Covariance Workshop Summary

Donald L. Smith

Argonne National Laboratory

Port Jefferson, NY, USA

27 June 2008

A Big Success!

Thank you for your attention!

… The End …

Tasting Room at a Long Island Winery

We won’t be allowed to “get off” that easily!

- The Workshop organizers would be very angry with me if my summary ended here
- So … during the next 30 minutes or so I will attempt to tell you what you undoubtedly already know … And - even worse – you will be subjected to my own interpretation of what you saw and heard during this Workshop just like the TV “talking heads” analyze the content of political speeches!

We appreciate those who made it happen!

Organizers: Pavel Oblozinsky, Mike Herman, Alejandro Sonzongi, and the NNDC staff

Program Committee: Mark Chadwick, Yaron Danon, Michael Dunn, Anatoly Ignatyuk, Makoto Ishikawa, Toshihiko Kawano, Arjan Koning, Dennis McNabb, Giuseppe Palmiotti, Massimo Salvatores, Don Smith

Conference Dinner: Brookhaven Science Associates & Yvette & Bob & Mike!

Venue: Danfords Hotel, Port Jefferson, USA

Some (pertinent?) quotes …

- Rodney Dangerfield (comedian): "… I don't get no respect! …"

For years nuclear data uncertainties (covariances) were a "back burner" issue that attracted "no respect" from data users

- George Santayana (historian): "Those who do not study history are doomed to repeat it"

Covariance matrices are a "hot" topic now, but will they be just as "trendy" and relevant in the future? Only time will tell …

- Edgar Allen Poe (poet)*:* "Ponder over many quaint and curious volumes of forgotten lore"

The literature on nuclear data errors is extensive! … While there are new things to discover, let's not reinvent the wheel!

A bit of relevant history …

- "*Nuclear Data Evaluation Methodology*", BNL, 1992 (almost 16 years ago!)

►67 participants, 77 papers published by World Scientific in 1993

►10 people attending the present Workshop were there!

► 9 papers dealt explicitly with covariance generation … But, other contributions touched on this subject in various ways

- "A *Covariance Workshop*", BNL, 1999

► Organized by Luis Leal and Don Smith (I almost forgot it!)

► 28 attendees, 7 of those people are here today

► Proceedings edited by Luis and published as an ORNL report

- Other smaller gatherings? … Certainly!

Some Workshop statistics …

- Registered participants: 53
  - ►United States: 37
  - ►Foreign Visitors: 16 from 10 countries

    Austria, Belarus, France, Germany, Israel, Japan, Netherlands, Slovenia, South Korea, United Kingdom
- Contributions: 39
  - ►Oral Talks: 32
  - ►Posters: 7

Contributions by Topic

- Introduction & Summary: 2
- User's Perspective: 4
- Methodology: 12
- Evaluations: 12
- Applications: 7
- Data Retrieval & Visualization: 2

Major part of the conference

Outline of this Summary Talk

- Some General Observations
- Covariance Methodology
- Covariance Evaluations
- Covariance Applications
- User's Perspective
- Data Retrieval & Visualization
- Some personal thoughts about the future

Some General Observations

Positive ☺

- The strong interaction between data producer and data user communities is unprecedented!
- Great progress has been made in developing and applying new evaluation methodologies
- Newer evaluations are including covariances
- Design of “smart” experiments is in progress

Negative 

- I would like to have seen more papers dealing with how to generate covariances for expt’s!

Some notes from Don's laptop …

- **Apology**: I will not be able to mention every point made in each talk and poster due to time limitations … and I may not interpret your points exactly as you intended in your presentations

… Anyway, each conference attendee will undoubtedly carry away a personal impression of what he (or she) saw, heard, and felt was important from the content of this Workshop

Covariance Methodology (1)

- There is a strong upsurge of activity in methods to obtain covariances from theory and modeling
  - ► The relationship between basic nuclear theory and phenomenological models for light nuclei, such as R-matrix formalism, and the practical impact of all this on evaluating covariances, was discussed (**Hofmann** & **Hale**)
  - ► Methods such as the Monte-Carlo, Kalman-filter, and GLS rely on including prior parameter & expt'l covariances. We were told that this can be done in a way that also takes model-defect uncertainties into account (**Leeb et al.**) … But, in doing this we must include systematic errors properly!
  - ► The brute force Monte Carlo approach offers a straightforward method to propagate errors and do evaluations, but this can be very computationally intensive … Two alternative ways to do this were mentioned: One is the Metropolis MC sampling scheme (**Capote et al.**) .. The other is a nonintrusive regression-based approach (**Dossantos-Uzarralde et al.**) … Both of these methods assess the relative importance of each parameter or combinations of them and can lead to a substantial speed-up in the analysis process compared with more "conventional" Monte Carlo techniques

Covariance Methodology (2)

- Large-scale evaluations of covariances from nuclear modeling have been facilitated by code enhancements … this is leading to new insight

  ► The need to produce covariance information on a mass scale has led to major enhancements of existing nuclear model codes such as EMPIRE … Covariance information can now be generated from thermal energy to many tens of MeV seamlessly using a single code (e.g., **Herman et al.**) … Similar evaluation code enhancements are being introduced for other N.M. codes

  ► Enhanced code capabilities are opening up opportunities for acquiring a better understanding of the inner workings of existing nuclear models … For example, distinct maxima and minima in evaluated neutron total cross section uncertainties have been observed in large scale calculations with the spherical optical model … These can be understood physically as resulting from partial wave effects at lower energies as well the Ramsauer effect at higher energy (**Pigni et al.** & **Herman et al.**) … This new insight offers a tool for exploring the uncertainties related to nuclear model deficiencies

Covariance Methodology (3)

- Investigations of the relationship between nuclear models and existing experimental data are offering some insight on how to estimate prior parameter errors and their correlations

  ► Information about correlations of nuclear model parameters emerges from exercises to filter possible choices for evaluations based only on nuclear modeling as a consequence of selection by comparison (**Rochman et al.**) or application of the Kalman filtering concept (**Pigni et al.** & **Kawano et al.**)

- Use of a Unified Monte Carlo (UMC) scheme for performing evaluations is being studied

  ► Properties of UMC have been explored with "toy" examples (**Capote et al.**) … Significant differences between UMC and GLS are seen for ratio experimental data while applicability of GLS for those cases that involve only "simple", non-linear data/parameter relationships has been demonstrated

Covariance Methodology (4)

- We were treated to interesting new ideas and timely reminders intended to “shake us up” and prevent us from falling into complacency

► A time honored pastime in the evaluation business is to “tweak” or “tune” evaluations to produce the best possible C/E agreement (usually to four significant figures) using data from fast critical benchmarks … We have been warned at this Workshop of the hidden risks of this approach in that it leads to a lack of traceability and “hidden” response parameter correlations result from using non-rigorous adjustment practices (**Wagschal** & **Maslov**)

► It appears that in principle it would be possible to start with a collection of well-validated nuclear model parameters and their estimated uncertainties and proceed without intermediate “stops” to estimates of the uncertainties of key reactor system operational parameters (e.g., k-eff) … The concept was demonstrated at this Workshop (**Rochman et al.**) … This is clearly a pretty controversial idea judging by discussion comments, but this tool has merit and deserves consideration for the detailed understanding it can contribute

Covariance Evaluations (1)

- The new ENDF/B-VII standards appear to have quite reliable covariance information

  ► The procedures used to produce the covariance matrices for ENDF/B-VII Neutron Standards Library were described at this Workshop (**Carlson et al.**)

  ► This standards library has been introduced into the GANDR system as a "pseudo experimental data set". GANDR is designed for a variety of tasks in the evaluation of nuclear reaction data, in assessing the status of existing nuclear data, and in guiding the planning of future experiments (**Muir et al.**)

- Extensive new covariance evaluations for the thermal and RR regions are being produced

  ► Work at the NNDC to estimate thermal & RR errors for 15 actinides and 20 structural and coolant materials was described (**Mughabghab et al.**)

  ► A new resonance module has been added to EMPIRE (**Cho et al.**)

  ► Thermal & RR covariances evaluated for ^{233,235,238}U & ^{239}Pu (**Leal et al.**)

  … Discussed novel new methods for handling the massive covariance info.

Covariance Evaluations (2)

- Extensive work is in progress on producing comprehensive neutron cross section evaluations that include covariances

► A collaboration to generate complete evaluations for isotopes of W has been undertaken … The methods used to produce these evaluations was described in a contribution to this Workshop along with results (**Trkov et al.**)

► LANL has an extensive program to produce evaluations in its region of specialization (light nuclei and actinides above the RR) … A paper at this conference described the methods used for the actinides (**Kawano et al.**)

► At the NNDC new evaluations for ^{55}Mn and ^{90}Zr have been completed … A paper at this Workshop describes the methodology used and discusses the results of this work including comparisons with earlier work (**Pigni et al.**)

► The JENDL Actinide File 2008 (JENDL/AC-2008) has been released … This file and plans for a future covariance evaluation of actinide fission and capture cross sections were described at this Workshop (**Iwamoto et al.**)

Covariance Evaluations (3)

- Work on producing covariances is extending beyond cross sections to neutron spectra due to its influence on system response errors

► If fission neutron spectra are represented by parameterized models then spectrum uncertainties can be estimated from the parameter uncertainties … Such a study has been carried out using the Watts and Kornilov spectrum formulations and a Monte Carlo method to propagate errors (**Trkov et al.**)

► The LANL group reported on its work to estimate prompt fission neutron spectra and neutron multiplicity uncertainties starting with the well-known Los Alamos model and merging experimental data uncertainties using the Kalman Bayesian filtering approach (**Kawano et al.**)

► When propagating fission spectrum uncertainties to system response uncertainties it is important that the spectrum be properly normalized and that all rows and columns of the covariance matrix sum to zero … Caution is also needed in scaling the sensitivity coefficients appropriately (**Yang et al.**)

Covariance Evaluations (4)

- Two additional papers at this Workshop dealt with issues associated with estimating errors in input data used for generating evaluations

  ► Uncertainties in non-elastic cross sections (~ 5-10%) are usually much larger than those for total cross sections … Work at LLNL has led to the development of a procedure to reduce these uncertainties based on the consideration of total and elastic cross sections and Wick's limit (**Dietrich**)

  ► Reliable evaluation of minor actinide neutron cross sections is extremely difficult to do … Guidance from measurements is often non-existent … Work at JINER, Minsk-Sosny, Belarus, investigates the manner in which the more extensive and better known information on major actinides can be used to provide reasonable estimates of MA data uncertainties … This paper discusses the influence of major actinide "tweaking" effects on estimating the cross section uncertainties and correlations for MA nuclei … The importance of performing evaluations and determining errors using good models as a means to reduce the assumed parameter errors was emphasized (**Maslov**)

Covariance Applications (1)

- Advances in data processing methods and use of covariances were reported at this Workshop

► The capabilities of the ORNL SCALE package to perform sensitivity and uncertainty analysis were described at this Workshop … Both Monte Carlo and deterministic approaches can be used … The latest version of this code system is SCALE-6 which is planned for release in 2008 (**Williams et al.**)

► Recent upgrades to the PUFF-IV processing code that will dramatically reduce the time needed to process evaluated ND files for heavy nuclei with large numbers of groups were described by the ORNL group (**Wiarda et al.**)

► The NNDC has been processing neutron cross section covariances in support of both the Criticality Safety Program and GNEP … This work has been done using both PUFF-IV and NJOY-99.259 … A contribution to this Workshop described this activity and anticipated benefits to users (**Arcilla**)

► The LANL group continues to upgrade and test the widely used nuclear data processing code NJOY, including the handling of covariances (**Kahler**)

Covariance Applications (2)

- Advances in sensitivity analysis methods that use data errors were reported at this Workshop

► A group at North Carolina State emphasized the need for a thoughtful assessment of nuclear data uncertainties … This group focuses on a novel method to reduce computational overhead by identifying and treating only parameters with significant sensitivity. This approach can help to prioritize nuclear data needs to meet design target accuracies (**Abdel-Khalik et al.**)

► An important collaboration involving BNL, LANL, ORNL, and ANL has generated an extensive library of "low fidelity" covariances that will be used to exercise the analysis codes used in the U.S. Nuclear Criticality Safety Program … This project was described at the Workshop (**Little et al.**)

► The use of covariance information for fast reactor analysis and design in Japan dates back to 1989 … A paper describing the current status of using covariance information in this context was presented at this Workshop … It discussed the adjustment of evaluated covariance information using results from integral studies to produce accurate applications libraries (**Ishikawa**)

User's Perspective (1)

- In recent years great strides forward have been made in user quantification of target accuracies for applications and – thus - for nuclear data

► The needs for covariance data for reactor system uncertainty analysis and data adjustment, i.e., provision of system-specific nuclear data libraries by adjusting ENDF-type libraries using integral data from critical facilities, can now be addressed in great detail … Method uses inverse approach, starting from target accuracies, to predict input data needs (**Salvatores et al.**)

► The currently available techniques for nuclear data evaluation and sensitivity analysis can be used to select certain experiments that – if carried out to the accuracies requested – would aid significantly in improving the applications libraries used for reactor design … A paper by the ANL group addressed this particular issue in the context of the U.S. GNEP advanced nuclear energy systems development program … Extensive numerical information obtained from the analysis of various benchmarks was presented (**Aliberti et al.**)

User's Perspective (2)

- Two perspectives on the use of nuclear data covariances for applications unrelated to reactor design were presented at the Workshop

► ORNL used TSUNAMI to perform sensitivity and uncertainty analyses for a generic spent fuel shipping/storage cask with 32 PWR assemblies … The model employs covariances for over 100 nuclides and produces information on the impact of these uncertainties … Paper described ORNL approach to Criticality Safety analyses and user training course program (**Rearden et al.**)

► One of the earliest uses of cross section covariances was for reactor dosimetry … A paper described the extensive current need for covariance information which has grown over the years due to developing sophistication of the methods … The fact that much of the earlier covariance information contained in ENDF/B-VI was not migrated to ENDF/B-VII was lamented… This is leading to some difficulties for reactor dosimetry community … The importance of neutron spectrum covariance data was also stressed (**Griffin**)

Data Retrieval & Visualization

- The ability visualize covariance matrices in order to subject them to the test by human of "reasonableness" is quite important … Work is in progress to provide this capability

  ► A new nuclear data user interface denoted by "Sigma" is under development at the NNDC … This is a Web rich application intended to offer user friendly access to and handling of archived nuclear data, including covariances … Eventually there will be on-line routines for manipulating and plotting nuclear data uncertainties and covariance matrix correlation profiles … Comparisons with experimental data will also be possible … One oral talk and one poster were presented to describe this capability (**Sonzogni et al.** and **Pritychenko et al.**)

  ► Similar covariance visualization routines are being developed and/or refined in the code packages from ORNL (**Dunn**) and LANL (**Kahler**)

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- It's a tradition for summary speakers to offer some future predictions (preferably mainly positive ones!)

but …

- It's also a risky enterprise in the Internet era because now the material (slides) can be retrieved from the Web years later with a few mouse clicks and could make the speaker look silly or naïve in retrospect, or worse be used for "blackmail" (just joking, of course!)
- I decided to accept that risk anyway for the sake of your entertainment and amusement

Looking into the “crystal ball” … (1)

- Nuclear modeling and derived system errors

  ► Models will continue to improve leading to smaller prior errors and better reliability of theoretical extrapolations to regions with few or no expt’l data

  ► Detailed system simulation studies to trace the impact of uncertainties in nuclear data will continue… This will lead to greater confidence in computed system parameters and in the design of advanced reactors by computers

- Experiments: Possibilities and limitations

  ► Efforts like WPEC Subgroup 30 will lead to improved confidence in the legacy database of experimental values … But, this work can only go so far!

  ► Detailed system sensitivity studies will lead to a steady refinement of data need specifications and thus spawn a new era of “smart” experiments

  ► Nuclear data work will continue to have trouble competing with basic N.P. research for the interest of young people and in obtaining support to acquire the resources that are necessary for this applied science effort. **Urgent!**

  ► Some data needs simply cannot be measured: samples, detectors, weak cross sections, low abundances ... Therefore it will be important to focus on expt’s that can serve to validate the nuclear models used for extrapolations!

Looking into the “crystal ball” … (2)

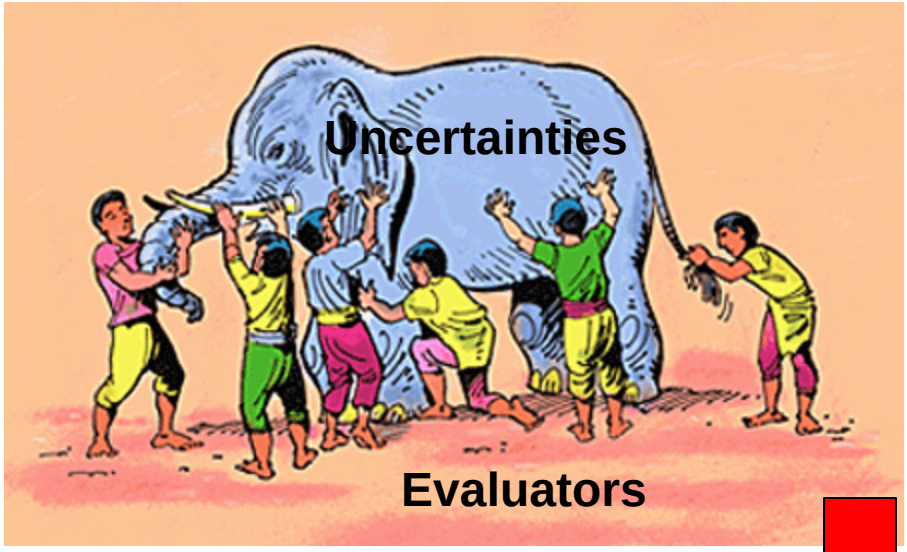
- Future course of evaluation methodology?
  - ► Improved knowledge of basic resonance parameters (energies, widths, strengths, spins…) will lead to better quality evaluations in the RR (Physics!)
  - ► The trend toward comprehensive evaluations (all energies and reaction channels for a particular nucleus) with complete covariances will continue
  - ► Modeling codes will be able to address wide energy ranges seamlessly
  - ► Improved knowledge of systematics (Z,A) will lead to better evaluations for minor isotopes and nuclei that are difficult to measure (extrapolation)
  - ► Evaluation tools will be chosen from a palette of validated approaches
- Preservation of information fidelity in passing evaluated data from producers to users
  - ► Limitations due to antiquated ENDF formats (precision, cumbersome formats, etc.) will be overcome by a migration to new database systems that are more flexible and user-friendly. The nuclear data community needs to begin thinking about how this evolution in data handling should take place
  - ► The task of “data processing” will eventually fade into history as newer applications codes should work directly from basic data files (parameters?)

Looking into the "crystal ball" … (3)

- Cross reaction and cross material issues
  - ► The newer evaluations that are emerging should at least include cross-reaction covariance information that is generated in a consistent manner
  - ► But, except for neutron standards, few ENDF's will offer information on cross-material covariances that could significantly affect system errors
- Differential and integral data: Will we reach a comfortable, beneficial working relationship?
  - ► Achievement of C/E ≈ 1 for some selected integral benchmarks by "tweaking" ENDF's is not equivalent to reducing the derived errors (i.e., "fuzziness") of calculated system parameters by reducing ENDF errors and doing this may lead to unintended and undesirable consequences
  - ► But, it is questionable whether nuclear data errors can ever be reduced sufficiently to satisfy user specifications for system design uncertainties
  - ► So … integral data testing (C/E comparisons), and also adjusted secondary nuclear data libraries, will continue to play a prominent role
  - ► But, libraries adjusted using integral data from typical benchmark systems should not be permitted to "unduly" influence the fundamental ENDF libraries since this primary information must serve all applications

Situation hopeless but not serious? …

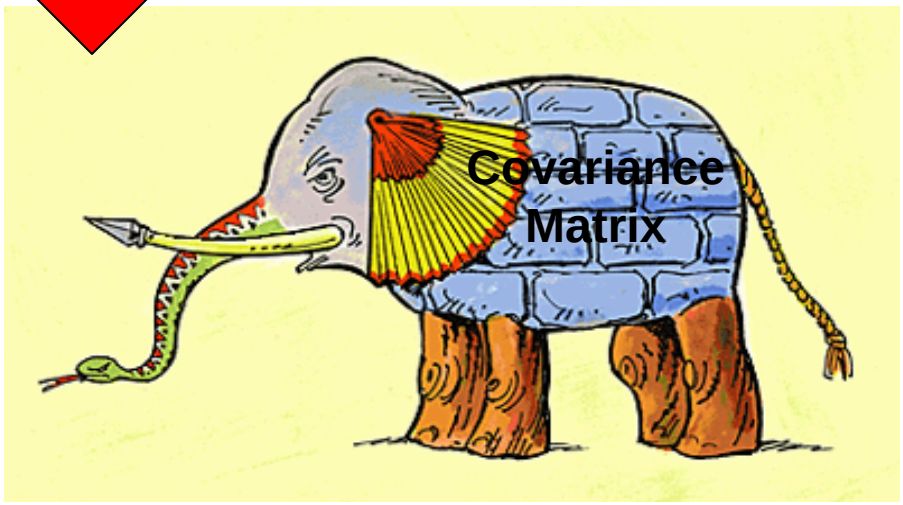
- Looking ahead with a critical eye, we certainly see significant problems in many directions … and its not at all clear how they will be resolved
- … But, look at how far we have progressed!
- Perfect convergence of C/E requirements with feasible data accuracies may not be possible
- … But, with the intelligent combination of error propagation and integral data adjustment we should be able to design reactors “on paper” that, with some modest added “safety” margins, will satisfy all the requirements placed upon us



Taming the beast!

The topic of nuclear data and related uncertainties is quite big & complex due to many different materials, reaction processes, energy regions, physics, etc. So, it's difficult for a single evaluator to have a complete perspective of the whole uncertainty situation

What we observe today when we examine any particular ENDF evaluation are often covariances generated from a patchwork of errors estimated from modeling, experiments, systematics, model defects?, and sometimes sheer guesswork! Can we do better? Perhaps, but let's be realistic…



We have made excellent progress, but we still don't have the whole picture in focus … Yet, I am confident that by the next Covariance Workshop (in a few years) the handling of nuclear data uncertainties will be far better understood and more routine!

Thank you for your attention!

… The End …

A Long Island Winery Tasting Room