Uncertainty Quantification

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Contents

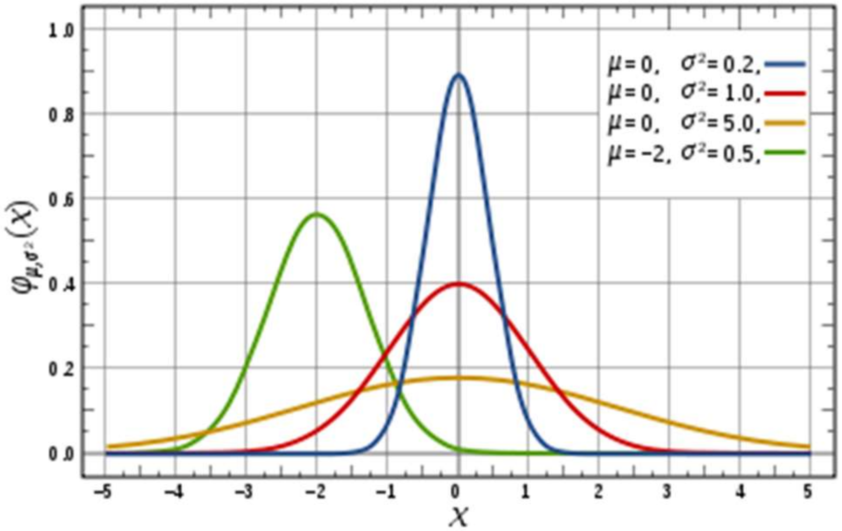
Gaussian Distribution

- Telescopes and sampling errors
  - The mathematician Gauss (1777-1855) was also a keen astronomer. He acquired a new telescope, and decided to use it to produce a more accurate calculation of the diameter of the moon.
  - To his surprise, he discovered that every time he took a measurement, his answer was slightly different.
  - He plotted the results and found that they formed a bell shaped curve, with most results close to the central average but the occasional one quite inaccurate.
  - Gauss quickly realized that any measurement he took was a 'sample' prone to error but which could be used as an estimate of the correct answer. The more readings he took, the closer the average would be to the correct reading.
  - He established that errors in readings belonged to a famous **bell curve** (or **normal distribution** or **Gaussian distribution**).

Normal Distribution

- The probability density function of the normal distribution with the mean value μ and the variance parameter σ^2 can be expressed as

$$f(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} = \frac{1}{\sigma}\phi\left(\frac{x-\mu}{\sigma}\right)$$



PDF of the normal distribution

- From the measurements Q_i (i=1,…,N), the variance can be estimated by

$$\sigma^2\left[\bar{Q}\right] = \frac{1}{N(N-1)}\sum_{i=1}^{N}\left(Q_i - \bar{Q}\right)^2; \quad \bar{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i$$

Error vs. Uncertainty

- When we measure a physical quantity with an instrument or obtain a numerical value, we want to **know how close the estimated value is to the true value**.

- The difference between the estimated and true values is the **error**.

$$\text{Error} = Q_{\text{est}} - Q_{\text{true}}$$

Unfortunately, the true value is unknown and unknowable.

- We can only **estimate** the error.
- The estimate of the error is called the **uncertainty**.

Uncertainty can be expressed in either absolute or percentage terms for typically 95% confidence interval, for example,

5 Volts $\pm$0.5 Volts, 5 Volts $\pm$10%, etc.

Types of Errors: Bias & Random Error

- **Random, Stochastic or Precision Error**
  - tend to be random in nature by effects of uncontrolled variables

- **Bias or Systematic Error (Accuracy)**
  - Error that remains with repeated measurements by a faulty equipment or consistent human errors
  - difference between your measurement (mean value) and the truth.

$$
\begin{aligned}
\sigma^2\left[\bar{Q}\right] &= E\left[\left(\bar{Q}-Q_{\text{true}}\right)^2\right] \\
&= E\left[\left\{\left(\bar{Q}-E\left[\bar{Q}\right]\right)+\left(E\left[\bar{Q}\right]-Q_{\text{true}}\right)\right\}^2\right] \\
&= E\left[\left(\bar{Q}-E\left[\bar{Q}\right]\right)^2\right]+E\left[\left(E\left[\bar{Q}\right]-Q_{\text{true}}\right)^2\right]+\cancel{2\,E\left[\left(\bar{Q}-E\left[\bar{Q}\right]\right)\left(E\left[\bar{Q}\right]-Q_{\text{true}}\right)\right]} \\
&= \sigma_S^2\left[\bar{Q}\right]+Bias^2
\end{aligned}
$$

Nuclear Data Uncertainty

- "It is now possible to model and analyze any nuclear system regardless of its complexity, to any degree of accuracy from the computational point of view. *The uncertainties that we do have today in analyzing nuclear systems are due to uncertainties in the nuclear data and not in the computational method.*" [1]

  [1] Yigal Ronen, (Ed.), *CRC Handbook of Nuclear Reactors Calculations*, CRC Press, Inc., Boca Raton, FL (1986).
- The nuclear data uncertainties are inevitable because they are generated from experimental results.
- Most of experimental uncertainties in the current measurements of nuclear data are systematic. Systematic uncertainties are characterized by inducing strong correlations in the nuclear data.
  - As an example, fission cross sections of some actinide nuclides are determined as relative values to those of ^{235}U, of which uncertainties are known 2-3%.
  - Thus, the uncertainties in the fission cross sections of these nuclides will be larger than and correlated to the uncertainties of ^{235}U.
  - The ν values of actinides are true with respect to ^{252}Cf ν which has an uncertainty of ~0.5-1%.

Estimated[a] Capabilities of LWR Parameter Accuracy

Parameter	Accuracy [%]
Steady-state power distribution	
• Within a fuel pin	±8
• Fuel pin relative assembly	±2-4
• Axial, within an assembly	±4-8
• Radial, between assemblies	±2-5
• Overall, pellet to average	±5-9
Steady-state reactivity	
• Initial k_{eff}	±0.3
• Reactivity lifetime	±2-6

Parameter	Accuracy [%]
Fuel burnup	
• Peak pellet	±5
• Fuel assembly	±4
• Discharge batch	±3-5
Isotopic composition[b] local (pellet)	
• ^{235}U depletion	±5
• ^{239}Pu/U ratio	±4
• Net fissile atoms produced/U	±4
Discharged batch	
• ^{235}U depletion	±5
• ^{239}Pu/U ratio	±5
• Net fissile atoms produced/U	±5

a. Estimates are for generic designs, not appropriate for any specific reactor.
b. Assuming that the burnup is known in predictive comparison.

<from C. R. Weisbin et al., Ann. Nucl. Energy, 9, 615 (1982) >

➡ *Theses uncertainties are mainly due to uncertainties in nuclear data dominated by experimental results.*

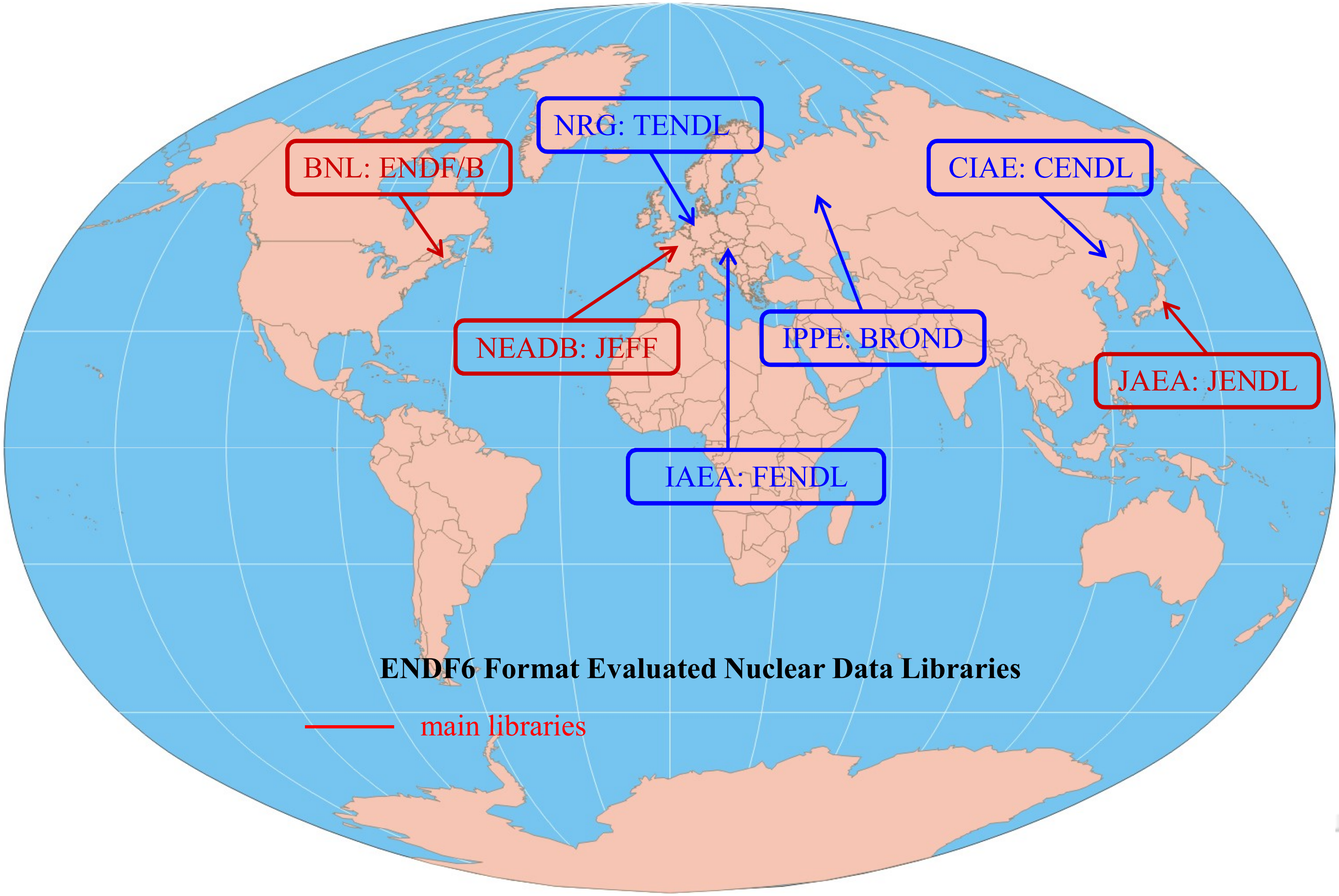
Uncertainties in the Design Parameters of Fast Demonstration Reactors

Parameter	Uncertainty[a] (%)		
	FRG (1972)	SNR-300 (1978)	CRBR (1980)
k_{eff}	1.1	0.4	0.7
Peak/average power	2.7	2.5	~4.7[b]
Control rod worth	6	4-10	5
Doppler coefficient	6-12	15	10[c]
Sodium void reactivity	12-18	15	20

a. 1 σ level.
b. Includes many engineering uncertainties; only about 2% comes from ability to calculate power dist.
c. Mainly from SEFOR experiments.

[1] Yigal Ronen, (Ed.), *CRC Handbook of Nuclear Reactors Calculations*, CRC Press, Inc., Boca Raton, FL (1986).

Evaluated Nuclear Data



ENDF/B-VII.1 Covariance Data

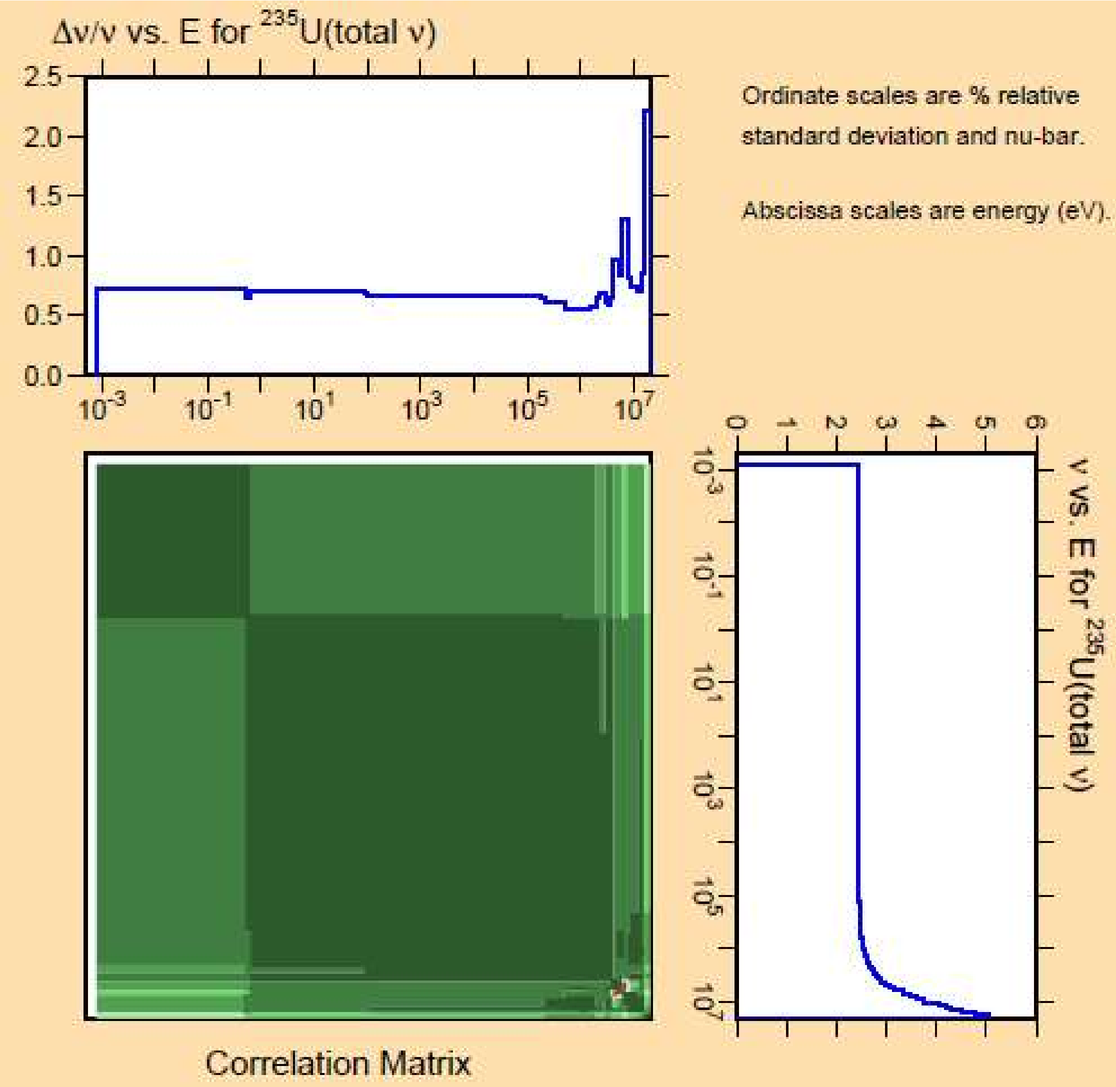
Source of covariances for ENDF/B-VII.1
New ORNL, LANL, BNL evaluations
IAEA/IJS evaluations
COMMARA-2.0
Neutron standards

Type	Number
Light materials	12
Structural & fission products	105
Actinides	20
Minor actinides	53
Total	190

MF	ENDF/B-VII.0	ENDF/B-VII.1
$\nu_{t,p,d}$ 31	2	73
Resonances 32	10	55
Cross-sections 33	24	183
Angular distr. 34	0	68
Energy distr. 35	0	64
Total	36	443

^{1,2}H, ^{4}He, ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{nat}C, ^{15}N, ^{16}O, ^{19}F, ^{23}Na, ^{24,25,26}Mg, ^{27}Al, ^{28,29,30}Si, ^{35,37}Cl, ^{39,41}K, $^{46,47,48.49.50}$Ti, ^{nat}V, ^{50,52,53,54}Cr, ^{55}Mn, ^{54,56,57}Fe, ^{59}Co, ^{58,60} Ni, ^{89}Y, ^{90,91,92,93,94,95,96}Zr, ^{95}Nb, ^{92,94,95,96,97,98,100}Mo, ^{99}Tc, ^{101,102,103,104,106}Ru, ^{103}Rh, ^{105,106,107,108}Pd, ^{109}Ag, ^{127,129}I, ^{131,132,134}Xe, ^{133,135}Cs, ^{139}La, ^{141}Ce, ^{141}Pr, ^{143,145,146,148}Nd, ^{147}Pm, ^{149,151,152}Sm, ^{153,155}Eu, ^{152,153,154,155,156,157,158,160}Gd, ^{166,167,168,170}Er, ^{169,170}Tm, ^{180,182,183,184,186}W, ^{191,193}Ir, ^{197}Au, ^{203,205}Tl, ^{204,206,207,208}Pb, ^{209}Bi, ^{225,226,227}Ac, ^{227,228,229,230,231,232,233,234}Th, ^{229,230,232}Pa, ^{230,231,233,234,235,236,238}U, ^{234,235,236,237,238,239}Np, ^{236,237,238,239,240,241,242}Pu, ^{240,241,242m,243}Am, ^{240,241,242,243,244,245,246,247,248,249,250}Cm, ^{245,246,247,248,249,250}Bk, ^{246,248,249,250,251,252,253,254}Cf, ^{251,252,253,254,254m,255}Es, ^{255}Fm

ν Uncertainty of ²³⁵U in ENDF/B-VII.1



The plots of the ENDF/B-VII.1 covariance matrices (44 & 187 energy groups) for **190** materials can be downloaded from http://www.nndc.bnl.gov/exfor/endfb7.1_covariances.jsp

Mission of Nuclear Data S/U Analysis

$$N^i(\mathbf{r},t)+\Delta N^i,\ x_r^i(\mathbf{r},E,\mathbf{\Omega})+\Delta x_r^i$$

$$\frac{1}{v}\frac{\partial\Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t}=-\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t)-\Sigma_t(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$
$$+\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E',\mathbf{\Omega}',t)f_s(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)$$
$$+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\chi(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\nu_f(E)\Sigma_f(\mathbf{r},E',\mathbf{\Omega}',t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)$$
$$+Q(\mathbf{r},E,\mathbf{\Omega},t)$$

$$k+\Delta k,\ \Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Delta\Phi,$$
$$\kappa\Sigma_f(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Delta P$$

Uncertainty Quantification – Sampling Method

$$\bar{x} \pm \sigma_x, \quad \bar{y} \pm \sigma_y \;\Rightarrow\; \boxed{z = f(x,y)} \;\Rightarrow\; \bar{z}, \sigma_z \;??$$

- Because of the input data uncertainties, there can be an infinitely different set of inputs, (x_i, y_i) (i=1,2,…). This may result in different z's as many as the number of input sets.

$$\begin{array}{cccc} (x_1,y_1) & \longrightarrow \; z = f(x,y) & \longrightarrow & z_1 \\ (x_2,y_2) & \longrightarrow \; z = f(x,y) & \longrightarrow & z_2 \\ \vdots & & & \vdots \\ (x_i,y_i) & \longrightarrow \; \boxed{z_i = f(x_i, y_i)} & \longrightarrow & z_i \\ \vdots & & & \vdots \end{array} \quad \cdots\cdots \; (1)$$

- Then from the results, the variance of z can be estimated by

$$\sigma_z^2 \equiv \sigma^2[\bar{z}] = \frac{1}{N(N-1)} \sum_i^N (z_i - \bar{z})^2; \; \bar{z} = \frac{1}{N} \sum_i^N z_i \quad \cdots\cdots \; (2)$$

- This methodology is called the **stochastic sampling method** or Brute force method.

Uncertainty Quantification – S/U Analysis

- Let's assume that $\bar{z}$ is determined from the best estimates of input variables as

$$\bar{z} = f(\bar{x}, \bar{y}) \qquad \cdots\cdots \quad (3)$$

- The Taylor series expansion of Eq. (1), $z_i = f(x_i, y_i)$ to the first order of input variations about their mean values, $(z_i - \bar{z})$ in Eq. (2), the sample variance formulation, leads to

$$z_i - \bar{z} \cong (x_i - \bar{x})\left(\frac{\partial f}{\partial x}\right) + (y_i - \bar{y})\left(\frac{\partial f}{\partial y}\right) \qquad \cdots\cdots \quad (4)$$

- The substitution of Eq. (4) into Eq. (2) results in

$$\sigma_z^2 \cong \frac{1}{N(N-1)} \sum_i^N \left((x_i - \bar{x})\left(\frac{\partial f}{\partial x}\right) + (y_i - \bar{y})\left(\frac{\partial f}{\partial y}\right) \right)^2$$

$$= \frac{1}{N(N-1)} \left\{ \sum_i^N (x_i - \bar{x})^2 \left(\frac{\partial f}{\partial x}\right)^2 + \sum_i^N (y_i - \bar{y})^2 \left(\frac{\partial f}{\partial y}\right)^2 + 2\sum_i^N (x_i - \bar{x})(y_i - \bar{y})\left(\frac{\partial f}{\partial x}\right)\left(\frac{\partial f}{\partial y}\right) \right\}$$

$$= \sigma_x^2 \left(\frac{\partial f}{\partial x}\right)^2 + \sigma_y^2 \left(\frac{\partial f}{\partial y}\right)^2 + 2\,\mathrm{cov}[x, y]\left(\frac{\partial f}{\partial x}\right)\left(\frac{\partial f}{\partial y}\right) \qquad \cdots\cdots \quad (5)$$

Error Propagation Examples

$$\sigma^2[f(x,y)] = \sigma_x^2\left(\frac{\partial f}{\partial x}\right)^2 + \sigma_y^2\left(\frac{\partial f}{\partial y}\right)^2 + 2\,\mathrm{cov}[x,y]\left(\frac{\partial f}{\partial x}\right)\left(\frac{\partial f}{\partial y}\right)$$

Function	Variance
$f = aA$	$\sigma_f^2 = a^2\sigma_A^2$
$f = aA \pm bB$	$\sigma_f^2 = a^2\sigma_A^2 + b^2\sigma_B^2 \pm 2ab\,\mathrm{cov}_{AB}$
$f = AB$	$\left(\frac{\sigma_f}{f}\right)^2 \approx \left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2 + 2\frac{\sigma_A\sigma_B}{AB}\rho_{AB}$
$f = \frac{A}{B}$	$\left(\frac{\sigma_f}{f}\right)^2 \approx \left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2 - 2\frac{\sigma_A\sigma_B}{AB}\rho_{AB}$

Current Nuclear Data UQ Approaches

- **Approach #1 Sensitivity and Uncertainty (S/U) Analysis**
  - Determination of sensitivity coefficients: $S_k = \dfrac{\Delta k / k}{\Delta \alpha / \alpha}$
  - k_{eff} uncertainty: $\sigma_k{}^2 = \sum_{(\alpha\alpha')} S_{k,\alpha}{}^T C_{\alpha\alpha'} S_{k,\alpha'}$
  - Examples:
    - ✓ McCARD based on Monte Carlo Perturbation Techniques for the sensitivity calculations
    - ✓ TSUNAMI, SUSD3D

- **Approach #2 Stochastic Sampling (S.S.)**
  - Probability procedure to sample input parameters (e.g. nuclear data) according to their variances/covariances
  - Examples:
    - ✓ GRS: initially Monte Carlo sampling for system codes by SUSA tool
      now also using XSUSA to make nuclear data sampling coupled with SCALE-6
    - ✓ NRG Total MC: sampling and perturbation are done directly to theoretical nuclear model parameters
    - ✓ AREVA: produce sets of randomly perturbed ENDF-formatted data libraries
      The TALYS and NUDUNA codes are available.

S/U vs. S.S

	Sensitivity / Uncertainty	Stochastic Sampling
Pros	- reveal individual uncertainty contribution to the total system uncertainty (in k_{eff})	- free of low-order approximations - easy to implement, existing statistical tools - applicable to any choice of "input → output"
Cons	- inherently "local" because of low-order Taylor expansions - implementation complexity increases dramatically if high-order expansion is required to account for non-linear effects	- high computational cost - decomposition of individual uncertainty contribution is not trivial