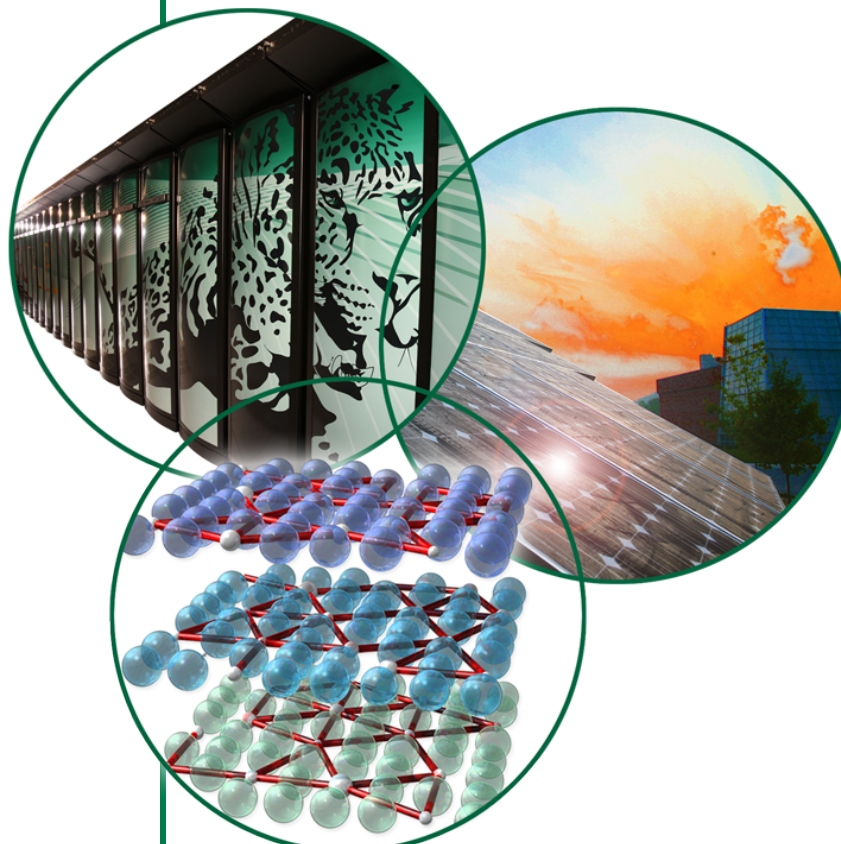
Unifying Nuclear Data Evaluations

CSEWG Meeting, BNL

November 15-17, 2011



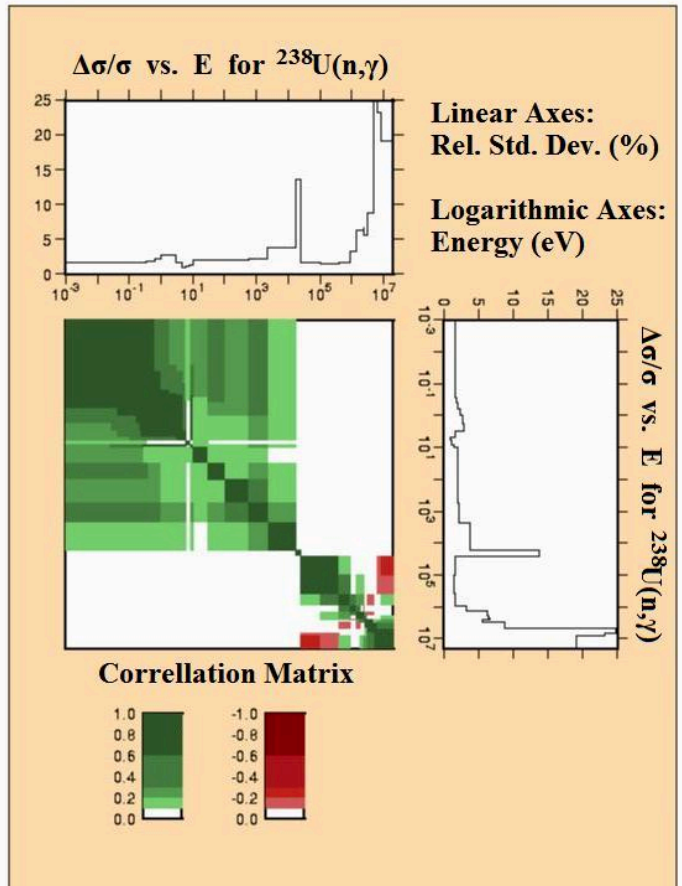
Goran Arbanas (ORNL)
Luiz Leal (ORNL)
Marco Pigni (ORNL)
Mark Williams (ORNL)

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Motivation

- Independent evaluation of RRR and HE ranges may cause
  - Mismatch between RRR and HE region evaluations
  - Large uncertainties near RRR and HE boundary
  - Absence of covariance between RRR and HE



Guiding principles for a unified method

- Expressible in a general data fitting framework
  - e.g. Generalized Least Squares (GLS)
- Away from the overlapping region the effect ought to be small
- Near the overlapping region the method would yield:
  - Covariance data where previously there was none
  - Parameter values that may differ from priors for a better *overall* fit
- Various limiting cases must yield the expected results, e.g.:
  - Unified fit of independent data/models/parameters = independent fits
  - Identical models treated as two distinct models = one model
  - Fits ought to vary smoothly between the extreme cases, e.g.
    - Between no-overlap and complete overlap of the data

Essential Generalized Least Squares

- **Using Froehner's JEFF Report 18 notation:**

$$Q(P) \equiv (P_0 - P)^T M_0^{-1} (P_0 - P) + (D - T(P))^T V^{-1} (D - T(P))$$

$$= Q(\hat{P}) + (P - \hat{P})^T M^{-1} (P - \hat{P})$$

$$\nabla Q(P) = 0 \quad \text{at} \quad P = \hat{P}$$

$$P_{n+1} = P_n - \frac{1}{\nabla \nabla^T Q(P_n)} \nabla Q(P_n)$$

How to extend GLS to two models?

- **An attempt:**

$$P \equiv \{p_1, p_2\}$$

$$T(P) \equiv \{t_1(p_1), t_2(p_2)\}$$

$$D \equiv \{d_1, d_2\}$$

$$M_0 = \begin{pmatrix} m_{0;11} & 0 \\ 0 & m_{0;22} \end{pmatrix} \qquad V = \begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix}$$

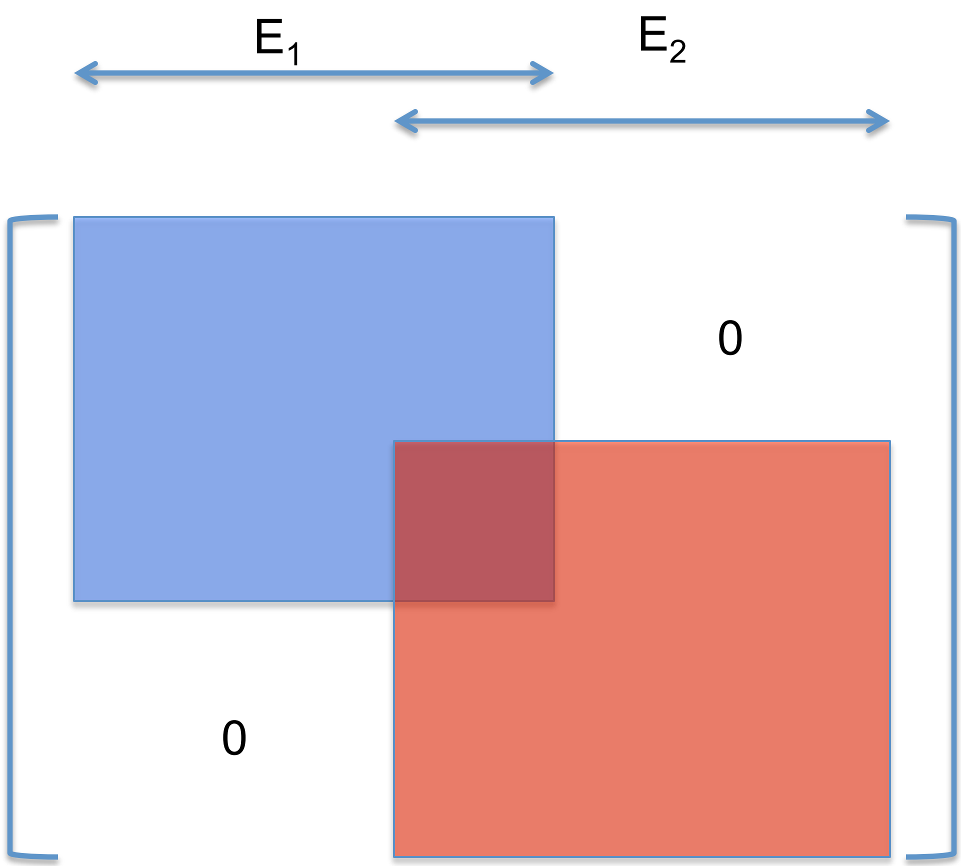
$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \qquad \begin{array}{l} v_{12} = 0 \Longrightarrow m_{12} = 0 \\ v_{12} \neq 0 \Longrightarrow m_{12} \neq 0 \end{array}$$

- **Covariance:** $\langle \delta T(P) \delta T(P) \rangle = (\nabla T)^T M (\nabla T)$

Graphic illustration:

- **Two data sets with overlapping energy ranges; two models**
  - **Data in the overlap energy range (at least) is correlated**

$$V =$$



Simple example

$t_1(n_1)=n_1x \quad , \quad t_2(n_2)=n_2x^2$

$x_1=\{0.8,\ 0.9,\ 1.0\} \quad , \quad x_2=\{1.0,\ 1.1\ ,\ 1.2\ \}$
$d_1=\{0.8,\ 0.9,\ 1.1\} \quad , \quad d_2=\{1.0,\ 1.21,\ 1.44\}$

$n_{01}=1.0 \qquad n_{02}=1.0$ (priors)

$$M_0 = \begin{bmatrix} 1.E+12 & 0.0 \\ 0.0 & 1.E+12 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.1 & 0.08 & 0 & 0 \\ 0 & 0 & 0.08 & 0.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.1 \end{bmatrix}$$

$n_1=1.05792 \quad n_2=0.985193$ (unified fit)
$n_1=1.04082 \quad n_2=1.0$ (independent fits)

$$M = \begin{bmatrix} 0.029 & 0.010 \\ 0.010 & 0.019 \end{bmatrix} \quad \text{cf.} \quad \begin{bmatrix} 0.040 & 0 \\ 0 & 0.022 \end{bmatrix}$$

Simple Example cont'd.

$$(\nabla T)^T M (\nabla T) =$$

0.019	0.021	0.023	0.008	0.010	0.012
0.021	0.024	0.026	0.009	0.011	0.013
0.023	0.026	0.029	0.010	0.012	0.015
0.008	0.009	0.010	0.019	0.024	0.028
0.010	0.011	0.012	0.024	0.028	0.034
0.012	0.013	0.015	0.028	0.034	0.040

cf. $\mathtt{t}_1(\mathtt{n}_1)$ fit to $\mathtt{d}_1$

0.026	0.029	0.033
0.029	0.033	0.037
0.033	0.037	0.041

cf. $\mathtt{t}_2(\mathtt{n}_2)$ fit to $\mathtt{d}_2$

0.022	0.027	0.032
0.027	0.032	0.038
0.032	0.038	0.046

- **Off-diagonal covariance between ranges no longer zero**
  - **and relatively smooth**
- **Covariance within ranges smaller than for independent fits**

Conclusions and Outlook

- A GLS method yields promising results in a simple test case
  - Covariance of the data in the overlapping range is a key input
  - Further study is required
  - More complex cases may validate the method or lead to a better one
- Attempts to unify data evaluations might provide new perspectives and improvements of evaluations and methods.
- Your feedback will be appreciated.