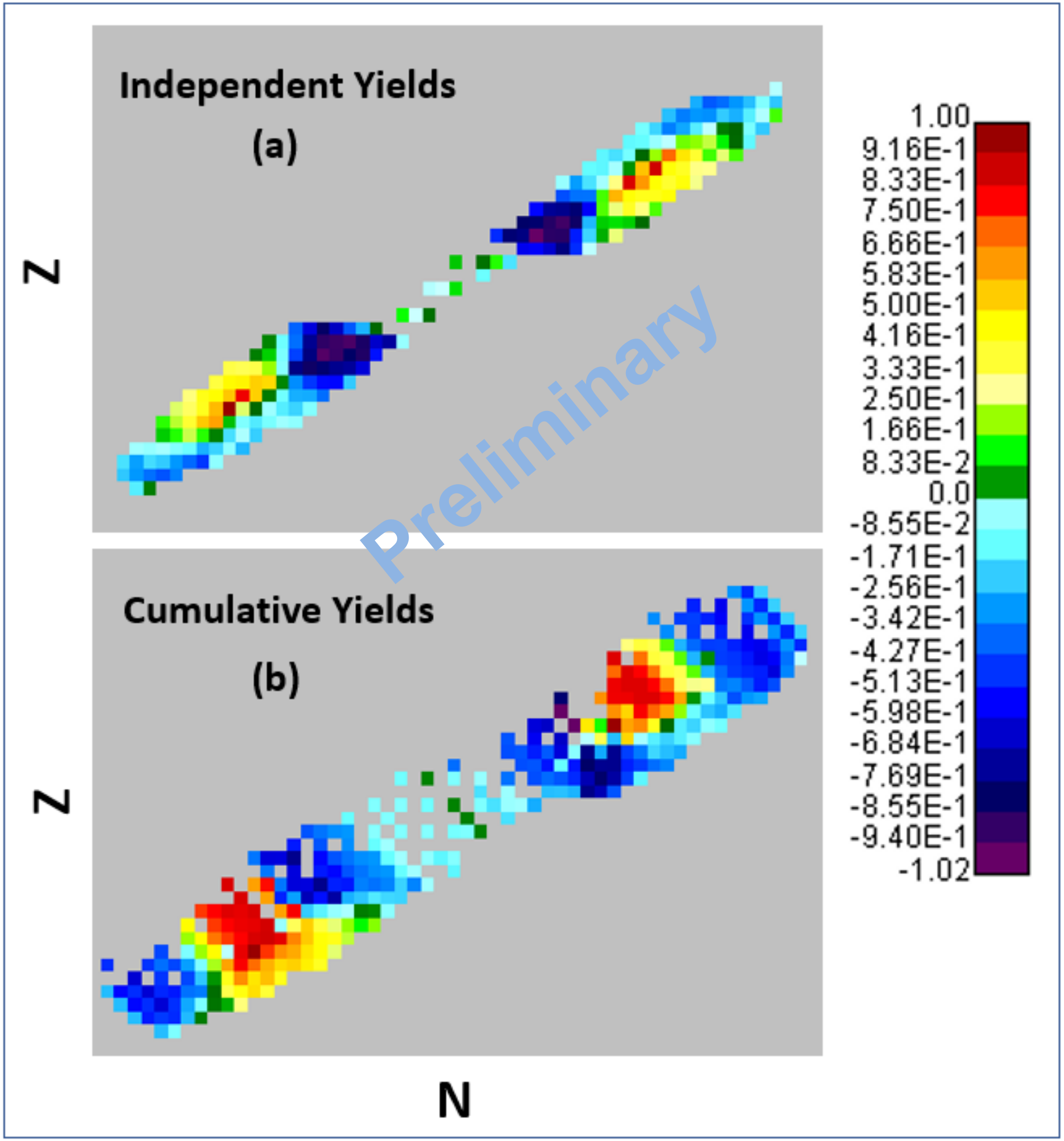
The CFY correlations get broader and shifted to lower Z values

Some issues combining GEF (Monte Carlo) with a JEFF-3.3 yields (deterministic)

Summation Method

Independent and cumulative fission yield correlations for ^{92}Rb in ^{235}U(n,f).

Cumulative fission yield correlations are considerable wider than the independent ones due to the link among different fission products provided by beta and IT decay.



ENDF/B-VIII.0 Augmented Covariance Data
The first iteration

V. Sobes, B.J. Marshall, D. Wiarda
F. Bostelmann, A. Holcomb, B. T. Rearden

31st WPEC Meetings
24-28 June, 2019
NEA Headquarters
Boulogne-Billancourt, France

The first iteration

Philosophy

1. 20/80 rule, start with only on the most impactful cross-correlations
2. Augment the ENDF/B-VIII.0 covariance matrix (not adjust)
3. Estimate the bulk correlation coefficient (coarse group structure)

Realization

1. ^{239}Pu, ^{235}U, ^{238}U $\sigma_{fis} - \bar{\nu}$
2. Only add new cross-correlations, do not adjust variances or existing correlations
3. Fast group 20 MeV - 50 keV*
   Inter. group 50 keV - 0.625 eV
   Thermal group 0.625 eV - 10^{-5} eV

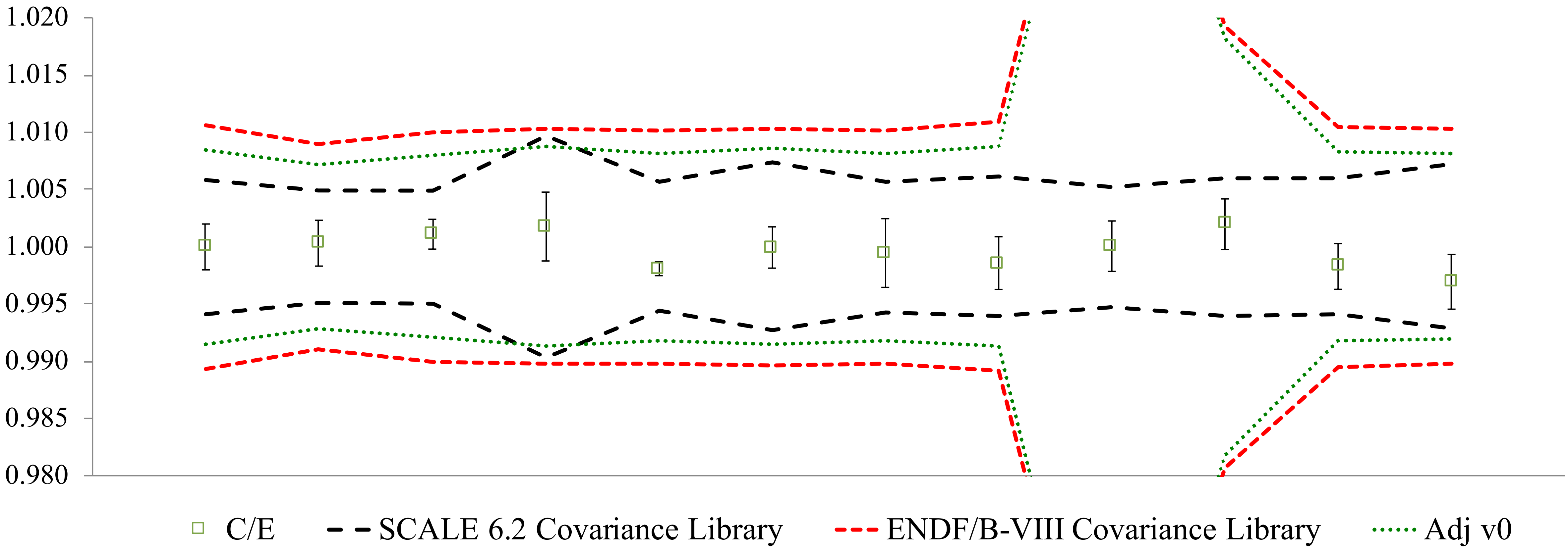
The goal of the first iteration was not to "solve" the problem outright, but to show conservative progress in the right direction

*Selected to match the boundary of the SCALE 56-group structure

^{235}U $\sigma_{fis} - \bar{\nu}$

INTER-MET-FAST (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-33	-37
fission intermediate	-28	-20	-23
fission thermal	-38	-26	-30
INTER-MET-FAST (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-34	-38
fission intermediate	-28	-20	-23
fission thermal	-39	-27	-31
LEU-COMP-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-10	-8	-13
fission intermediate	-24	-17	-32
fission thermal	-23	-13	-36
LEU-COMP-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-9	-9	-11
fission intermediate	-23	-18	-30
fission thermal	-23	-13	-36

Results for PU-MET-FAST systems



OAK RIDGE National Laboratory

DE LA RECHERCHE À L'INDUSTRIE

STATUS AND REQUIREMENTS OF NUCLEAR DATA VARIANCE-COVARIANCE MATRICES FOR THE NEUTRONIC ASSESSMENT OF FAST REACTOR CORES.

G. Rimpault, G. Noguère, L. Buiron

CEA, DEN, DER, CADARACHE, FRANCE

WPEC 44 :
"Investigation of Covariance Data in General Purpose Nuclear Data Libraries"

OECD NEA HQ, Boulogne-Billancourt,
June 25-26, 2019

k_{EFF} UNCERTAINTIES

Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	0.00565	0.00252	0.00068	0.00403	0.00023	0.00156	0.00758
ENDF-BVII	0.00220	0.00418	0.00150	0.01137	0.00007	0.00175	0.01253
JENDL-4	0.00281	0.00451	0.00076	0.00601	0.00009	0.00156	0.00821

✓ By comparing Uncertainties on Keff using different covariances: COMAC, ENDF BVII.1 and JENDL4.0, one can notice significant differences

*SFR Core

$\rho_{Doppler}$ UNCERTAINTIES

Library	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	NU	SUM
COMAC	1.47%	1.82%	1.23%	1.35%	0.05%	0.20%	2.97%
ENDF-BVII	0.46%	1.47%	2.07%	2.44%	0.02%	0.21%	3.56%
JENDL-4	0.56%	1.20%	1.76%	1.52%	0.03%	0.20%	2.68%

- ✓ By comparing Uncertainties on Keff using different covariances: COMAC, ENDF BVII.1 and JENDL4.0, one can notice significant differences

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The identification and treatment of unrecognized uncertainties and the impact on evaluated uncertainties– SG44

Henrik Sjöstrand, Georg Schnabel

Department of Physics and Astronomy
Division of Applied Nuclear Physics Uppsala University

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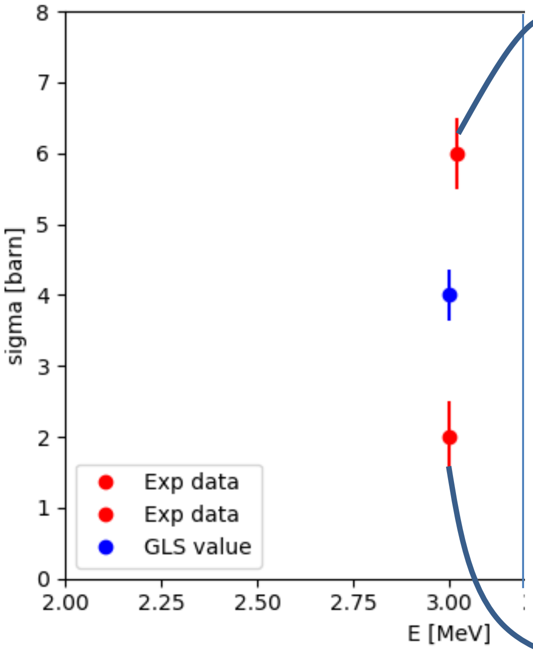
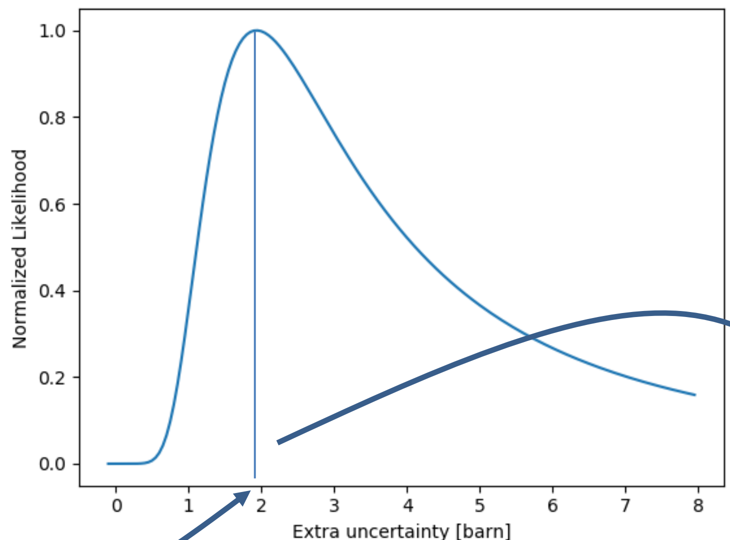
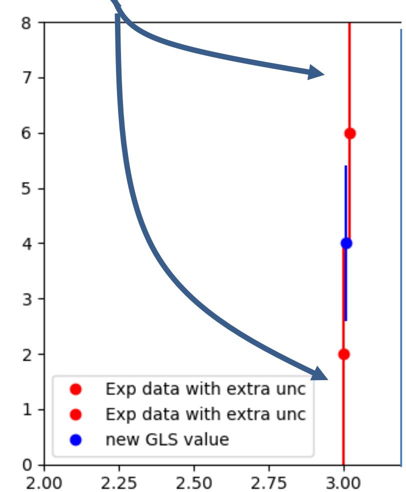
Toy example and L- function

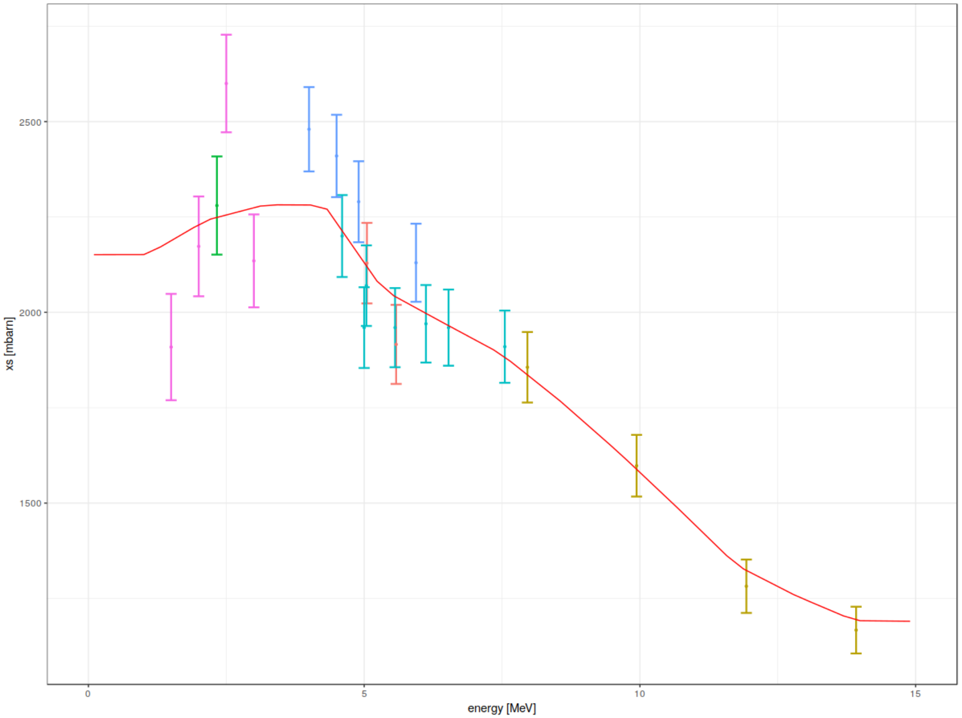


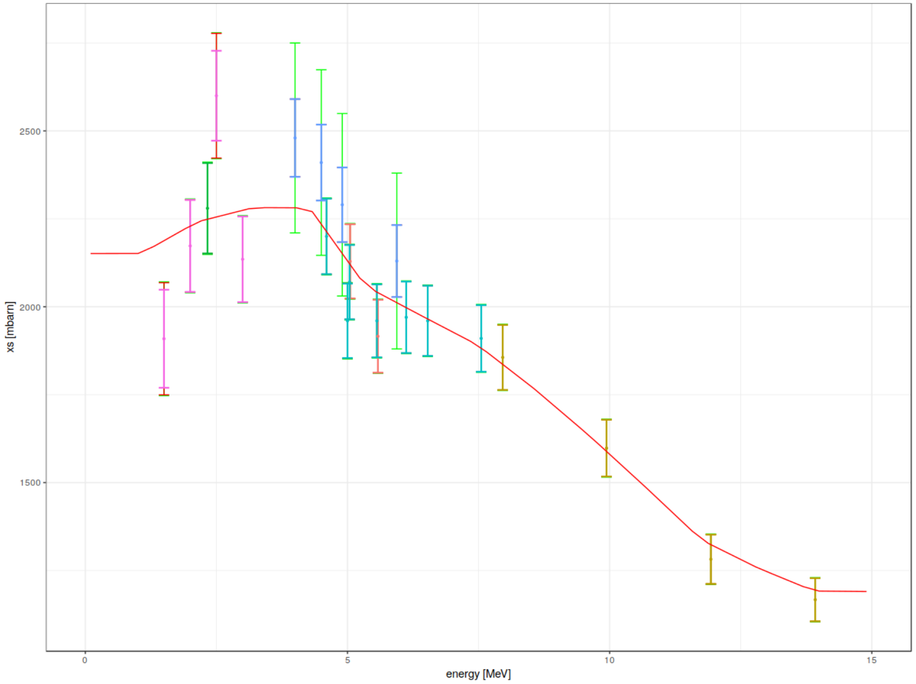


$$L = \frac{1}{\sqrt{2\pi n \left| S A_0 S^T + \mathrm{cov}_{rep} + \mathrm{cov}_{extra} \right|}} e^{-\frac{\chi^2}{2}} e^{-\beta \sum \kappa_{extra}^2}$$



Fe56 results





Fe56(n,el)

Improved Calibration of Nuclear Resonance Parameters

MTV Kickoff Meeting

May 20th, 2019

Chris Perfetti
University of New Mexico

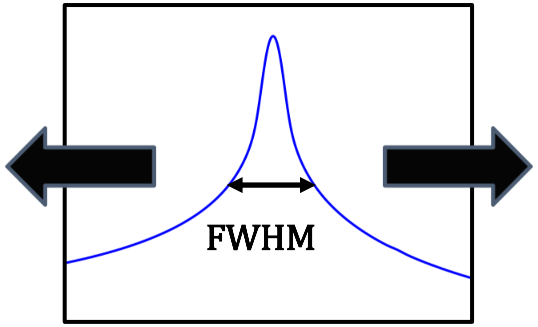
Technical Work Plan

- **Task 1:** Develop a resonance parameter sensitivity capability.
- **Task 2:** Modify TSURFER to assimilate experimental data by adjusting fundamental nuclear data.
- **Task 3:** Evaluate the accuracy of nuclear data and nuclear covariance adjustments.

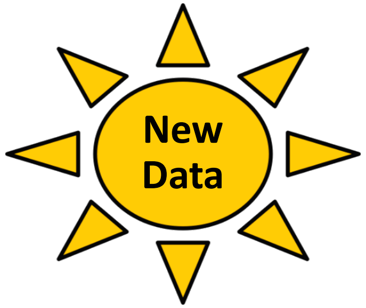
Task 1:

$$S_{f(x),\,FWHM} = \frac{\partial f(x) / f(x)}{\partial FWHM / FWHM}$$

Task 2:



Task 3:



Technical Work Plan

Year 1:

- Develop resolved resonance sensitivity capability.

Year 2:

- Modify TSURFER to allow resolved resonance data adjustment.
- Demonstrate capability.

Year 3:

- Develop unresolved resonance sensitivity capability.

Year 4:

- Develop sensitivity capability for fast energy model parameters.

Year 5:

- Modify TSURFER to allow adjustment of all nuclear data parameters.
- Demonstrate capability.

Report on the CSEWG covariance and measurement session initiative on creating templates of expected measurement uncertainties

Denise Neudecker WPEC-SG44, 6/22/19

Thanks to: Y. Danon, A. Lewis, P. Talou, M.C. White, R.C. Haight, B. Pritychenko, P. Schillebeeckx, D.L. Smith, A. Sonzogni and all mini-CSEWG 2019 participants.

What is a template?

Unc. Source	Absolute	Clean Ratio	Indirect Ratio
Sample Mass	> 1%	Both Samples	Both samples
Counting Statistics	Sample-dependent	Both, combined	Both samples
Attenuation	0.2-2%	0.02-0.2%	0.2-2%
Detector Efficiency	1-2%	0-0.3%	1-2%, 0.5-1%
FF Angular Distrib.	~0.1%	Less than for abs.	~0.1%
Background	0.2 - >10%	0.2 - >10%	0.2 - >10%
Energy Unc.	1%, 1-2 ns	Combined	Both detectors
Neutron Flux	>1%	Cancels or small	Cancels or small
Multiple Scattering	0.2-1%	Reduced for abs.	0.2-1%
Impurit. in Sample	Sample-dependent	Both samples	Both samples
Dead Time	>0.1%	Both, combined	Both detectors

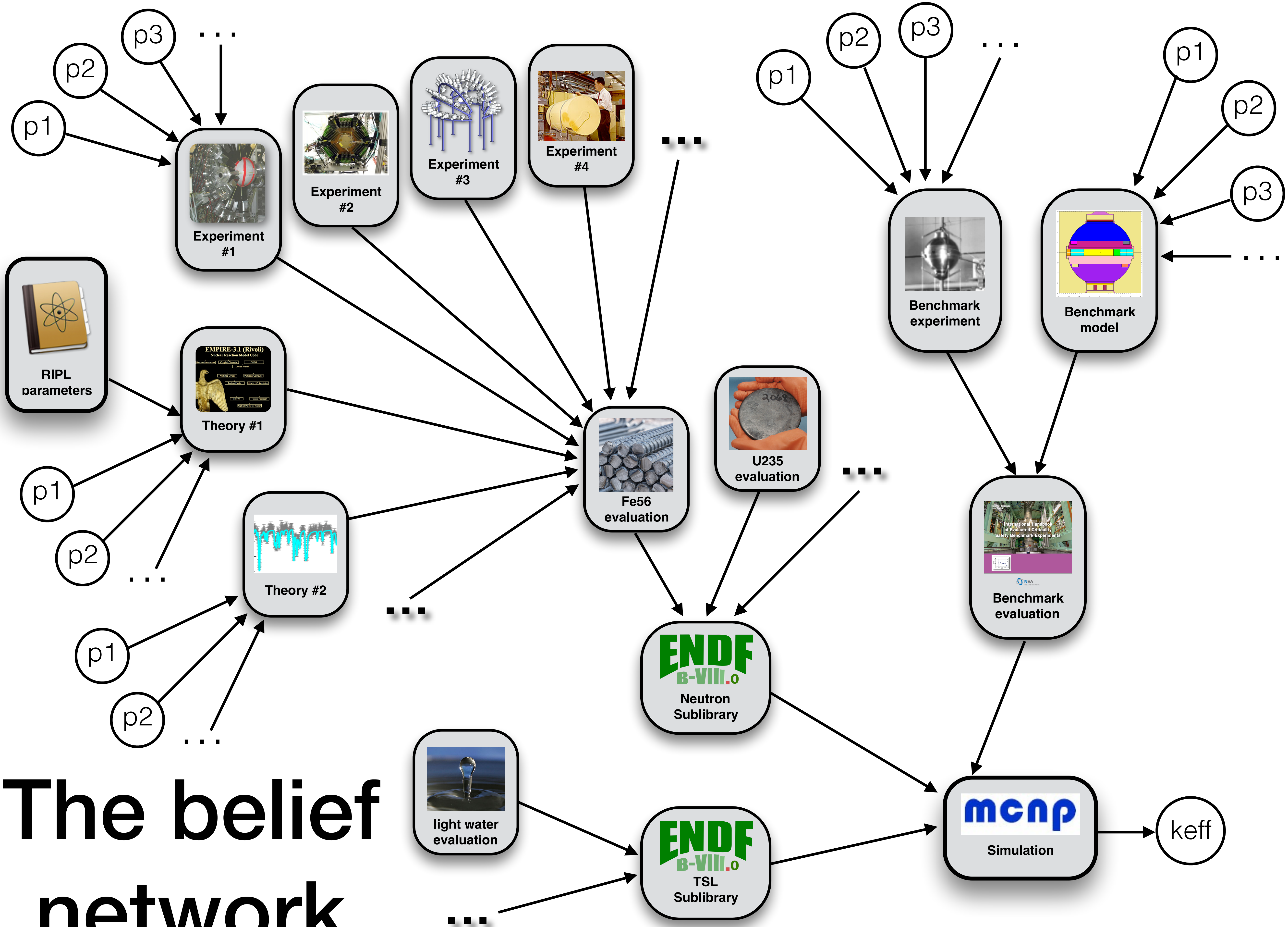
The (n,g) template needs more work:

Unc. source	Range (%)	Correlations	Cor(Exp_1,Exp_2)
Normalization	0.3-2%	full	Possible
Background	3%	full	0
Attenuation	2-5%	?	?
Reaction and Fluence counts	Should be given, otherwise reject	diagonal	0
Nuclear Data	Take from library	Take from library	Take from library
Detector efficiency	Part of normalization	full	possible

Session lead: P. Schillebeeckx

The Nuclear Data Belief Network

The belief network

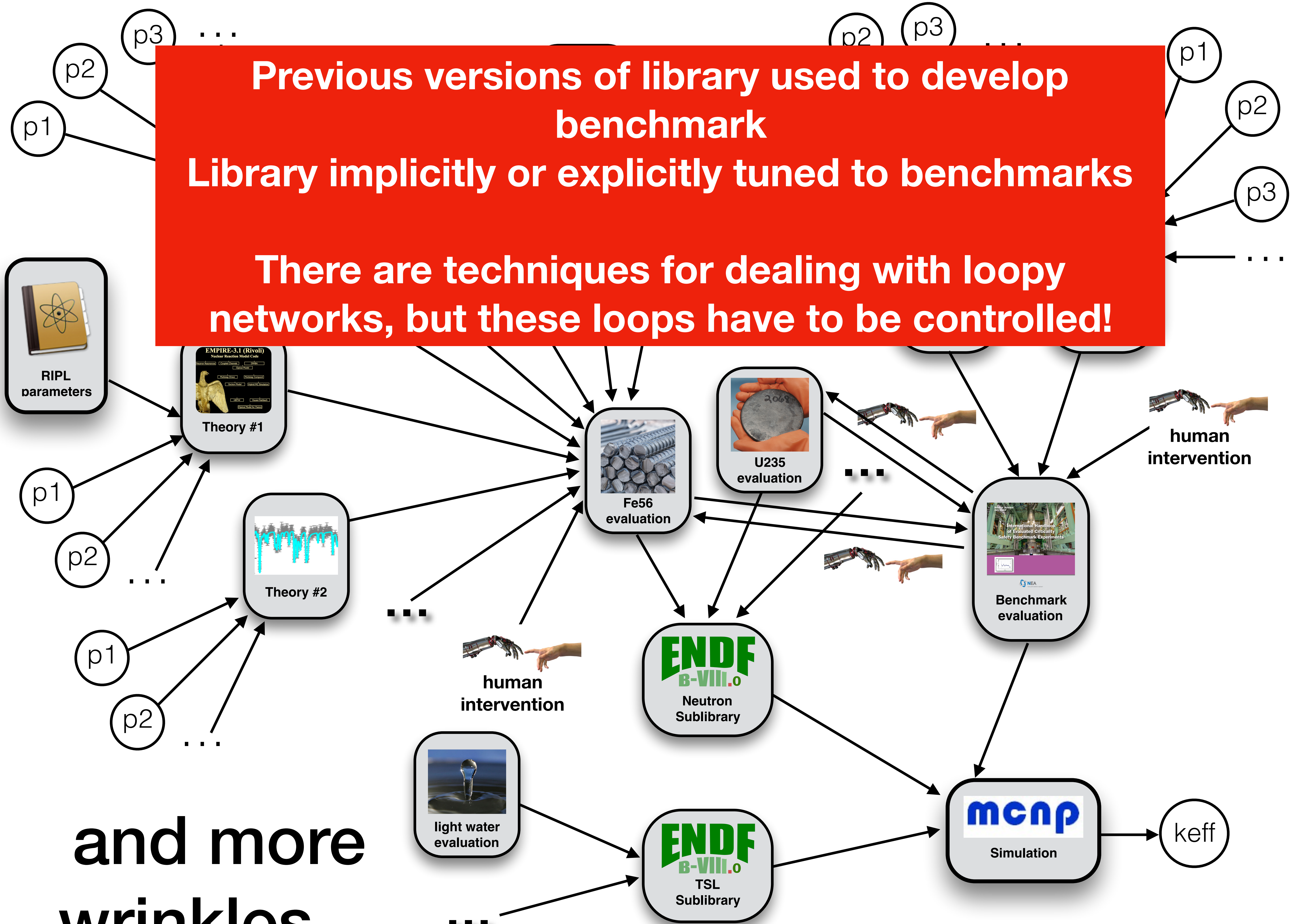


Slide from D. Brown (Nuclear Science and Technology)

Previous versions of library used to develop benchmark

Library implicitly or explicitly tuned to benchmarks

There are techniques for dealing with loopy networks, but these loops have to be controlled!



and more wrinkles…

Slide from D. Brown (Nuclear Science and Technology)

WPEC sub-group report

(Cyrille de Saint Jean (CEA, France) and Vladimir Sobes (ORNL, USA))

Title:

Investigation of Covariance Data in General Purpose Nuclear Data Libraries

Subgroup Mandate

The motivation for the subgroup is to bring together the international covariance community to understand how the covariance data can be so different between the different evaluated nuclear data files, ENDF, JEFF, JENDL, CENDL, etc., while the mean values (cross sections, nu-bar, etc.) are generally very similar. Many questions have emerged from the groups applying covariance data for analysis, such as the Working Party on Nuclear Criticality Safety (WPNCS) Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA), on how the use of different covariance libraries (e.g. ENDF, JEFF, JENDL, etc.) affects uncertainty quantification and similarity assessment. Further, significant differences in covariance libraries lead to differences in the adjustment of parameters for fast reactors, which is an important topic for WPEC sub-group (SG) 39.

The CIELO project, WPEC SG-40, established an international effort of nuclear data evaluators from different nuclear data projects to provide nuclear data evaluations that may be consistently accepted by all major nuclear data projects. This work has certainly driven the progress towards minimizing the disagreement in the mean values (cross sections, nu-bar, etc.) between different nuclear data libraries. However, with that project coming to a close in the coming year, there has not yet been a concentrated effort on providing consistent covariance evaluations across the different nuclear data libraries. The maturity of the nuclear data evaluation process is such, at this time, that it is warranted to create an international collaboration on cross section covariance evaluation methodologies.

This sub-group will be tasked with the goal to investigate covariance data for a broad range of system types, not just fast reactors as is the focus of WPEC SG-39. This sub-group will leverage the work of previous sub-groups which investigated the generation of covariance data for specific physical regions, such as WPEC SG-24 and SG-36, which focused on evaluations of fast neutron region and the resolved resonance region, as well as WPEC SG-42 which focused on the evaluation and covariance generation for thermal scattering. This sub-group will focus its attention on providing guidance to the international community on methods for systematic and consistent evaluation of covariance data for the whole energy range, paying special attention to energy domain interface (resolved resonance/unresolved resonance/continuum). The group will also deliver examples of the application of the proposed methodology on a few selected isotopes. The ultimate goal of the subgroup is to provide an overview of the best practices of how to generate more consistent covariance data sets.

1. Introduction [Sobes]
2. Evaluation techniques proposed to break into two sections:
    a. (I) main techniques used [Cyrille]
    b. (II) synthesize discussion from previous meetings/discussions on known problems (model defects/biases, (R/U)RR uncertainties) [Denise/Schnabel?/Henrik?/ Leeb?]
        i. Model defects: phenomenological models can be poor but with very low evaluated uncertainties
        ii. Model biases: inference of biases from advanced models
        iii. Treatment and representation of uncertainties in the unresolved resonance region where self-shielding is important for reactors
3. Analysis of experimental data results from the mini-CSEWG [Denise/Lewis], including experimental cross-correlations
    a. Sources of experimental uncertainty
        i. Catalogue
        ii. Publication requirements (not only numbers)
        iii. Recommendations for EXFOR database IAEA contribution on evaluated EXFOR [Zerkin]
        iv. Algorithms/methods Ni evaluation example [Sjostrand/Schnabel]
    b. Commenting on autonomous/automatic methods. See previous bullet [Sjostrand/Schnabel]
    c. Commenting on handling of discrepant data sets discrepant experiments work [Sjostrand/Schnabel]
4. Propagation of uncertainty and integral experiments - Collaboration with SG46
    a. Use of integral experiments in evaluations, documentation not guidance for whether or not to utilise IE, but comments regarding documentation [Sobes]
    b. Other probability distributions for nuclear data uncertainty review paper from CW to consider inclusion [Sobes]
        i. Document
        ii. Format
    c. Testing/comparison/consistency of covariance data pub methodology [Denise]
    d. IE cross-correlation [Hill]
5. Cross-correlation
    a. Cross-isotope and when to neglect [Sobes]
    b. Fission yields [Sonzogni/Fiorito?/Serot?/Rochman?]
6. New computational benchmark [Sobes]
7. Formats and interpretation [Denise reformat LANL report]
    a. Documentation of covariance evaluation technique
        i. Clear interpretation by evaluator
        ii. Model parameters and code
        iii. Reporting known unknowns vs estimating unknown unknowns
        iv. Clear interpretation by user
    b. Angular distribution covariance format and evaluation [Fiorito, Trkov]
    c. Verification: positive definite, robust, stable to numerical errors. How to deal with negative eigenvalues? [write eigenvalue decomp, Caleb]
    d. Thermal scatter law covariance methods [Sobes]
8. Processing codes wish list – Collaboration with SG43
    a. Prompt fission neutron spectra (PFNS) correlations to cross section [short note, Sobes, Denise]

b. Covariances of secondary distributions (e.g., inelastic) Legendre covariances [Trkov?]
c. S(α,β) format [Sobes]
d. Random files cases where limitations of covariances are overcome via random files [Sjostrand/Schnabel]

9. Conclusion
10. References
11. Appendices

Computational Benchmark Proposal

ENDF/B-VIII.0 Covariance Disclaimer

Comments about the covariance in current ENDF evaluations

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2. The use of this covariance to calculate uncertainties for integral quantities such as Keff will usually result in an overestimate of the uncertainty. That said, comparisons to integral data are essential during the evaluation process and users should not be surprised if the *mean value* nuclear data allow for the accurate prediction of Keff, even if the covariances to not reflect this consideration.

Proposal

It is proposed to estimate the missing cross-correlations from nuclear data libraries.

Hypotheses:

1. Some correlations, e.g. Pu-239 fission vs. nu, will be "stable" regardless of which integral benchmarks are used, therefore they can be reliably estimated.
2. These correlations will have a significant impact on reducing the propagated nuclear data uncertainty.