Covariance work at BNL

(0.0253 eV to 20 MeV, BNL-LANL approach)

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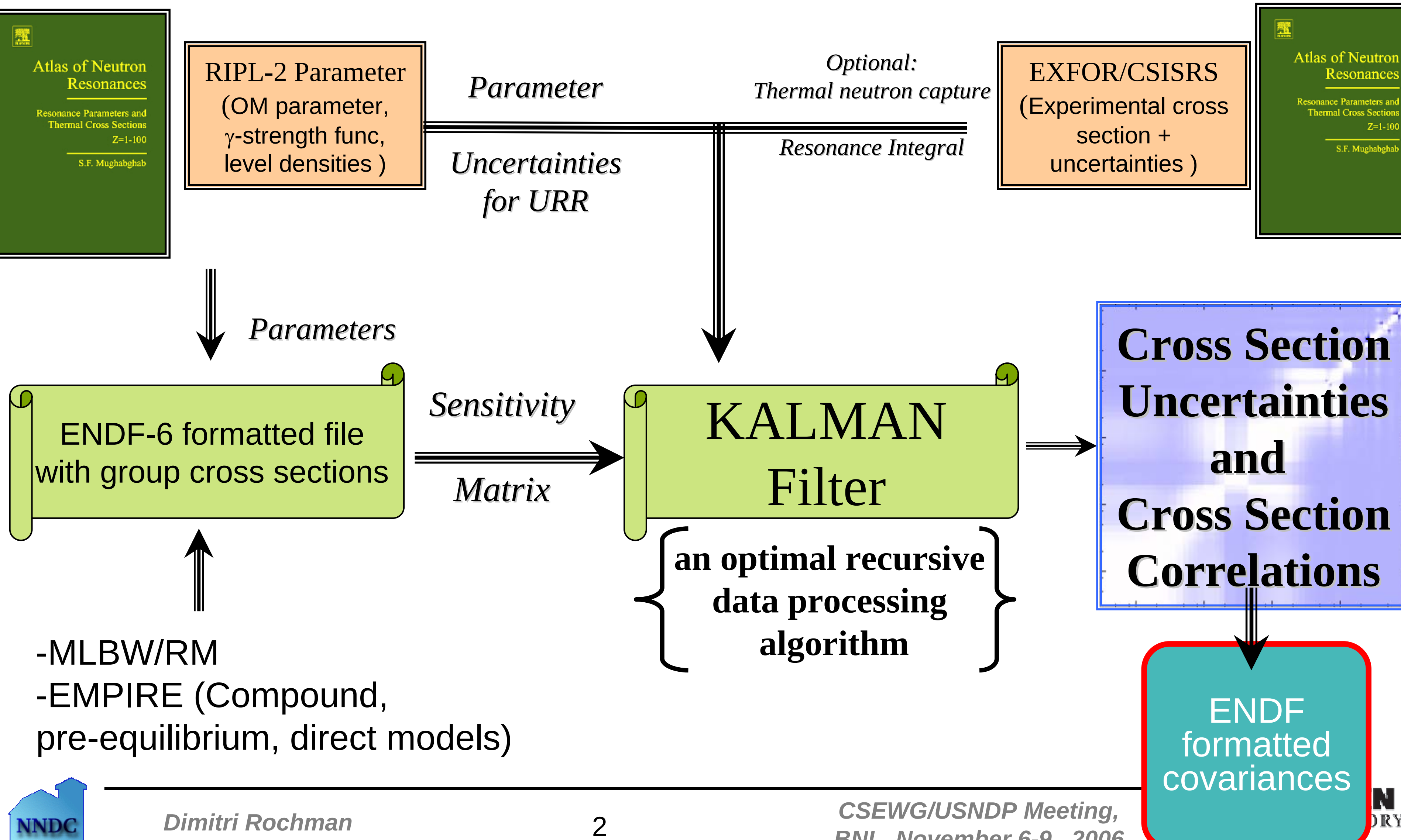
Covariance generation in the resonance neutron region (RRR+URR) and or (URR+Fast)



Sensitivity Matrix calculation

- A cross section Y_j is approximated by a linear function, obtained by a Taylor-Young expansion:

$$
\begin{aligned}
Y_j &= f_j(X_1, ..., X_p) \\
&\approx f_j(\mu_1^X, ..., \mu_p^X) + \sum_{i=1}^{p} \left(\frac{\partial f_j}{\partial X_i}(\mu_1^X, ..., \mu_p^X) \right) (X_i - \mu_i^X) \\
&\quad + \frac{1}{2} \sum_{i=1}^{p} \sum_{i'=1}^{p} \left(\frac{\partial^2 f_j}{\partial X_i \partial X_{i'}}(\mu_1^X, ..., \mu_p^X) \right) (X_i - \mu_i^X) \left(X_{i'} - \mu_{i'}^X \right)
\end{aligned}
$$

- From this relation, one can derive the sensitivity matrix S_X :

$$
\begin{aligned}
S_X &= F_X + \frac{1}{4} F_X^2 \\
&= \begin{pmatrix} \frac{\partial f_1}{\partial X_1} & \cdots & \frac{\partial f_1}{\partial X_p} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \frac{\partial f_s}{\partial X_1} & \cdots & \frac{\partial f_s}{\partial X_p} \end{pmatrix} + \frac{1}{4} \begin{pmatrix} \frac{\partial^2 f_1}{\partial X_1^2} & \cdots & \frac{\partial^2 f_1}{\partial X_p^2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \frac{\partial^2 f_s}{\partial X_1^2} & \cdots & \frac{\partial^2 f_s}{\partial X_p^2} \end{pmatrix}
\end{aligned}
$$

$$
\frac{\partial f_j}{\partial X_i} \approx \frac{f_j(\mu_i^X + \delta x_i) - f_j(\mu_i^X - \delta x_i)}{2 \delta x_i}
$$

$$
\frac{\partial^2 f_j}{\partial X_i^2} \approx \frac{f_j(\mu_i^X + \delta x_i) - 2 f_j(\mu_i^X) + f_j(\mu_i^X - \delta x_i)}{\delta^2 x_i}
$$

Discrete Kalman Filter

- Definition:

…a set of mathematical equations that implement a predictor-corrector type estimator that is optimal in the sense that it minimizes the estimated error covariance…

- Three basic assumptions:

(1) A linear system:
Often adequate even if nonlinearities exist, easily manipulated by computational tools

(2) White measurement noise:
Implies that the noise is not correlated in time

(3) Gaussian noise:
The measurement noise is caused by a number of small sources (independent random variables)

Discrete Kalman Filter

The Kalman filter addresses the general problem of trying to estimate the state of a discrete-time controlled process [11] that is governed by the linear stochastic difference equation $x \in \Re^n$:

$$x_k = Ax_{k-1} + Bu_k + w_{k-1} \tag{1}$$

with a measurement $Z \in \Re^m$ that is:

$$z_k = Hx_k + v_k \tag{2}$$

Discrete Kalman filter time update equations

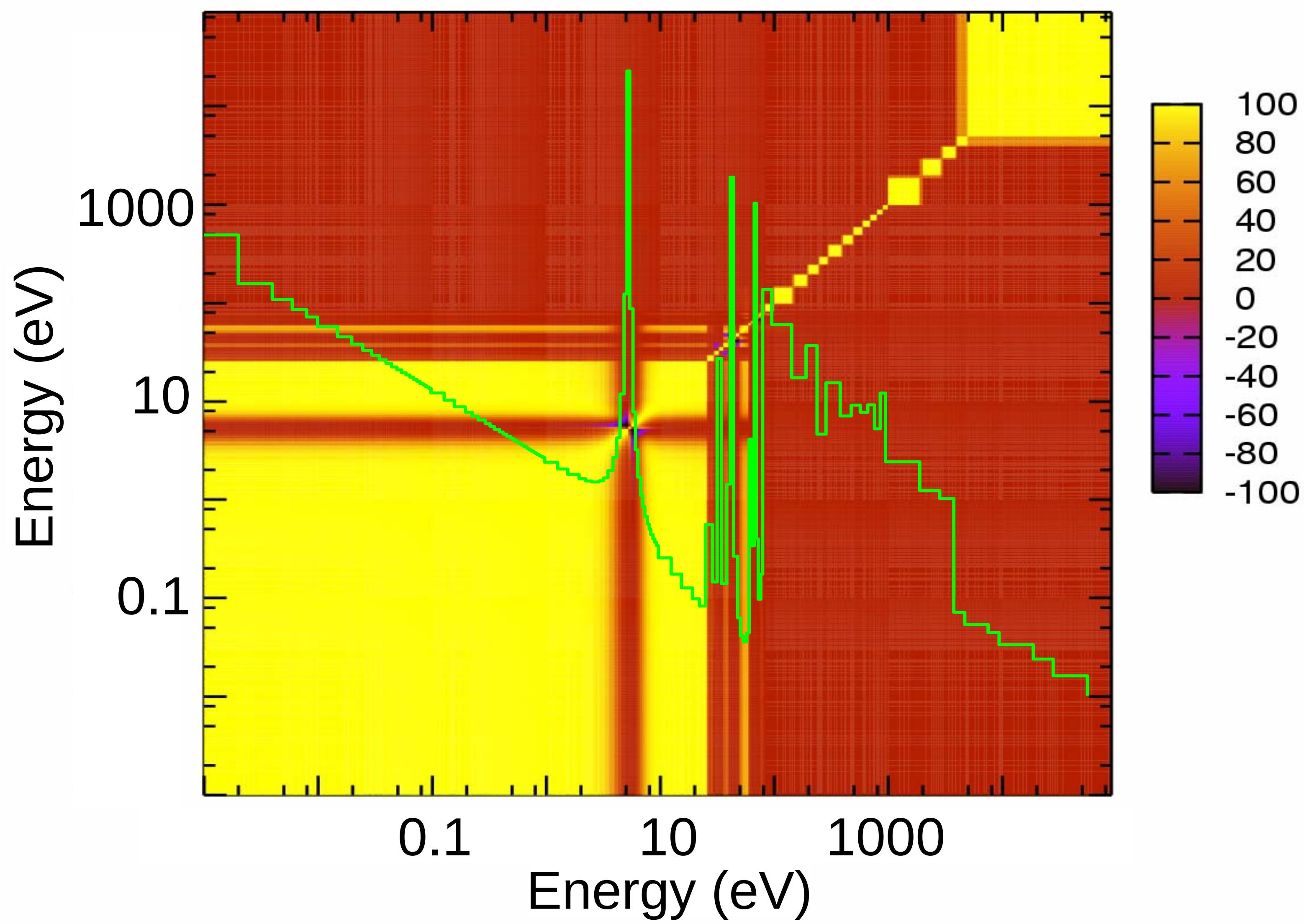
$$\hat{x}_k^- = A\hat{x}_{k-1} + Bu_k$$
$$P_k^- = AP_{k-1}A^T + Q$$

Discrete Kalman filter measurement update equations

$$K_k = P_k^- H^T \left(HP_k^- H^T + R\right)^{-1}$$
$$\hat{x}_k = \hat{x}_k^- + K_k \left(z_k - H\hat{x}_k^-\right)$$
$$P_k = (I - K_k H)P_k^-$$

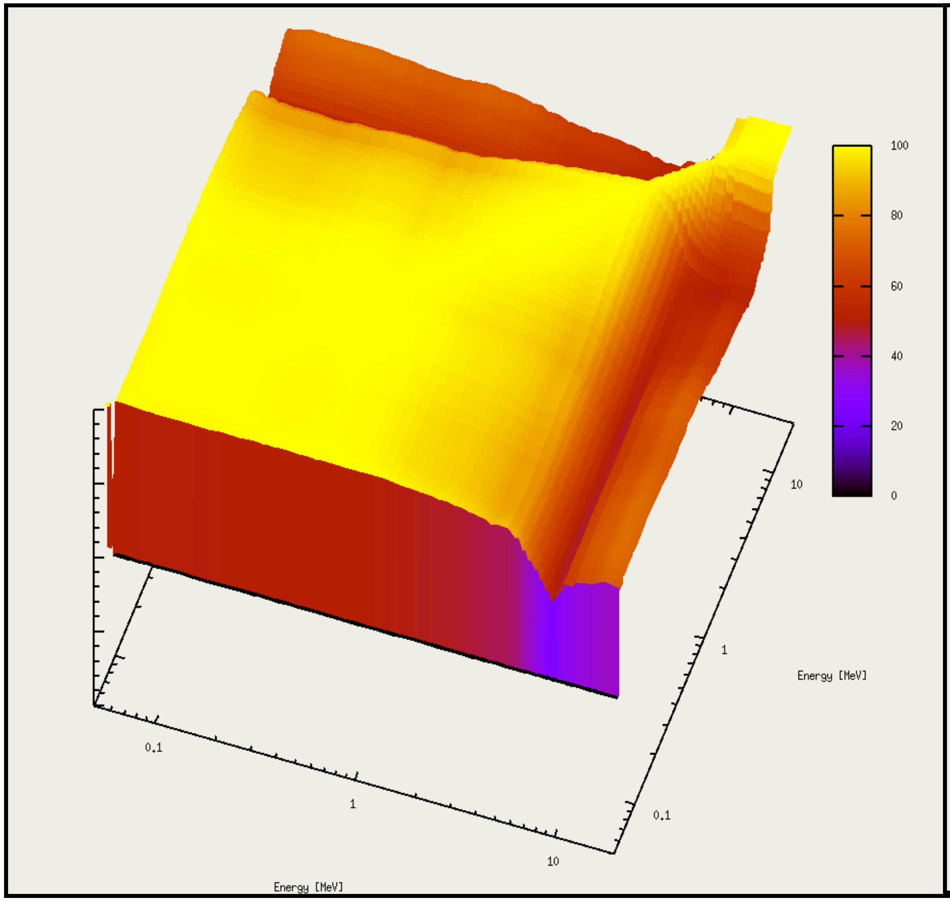
X_k = resonance parameters, OM parameters…
u_k= uncertainties on parameters
z_k = cross section
H = sensitivity matrix
…

RRR+URR: Uranium-236(n,f) correlation

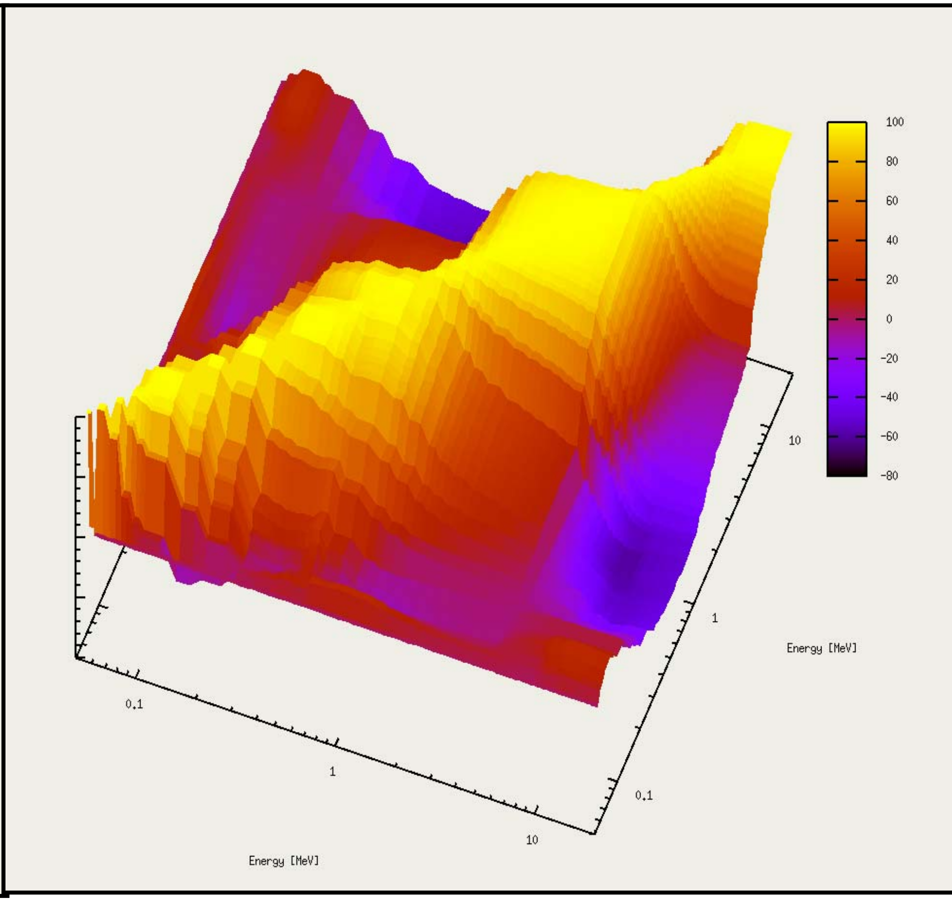


URR+Fast: Gd-155(n,γ) correlation

✓ Without/With experimental data

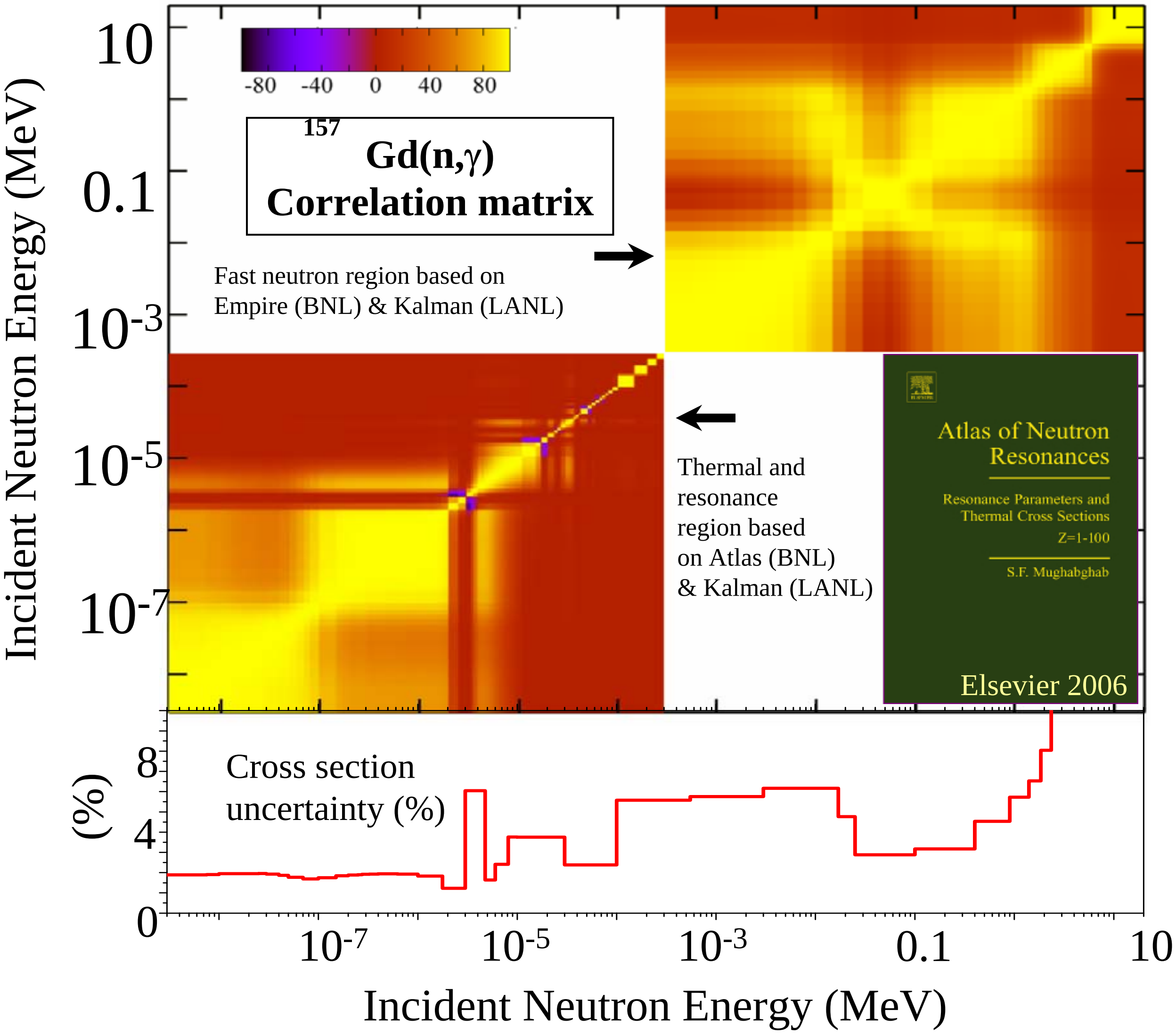


No experimental data



With experimental data

Merging and formatting



- RRR, URR and Fast neutron region merged together under one file
- Covariance formatted in MF-33 format and merged to the ENDF-6 evaluation
- ENDF-6 files tested with NJOY99.161, PUFF-IV, ERRORJ, MCNP5

Conclusion

- Collaboration between BNL and LANL
- Methodology for energy-energy covariance calculations from thermal energy to 20 MeV
- Results in ENDF/B-VII.0 for ^{89}Y, ^{191,193}Ir and ^{99}Tc and for Gd isotopes the fast region (see beta3 for testing).
- Processing: results tested with NJOY/ERRORJ and PUFF-IV
- Produce covariances for WPEC/SG-26 (Salvatores)
- Further development needed for "low fidelity" covariances