SENSITIVITY, UNCERTAINTY, AND ADAPTIVE SIMULATION METHODS

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Objectives

- Provide rigorous framework for uncertainty management for general analysis codes used routinely in design:
  - Estimate uncertainties, (via UQ)
  - Understand uncertainties, (via SA coupled with UQ)
  - Reduce uncertainties (Inverse/Adaptive Analysis)
- Realize potential of increasingly promoted role of modeling and simulation in design of nuclear systems

Objectives

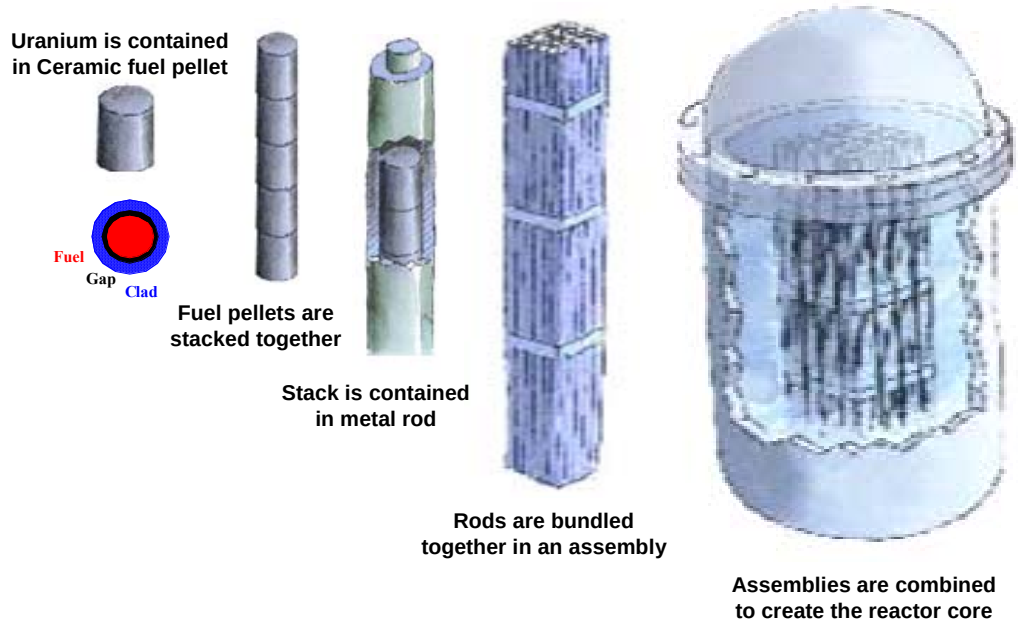
- Predict best-estimates responses and their uncertainties originating from:
  - Input data (including correlations) epistemic (reducible) and aleatory (irreducible) uncertainties
  - Initial and boundary conditions errors
  - Homogenization theory errors
- *Currently not treating modeling errors, numerical errors, interaction between various error sources*
- Efficiency, ease of implementation, and transferability to different codes systems

Relevance

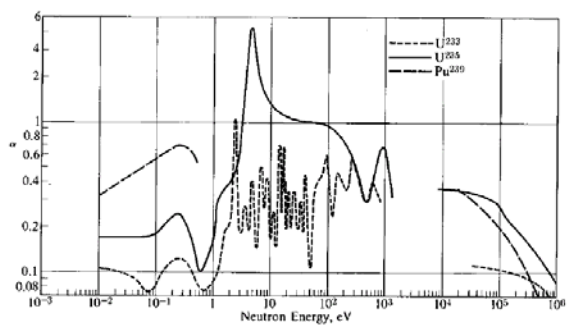
- Define required system design margins
- Identify key input data and associated models contributing most to quantified uncertainties
- Alter design to make it less sensitive to identified key sources of uncertainties
- Optimize experiments design to reduce uncertainties
- Increase design freedom by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

Nuclear Reactors Modeling

- Nuclear models involve a wide range of energy and length scales varying by several orders in magnitude
- 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



Spatial Heterogeneity of nuclear reactor core



Cross-Sections dependence on neutron energy

Mathematical Description

- The ensemble average of neutron distribution in a reactor can be described by Boltzmann Equation:

$$\frac{1}{\upsilon}\frac{\partial\varphi}{\partial t}+\vec{\Omega}\bullet\nabla\varphi+\Sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega},t)=$$

$$\int_{4\pi}d\vec{\Omega}'\int_0^{\infty}dE'\Sigma_s(E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega})\varphi(\vec{r},E',\vec{\Omega}',t)+$$

$$\frac{\chi(E)}{4\pi}\int_{4\pi}d\vec{\Omega}'\int_0^{\infty}dE'v(E')\Sigma_f(E')\varphi(\vec{r},E',\vec{\Omega}',t)+$$

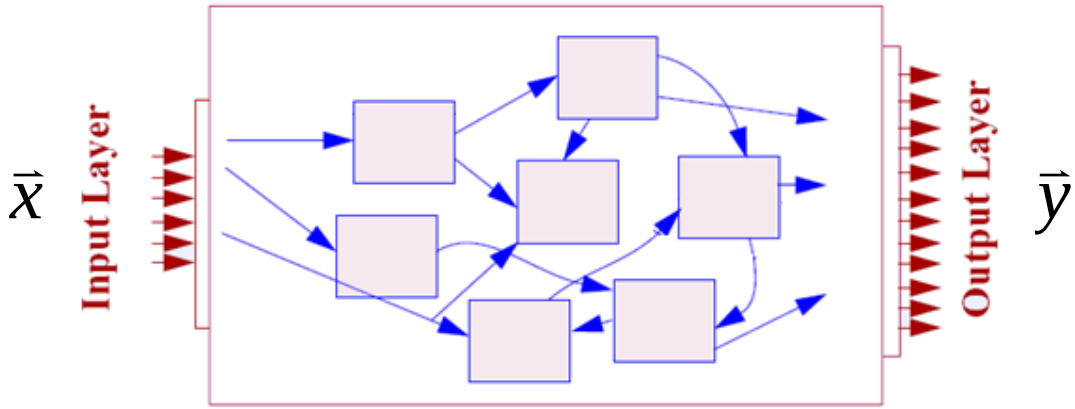
$$s(r,E,\vec{\Omega},t)$$

Framework Requirements

- Consider a computational model describing an engineering system:

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

- **<u>Sensitivity:</u>** Rate of Change of output with respect to input
- **<u>Uncertainty:</u>** Confidence in calculated results
- **<u>Adaptive Simulation:</u>** Reduction of calculations uncertainties and meeting target accuracy requirements



Sensitivity Analysis

- Characterize responses' variations w.r.t various error sources to as many degrees as computationally possible.

$$\vec{y} = \Theta(\vec{x}); \quad \vec{x} \in \mathbb{R}^n; \vec{y} \in \mathbb{R}^m$$

$$y_i = y_{i0}\left(\vec{x}_0\right) + \vec{g}_i^T\left(\vec{x} - \vec{x}_0\right) + \frac{1}{2}\left(\vec{x} - \vec{x}_0\right)^T \mathbf{H}_i\left(\vec{x} - \vec{x}_0\right) + \ldots.$$

$$\left\{ g_{ij} = \frac{\partial y_i}{\partial x_j} \right\} \in \mathbb{R}^{m \times n}; \left\{ \mathbf{H}_{ijk} = \frac{\partial^2 y_i}{\partial x_j \partial x_k} \right\} \in \mathbb{R}^{m \times n \times n}$$

- Challenges: *m*,*n* very large for nuclear codes; thus leading to intractable computational burdens

Linear-Based Uncertainty Management Requirements

- One Code:

$$SA: \ \mathbf{G} = \left[\frac{\partial y_i}{\partial x_j} \right]^{m \times n} ;$$

$$UQ: \ \mathbf{G}\mathbf{C}_x\mathbf{G}^T; \qquad DA: \ \left(\mathbf{G}^T \mathbf{C}_{y(m)}^{-1} \mathbf{G} + \mathbf{C}_x \right)^{-1}$$

- Multiple codes:

$$SA: \ \mathbf{G}^{m \times n} = \mathbf{G}_1^{m \times l_1} \times \mathbf{G}_2^{l_1 \times l_2} \times \ldots\ldots \times \mathbf{G}_k^{l_{k-1} \times n};$$

Sensitivity Forward Approach

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

- 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

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

Sensitivity Reverse Approach

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

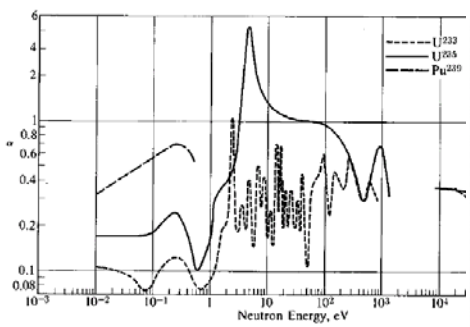
- Generalized Perturbation Theory
  - Based on select output response, constructs adjoint model to calculate the response sensitivities with respect to all input data
  - Suited for problems with many inputs and few outputs
  - Difficult to implement for legacy codes, particularly for coupled code systems

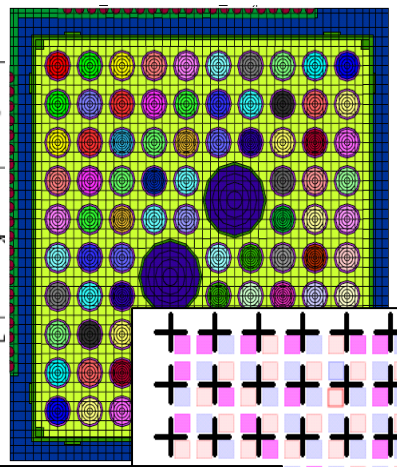
$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & .. & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_r}{\partial x_1} & \frac{\partial y_r}{\partial x_2} & .. & \frac{\partial y_r}{\partial x_n} \end{bmatrix}$$

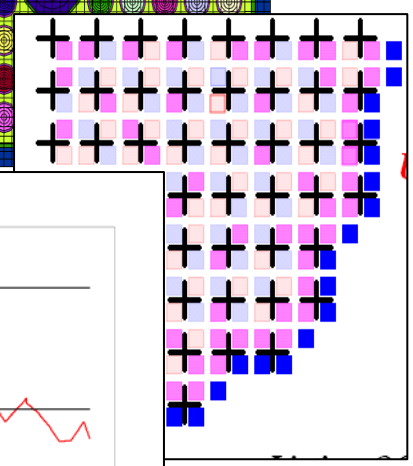
Structure of Typical LWR Models

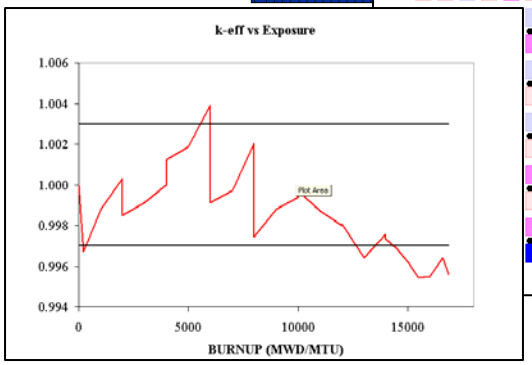
of Data > 10^6 Runtime ~ mins 10^4

ENDF → MG Gen Codes → MG XS









Lattice Calcs — hrs

FG XS — 10^6

Core Calcs — mins

k_{eff}, power, flux, margins, etc. — 10^5

Philosophy of Subspace Methods

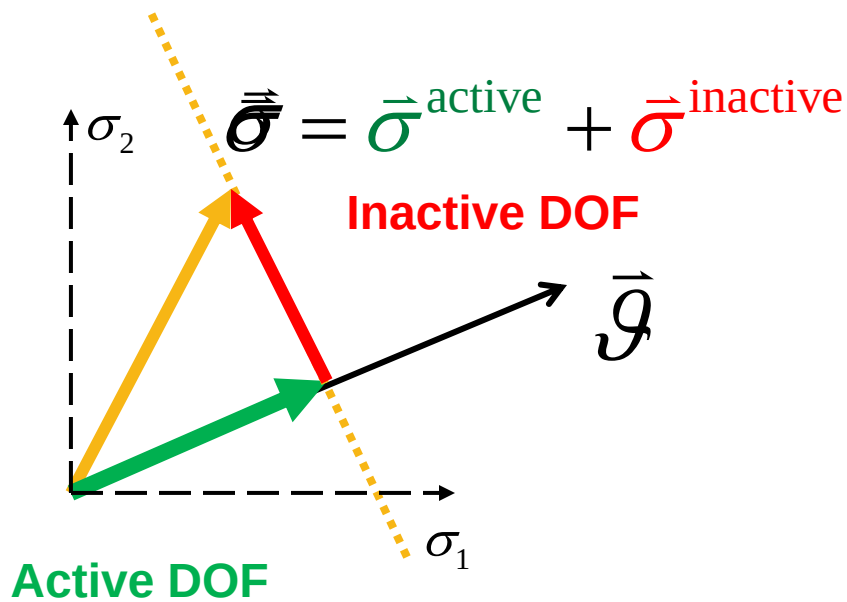
- In Euclidean sense, one can change n inputs to a computational model in n different ways, however, for most complex codes, only a subset $r<<n$ leads to **noticeable** changes in outputs.
- **Active Degrees of Freedom** denote the various changes in inputs leading to changes in outputs.
- Most outputs 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)

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

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



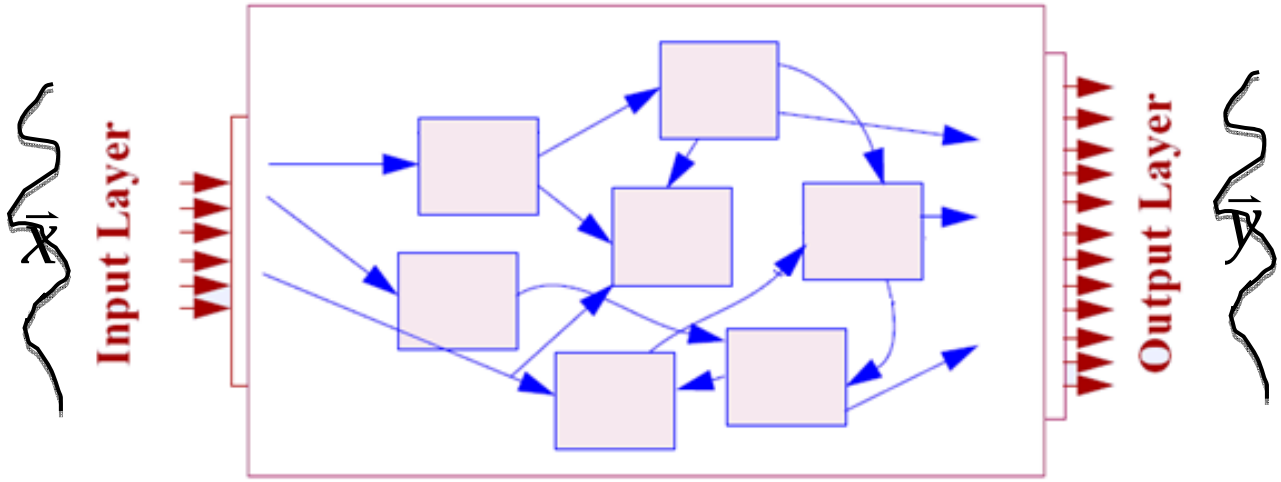
- Consider **inverse problem:** How to select $\vec{\sigma}$ for some ***E***?

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

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



$$\left\| \vec{x} - \vec{x}_{DOF} \right\| \prec \varepsilon \qquad \left\| \vec{y} - \vec{y}_{DOF} \right\| \prec \eta$$

$$\vec{x}_{DOF} = \Phi_x(\vec{v}_{DOF}) \qquad \vec{y}_{DOF} = \Phi_y(\vec{u}_{DOF})$$

$$\vec{v}_{DOF} \in \mathbb{R}^r \qquad \vec{y}_{DOF} = \Theta_r(\vec{x}_{DOF}) \qquad \vec{u}_{DOF} \in \mathbb{R}^r$$

Active DOFs

$$\left[\vec{x}_{DOF}\right]_k = \sum_{i=1}^{n} \alpha_{ki} x_i = \vec{\alpha}_k \vec{x}$$

$$\left[\vec{y}_{DOF}\right]_k = \sum_{j=1}^{m} \beta_{ki} y_j = \vec{\beta}_k \vec{y}$$

$$\vec{y}_{DOF} = \mathbf{\Theta}_r \vec{x}_{DOF}$$

Subspace Methods:

Rank Revealing Decomposition

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{bmatrix} \begin{bmatrix} \cdot & \\ & \cdot \end{bmatrix} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

Determined via *r* Forward runs

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

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

Determined via *r* adjoint runs

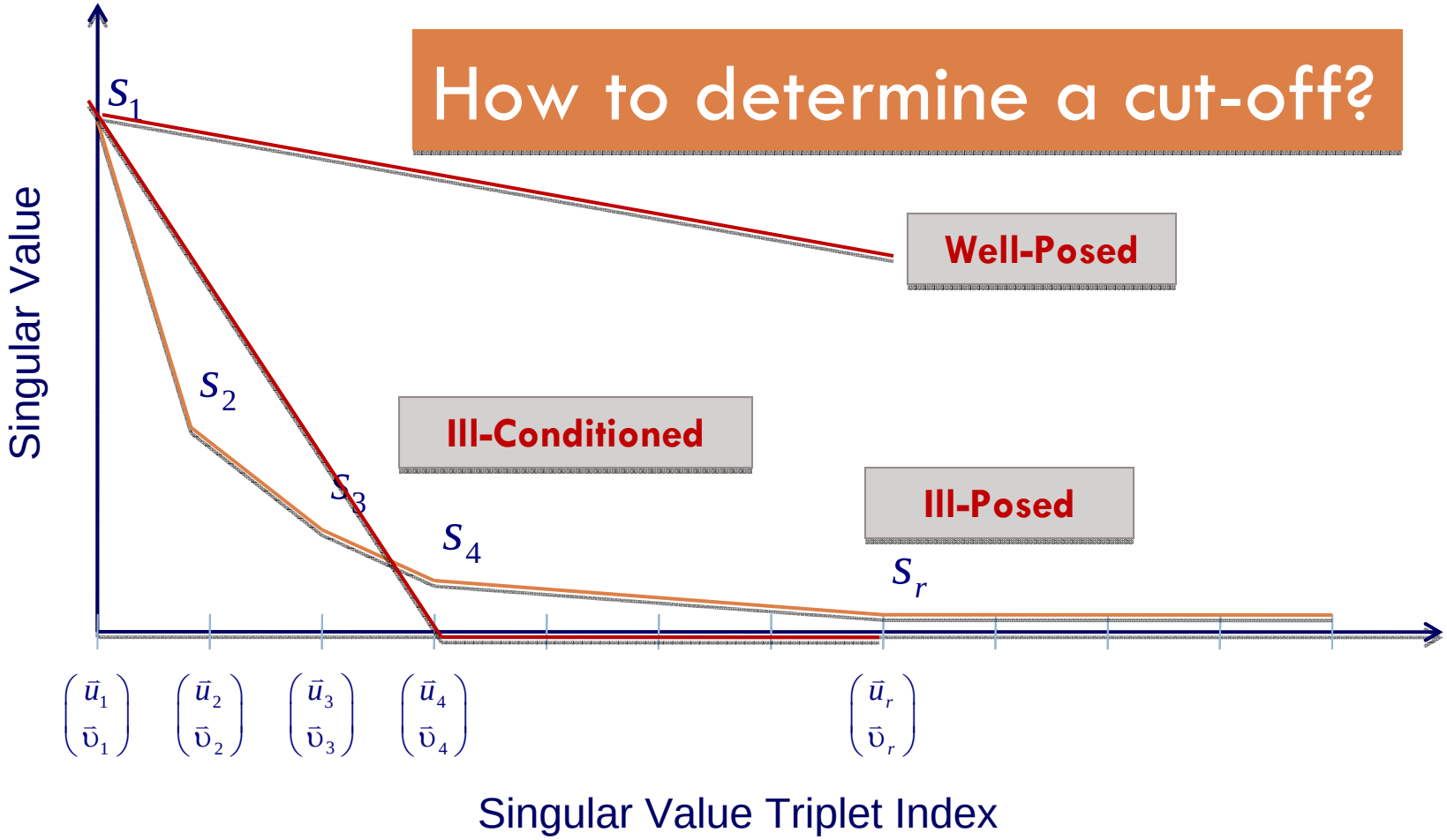
$$\mathbf{\Theta}^* \times \delta \vec{y} \in \text{span}\{\vec{v}_1, .., \vec{v}_r\}$$

Active output subspace
Active output DOFs

Active input subspace
Active input DOFs

```
>> X=rand(n,r); % only r columns, since rank of A is r.
>> Y=A*X;   % Columns of Y span R(A)
>> Z=B'*X;  % Columns of Z span R(A')
>> G=Z*inv(Z'*Z)*Z';
>> x=G*X*inv(Y'*Y)*Y'*y;  % x is the minimum norm solution
>> % Now, compare this solution with the minimum norm solution
>> % obtained by tranditional SVD techniques.
>> x_ls=V(:,1:r)*inv(S(1:r,1:r))*U(:,1:r)'*y;
>> maxerr_x=max(abs(x_ls-x));
>> % The matrix A may be reconstructed as follows:
>> [Q,R]=qr(G*X,0);
>> A_recon=Y*inv(R)*Q';
>> Now, compare the reconstructed A with the original A.
>> maxerr A=max(max(abs(A recon-A)));
```

Singular Values Spectrum



Relation to Past Work?

- The idea of dimensionality reduction has been exploited by mathematicians, scientists and engineers from various scientific backgrounds, e.g. *Taylor Series Expansion, Nodal (Polynomial) Expansion Methods, Principal Component Analysis, rank of matrix operator, information capacity in communication, principal component analysis in statistics, etc.*
- **Challenge:** How to choose the 'optimum subspace'

$$\left(\vec{\phi}(x_j) = \sum_{i=1}^{r} a_i \vec{\psi}_i(x_j) \right)_{j=1}^{n} \in \mathbb{R}^n$$

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

$$\delta y(\varpi) = \int \boxed{\vartheta(\varpi, t)} \, \delta x(t) \, dt$$

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

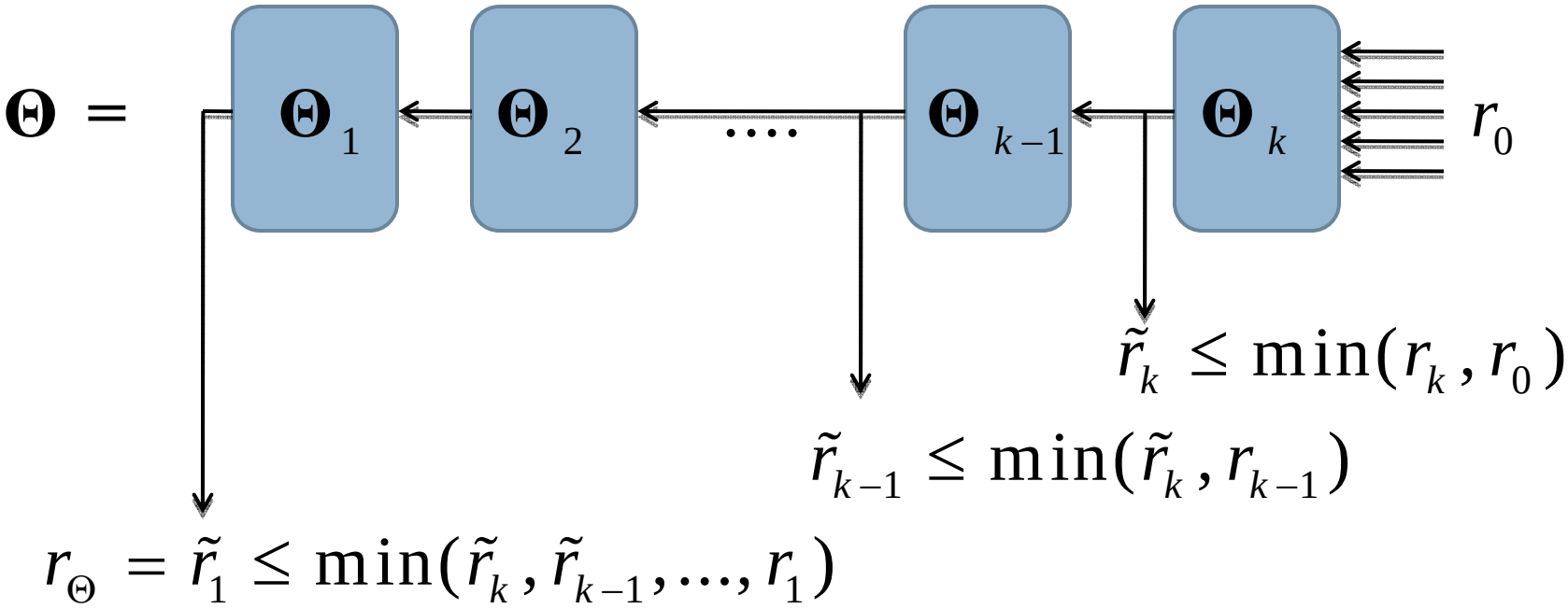
$$\vartheta(\varpi, t) = \sum_{i=1}^{\infty} \mu_i u_i(\varpi) \upsilon_i(t)$$

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 for Chained Codes

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



Active DOFs in Complex Modeling

- Small active DOFs implies high degrees of correlations among input data and output responses.
- Many modeling strategies of complex systems rely on concept of multi-level homogenization, where series of models varying in complexity (high resolution vs. low resolution models) are linked to model system macroscopic behavior starting from very detailed microscopic level. At each modeling stage, a certain reduction in problem dimensionality is achieved.

Uncertainty Management for BWR:

Based on PhDs of Abdel-Khalik and Jessee

Phase 1: Methodology Development

- Quantification of uncertainties at various stages of calculations
- Sensitivity study for importance ranking of indentified sources of uncertainties
- Virtual adaption: simulate core measured responses, i.e. adapt one core simulator code to match predictions of another version of the same code, or an entirely different code
- Ability to check robustness of developed methods by knowing exactly sources of calculations errors (modeling, data, etc.)
- Adaption at few-group, multi-group, and basic input data level

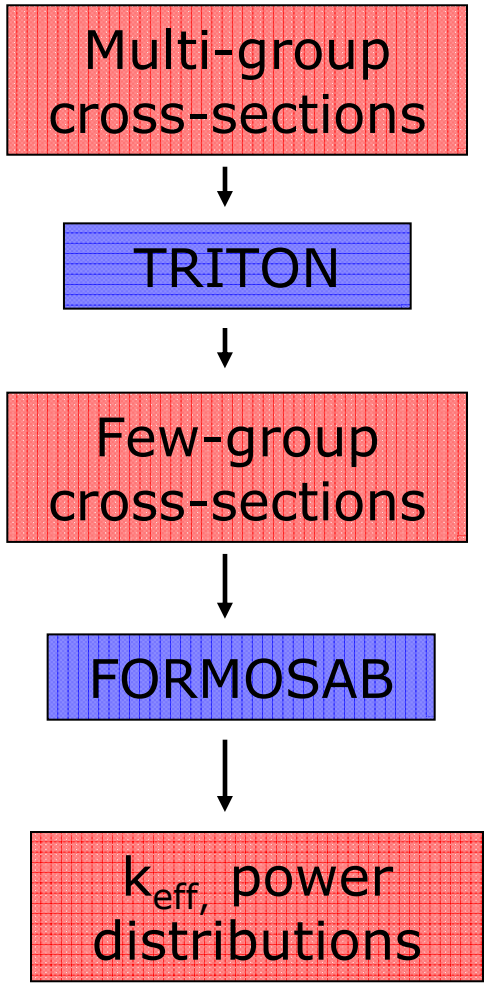
Phase 2: Application to Real Plant Data

- A fuel vendor's supplied core follow data, start-up physics measurements, in-core instrumentations models will be used as basis for cross-section adaption

BWR Case Study:

Based on work of Dr. Matthew Jessee

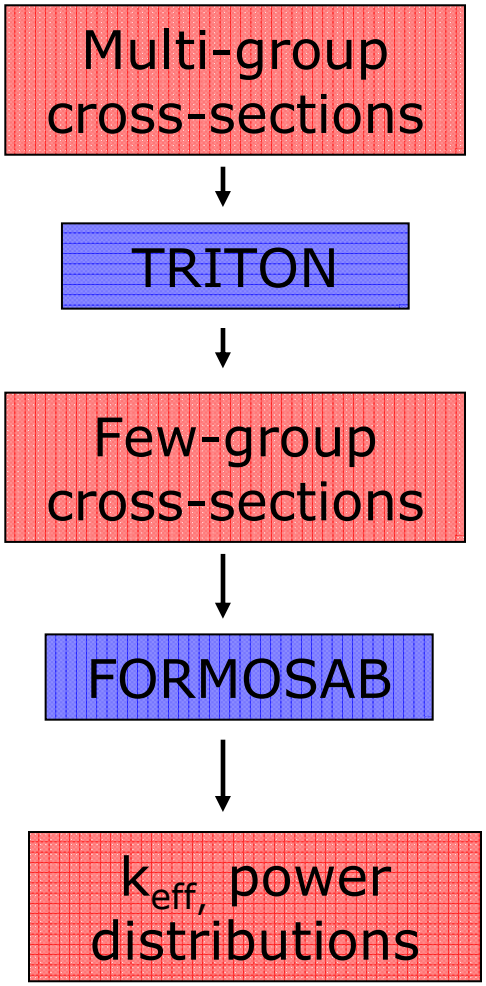
- **AMPX** – ORNL ENDF Processing Code System
  - Processes ENDF covariance data into 44 group energy structure
  - SCALE5.0 libraries (PUFF3)
    1. **44GROUPV5COV** - 29 isotopes including H, B, Al, U, Pu, and Minor Actinides et al.
    2. **44GROUPANLCOV** - 30 additional isotopes including Gd, Sm,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



BWR Case Study

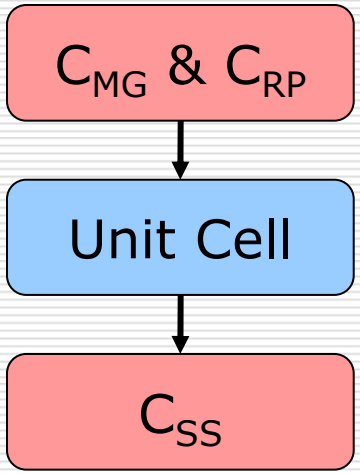
- **Few-Group Cross Sections –** lattice-averaged few-group cross-section functionalized for various fuel colors, void fractions, and branch cases

- **FORMOSAB –** NCSU's core simulator
  - GE BWR/3 reload core design
  - Cycle Exposure ~16 GWD/MTU
  - Number of FAs = 560



Uncertainty Propagation (Part 1)

GOAL: propagate infinitely-dilute MG cross-sections covariances and Resonance Parameter covariances to a self-shielded MG covariance matrix

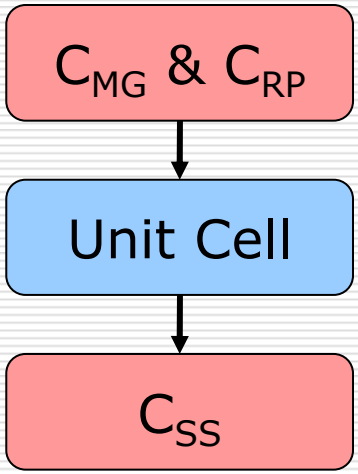


- Provided covariance data:
  - 44-group cross-section covariance matrices for infinitely-dilute cross-sections (44GROUPV6REC library from ORNL)
  - Majority of High fidelity covariance data generated from ENDFBV6 data files
  - Low fidelity covariance data processed from tabulated covariance data in Atlas of Resonance Parameters (Mughabghab)
  - Resonance Parameter Uncertainties for U-235, U-238, Pu-239, Pu-240, Pu-242, Am-241, and Gd Isotopes
  - Resonance Parameter covariance data in multiple formats (SLBW,Reich-Moore) from multiple libraries (ENDFB5V5,V6,V7)
  - Covariance data is used to construct a **relative** covariance matrix
  - Using **relative** covariance data, differences in formats and libraries are assumed negligible

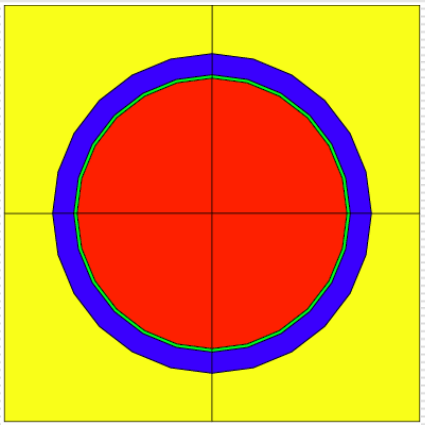
Uncertainty Propagation (Part 1) (cont.)

- Unit Cell Calculation:
  - Bondarenko factor treatment (unresolved resonance energy range) (BONAMI code)
  - Nordheim Integral Treatment (resolved resonance energy range (NITAWL code)
  - Limited to SLBW or MLBW resonances
  - Cannot treat resonance interference effects
  - Self-shielded MG cross-sections are calculated as:

$$\overline{\sigma}_{SS} = \overline{\sigma}_{ID} + \overline{\Delta}$$



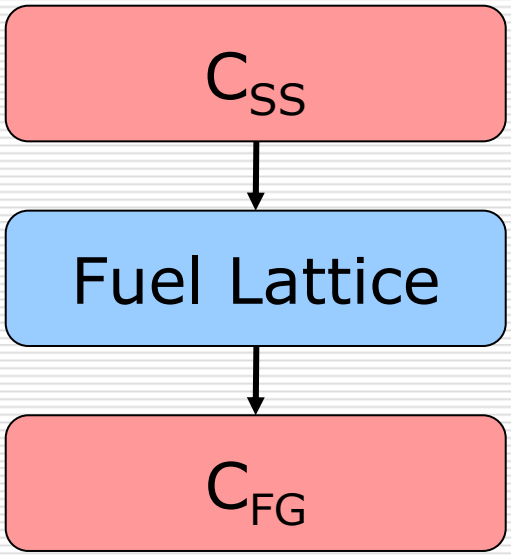
- The correction factor (Δ) is strongly dependent on:
  - Resonance Parameter
  - Number Density of the Resonance Absorber
  - Fuel Temperature
  - Background Moderating Power in the fuel region
  - Dancoff factor

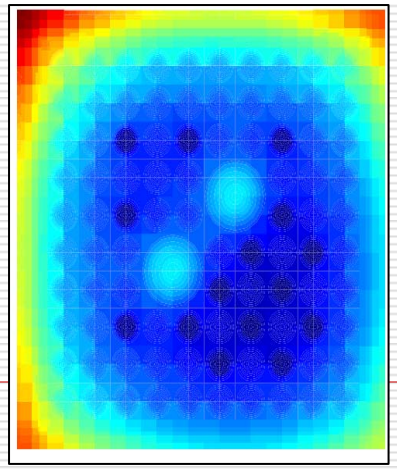


Uncertainty Propagation (Part 2)

GOAL: Calculate few-group cross-section covariance matrix from self-sheilded cross-section covariance matrix

- 2000 singular vectors of C_{SS} –> too many lattice physics calculations
- 1500 singular vectors were discarded based on a sensitivity analysis of lattice k-infinity and power peaking factor at BOL and EOL
- **The remaining 500 singular vectors are used to adjust the Δ's for adaptive simulation**
- 10 Lattice designs used to compute FG cross-section covariance data for all possible pin-by-pin enrichment distributions

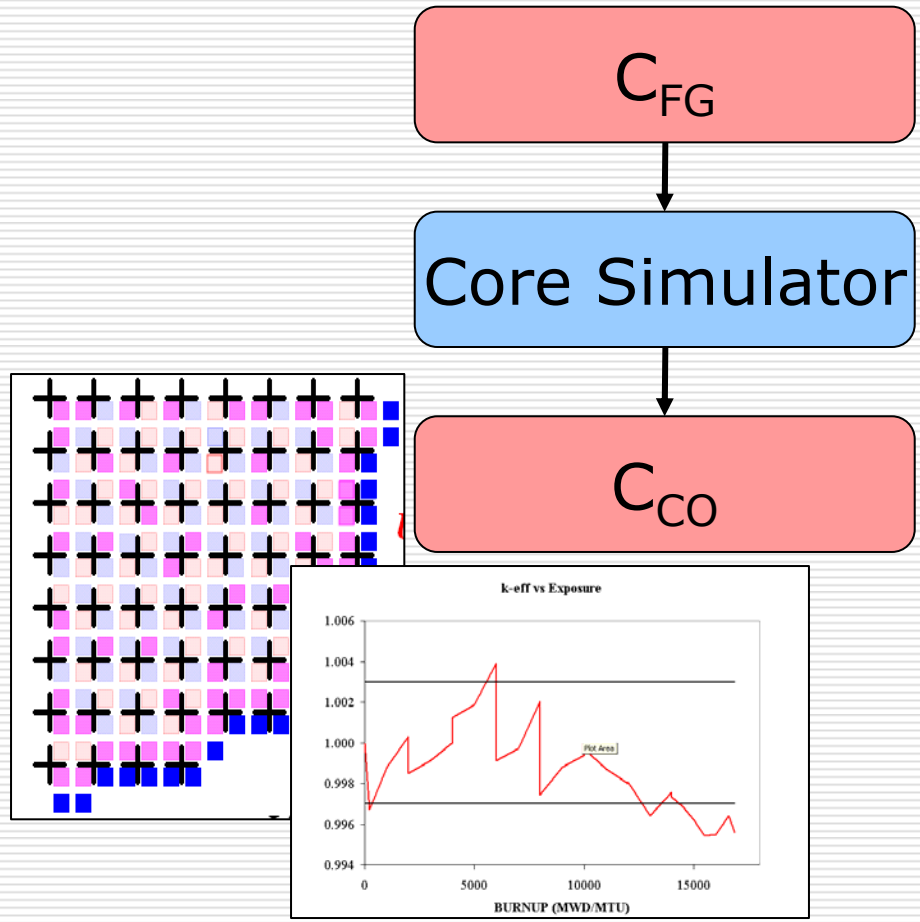




Uncertainty Propagation (Part 3)

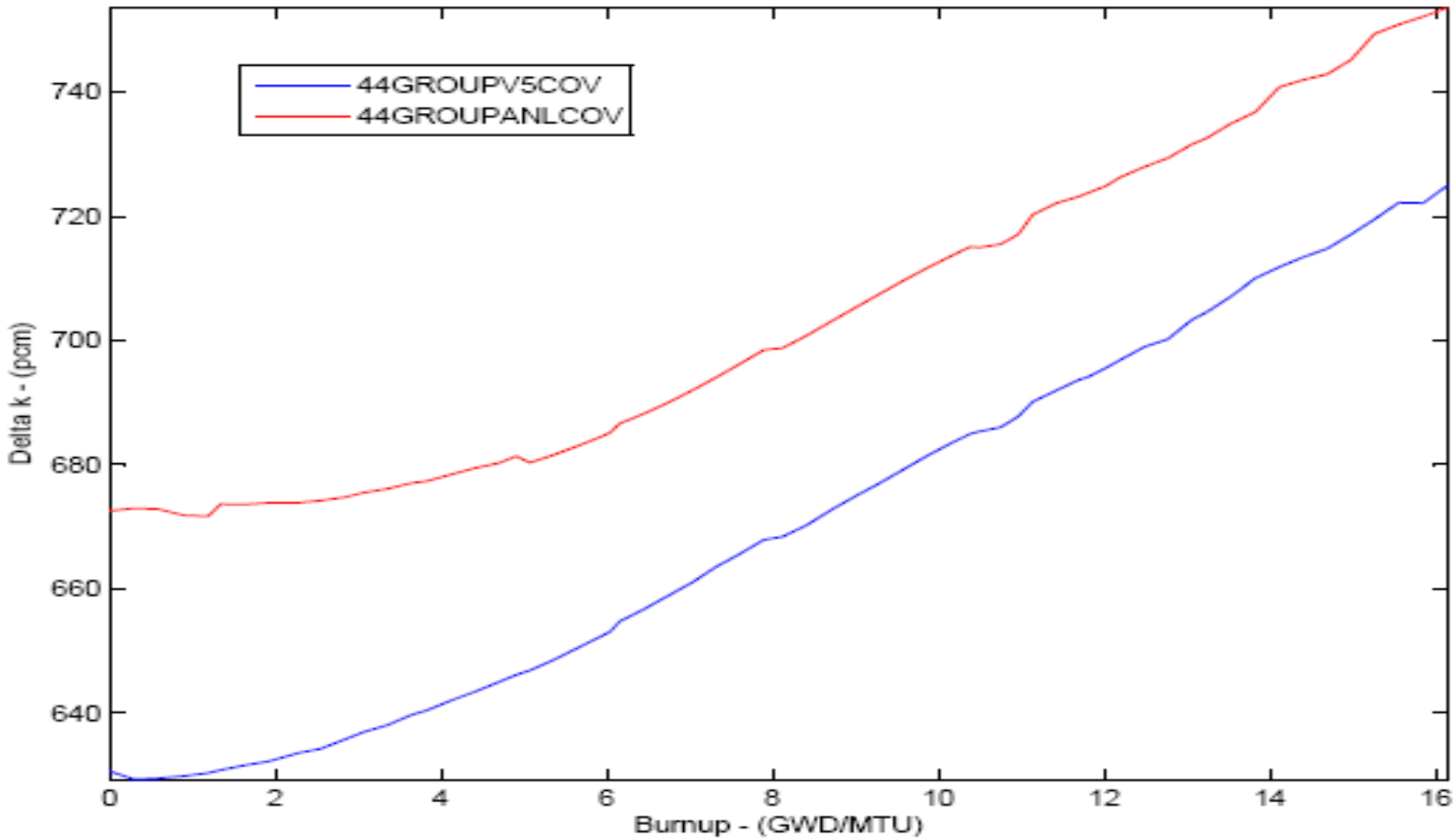
GOAL: Calculate core-observables covariance matrix from few-group cross-section covariance matrix

- rank of C_{FG} is 350
- Calculate C_{CO} using matrix-free approach
  - 350 core simulator calculations
  - ~5 min / FORMOSA-B run

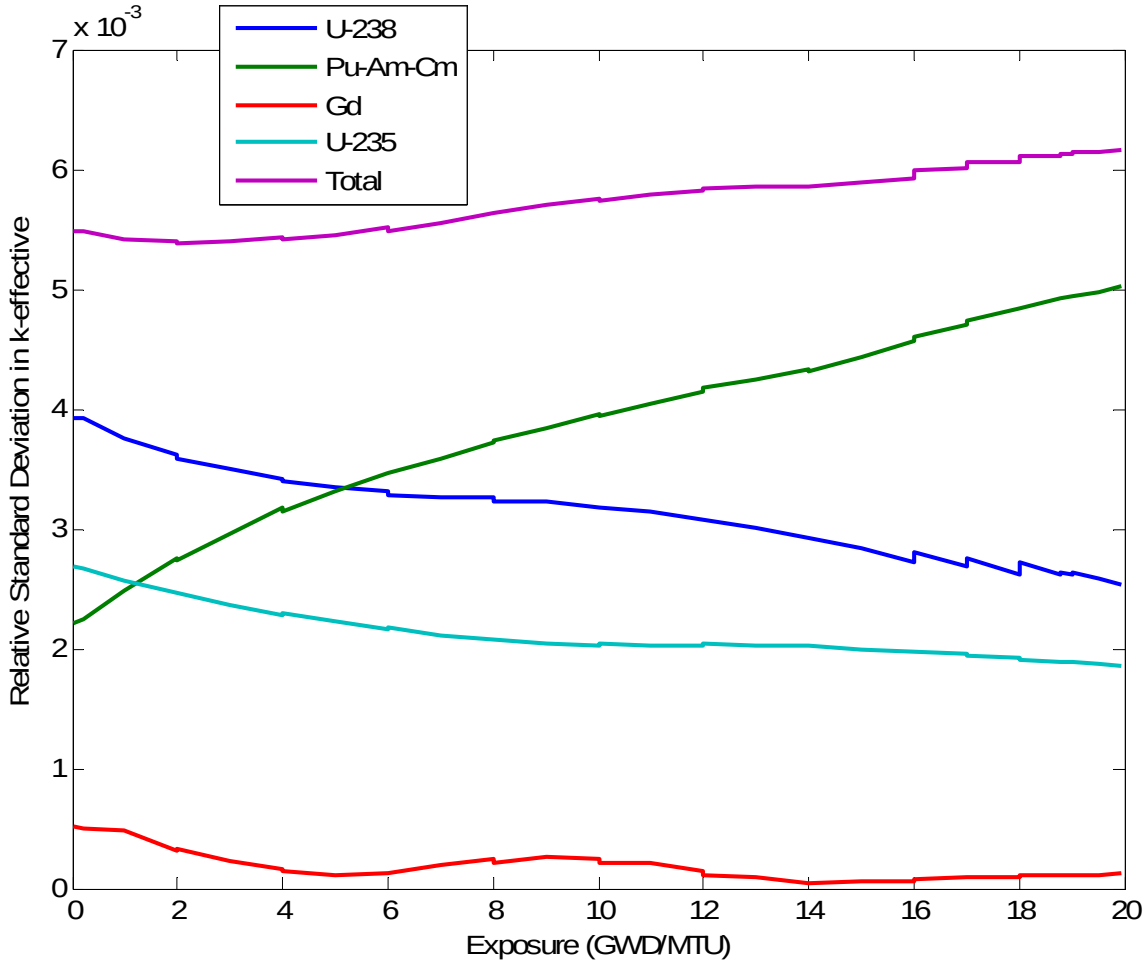


Propagated BWR Attributes Uncertainties

Core k_{eff} Uncertainty

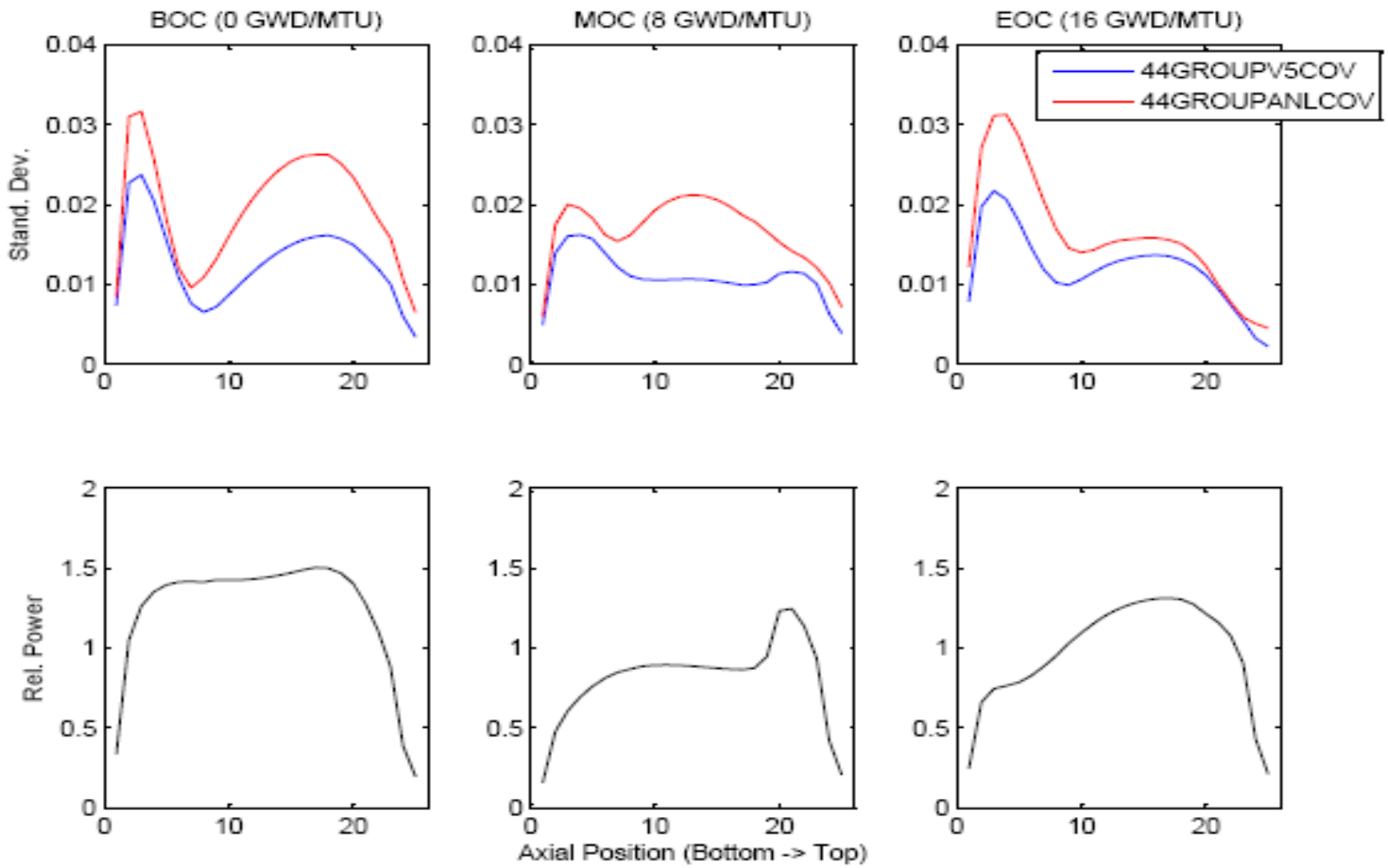


Core k-eff uncertainty

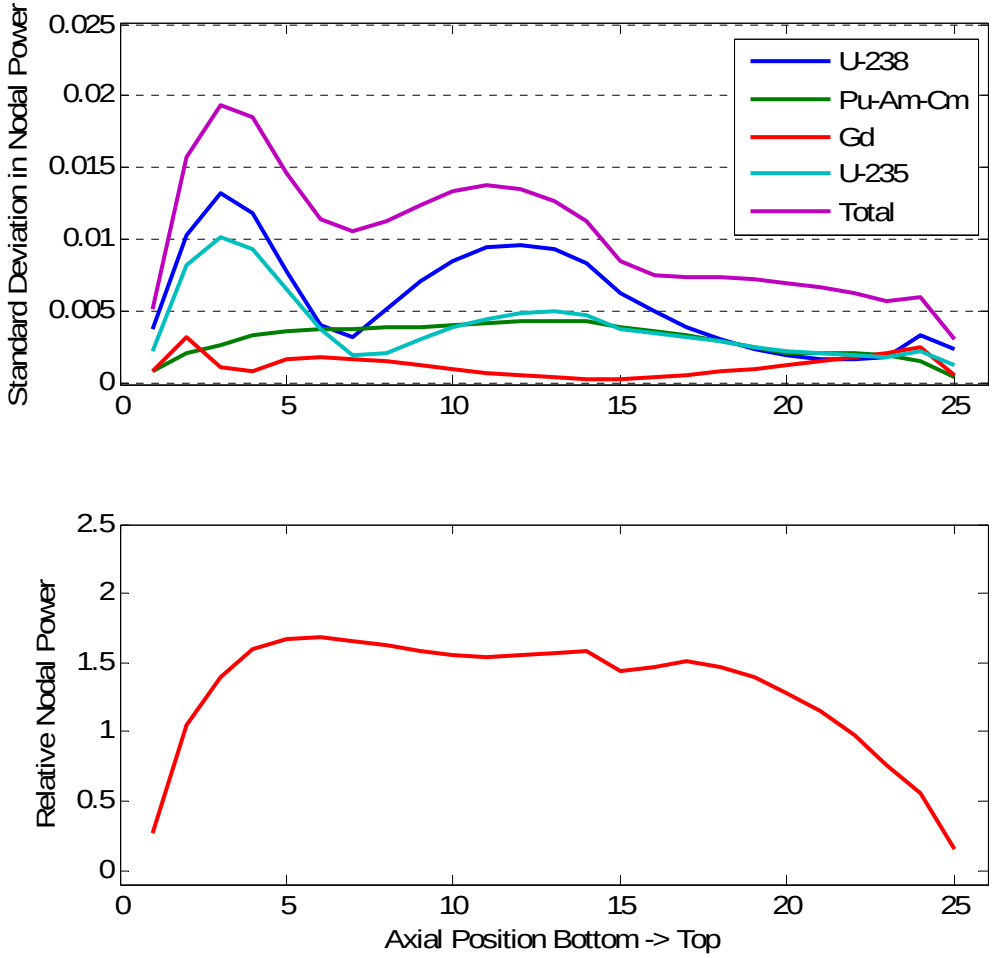


Propagated BWR Attributes Uncertainties

Nodal Power Uncertainty

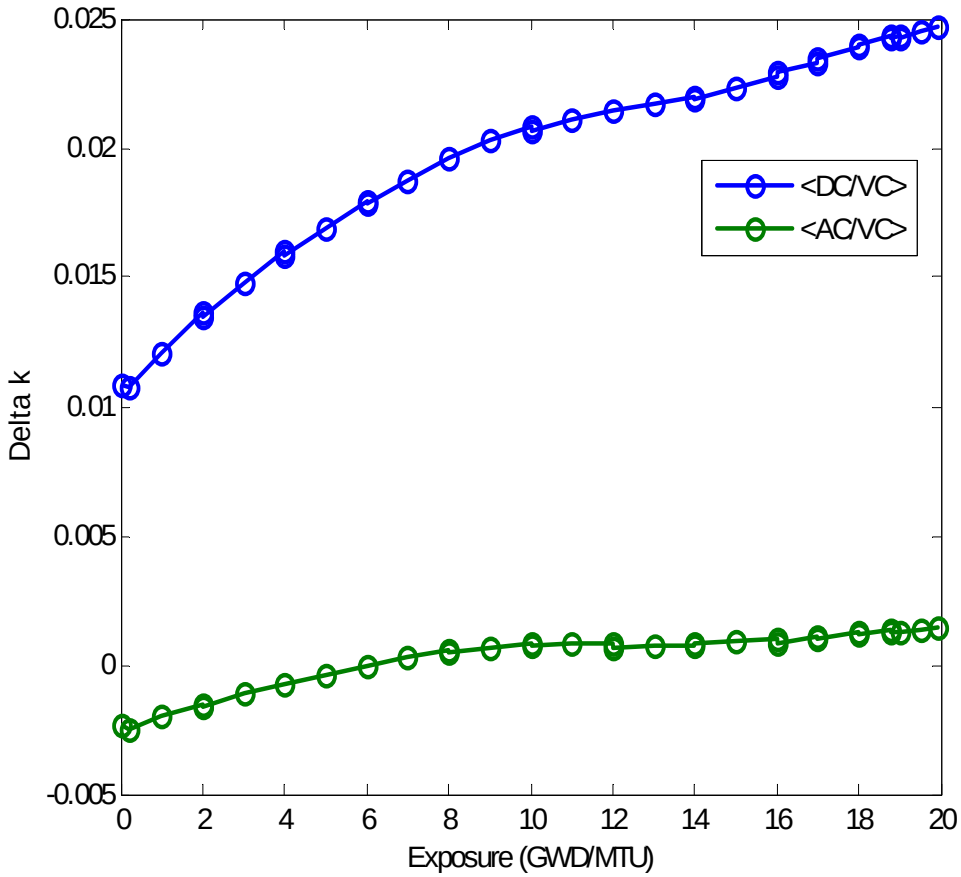


Core Nodal Power Uncertainty

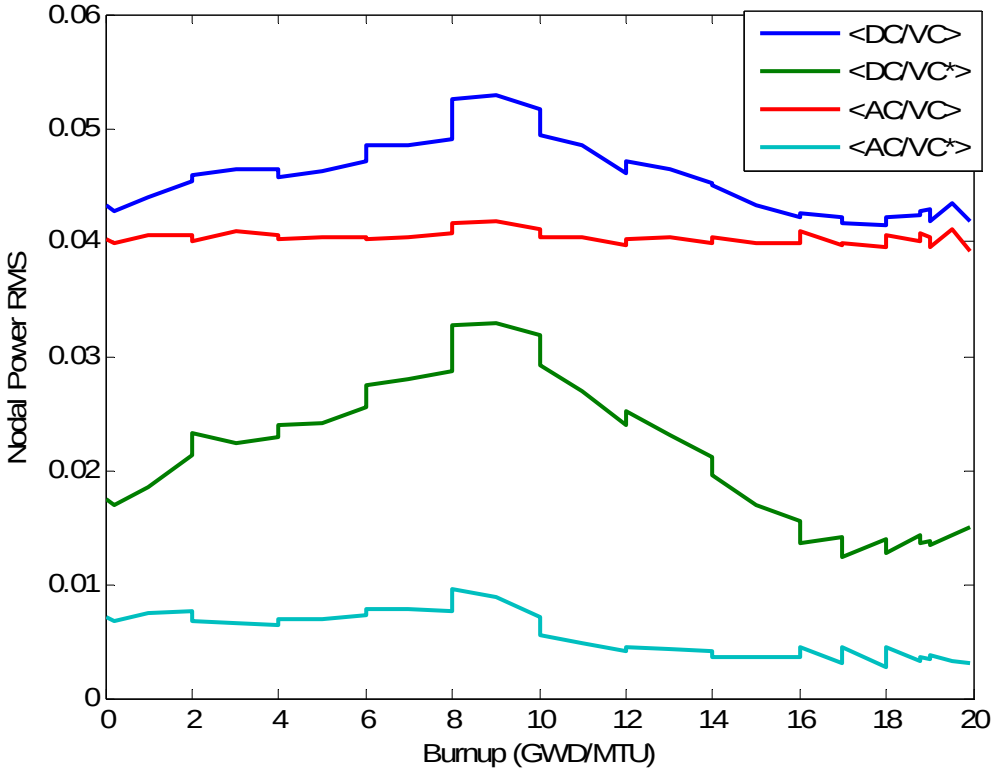


BOC Uncertainty Profile

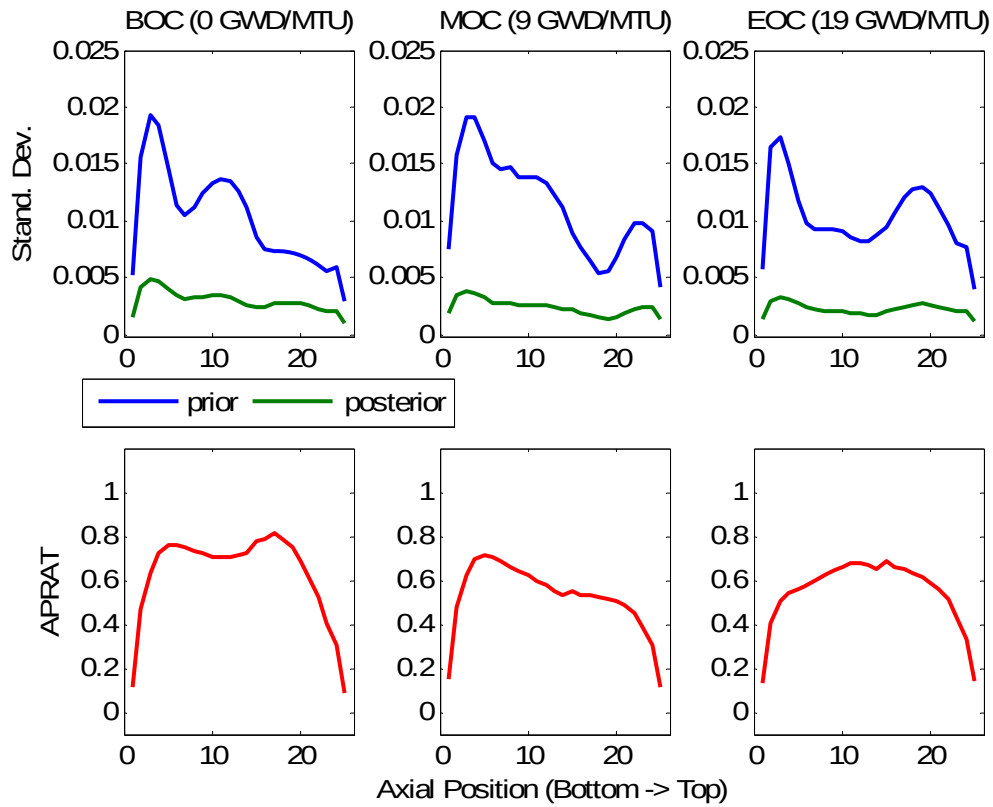
Adaptive Core Simulation



Adaptive Core Simulation

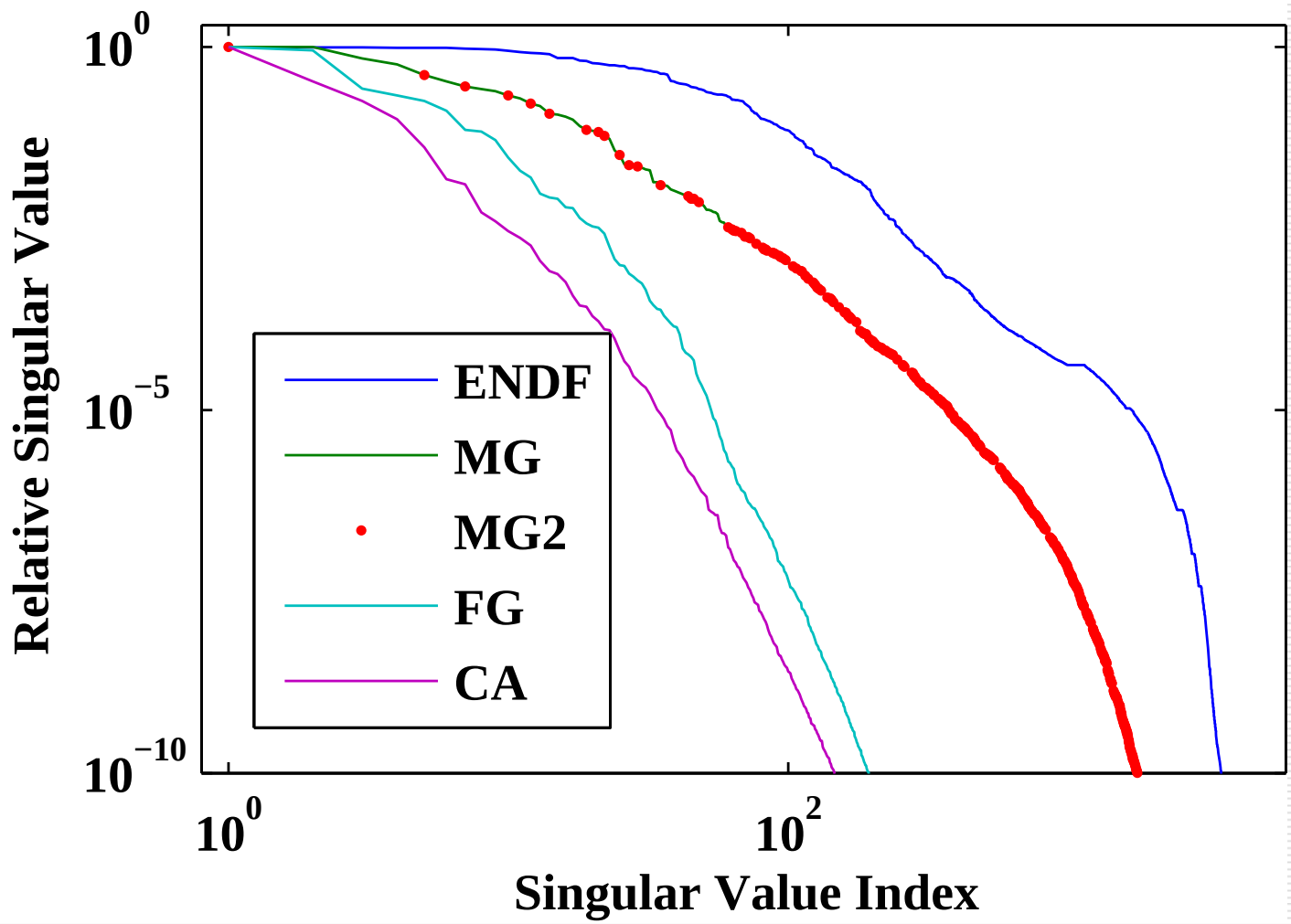


Adaptive Core Simulation



APRAT: Average Linear Power Density Ratio

BWR: I/O Streams SVDs



Conclusions

- Can do:
  - Linear model with many inputs and few outputs (adjoint)
  - Linear model with many outputs and few inputs (forward)
  - Nonlinear and bifurcated models with few inputs (higher order statistical sampling techniques)
  - Linear model with many inputs and many outputs (ESM)
- Trying to do:
  - Nonlinear models with few inputs coupled with linear model with many inputs/outputs (Extension of ESM)
  - Application to Monte Carlo models
- Cannot do yet:
  - Nonlinear/bifurcated models with many inputs
  - Understand interaction between numerical/modeling errors and input data errors