Formal Statistical Methods and Uncertainty Quantification Considerations Regarding Covariances

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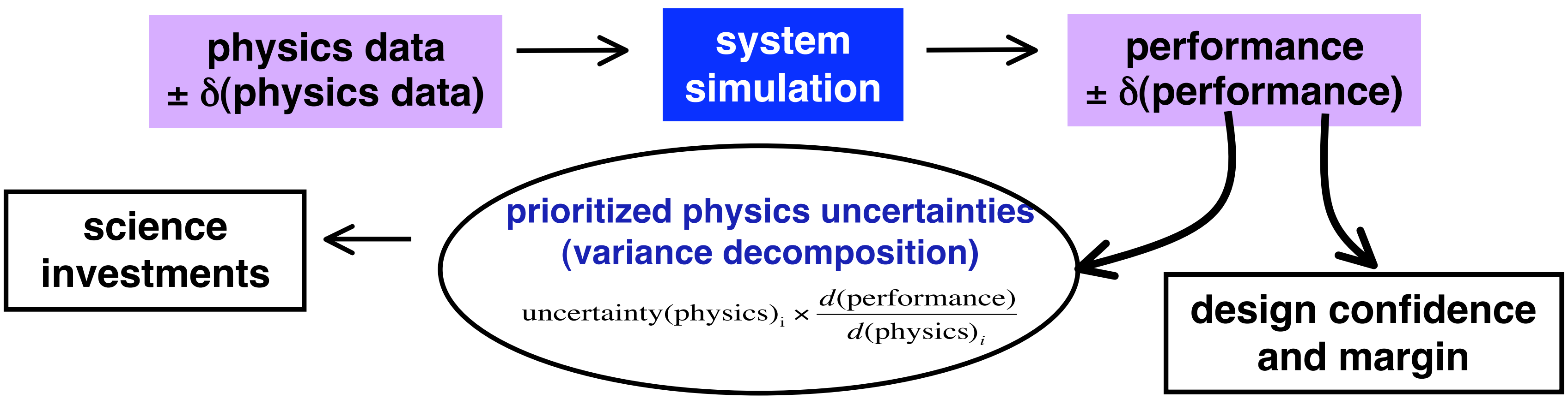
Quantifying the relation between physics uncertainties and system performance can benefit applications and guide science investment

Flow of physics processes: input experimental data with measurement uncertainties and/or model input with physics uncertainties used to simulate the system in question --> output of model reveals information about the performance of the system and its related uncertainties

Quantitative information on system performance gives a two-fold result: some level of confidence in the system design and and indication of areas where improvement needed

Allows prioritization of uncertainties --
Where do you put your money to make science investments that will actually reduce the uncertainties?



These methods have seen some use in nuclear applications. (The JASON's recommended against it for weapons: the model should be the focus).

Specifying probabilities for nuclear data is hard because of poorly understood model inputs and complicated external data

How do we quantify the probability for a given set of input data to give the right output?
(Probability for a certain outcome should be proportional to probability of the inputs being correct.)
Improvement of the model should be the focus of this exercise…

fixed model inputs:
level densities, strength functions, fission barriers, mass tables …

A-priori we have little understanding of the probability distributions for the inputs aside from experiments and model

Microscopic model : reaction code
Monte-Carlo or deterministic

Outputs

Models don't explicitly relate output dependence on microscopic external data to that on integral experiments, e.g. relation between cross section and k_{eff}

external data:
spectra, multiplicities, kinetic energies, $\nu(A)$…
variable model inputs: parameters tuned to data

Microscopic (directly comparable to data)
- cross section measurements
- spectral measurements
- multiplicity distributions, correlations…

Integral experiments (indirect)
- k_{eff} eigenvalues
- pulsed sphere outputs
- ...

The same statistical assumption used for system assessment can be used for quantifying the probability for a nuclear data set to be correct

The probability for a given set of inputs to produce a correct output can be factorized in three components

$$P(\text{data} = \text{correct}) \propto P(\text{output}|\text{input}) = P(\text{model inputs}) \times P(\text{microscopic}) \times P(\text{integral})$$

For many problems where experimental data are available the probability for a set of parameters is not important since it can be understood from the data to begin with

We can calculate the uncertainties (covariances) and correlations in inputs/outputs in a fairly simple way using moments of an input or an output observable

$$\langle \mathcal{O}^n(E) \rangle = \sum_i P_i \mathcal{O}_i^n(E) \qquad \mathcal{O} = \overline{\nu}...$$

$$\langle \mathcal{O}^n(E,E') \rangle = \sum_i \sum_j P_i P_j \mathcal{O}_{ij}^n(E,E') \quad \mathcal{O} = C, R...$$

n = 1, 2 for averages, variances
C is covariance matrix, I=j diagonal elements, I.ne.j off-diagonal
R is correlation matrix, I = j = 1, R>0 correlation, R<0 anticorrelation

We applied this method to our fission neutron spectrum evaluation

- FREYA (Fission Reaction Event Yield Algorithm) studies fission event-by-event (see my fission talk for details)
  - Samples spectra for different physics input parameters
  - Up to 4 microscopic model parameters used in evaluation for incident energy less than 3.5 MeV
    - d, tip separation distance in Coulomb approximation to total kinetic energy of fragments
    - a_L, asymptotic level density parameter, 'temperature' of excited fragment
    - x, relative balance between excitation of light and heavy fragments
    - ε_d, parameter to introduce fragment mass dependence to distance between fragments
  - Calculate spectra and multiplicity for each parameter set (1-4) sampled
  - Generate probabilities from known data where the χ^2 includes that of the fission spectrum and average multiplicities

Parameter values obtained from spectral fits

E_n (MeV)	d (fm)	$\overline{\nu}$
0.5	4.053 ± 0.026	2.943
1.5	4.131 ± 0.013	3.091
2.5	4.170 ± 0.017	3.246
3.5	4.197 ± 0.014	3.374

E_n (MeV)	d (fm)	a_L (MeV^{-1})	$\overline{\nu}$
0.5	4.060 ± 0.028	6.651 ± 0.093	2.958
1.5	4.155 ± 0.021	8.179 ± 0.582	3.087
2.5	4.202 ± 0.022	8.214 ± 0.482	3.239
3.5	4.236 ± 0.024	8.441 ± 0.625	3.375

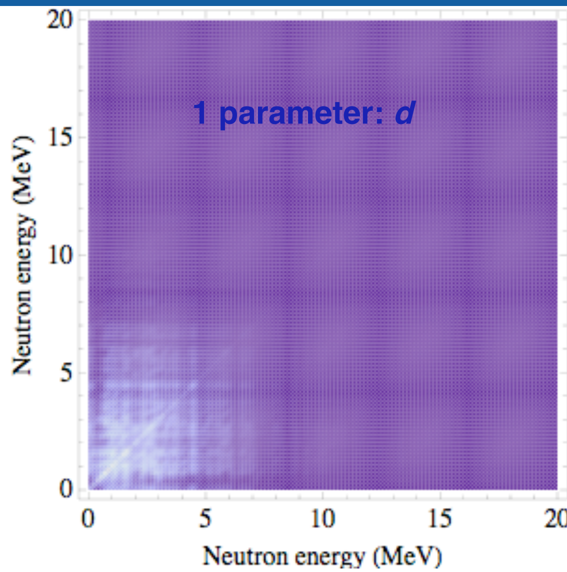
Parameter values obtained from spectral fits to data using 1-4 parameters
Most convenient to extrapolate to other energies with fewest parameters needed

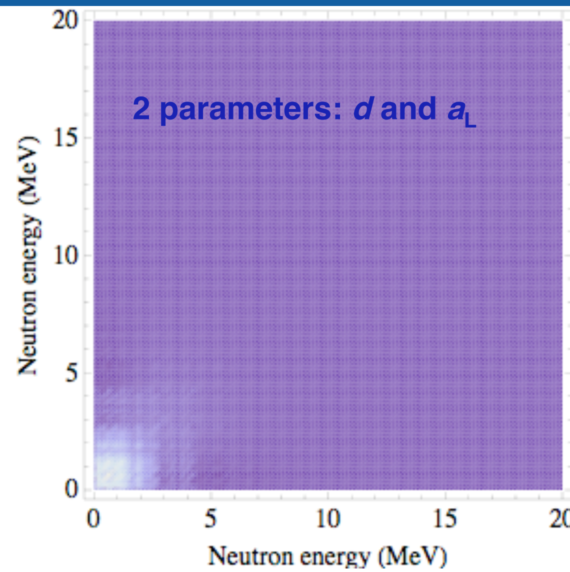
E_n (MeV)	d (fm)	x	$\overline{\nu}$
0.5	4.102 ± 0.047	0.863 ± 0.069	2.936
1.5	4.101 ± 0.036	1.115 ± 0.112	3.090
2.5	4.141 ± 0.045	1.103 ± 0.123	3.242
3.5	4.154 ± 0.041	1.140 ± 0.115	3.373

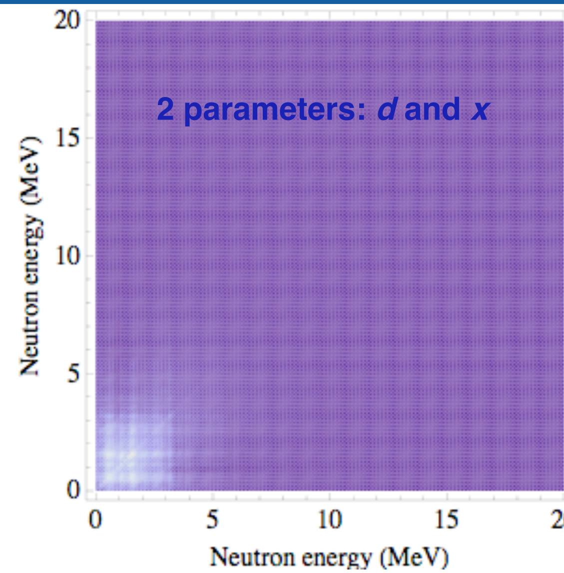
E_n (MeV)	d (fm)	x	ϵ_d	$\overline{\nu}$
0.5	4.055 ± 0.061	0.917 ± 0.087	0.0125 ± 0.0230	2.940
1.5	4.092 ± 0.093	1.136 ± 0.107	0.0014 ± 0.0288	3.087
2.5	4.119 ± 0.094	1.103 ± 0.115	0.0077 ± 0.0291	3.242
3.5	4.149 ± 0.082	1.135 ± 0.101	0.0014 ± 0.0270	3.371

E_n (MeV)	d (fm)	a_L (MeV^{-1})	x	ϵ_d	$\overline{\nu}$
0.5	4.107 ± 0.056	7.328 ± 0.351	0.960 ± 0.105	-0.0149 ± 0.0189	2.942
1.5	4.145 ± 0.084	8.011 ± 0.557	0.992 ± 0.145	0.0059 ± 0.0256	3.090
2.5	4.157 ± 0.087	7.962 ± 0.728	1.015 ± 0.134	0.0104 ± 0.0272	3.236
3.5	4.199 ± 0.055	8.305 ± 0.706	1.059 ± 0.137	0.0058 ± 0.0205	3.373

A simple example with the fission spectrum



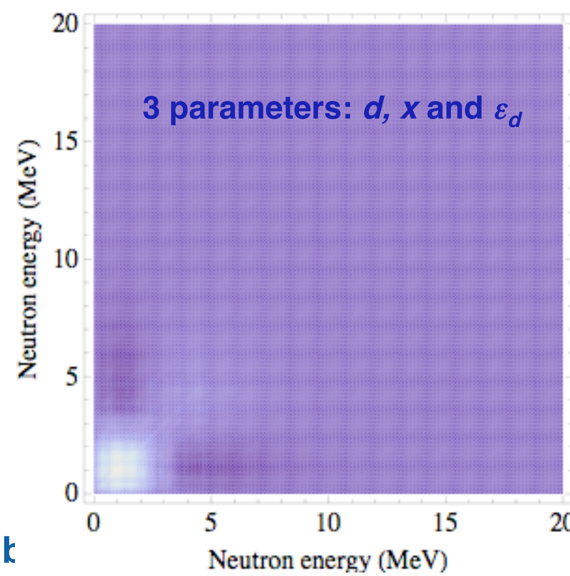


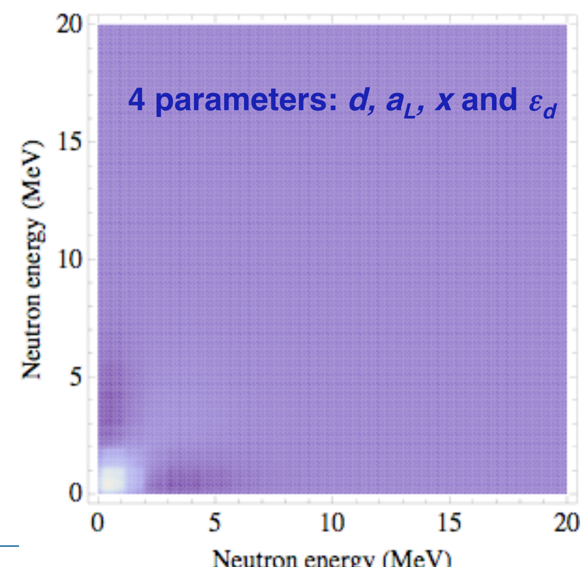


Density plots of spectral covariances for different parameter sets
Incident neutrons at 0.5 MeV
Parameters: *d* is separation distance,
a_L is level density parameter,
x is balance between excitation energies of light and heavy fragments
and ε_d is the *A*-dependent change in *d*)

Lighter areas imply higher covariance

Other energies look about the same





Correlations in the Model Inputs

- Up to 4 parameters in fission spectra calculation gives a 4x4 matrix of correlations:

$$\begin{pmatrix} R_{d\,d} & R_{d\,a_L} & R_{d\,x} & R_{d\,\epsilon_d} \\ R_{a_L\,d} & R_{a_L\,a_L} & R_{a_L\,x} & R_{a_L\,\epsilon_d} \\ R_{x\,d} & R_{x\,a_L} & R_{x\,x} & R_{x\,\epsilon_d} \\ R_{\epsilon_d\,d} & R_{\epsilon_d\,a_L} & R_{\epsilon_d\,x} & R_{\epsilon_d\,\epsilon_d} \end{pmatrix} \quad R_{ij} = \frac{C_{ij}}{\sigma_i \sigma_j}$$

C_{ij} is covariance matrix element
σ_i is uncertainty on one parameter
Only off-diagonal terms shown in tables below, $R_{ii} = 1$

Correlation for 2 parameter fits to *(d, a_L)* and *(d, x)*

E_n (MeV)	$R_{d\,a_L}$	E_n (MeV)	$R_{d\,x}$
0.5	-0.360	0.5	-0.767
1.5	0.704	1.5	-0.913
2.5	0.619	2.5	-0.927
3.5	0.766	3.5	-0.905

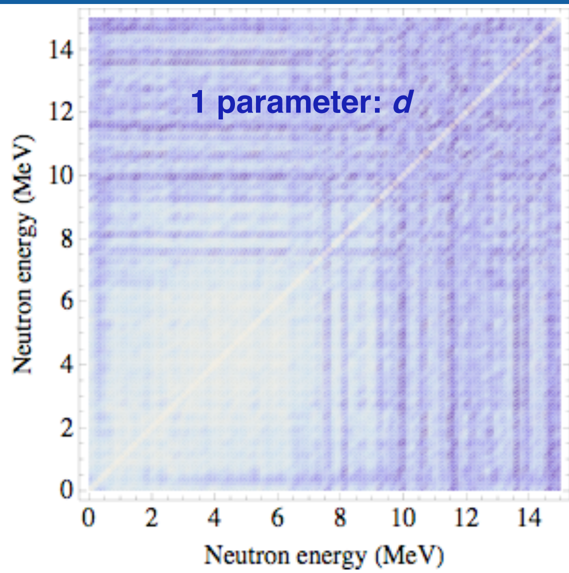
Correlation for 3 parameter fits to *d, x* and ε_d

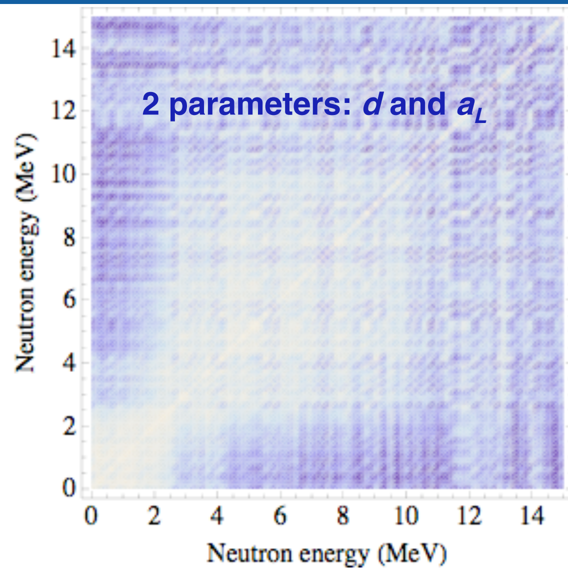
E_n (MeV)	$R_{d\,x}$	$R_{d\,\epsilon_d}$	$R_{x\,\epsilon_d}$
0.5	-0.298	-0.788	-0.280
1.5	-0.351	-0.921	-0.007
2.5	-0.395	-0.903	0.064
3.5	-0.201	-0.893	0.202

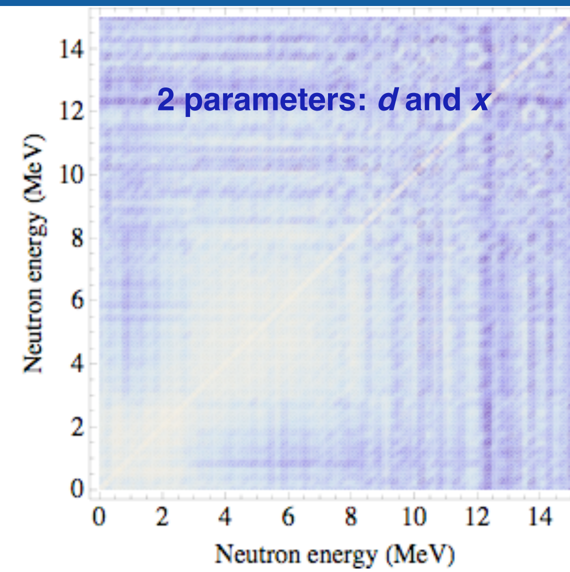
Correlation for 4 parameter fits

E_n (MeV)	$R_{d\,a_L}$	$R_{d\,x}$	$R_{a_L\,x}$	$R_{d\,\epsilon_d}$	$R_{a_L\,\epsilon_d}$	$R_{x\,\epsilon_d}$
0.5	0.674	-0.562	-0.653	-0.498	-0.156	-0.379
1.5	0.351	-0.406	-0.491	-0.733	0.126	-0.268
2.5	0.313	-0.361	-0.426	-0.726	0.166	-0.321
3.5	0.482	-0.390	-0.390	-0.496	0.224	-0.492

Correlations in the fission spectra



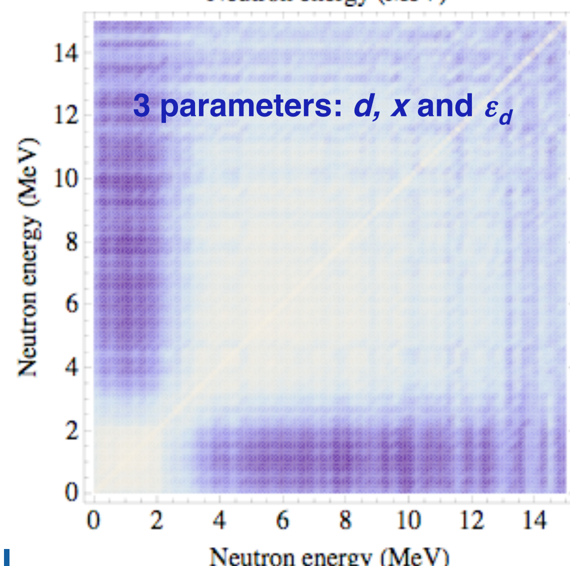


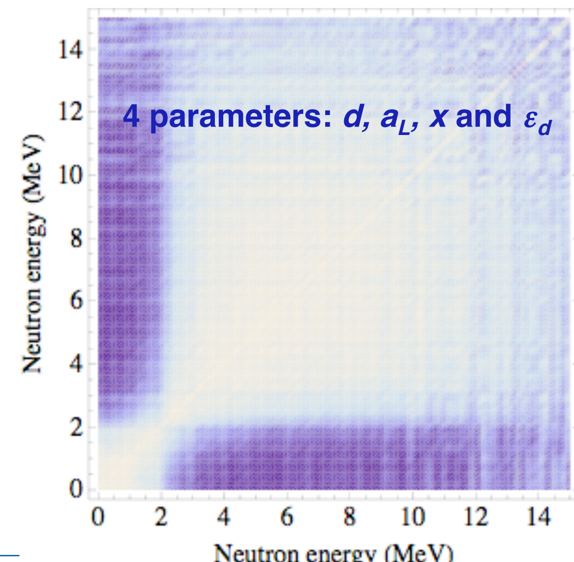


Correlation matrix R with limits restricted due to poor FREYA statistics

Weak correlation at all energies with a single parameter, adding more parameters introduces greater anticorrelation

Low energy region (E < 2 MeV) tightly correlated, weak correlation at E > 2 MeV





The factorizability of the probability gives a great freedom in accounting for integral experiments

- **Integral experiments imply complicated indirect constraints on data**
  - e.g. k_{eff} relates $\sigma(n,f)$, spectra, $\sigma(n,\gamma)$, $\sigma(n,n')$.... for all isotopes in an assembly
- **Tedious to directly account for all possible constraints**
  - changes every time consider a new integral experiment or configuration
  - covariance files are not intrinsically interesting outside applications
- **because *P* factorizes we have great freedom**

- **We have**

$$P = P(\text{model inputs}) \times P(\text{microscopic}) \times P(\text{integral}) = \tilde{P} \times P(\text{integral})$$

  - $\tilde{P}$ typically simple correlations
  - *P*(integral) generally complicated
  - for example, Gaussian *P*(integral)

$$P(\text{integral}) = \Pi_k \exp\left[-\frac{|k-k_{\text{eff}}|^2}{2\sigma_k^2} \right]$$

- **Define and store $\tilde{P}$**
- **Account for integral experiments at run time:**
  - sample from $\tilde{P}$
  - calculate interesting integral quantities and *P*(integral)
- **Convenient because you can always add more integral experiments and no information lost in defining correlations**

This leads us to the 'weak criticality conjecture'

- **A conjecture:**
  - **For near-critical systems constrained by integral experiments, the details of $\tilde{P}$ are not important - it suffices to specify approximate uncertainties and a covariance correlation length**
- **Why?**
  - ***P*(integral) provides constraints that are about an order of magnitude stronger than *P*:**
  - **For example, we know k_{eff} for Jezebel to 0.2% while the cross sections are only known to 1-2% or less. For a Jezebel-like system, the uncertainty cannot be further reduced until the cross sections are known to the same precision as k_{eff}**
- **Why is it useful?**
  - **It means it is not necessary to specify the actinide covariances in detail for criticality applications**

Summary

- At LLNL, we are developing formal uncertainty quantification tools:
  - Library of evaluated uncertainties, on the fly data processing, dynamic checking for integral systems
  - Used in programmatic applications for several years now
- A fairly simple formalism gives uncertainties in neutron spectra
  - Depending on parameters, mean neutron spectra and multiplicity is unchanged but correlations are
- Factorization of probability gives great freedom
  - consider storing only $\tilde{P}$
    - integral constraints can be accounted for at run time
    - simulations of integral constraints are almost always cheap compared to full system simulations