INL Methods and Data for SG33 Adjustment Exercise

G. Palmiotti

www.inl.gov

Idaho National Laboratory

Methods and Data for Experiment Analysis

Codes:

- Deterministic: ERANOS code with 2D (Sn) and 3D (Variational Nodal Transport)
- Stochastic: MCNP (Monte Carlo Continuous Energy)

Data:

- ENDF/B-VII
- Also available: ENDF/B-VI, JEFF 2.2, JEFF 3.1

- For this study, whenever possible use of MCNP with ENDF/B-VII

Methods and Codes for Sensitivity Analysis

Methods:

- Classical Perturbation Theory for K_{eff}
- GPT (General Perturbation Theory) for reaction rates ratios
- EGPT for Reactivity Coefficients
- Time dependent perturbation theory for burn up and irradiation

Codes:

- ERANOS

Theory

We can calculate the variation of the integral parameter for the indirect effect as:

$$\delta R_S = R'_S - R_S = \left\langle \tilde{\Psi}^*, (\partial A - \partial F)\Phi' \right\rangle$$

In the case of a reaction rate ratio:

$$I_S = \frac{\left\langle \sigma_f \Phi_1 \right\rangle}{\left\langle \sigma_f \Phi_2 \right\rangle}$$

The adjoint importance satisfies the following equation:

$$\left(A^* - F^*\right)\tilde{\Psi}^* = \frac{\sigma_f(r,E)}{\left\langle \sigma_f \Phi_1 \right\rangle} - \frac{\sigma_f(r,E)}{\left\langle \sigma_f \Phi_2 \right\rangle}$$

Theory

Sensitivity Coefficients : The Case of Reactivity Coefficients (EGPT)

For the Equivalent Generalized Perturbation Theory the integral parameter is defined as:

$$I_s = \frac{1}{k'} - \frac{1}{k} = \frac{\left\langle \Phi^*, (\partial A - \partial F)\Phi' \right\rangle}{\left\langle \Phi^*, {}^{1}\!/_{k'} F'\Phi' \right\rangle}$$

Where $(\partial A - \partial F)$ characterizes the reactivity coefficient and the sensitivity coefficients are calculated using the fact that changing the order of the derivatives does not change the results:

$$\frac{\sigma}{I_s}\frac{dI_s}{d\sigma} = \frac{\left\langle \Phi'^*, (\partial A' - \partial F')\Phi' \right\rangle}{\left\langle \Phi'^*, {}^{1}\!/_{k'} F'\Phi' \right\rangle} - \frac{\left\langle \Phi^*, (\partial A - \partial F)\Phi \right\rangle}{\left\langle \Phi^*, {}^{1}\!/_{k} F\Phi \right\rangle}$$

Theory

Sensitivity Coefficients : The Case of Nuclide Transmutation (i.e. nuclide densities at end of irradiation)

The generic nuclide K transmutation during irradiation can be represented as the nuclide density variation between time t_0 and t_F. If we denote n_F^K the “final” density, the appropriate sensitivity coefficients are given by :

$$S_j^K = \frac{\partial n_F^K}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^K} = \frac{1}{n_F^K} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \quad dt$$

where the time dependent equations to obtain n* and n are the classical Bateman equation and its adjoint equation, with appropriate boundary conditions:

$$\frac{dn_k(t)}{dt} = \sum_{j=1}^{K-1} C_{kj} n_j(t) - C_{kk} n_k(t)$$

Theory

Sensitivity Coefficients : The Case of the Reactivity Loss during Irradiation, $\Delta\rho^{cycle}$

At first order:

$$\Delta\rho^{cycle} = \sum_{K} \Delta n^{K}\, \rho_{K} \qquad \Delta n^{K} = n_{F}^{K} - n_{0}^{K}$$

and ρ_K is the reactivity per unit mass associated to the isotope K. The related sensitivity coefficients associated to the variation of a σ_j, are given by :

$$S_j^{cycle} = \frac{\sigma_j}{\Delta\rho^{cycle}} \frac{\partial\Delta\rho^{cycle}}{\partial\sigma_j} = \frac{\sigma_j}{\Delta\rho^{cycle}} \left(\sum_K \frac{\partial n^K}{\partial\sigma_j} . \rho_K + \sum_K \Delta n_K \frac{\partial\rho_K}{\partial\sigma_j} \right)$$

or:

$$S_j^{cycle} = \frac{\sigma_j}{\Delta\rho^{cycle}} \frac{\partial\Delta\rho^{cycle}}{\partial\sigma_j} = \frac{\sigma_j}{\Delta\rho^{cycle}} \left(\sum_K \frac{\partial n^K}{\partial\sigma_j} \cdot \rho_K + \sum_K \Delta n_K \frac{\partial\rho_K}{\partial\sigma_j} \right)$$

ERANOS Sensitivity Capabilities

- 1, 2, and 3D adjoint capability for calculation of adjoint flux and generalized importance function.
- Calculation of source term for functionals linear in the real or adjoint flux (e. g. reaction rate, reaction rate ratio, power density, etc.)
- Elimination of fundamental mode contamination, higher eigenfunctions calculation.
- Perturbation components, sensitivity coefficients in diffusion and transport theory for any possible change of cross sections, fission spectra, nuclide densities, or macroscopic variation.
- Sensitivity coefficients to bilinear functionals (e. g. reactivity coefficients, β_{eff}) using equivalent generalized perturbation theory.

ERANOS Sensitivity Capabilities (cont.)

- Direct and indirect effects calculations.
- Inhomogeneous solutions for ADS (φ^*, inhomogeneous reactivity).
- Representativity factors between reference design and experiments.
- Special treatment of positive and negative source for S_n transport calculations.
- Time dependent perturbation theory in the nuclide evolution field for burn up and fuel cycle calculations (neutron sources, decay heat in the repository, radiotoxicity, etc.).
- Target accuracy assessment in connection with optimization code.

Covariance Matrix

Work has been performed mostly at BNL (in collaboration with LANL and ORNL). A methodology for evaluating cross section covariance data has been developed within the EMPIRE code system. The methodology covers the thermal energy, resolved resonance, unresolved resonance and fast neutron regions and builds on the following major components:

- Nuclear reaction model code EMPIRE
- Atlas of Neutron Resonances
- Kalman filter code and Monte Carlo sampling

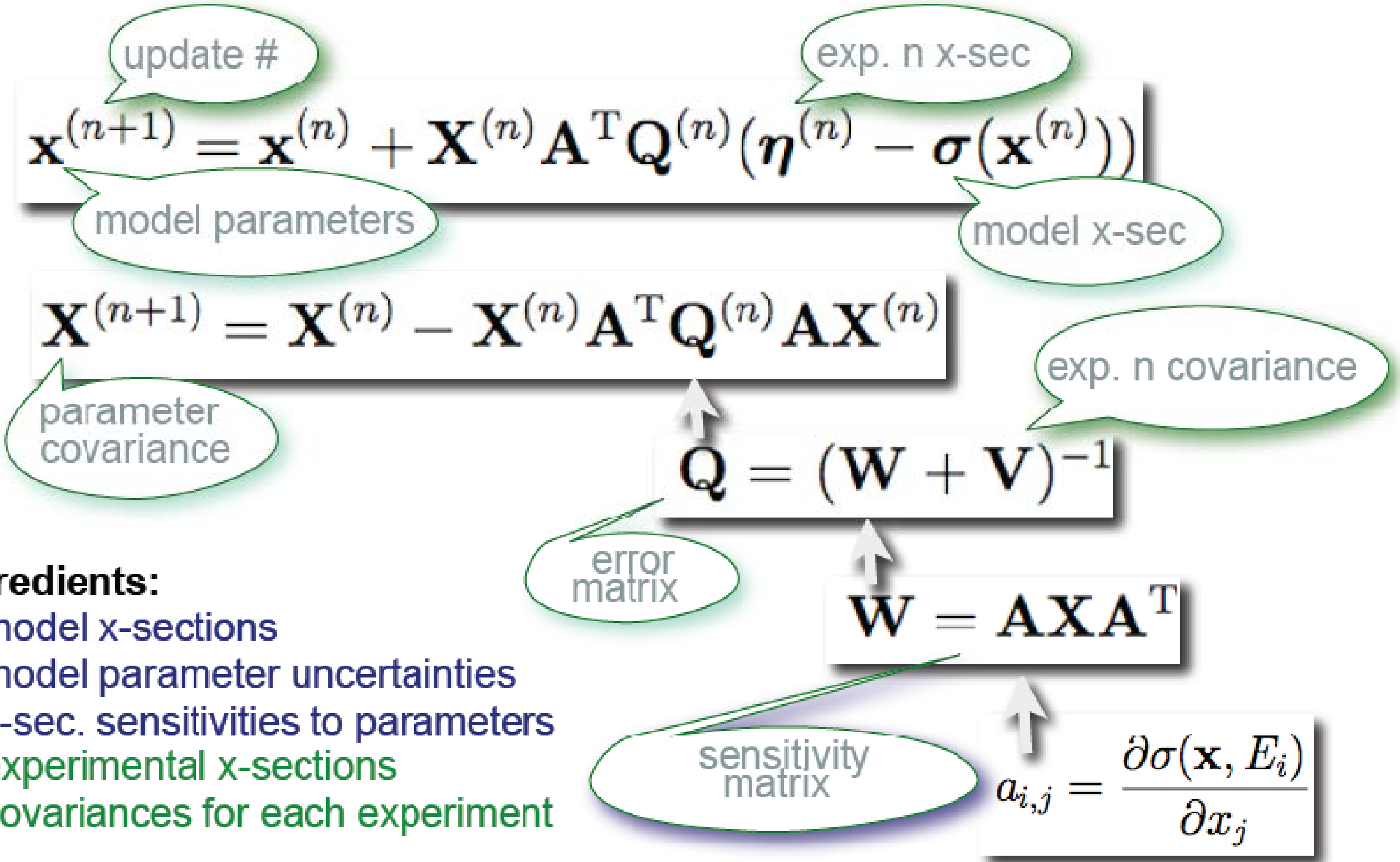
Covariance Matrix

- The generation of covariances is based on the deterministic Kalman filter technique, which is used in the thermal and resonance range as well as in the fast neutron range.
- The stochastic Monte Carlo approach propagates uncertainties of model parameters by means of random sampling.
- The two approaches currently differ regarding treatment of experimental data; it is naturally included in Kalman whereas a generalized least squares code GANDR must be run with the MC generated model-based prior as input.

From M. Herman BNL

Fast neutron region

Kalman: Bayesian, Generalized Least Squares approach



$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + \mathbf{X}^{(n)}\mathbf{A}^{\mathrm{T}}\mathbf{Q}^{(n)}(\boldsymbol{\eta}^{(n)} - \boldsymbol{\sigma}(\mathbf{x}^{(n)}))$$

$$\mathbf{X}^{(n+1)} = \mathbf{X}^{(n)} - \mathbf{X}^{(n)}\mathbf{A}^{\mathrm{T}}\mathbf{Q}^{(n)}\mathbf{A}\mathbf{X}^{(n)}$$

$$\mathbf{Q} = (\mathbf{W} + \mathbf{V})^{-1}$$

$$\mathbf{W} = \mathbf{A}\mathbf{X}\mathbf{A}^{\mathrm{T}}$$

$$a_{i,j} = \frac{\partial\sigma(\mathbf{x}, E_i)}{\partial x_j}$$

Ingredients:

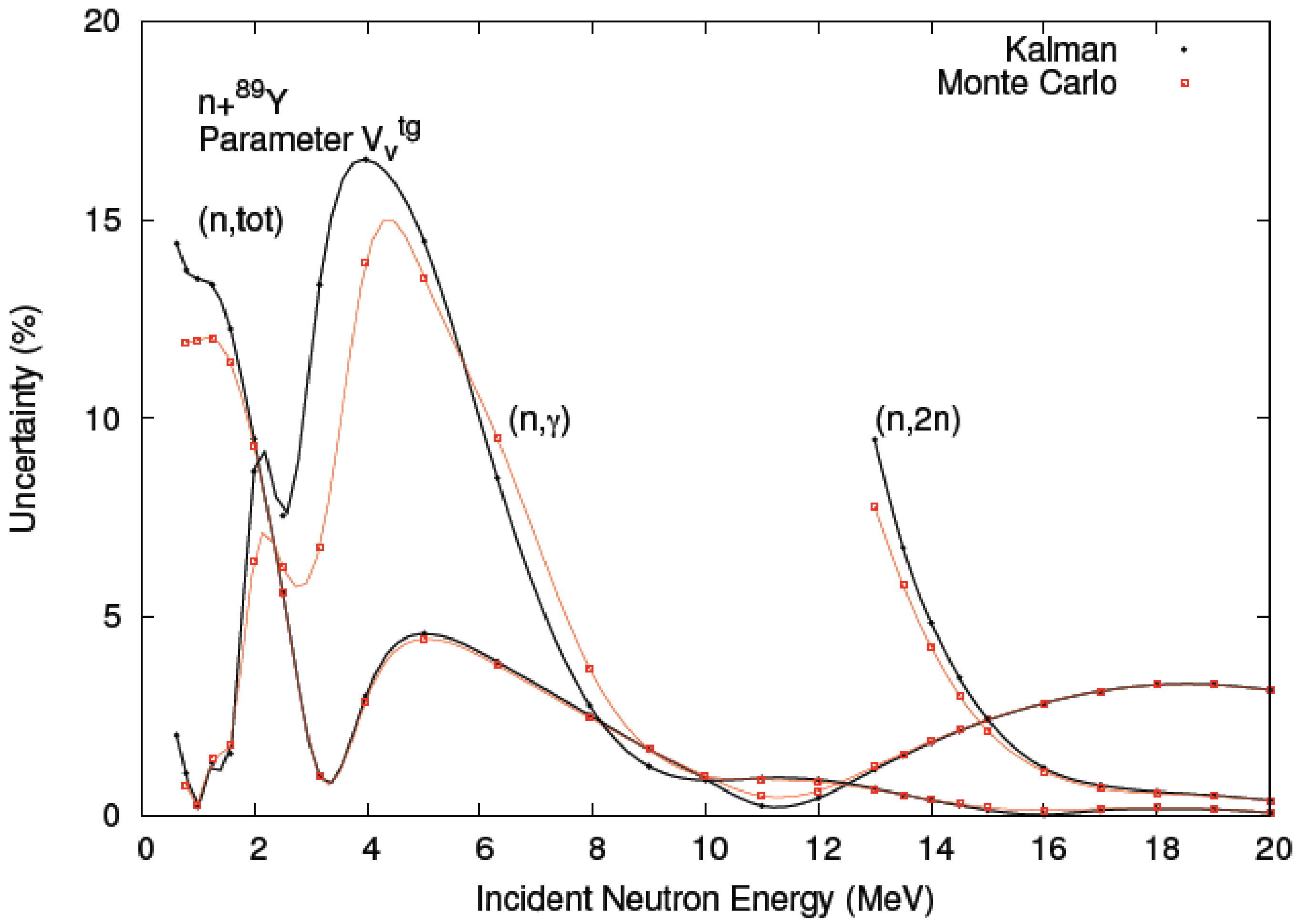
- model x-sections
- model parameter uncertainties
- x-sec. sensitivities to parameters
- experimental x-sections
- covariances for each experiment

Unifies model parameters, experiments, x-sections, covariances

From M. Herman BNL

n + ^{89}Y

comparison of uncertainties due to OMP real volume depth



AFCI covariance library

- 110 materials (20 Actinides, 12 Light materials, 78 structural + FP)
- Important materials treated individually at several institutions.
- Bulk of library (approximately 70 of 110 files, FPs and structural) based on the 'low-fidelity' covariance estimates from LANL,ORNL,BNL
  - Experimental uncertainties in thermal, resonance regions, model-based covariances from EMPIRE +KALMAN in fast region

AFCI covariance library

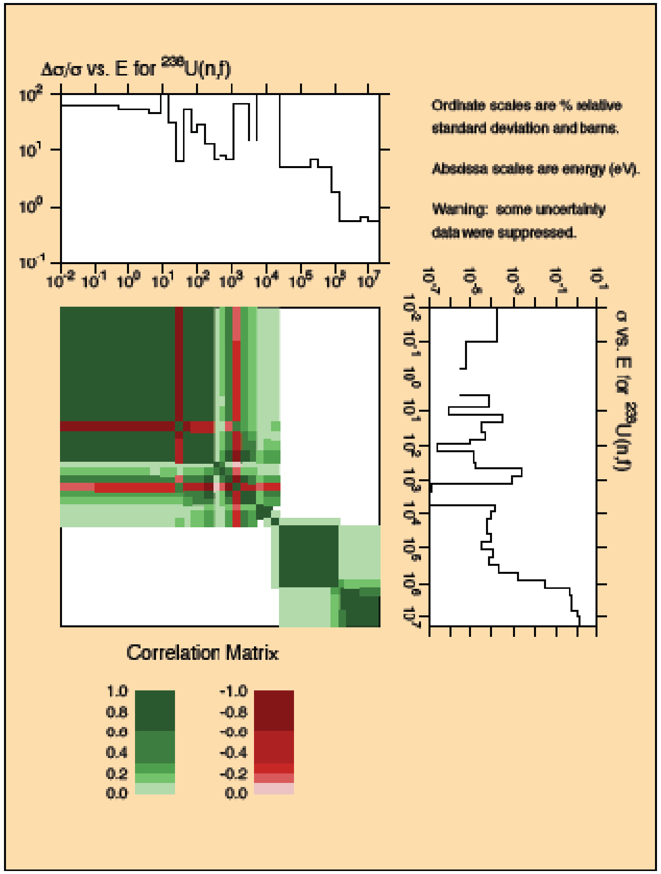
- Initial version (GNEP 1.0) released October 2008
- GNEP 1.1 April 2009, mainly fixes for structural materials
- AFCI 1.2 August 2009, many fixes for minor actinides, structural and fission products

Major Actinides

- Produced by LANL and ORNL, using GNASH +KALMAN methodology in fast region, SAMMY for resonances

1	90-Th-232	ENDF/B-VII
2	92-U-233	ENDF/A, LANL/ORNL 2008
3	92-U-235	ENDF/A, LANL/ORNL 08/09
4	92-U-238	ENDF/A, LANL/ORNL 2008
5	94-Pu-239	ENDF/A, LANL/ORNL 08/09

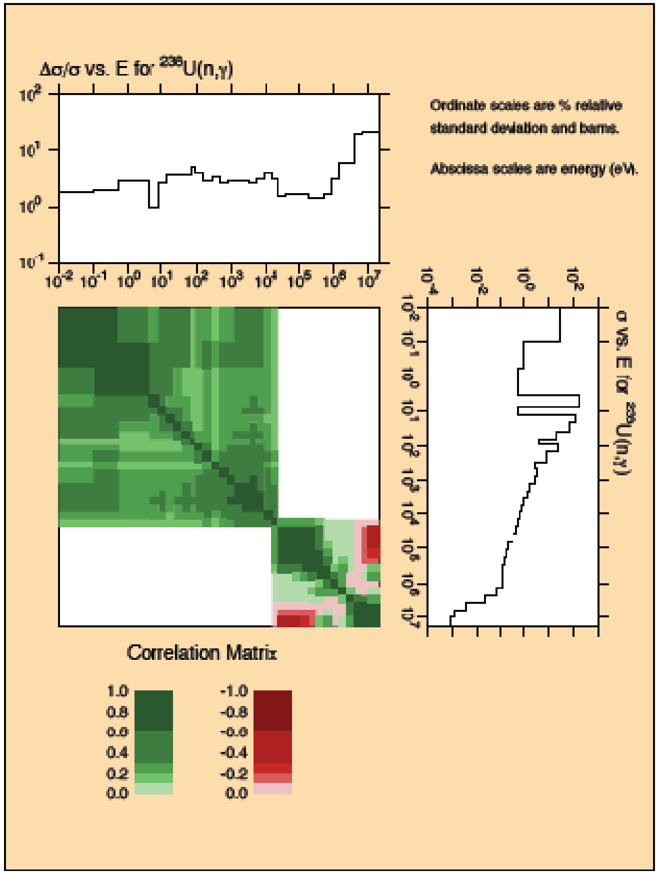
^{238}U



Ordinate scales are % relative standard deviation and barns.

Abscissa scales are energy (eV).

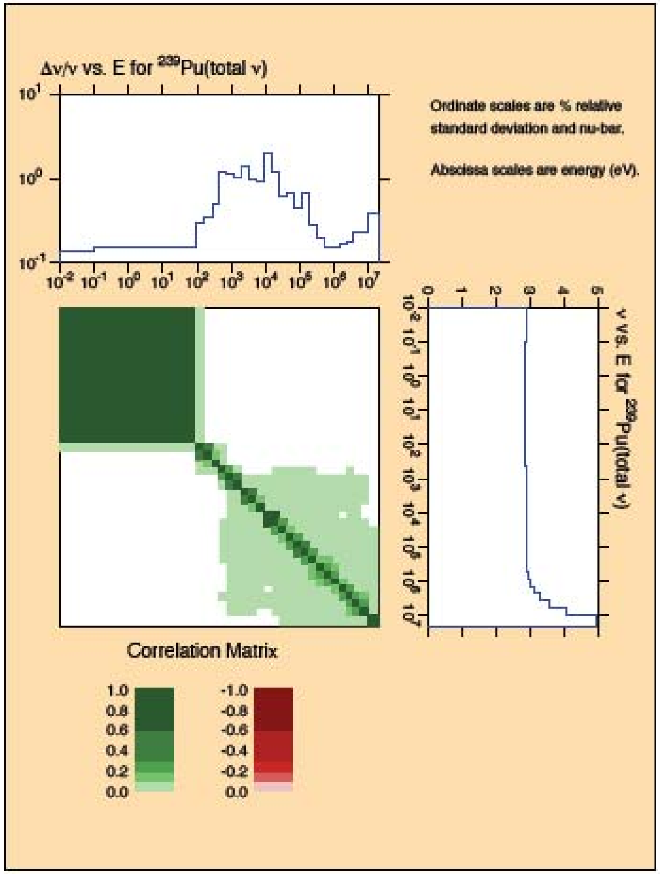
Warning: some uncertainty data were suppressed.



Ordinate scales are % relative standard deviation and barns.

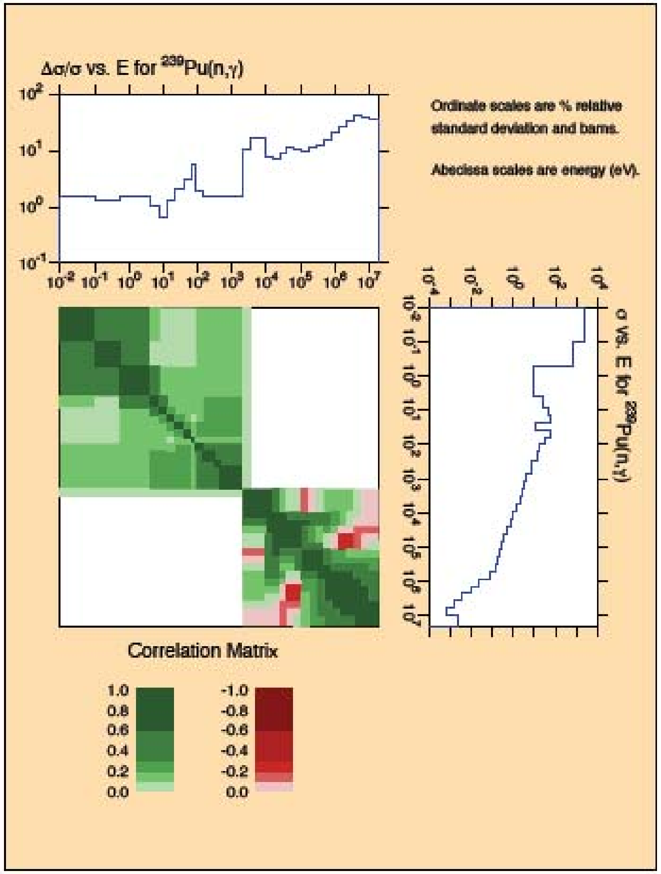
Abscissa scales are energy (eV).

^{239}Pu



Ordinate scales are % relative standard deviation and nu-bar.

Abscissa scales are energy (eV).



Ordinate scales are % relative standard deviation and barns.

Abscissa scales are energy (eV).

Minor Actinides:

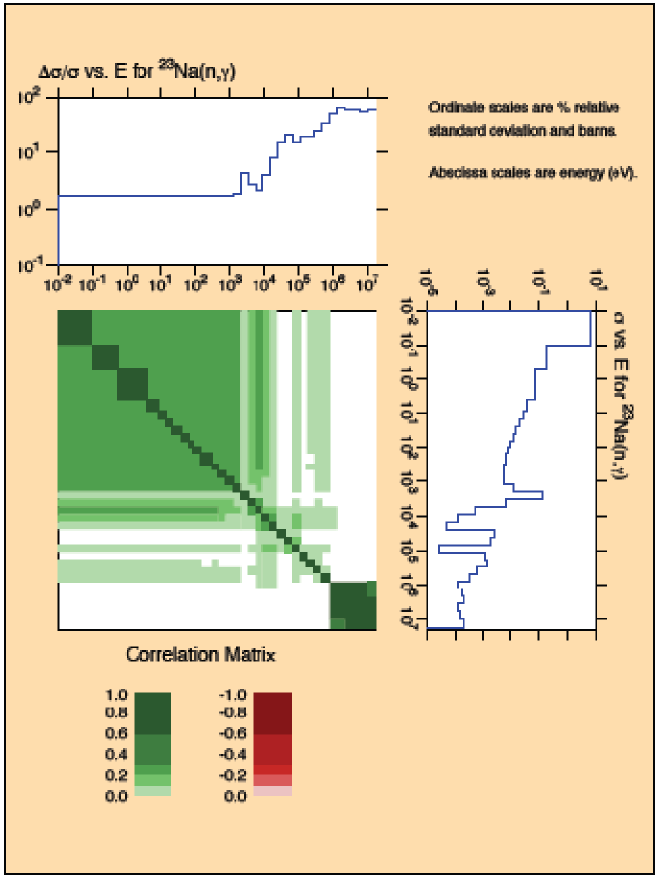
- For 1 Minor Actinide (^{246}Cm) covariances came from ENDF/B-VII
- Covariances for 14 MA previously produced using EMPIRE+KALMAN approach for SG26, adapted to current work
  - *Do not* correspond to processable ENDF files! Needs improvement

Structural Materials

- From several sources, include:
  - 23Na from M.Pigni (BNL), produced for Data Assimilation project
  - 56Fe adopted from JEFF-3.1 / BROND (Tagesen, Pronyaev, Vonach, 1995)
  - 52Cr, 53Cr and 58Ni, produced at BNL using EMPIRE+KALMAN in fast region, Atlas for resonance region.

^{23}Na:

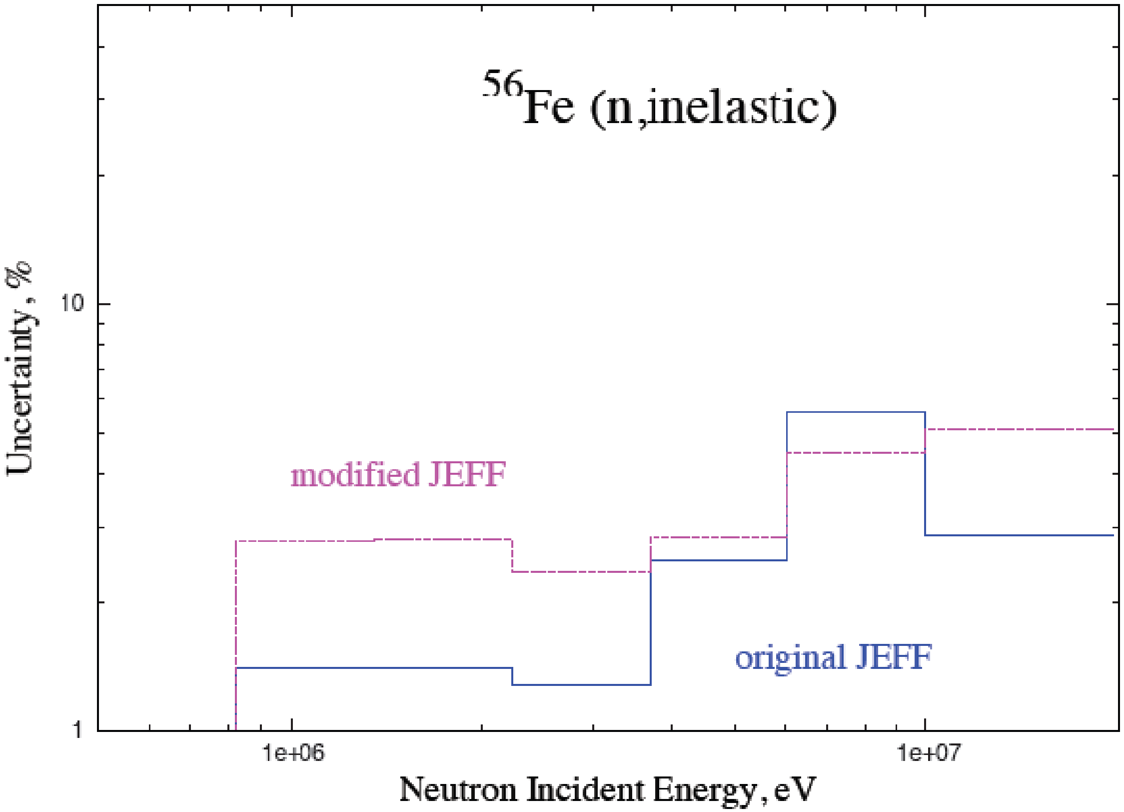
- Using new BNL evaluation by M. Pigni, created for AFCI Data Assimilation effort



^{56}Fe:

- Two ‘recent’ (mid-nineties) evaluations contain covariances: Shibata et al. in JENDL3.3 and Pronyaev/Vonach in JEFF3.1 (also adopted by BROND)
- Trouble in both: surprisingly low values for elastic uncertainties in JENDL, inelastic in JEFF
- Currently using JEFF/BROND version, some changes introduced

^{56}Fe cont.


^{56}Fe (n,inelastic)
modified JEFF
original JEFF
Uncertainty , %
10
1
1e+06
1e+07
Neutron Incident Energy, eV

Low-fidelity

- Low-fidelity project [1] tries to address growing need for covariances. Takes uniform approach:
  - experimental basis in thermal, resonance regions (Atlas of Neutron Resonances)
  - EMPIRE+KALMAN approach in fast region
- Covariance estimates for >300 isotopes generated

[1] R.Little et al, Nuclear Data Sheets vol.**109**, 2008

Statistical Adjustment Method

The method makes use of Lagrange multipliers with most likelihood function, and:

- **"a priori" nuclear data covariance information,**
- **integral experiments analysis to define C/E values**
- **integral experiment uncertainties**
- **sensitivity coefficients**

If we define: $y_j=(\sigma_j^{adj}-\sigma_j)/\sigma_j$ and $y_{Qi}^{exp}=(Q_i^{exp}-Q_i)/Q_i$, the y_i are given by:

$$y_i=\left(S^T D_Q^{-1} S + D^{-1}\right)^{-1} S^T D_Q^{-1}\, y_{Qi}^{exp}$$

where D_Q is the covariance matrix of the experiments, D the covariance matrix of the cross sections and S is the sensitivity vector. It will also result an adjusted covariance matrix for the nuclear data:

$$\left(D^{adj}\right)^{-1}=D^{-1}+S^T D_Q^{-1}\, S$$