Uncertainty Management for Nuclear Systems Simulation

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Acknowledgement and Research Team

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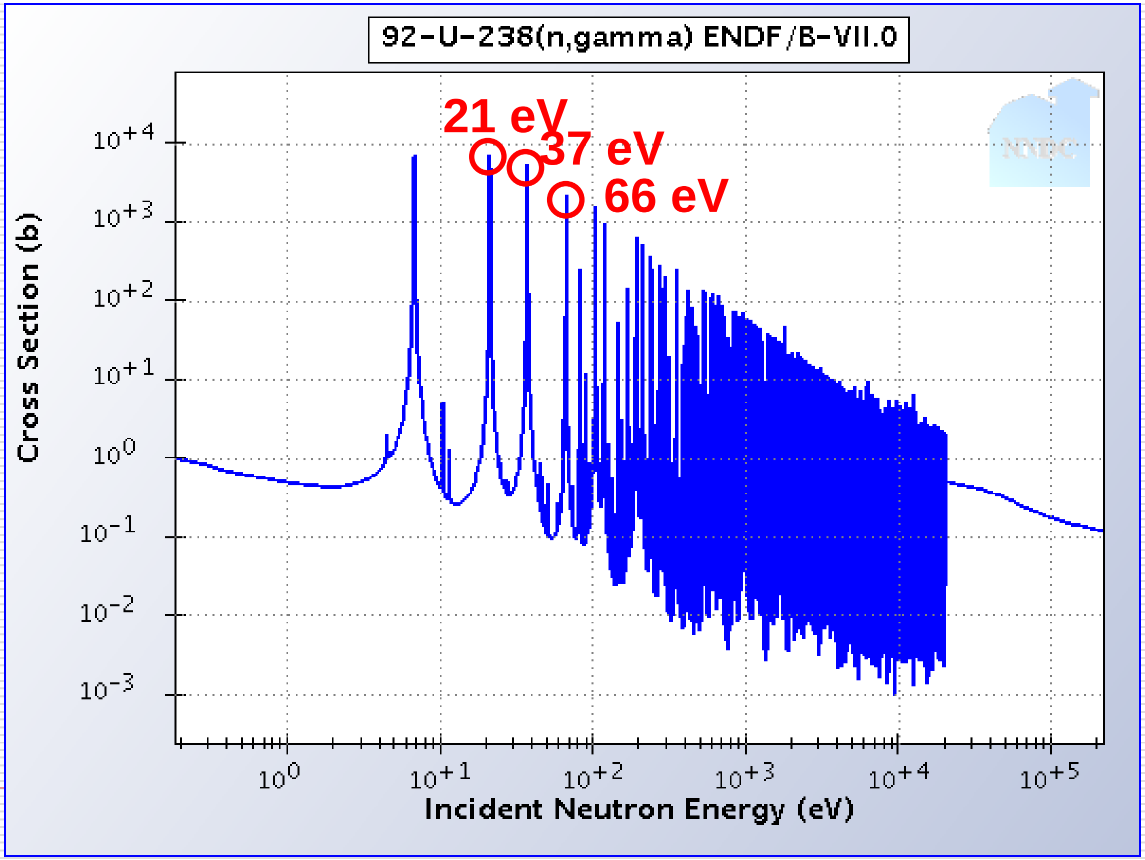
Introduction

- Recently, modeling and simulation (M&S) recognized as viable tools to achieve optimal design and operation of existing and next generation reactor systems (Gen-IV)
- Design and evaluation strategies projected to reduce reliance on expensive validating experiments and employ accurate M&S as primary design and analysis tool
- M&S must have uncertainty management framework
  - Quantifiable error bounds on simulation results
  - Means to understand various sources of errors
  - Mean to reduce identified sources of errors
  - Means to integrate experiments, and devise their optimal design

Neutron Cross-Section

- Many studies proved that nuclear data uncertainties constitute major source of errors in neutronics design calculations

Resonance Parameter Uncertainty leads to 0.15% uncertainty in EOC k-effective ($600K in FCC)



Importance of Uncertainty Management

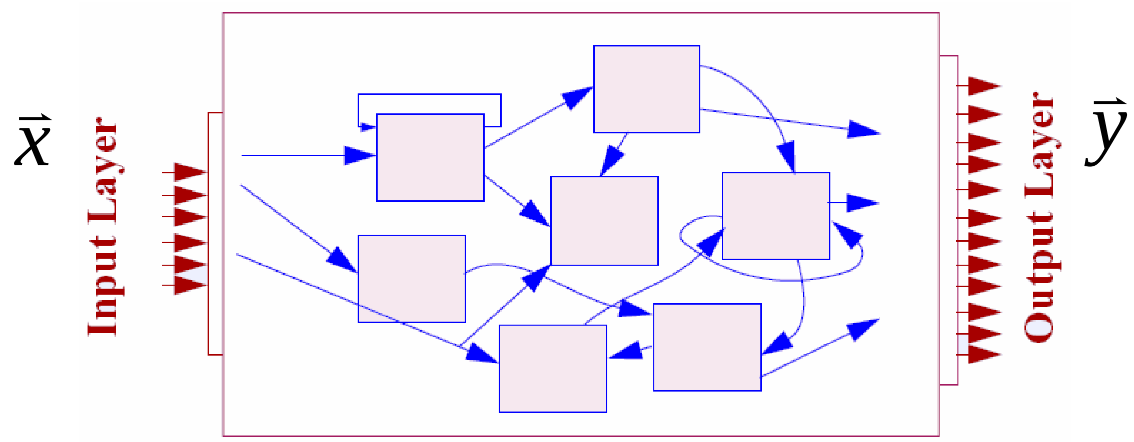
- Define required system design margins
- Identify key input data and associated models contributing most to quantified uncertainties
- Alter design to make it less sensitive to identified key sources of uncertainties
- Optimize experiments design to reduce uncertainties
- Increase design freedom by reducing design margins realized by higher fidelity calculations
- These goals to be achieved via **simulation to minimize reliance on expensive experiments**

Definitions

- Consider a computational model describing an engineering system:

$$\vec{y} = \Theta(\vec{x})$$

- **Sensitivity:** Rate of Change of output with respect to input
- **Uncertainty:** Confidence in calculated results
- **Data Assimilation:** Reduction of calculations uncertainties



Sensitivity Analysis Goal

- Given a system model:

$$\vec{y} = \vec{\Theta}(\vec{x})$$

where $\vec{x} \in \mathbb{R}^n$ are input data (physical constants, operating conditions, control parameters, etc.), and $\vec{y} \in \mathbb{R}^m$ are output responses (system attributes of interest to design, operation, and safety)

- Calculate *at a minimum* first order derivatives of output responses with respect to input data

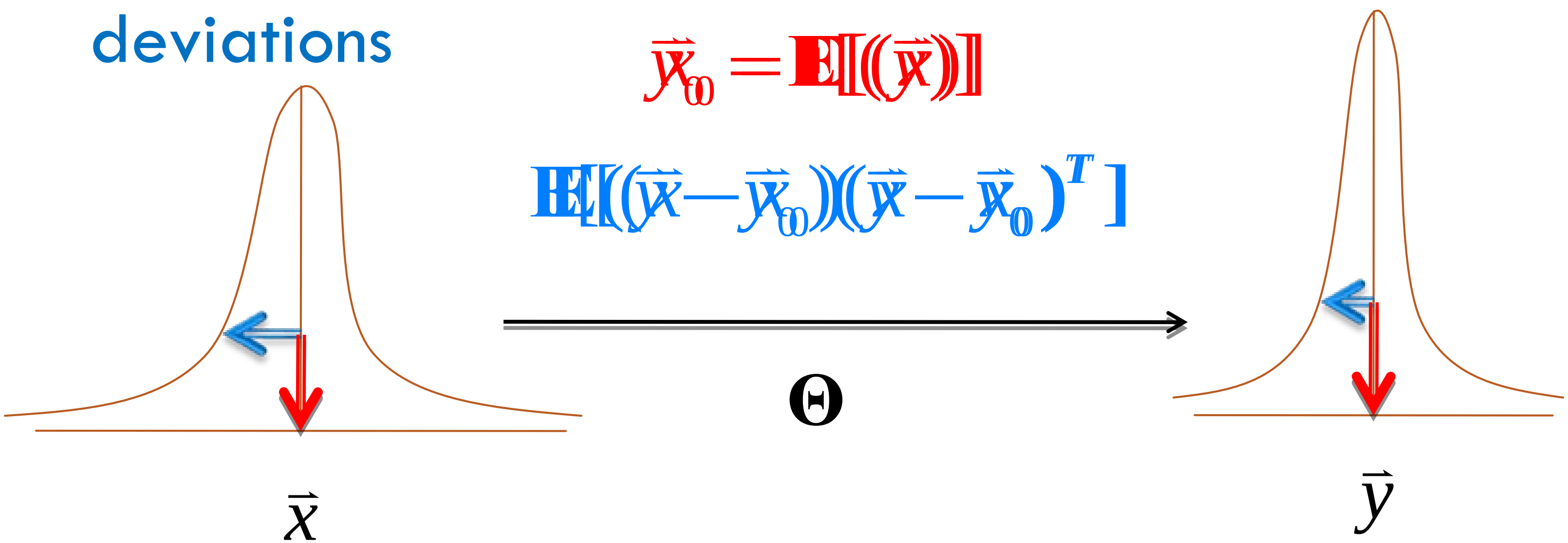
$$\mathbf{\Theta}_{ij} = \frac{\partial y_i}{\partial x_j}, i = 1, \ldots, m, \; j = 1, \ldots, n$$

Uncertainty Analysis Goal

- Given system model and input data uncertainties calculate output responses uncertainties.
  <u>Need:</u> Sensitivity Analysis
- Data uncertainties described *<u>at a minimum</u>* by probability distributions' means and standard deviations

$$\vec{x}_0 = E[\vec{x}] \qquad \vec{y}_0 = E[\vec{y}]$$

$$E[(\vec{x}-\vec{x}_0)(\vec{x}-\vec{x}_0)^T] \qquad E[(\vec{y}-\vec{y}_0)(\vec{y}-\vec{y}_0)^T]$$



Data Assimilation Goal

- Given measured system responses, adapt model to increase simulation fidelity by accounting for:
  - Modeling errors due to simplifying assumptions
    (Unclear how to accomplish?)
  - Numerical errors due to discretization
    (Emerging posterior and goal-oriented techniques)
  - **Boundary Conditions** characterizing interaction between various modeling stages: (calls for rigorous approaches)
  - **Input data errors**
    (well-established approaches: requires model inversion, sensitivity analysis, and input data uncertainties)

$$\min_{x} \left\| \vec{y}^{m} - \vec{\Theta}(\vec{x} + \delta\vec{x}) \right\|^{2} + \alpha^{2} \left\| \delta\vec{x} \right\|^{2}$$

Uncertainty Management Steps

Linear Approximation

- Evaluate sensitivity information

$$\boldsymbol{\Theta}_{ij} = \frac{\partial y_i}{\partial x_j}, i = 1, \ldots, m,\ j = 1, \ldots, n \Rightarrow \boldsymbol{\Theta} = \begin{bmatrix} \boldsymbol{\Theta}_{11} & . & \boldsymbol{\Theta}_{1n} \\ . & . & . \\ \boldsymbol{\Theta}_{m1} & . & \boldsymbol{\Theta}_{mn} \end{bmatrix}$$

- Obtain input data covariance matrix

$$\mathbf{C}_x = E\left[(\vec{x} - \vec{x}_0)(\vec{x} - \vec{x}_0)^T\right]$$

- Calculate of output data covariance matrix

$$\mathbf{C}_y = E\left[(\vec{y} - \vec{y}_0)(\vec{y} - \vec{y}_0)^T\right] = \boldsymbol{\Theta}\mathbf{C}_x\boldsymbol{\Theta}^T$$

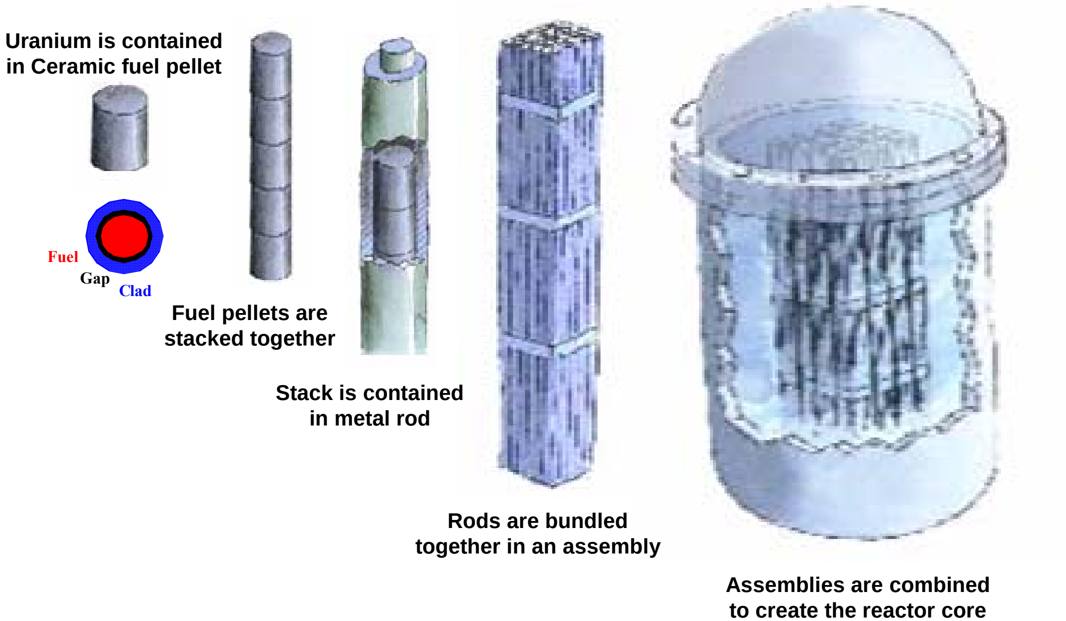
- Identify key sources of errors:

$$\left(\mathbf{C}_x + \boldsymbol{\Theta}^T\boldsymbol{\Theta}\right)^{-1}$$

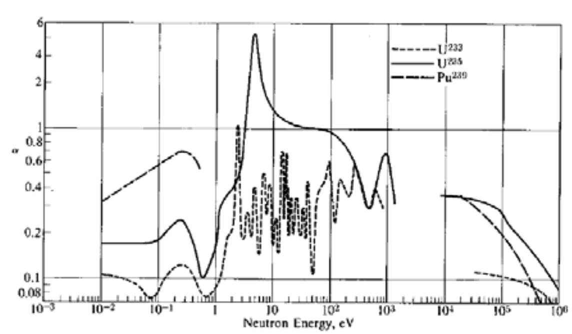
Why UQ Challenging?

<u>Example:</u> Nuclear Reactors Modeling

- Fully resolved description of reactor is not practical even with anticipated growth in computer power over foreseeable future
- Multi-level homogenization theory adopted to render reactor calculations in practical run times with reasonable accuracy
- Input data: cross-sections, design data, etc.
- Output data: criticality, power, thermal margins, reactivity coefficients, etc.



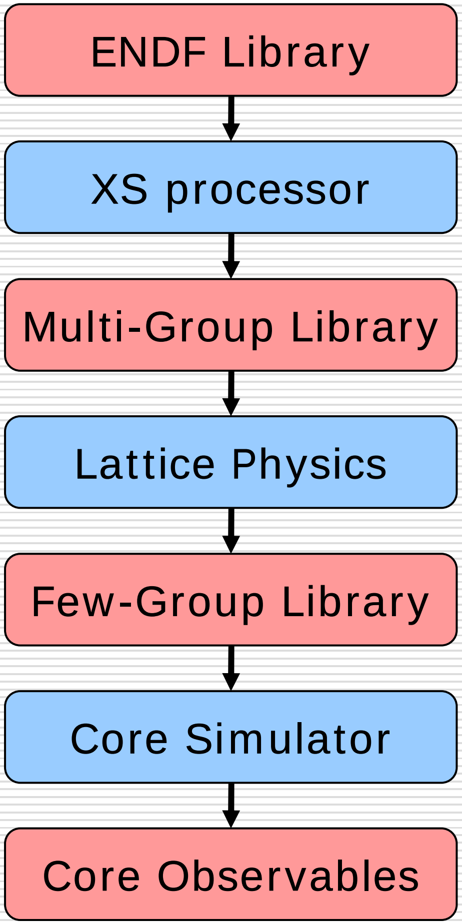
Spatial Heterogeneity of nuclear reactor core



Cross-Sections dependence on neutron energy

BWR Example (Size of I/O streams)

$\bar{\bar{\mathbf{C}}}_{ENDF}$	$10^4 \times 10^4$	--
$\bar{\bar{\mathbf{S}}}_{XP}$	$10^7 \times 10^4$	--
$\bar{\bar{\mathbf{C}}}_{MG} = \bar{\bar{\mathbf{S}}}_{XP} \bar{\bar{\mathbf{C}}}_{ENDF} \bar{\bar{\mathbf{S}}}_{XP}^{T}$	$10^7 \times 10^7$	--
$\bar{\bar{\mathbf{S}}}_{LP}$	$10^6 \times 10^7$	6.7 hr/ 51 days
$\bar{\bar{\mathbf{C}}}_{FG} = \bar{\bar{\mathbf{S}}}_{LP} \bar{\bar{\mathbf{C}}}_{MG} \bar{\bar{\mathbf{S}}}_{LP}^{T}$	$10^6 \times 10^6$	--
$\bar{\bar{\mathbf{S}}}_{CS}$	$10^5 \times 10^6$	5 min
$\bar{\bar{\mathbf{C}}}_{CO} = \bar{\bar{\mathbf{S}}}_{CS} \bar{\bar{\mathbf{C}}}_{FG} \bar{\bar{\mathbf{S}}}_{CS}^{T}$	$10^5 \times 10^5$	--



Sensitivity Forward Approach

$$\mathbf{\Theta}\,\delta\vec{x} \approx \vec{\Theta}(\vec{x}_0 + \delta\vec{x}) - \vec{\Theta}(\vec{x}_0)$$

- Perturb input data one-at-a-time to calculate sensitivities of all outputs with respect to the perturbed input
- Suited for problems with few inputs and many outputs
- *Variations*:
  - Simultaneously perturb all inputs based on their prior PDFs; repeat until the output PDFs converge
  - Suitable for non-Gaussian distributions, and nonlinear systems.
  - Difficult to infer sensitivity information

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_r} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_r} \\ \vdots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_r} \end{bmatrix}$$

Sensitivity Reverse Approach

$$\boldsymbol{\Theta}^{T} \delta \vec{y} \;\square\; ???$$

- Generalized Perturbation Theory
  - Based on select output response, constructs adjoint model to calculate the response sensitivities with respect to all input data
  - Suited for problems with many inputs and few outputs
  - Difficult to implement for legacy codes

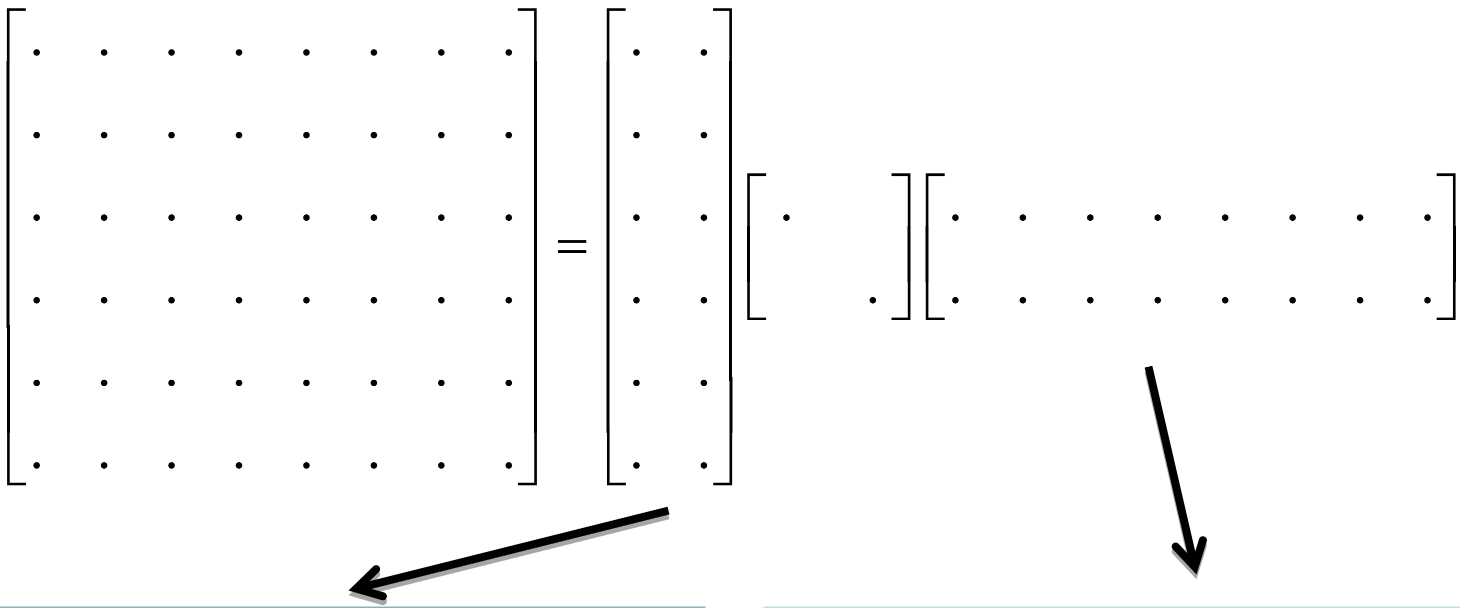
$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & .. & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_r}{\partial x_1} & \frac{\partial y_r}{\partial x_2} & .. & \frac{\partial y_r}{\partial x_n} \end{bmatrix}$$

Subspace Methods

- Replace original I/O streams by mathematical subspaces
- Subspaces are mathematical abstractions denoting change of basis in the I/O streams:
  - Create new I/O variables (called active DOFs).
  - Dimensions of subspaces are much smaller than original I/O streams
  - Each variable (active DOF) is a linear combination of all original variables, with weights reflecting importance of original variables
  - Subspaces identified by means of stochastic approach involving randomized matrix-vector and matrix-transpose-vector products
  - Mathematically, this process is equivalent to finding rank revealing decomposition of sensitivity and uncertainty matrices
  - Requirement: matrices be ill-conditioned

Subspace Methods:

Rank Revealing Decomposition



Determined via ***r*** Forward runs

Determined via ***r*** adjoint runs

$$\mathbf{\Theta} = \left[\vec{u}_1 \ldots \vec{u}_r\right]\begin{bmatrix} s_1 & \\ & s_r \end{bmatrix}\begin{bmatrix} \vec{v}_1 \\ \vec{v}_r \end{bmatrix}^T$$

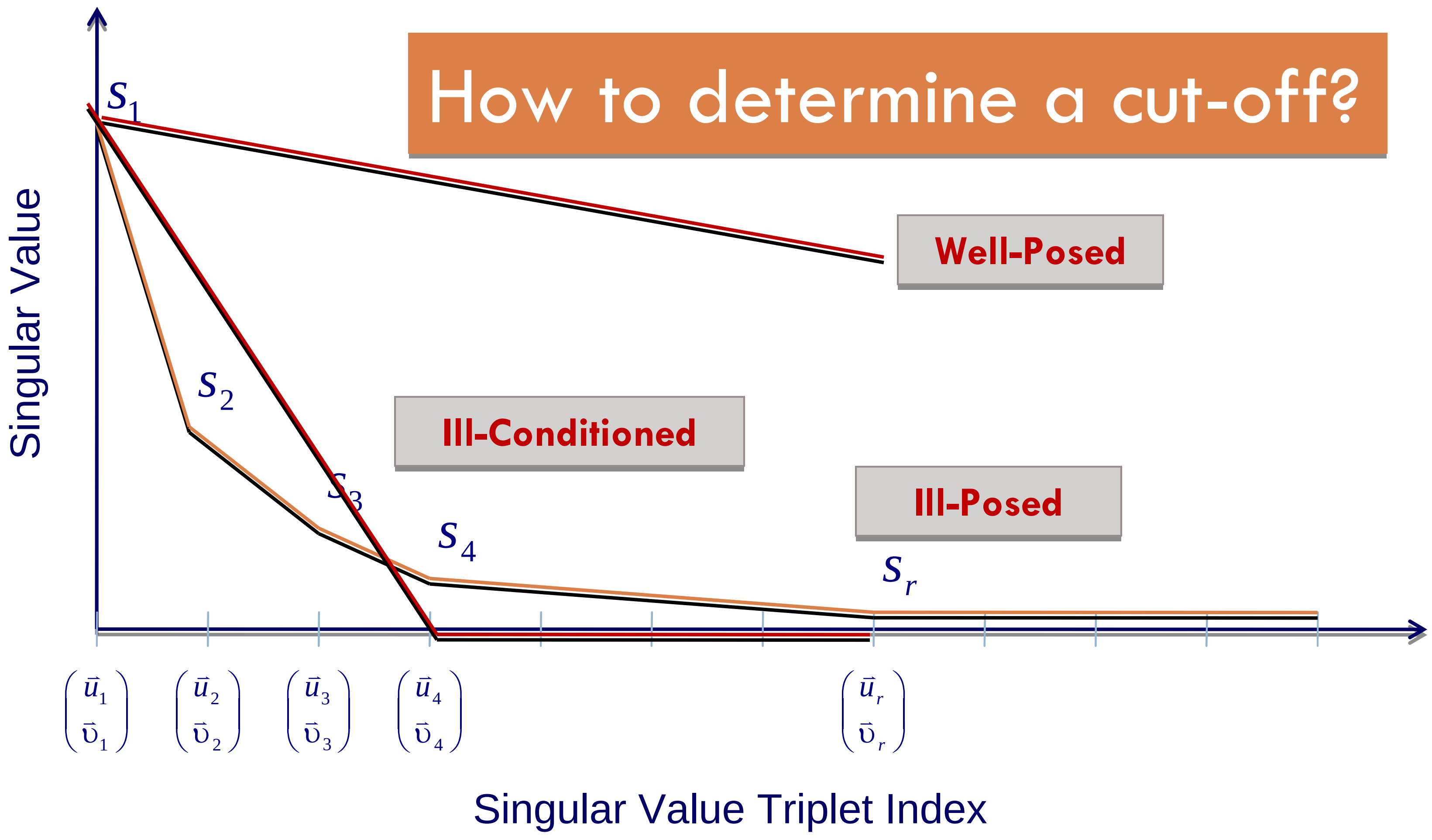
$$\mathbf{\Theta} \times \delta\vec{x} \in \text{span}\left\{\vec{u}_1,..,\vec{u}_r\right\}$$

$$\mathbf{\Theta}^* \times \delta\vec{y} \in \text{span}\left\{\vec{v}_1,..,\vec{v}_r\right\}$$

Active output subspace
Active output DOFs

Active input subspace
Active input DOFs

Singular Values Spectrum



Philosophy of Subspace Methods

- In Euclidean sense, one can change n inputs to a computational model in n different ways, however, for most complex codes, only a subset $r \ll n$ leads to **noticeable** changes in outputs.
- **Active Degrees of Freedom** denote the various changes in inputs leading to changes in outputs.
- Most outputs of interest to designers and operators are often **integral quantities**, e.g. power, reactivity, thermal margins, etc., (hence dimensionality reduction)

Active and Inactive DOFs: Example

- Consider a simple model with one output response (energy produced from fission) and ***n*** input data (fission cross-sections of ***n*** different isotopes)

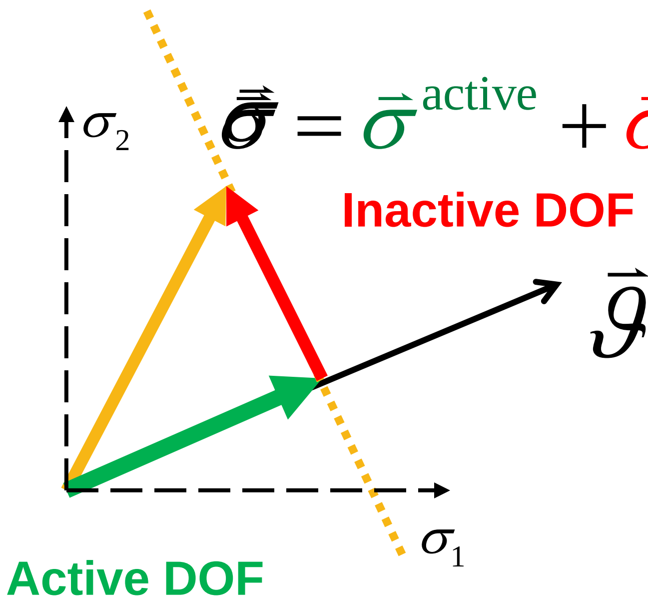
$$E = \sum_{i=1}^{n} \kappa_i N_i \sigma_i \Phi = \vec{\vartheta}^T \vec{\sigma}$$

$$\vartheta_i = \frac{\delta E}{\delta \sigma_i} = \kappa_i N_i \Phi$$

- Consider **inverse problem:** How to select $\vec{\sigma}$ for some ***E***?

$$\delta\vec{\sigma} \propto \vec{\sigma}^{\text{active}}$$

$$\vec{\sigma} = \vec{\sigma}^{\text{active}} + \vec{\sigma}^{\text{inactive}}$$



Background for Subspace Methods

Dimensionality reduction induced by a multi-level homogenization-type model can be described by Fredholm integral Equation of the first kind

$$\delta y(\varpi) = \int \vartheta(\varpi, t) \cdot \delta x(t)\, dt$$

Every square-integrable *kernel* has mean convergent singular value expansion of the form (Schmidt 1907-1908):

$$\vartheta(\varpi, t) = \sum_{i=1}^{\infty} \mu_i u_i(\varpi) \upsilon_i(t)$$

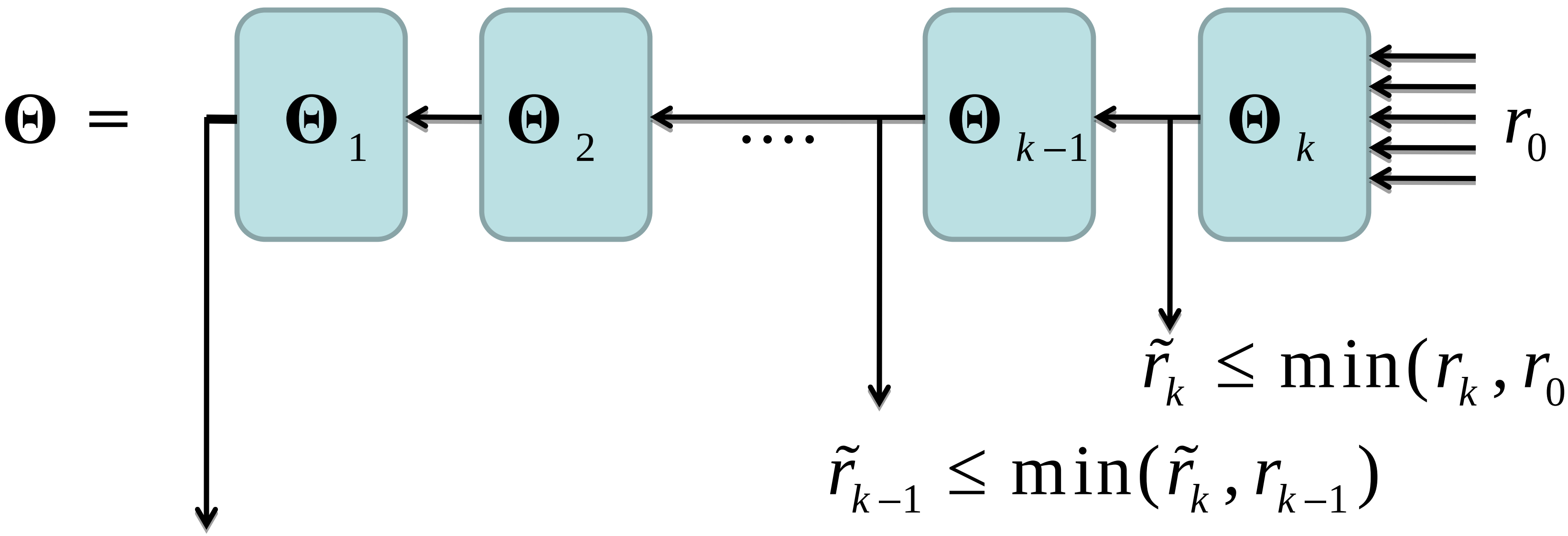
Singular Value Decomposition (SVD) is the algebraic version of SVE (Eckart and Young 1936-1939):

$$\boldsymbol{\theta}^{m \times n} = \sum_{i=1}^{r} s_i \vec{u}_i \vec{\upsilon}_i^{T} = \mathbf{U}_{m \times r} \boldsymbol{\Sigma}_{r \times r} \mathbf{V}_{n \times r}^{\mathbf{T}}$$

Subspace Methods

Consider a multi-level model composed of ***k*** sub-models (*also applies to various components of a single sub-model*):

<u>1. Forward Runs:</u>



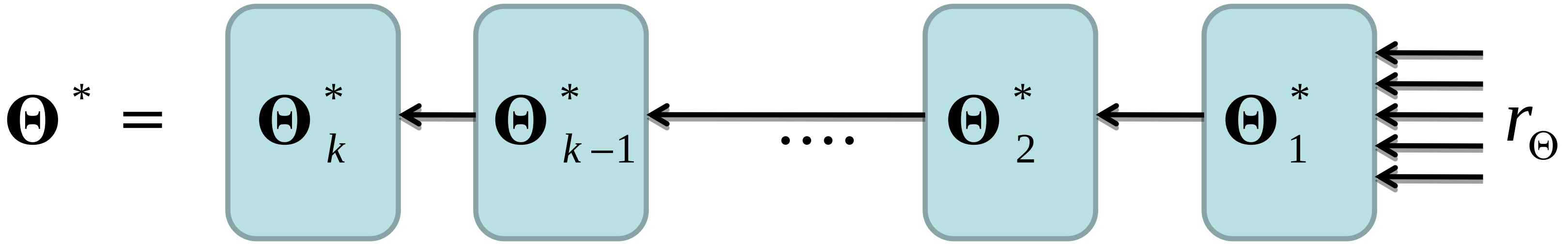
$$\tilde{r}_k \le \min(r_k, r_0)$$

$$\tilde{r}_{k-1} \le \min(\tilde{r}_k, r_{k-1})$$

$$r_\Theta = \tilde{r}_1 \le \min(\tilde{r}_k, \tilde{r}_{k-1}, \ldots, r_1)$$

Subspace Methods

<u>2. Reverse Runs (ex. Adjoint):</u>

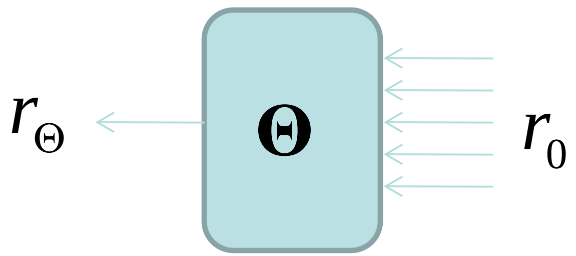


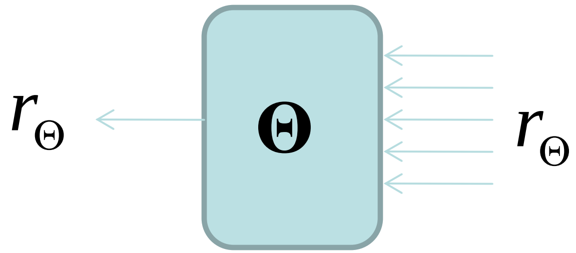
-Reverse model runs only $\boldsymbol{r_{\Theta}}$ times, i.e. rank of overall model.

-Reverse runs only required for rank-deficient sub-models.

Subspace Methods

Q: What if reverse model infeasible for a sub-model or component?
A: Given input subspace of dimension $\boldsymbol{r_0}$, run forward model $\boldsymbol{r_0}$ times, and via a RVD, reduce the input subspace to $\boldsymbol{r_\Theta}$



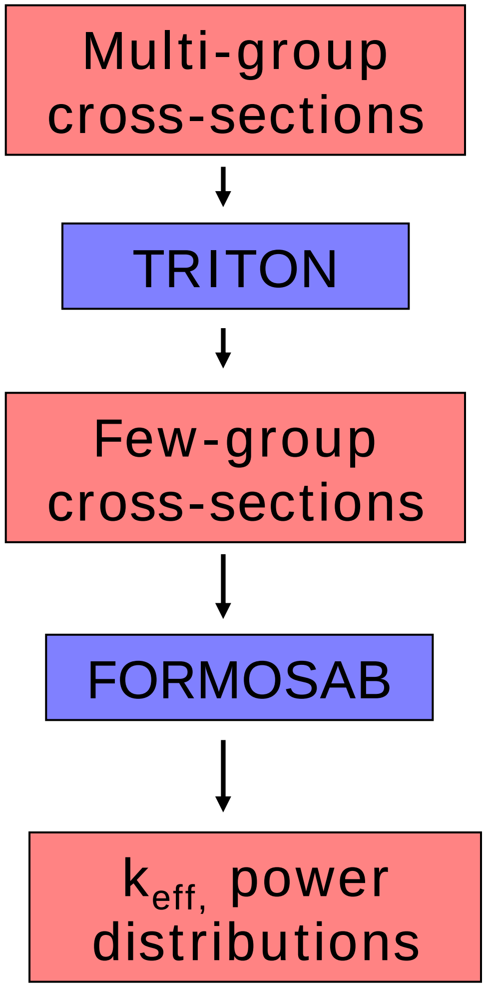


Example 1: Boiling Water Reactor

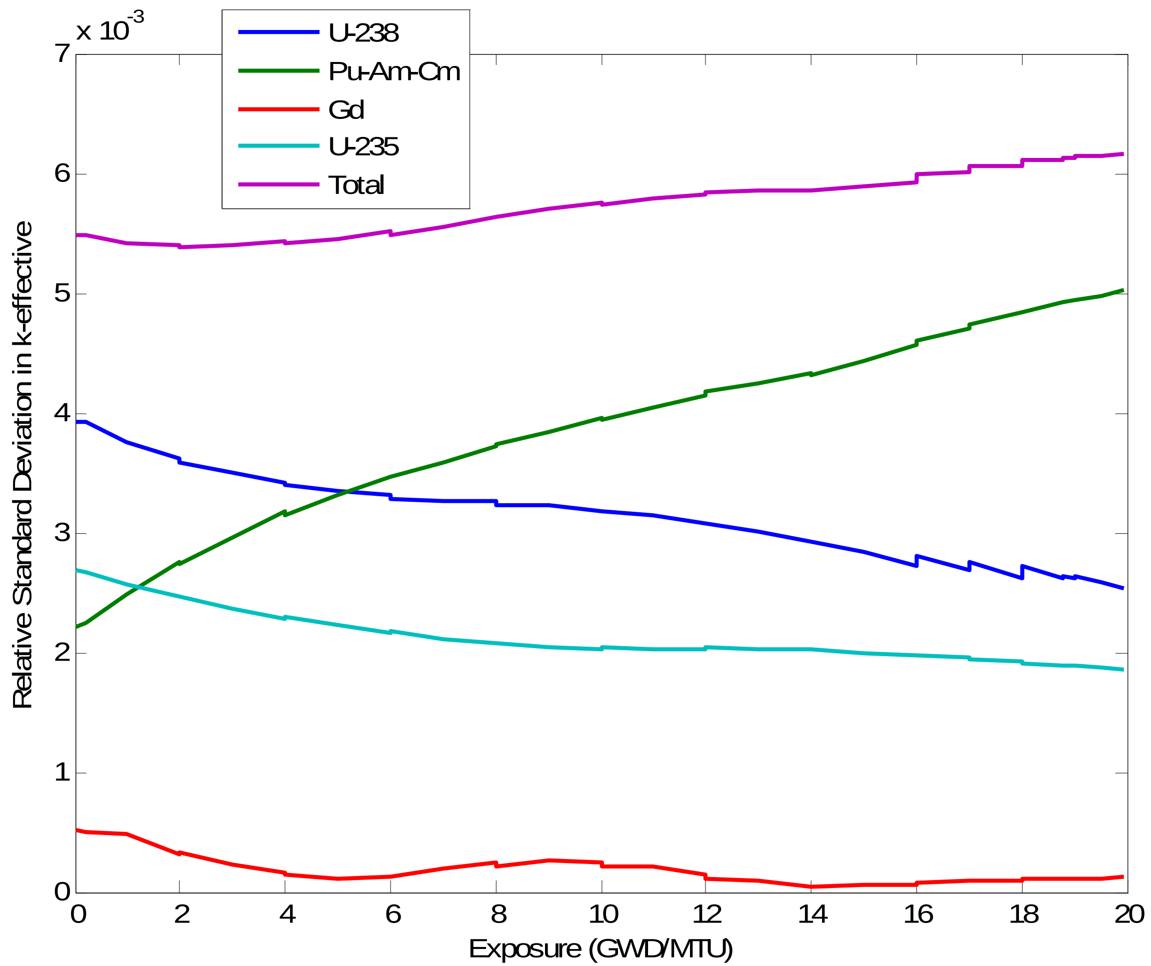
- Part of GE-Hitachi funded research on ‘Development of Adaptive Simulation Algorithms for BWRs’
- Given voluminous amount of data routinely collected from operating nuclear power plants, and maturity of neutronics calculations over past five decades, can one use a data assimilation to enhance agreement between measurements and predictions by adjusting cross-sections?

BWR Case Study

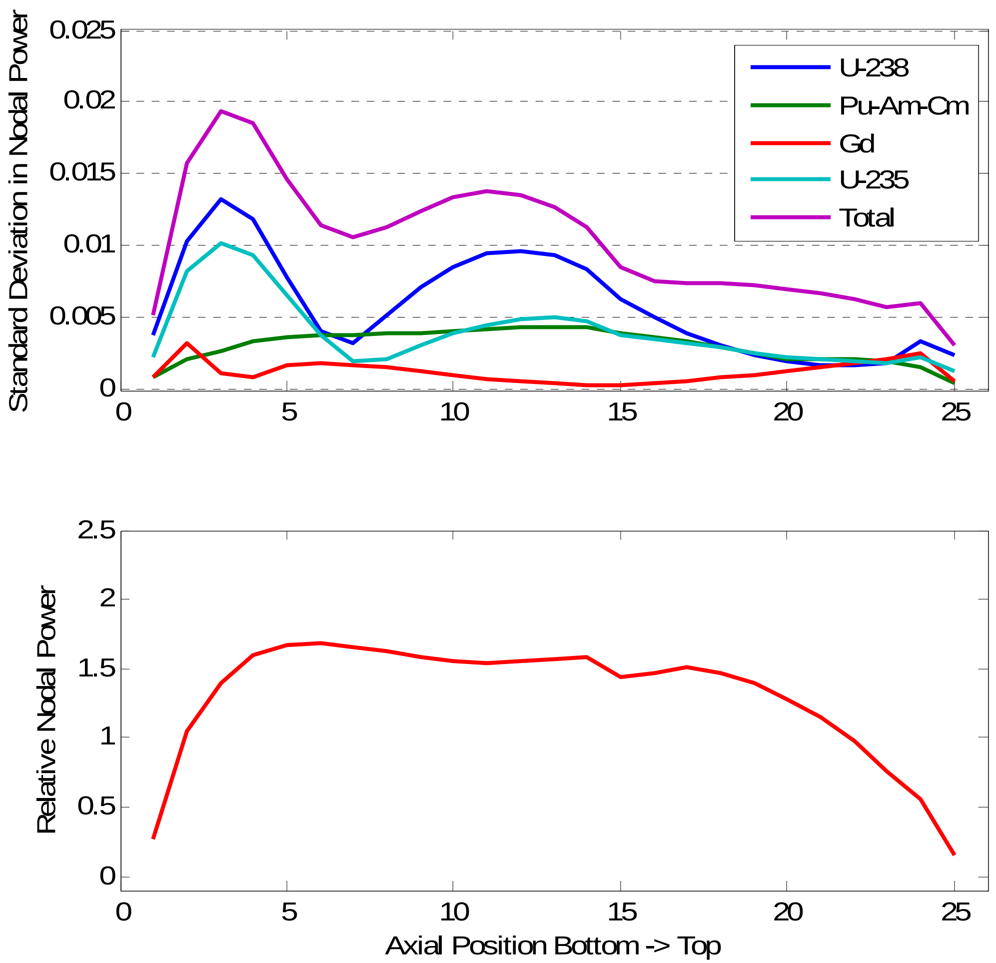
- **AMPX** – ORNL ENDF Processing Code System
  - Processes ENDF covariance data into 44 group energy structure
  - SCALE5.0 libraries (PUFF3)
    1. **44GROUPV5COV** - 29 isotopes including H, B, Al, U, Pu, and Minor Actinides et al.
    2. **44GROUPANLCOV** - 30 additional isotopes including Gd, Sm, Zr, et al.
  - SCALE5.1 libraries - Evaluations for V5 and V6 covariance data
- **TRITON -** ORNL lattice physics code
  - GE14 10x10 lattice design



BWR: Few-Group Cross-section Uncertainties

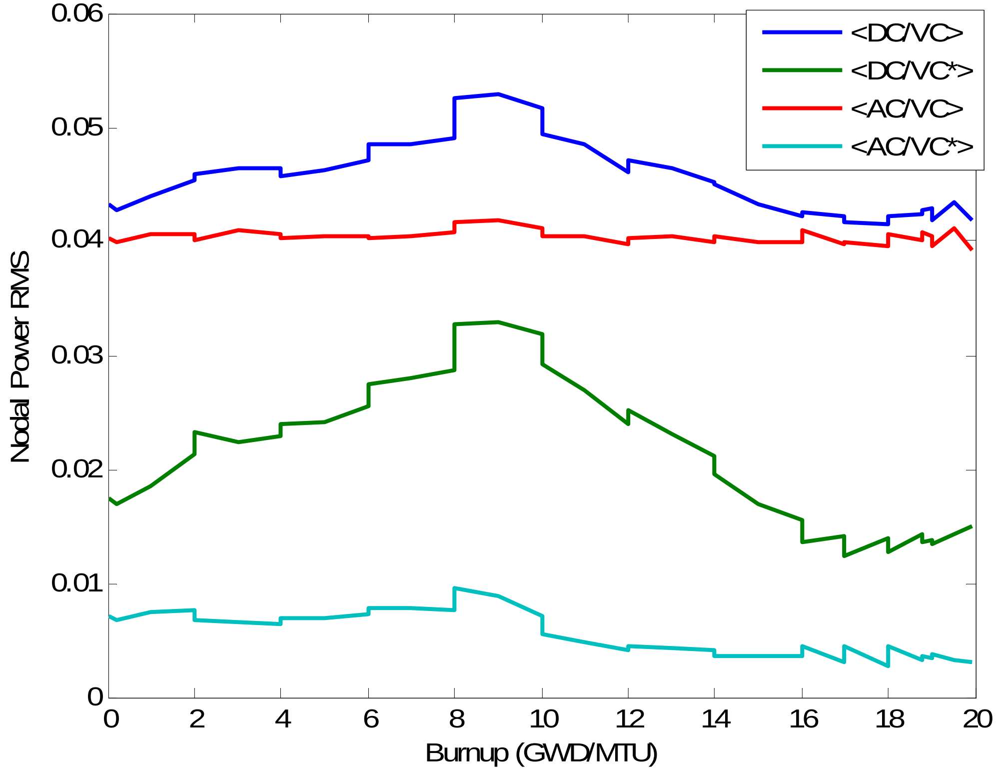


BWR: Power Distribution Uncertainties

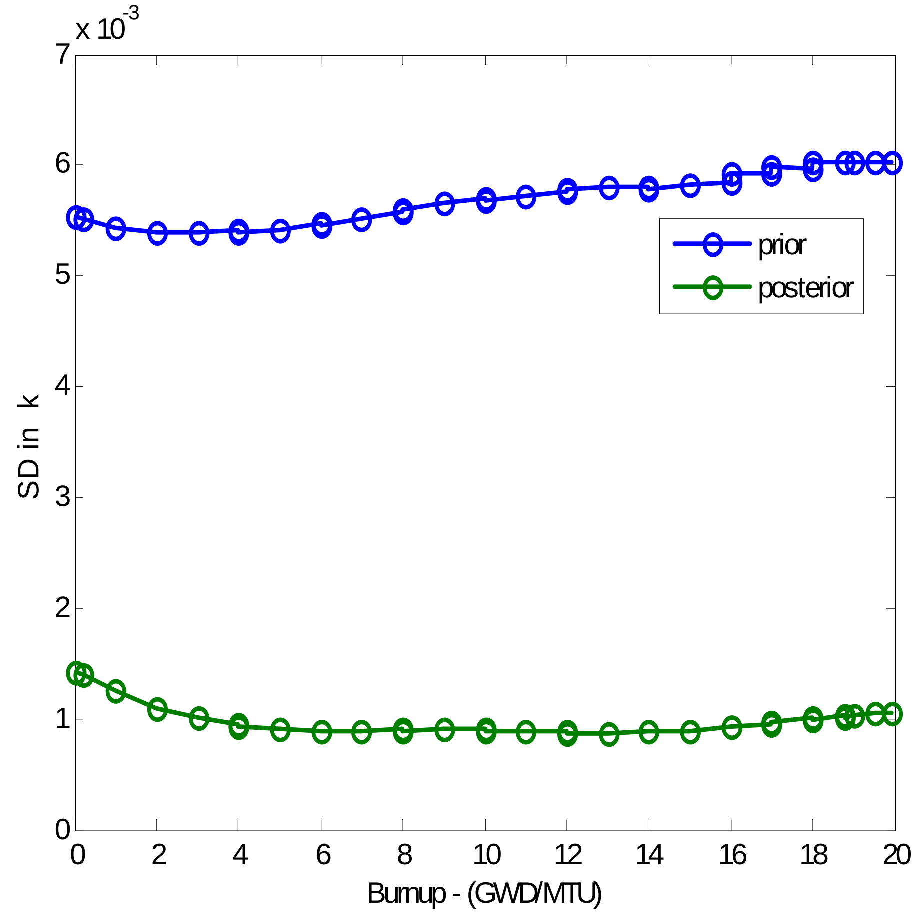


BOL Uncertainty Profile

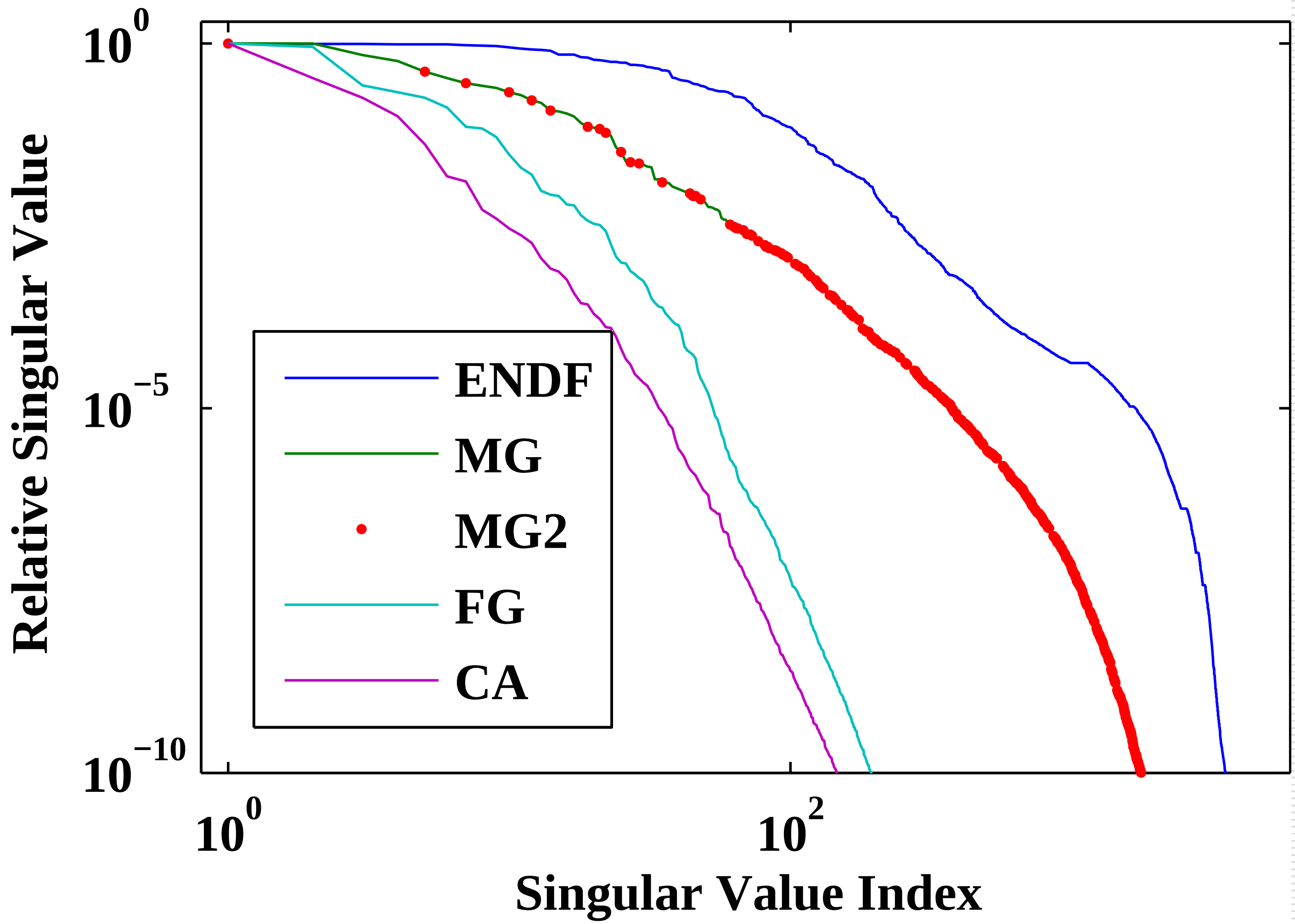
BWR: Data Assimilation "Virtual Approach"



BWR: Data Assimilation “Virtual Approach”



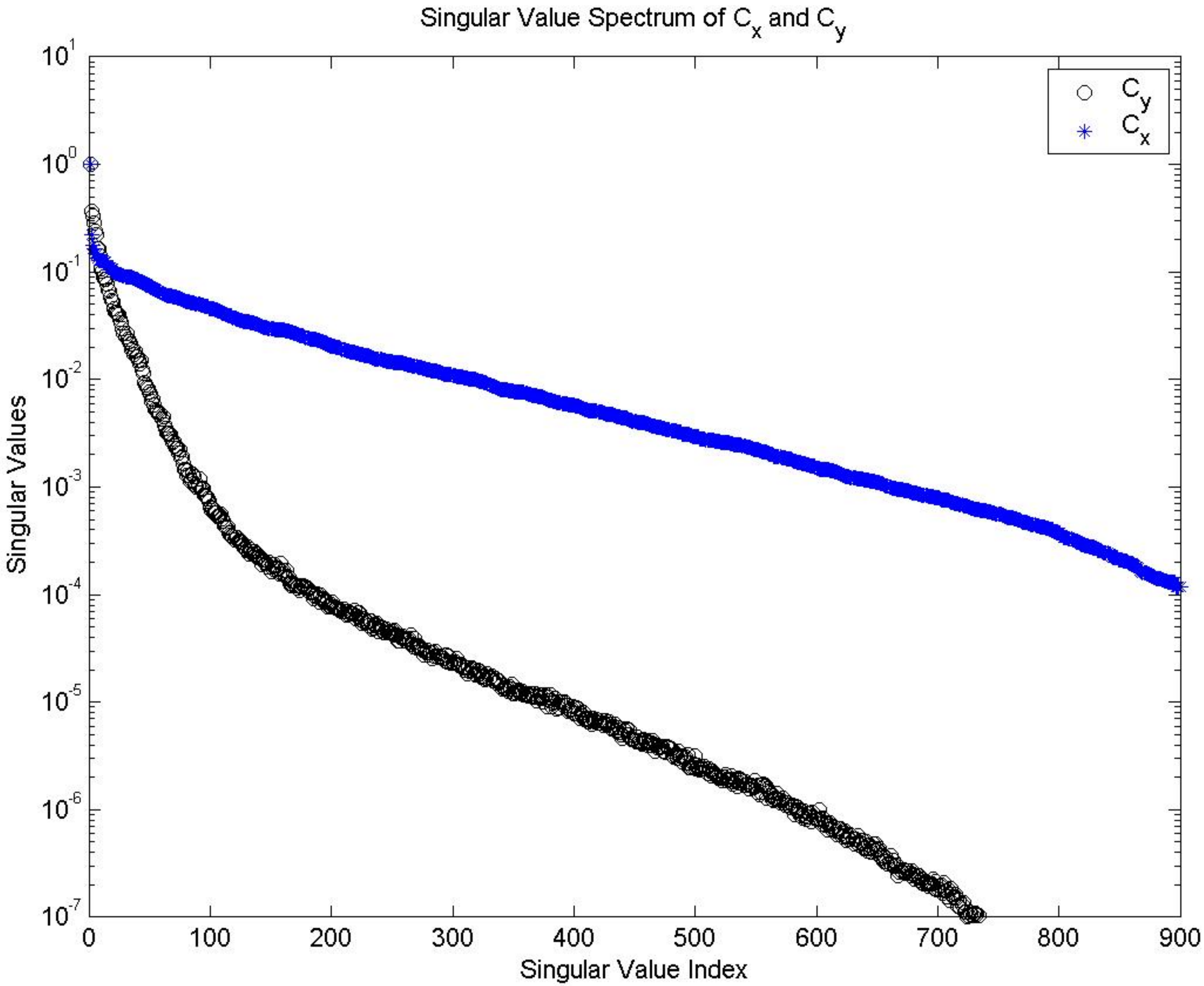
BWR: I/O Streams SVDs



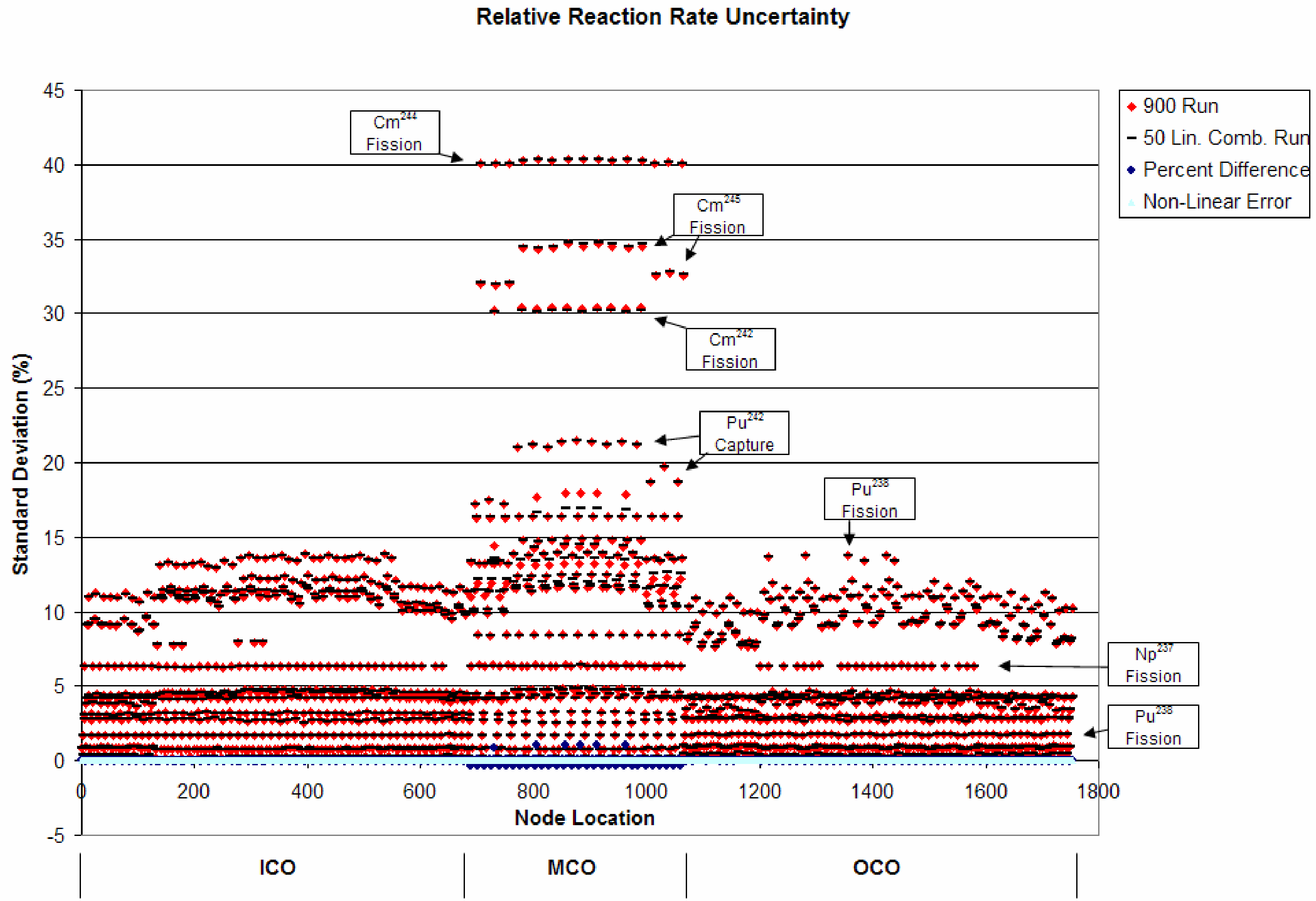
Example 2: Sodium Fast Reactor

- Work part of NERI on 'Management of Data Uncertainties and Optimum Design of Experiments for Gen-IV systems'
- Selected for analysis: ABTR core + ZPR experiments
- Research requires following capabilities:
  - Availability of group x-section uncertainties
  - Propagation of group x-section uncertainties to ABTR key attributes uncertainties
  - Data assimilation for x-sections using ZPR measurements
  - Reevaluation of ABTR's uncertainties using adjusted x-sections

ABTR: I/O Streams SVD



Results:
Relative Reaction Rate Uncertainty Data



Conclusions

- For multi-level models exhibiting reduction in dimensionality through various levels, significant computational savings are possible via a subspace approach
- Only information belonging to ‘**active**’ subspaces are communicated between various levels.
- Reverse models only required for the rank-deficient sub-models, thus relaxing need for full adjoint capability, which can be quite challenging for linked code system.
- If reverse model infeasible, use a two-step reduction process to identify the active I/O subspace.
- Result is a framework for uncertainty management that can be applied effectively on a routine basis

Future Work

- Extend methodology to adjust resonance parameters directly using a probabilistic Monte Carlo model
- Develop methodology to situations when nonlinear behavior must be considered
  - Weak nonlinearities: Guide deterministic calculations for second order derivatives, i.e. Hessian operators, using active DOFs (r) from linear model (Computational cost ~ r^2)
  - Strong nonlinearities: Hybrid deterministic-probabilistic approach to bias stochastic samples using active DOFs from linearized model
  - Implicit assumption of these developments is that higher order derivatives may be ignored if first order derivatives are small

Questions?