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Stochastic Finite Element Approaches in Nuclear Reactor Applications

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ICCOPT-MOPTA 2007

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NOTE: Figures, not authored by the presenter, from various public domain web sites were used in this presentation.

Outline

1. New initiative in Nuclear Research and Development: GNEP to “close” the nuclear fuel cycle.
2. Economics of and coupled physical phenomena in nuclear reactors; sources of parameter uncertainty.
3. Stochastic Finite Element Methods (SFEM)
4. Application of SFEM to parametric optimization problems.
5. Numerical examples of SFEM application in one dimensional reactor models.

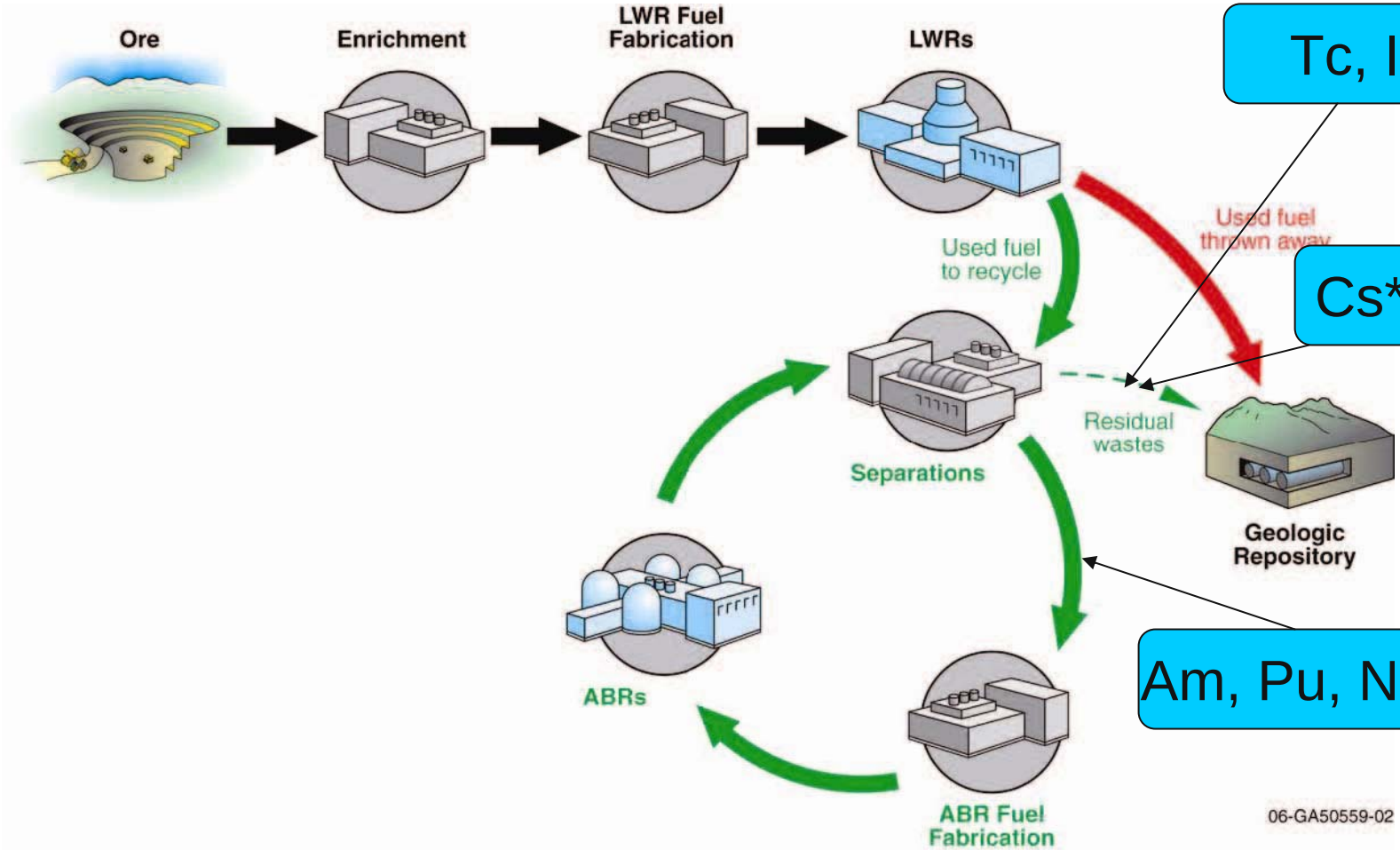
What is GNEP? Program Mission

- GNEP: Global Nuclear Energy Partnership
- A new Department of Energy initiative, started in 2006 with $250 million per year, and plans for increase.
- Use scientific computing (among other things) to “close the nuclear cycle”, reduce radioactivity of nuclear waste from nuclear reactors.

Sources: DOE GNEP fact sheet,

DOE GNEP implementation Plan (June 07)

The open-closed nuclear fuel cycle



Source: DOE ONE “Recycling spent nuclear fuel”

Separation-reprocessing for the closed fuel cycle

- The main candidate separation technology UREX+ (Uranium extraction plus- developed primarily at ANL).
- The current target site for geological storage (Yucca Mountain) is rated in terms of total radiation; closing fuel cycle may increase its effective capacity by 10,000%.

Source: DOE GNEP fact sheet

Computing goals for GNEP

- "The final goal will be optimization in the presence of modeling and input uncertainty in order to design safe, reliable, economical, and socially acceptable end-to-end solutions for nuclear energy production"—stochastic (robust?) optimization.
- Crosscutting technologies R&D needs identified
  - Multi-physics coupling
  - Optimization and confidence analysis
    - Considering higher order uncertainty analysis ("Nonlinearities can cause problems with first-order perturbation theory methods")
    - The sensitivity and uncertainty methods should be able to address 3D system designs, possibly with multi-physics coupling.

Major sources of uncertainty in the "normal" functioning closed fuel cycle

- In the reprocessing plant
  - The chemical composition and state of the waste.
  - Measurements.
  - Parameters associated with reactions in aequeous environments
- In nuclear reactor (LWR and ABR):
  - The composition of the fuel (it is well known at loading; but it is time-dependent, **contains the entire periodic table**, and cannot be directly tested for months or years, and even then not completely (for reprocessing calibration)).
  - The physical parameters governing neutron scattering and fission.

Source: GNEP development plan- June 07

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Design under uncertainty of nuclear reactors

- A huge, multiphysics, multiple time scales, complex systems stochastic optimization problem.
- The workhorse technique has been first-order sensitivity analysis with Gaussian pdf (Cacuci et al., 1981, 2005). Probably a precursor for many other fields – the favorite complex system example.
- It has been undertaken for more than 5 decades (even for ABR) … so is there something to still do here?
- To answer this, we look at the economics of nuclear power.

About our choice of justification

- A lot of the extra work solicited by GNEP is in safety of nuclear reactors (safe response to abnormal functioning) and not in maintaining safety margins under “normal” working assumptions.
- Most of the computational tools developed here are usable in answering safety questions in any case.
- We use economics since it is easier to convey to a multidisciplinary audience.
- We present US only because of the amount of data available to us. In many ways US nuclear R&D is not the leader (see recent IBM Global Center of Excellence for Nuclear Power announcement)

Nuclear Power Economics 101

- US Nuclear Business in FY06 sales: $64B
- Annual costs for a **new** 1000 MWe power plant
  - Total = $391M (4.9 cents/KWh)
  - Capital = $254M (3.2 cents/KWh)
  - O&M = $101M (1.27 cents/KWh)
  - Fuel = $36M (0.45 cents/ KWh)

Source: Paul Turinsky – MCSNA 07

Nuclear Power Economics 101.

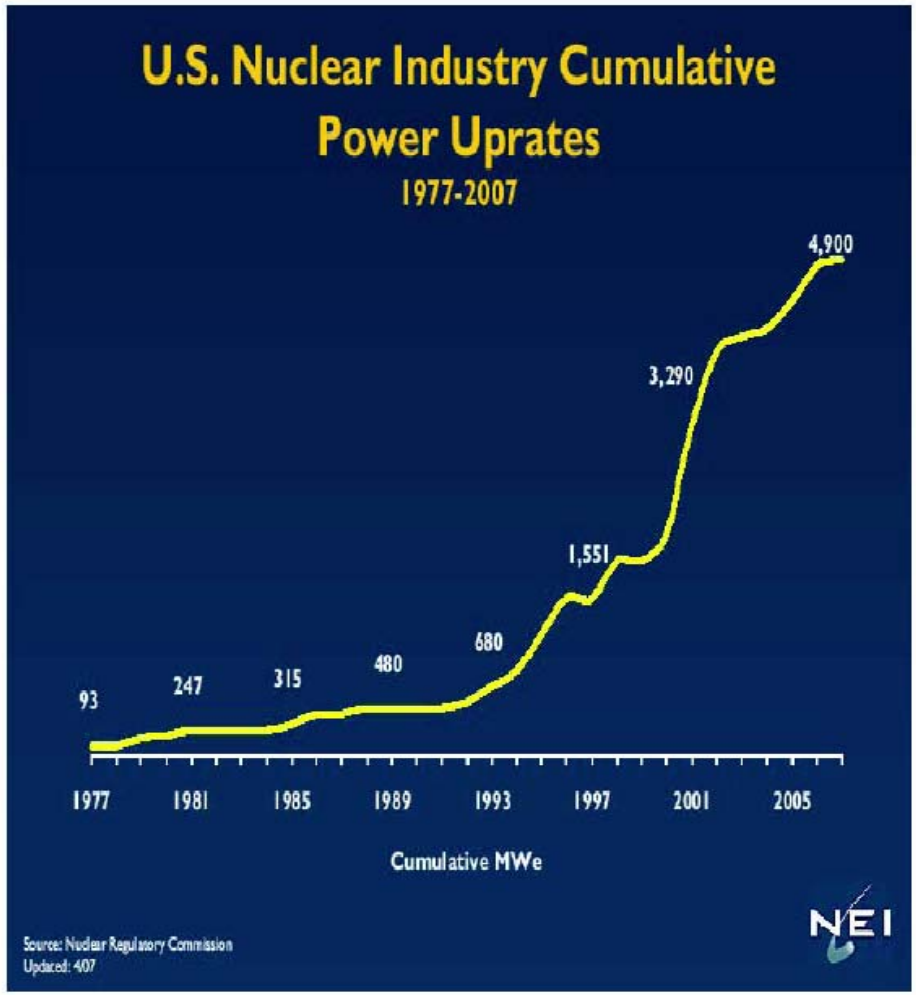
- Annual savings in bus-bar electrical energy cost for 1% power uprate of one 1000 MWe LWR (assuming annual capital and O&M costs fixed) = $3.55M/year
  - *OR*
- A 0.3% power uprate of one 1000 MWe LWR results in bus-bar electric energy cost savings of $1M/year

- Annual savings in bus-bar electrical energy cost for 1% reduction in fuel cost for one 1000 MWe LWR = $0.36M/year
  - *OR*
- A 2.8% reduction in fuel cost for one 1000 MWe LWR results in bus-bar electric energy cost savings of $1M/year

Source: Paul Turinsky – MCSNA 07

How are power uprates achieved?

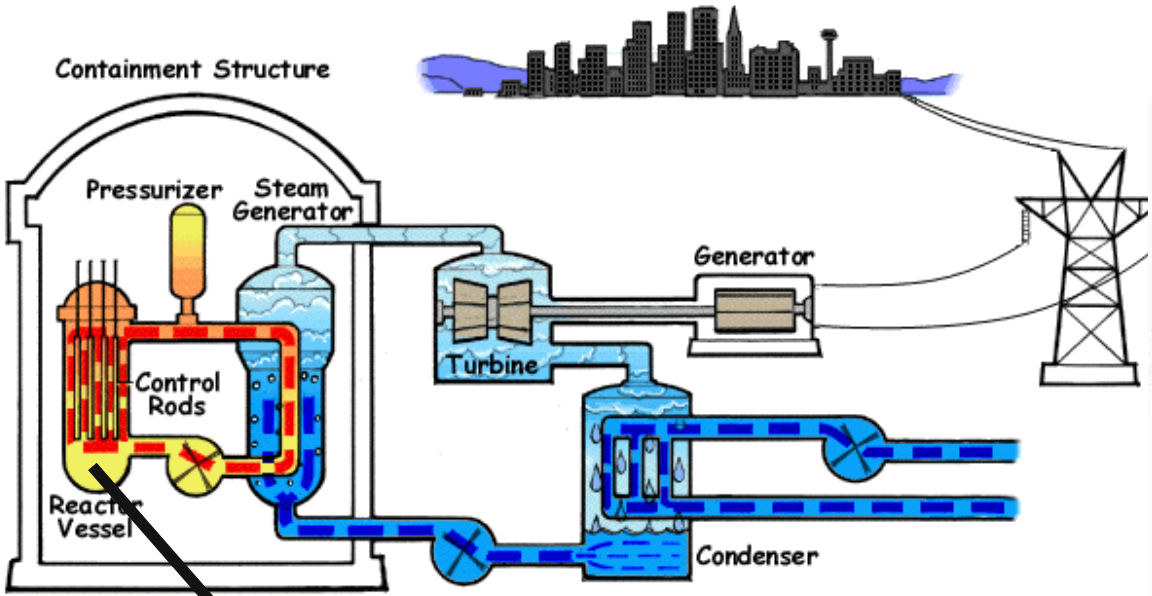
- Modification of nuclear fuel design to extract higher power with the same thermal margins. design margin,e.g. BWR 7x7 lattice => 10x10 lattice = 15-20% power uprates
- The power uprates in the last 3 decades amount to about 5 new reactors!



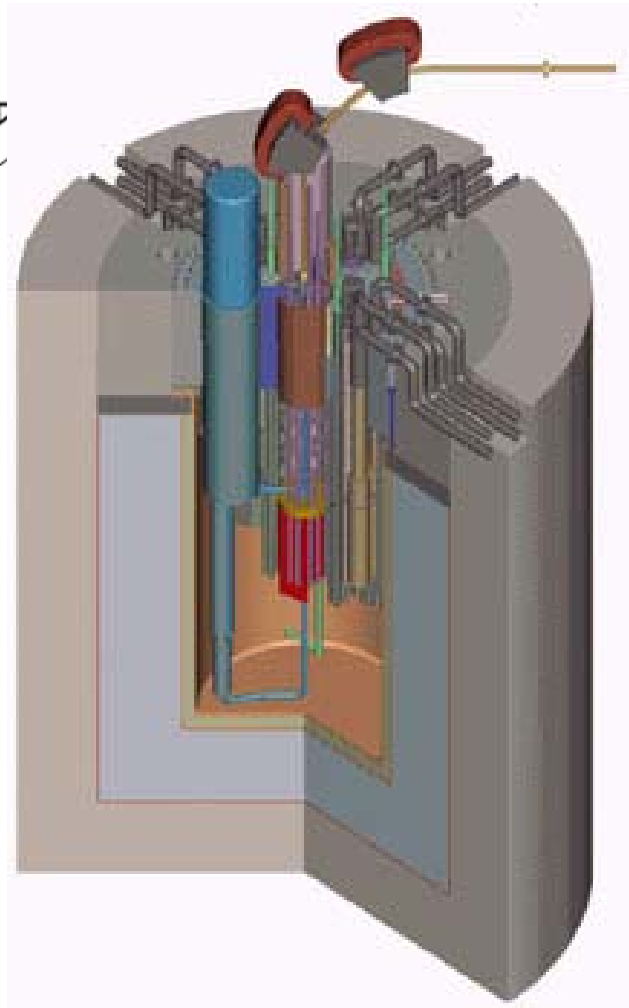
How can computing help for ensuring power uprates while maintaining safety margins?

- Due to limited computational power the design problem was decomposed in subcomponents, and conservative margins are imposed on intermediate criteria to satisfy the all-important, NRC-mandated safety margins.
- An “all-at-once” design will increase performance (and design complexity) while preserving the NRC safety margins.
- Reduction of uncertainty effects in simulator predictions of limiting nuclear plant attributes via
  - More accurate simulator models
  - More accurate physics input data
  - More rigorous treatment of uncertainties.
- But now we must take on increased model complexity, and in particular effects of uncertainties on nonlinear models

Nuclear Reactors

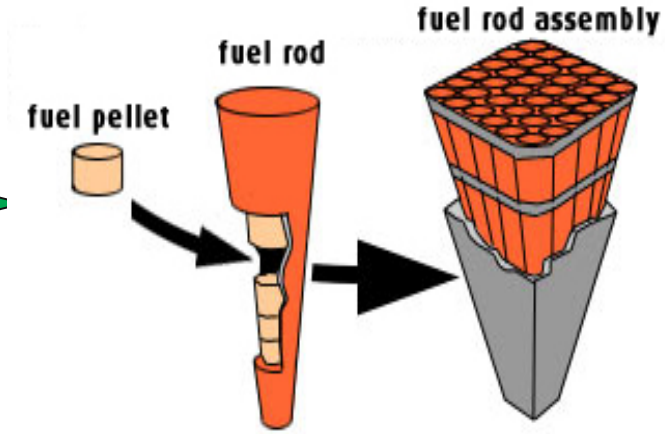


The largest modeling complexity by far: the core



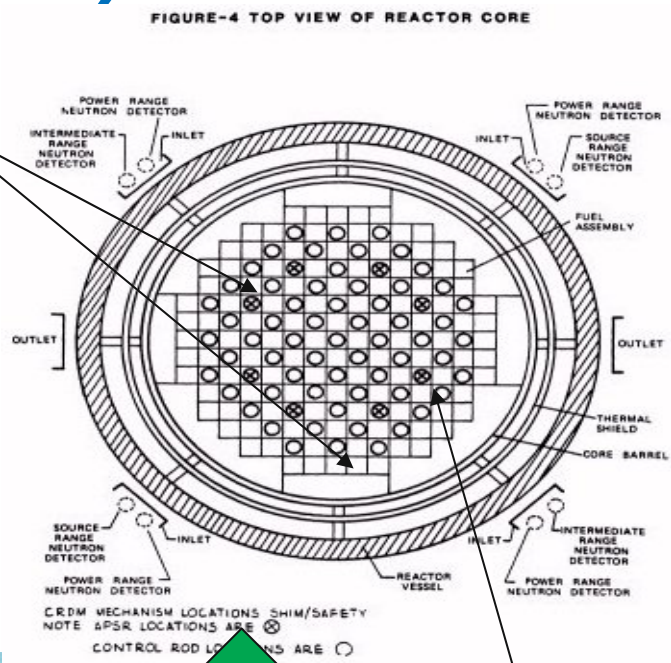
Physical Structure of the Nuclear Reactor Core of a PWR (I) the fuel assembly (bundle)

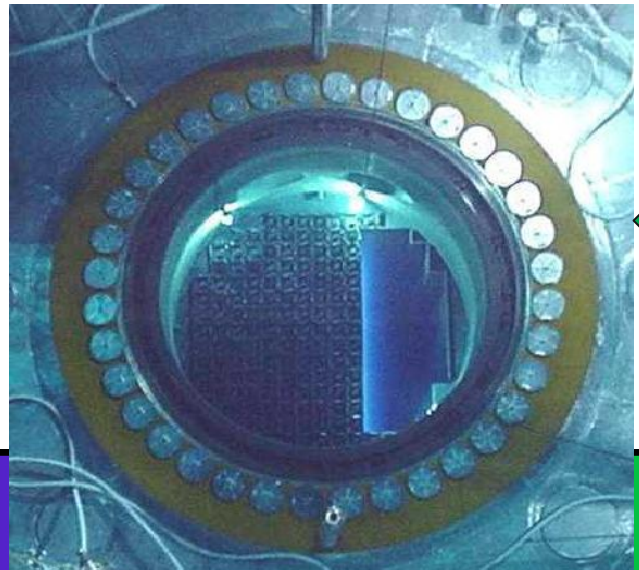
Energy : 3.5 barrels of oil, 17,000 cubic feet of natural gas, or 1,780 pounds of coal.



Physical Structure of the Nuclear Reactor Core of a PWR (II) the core (bundle)

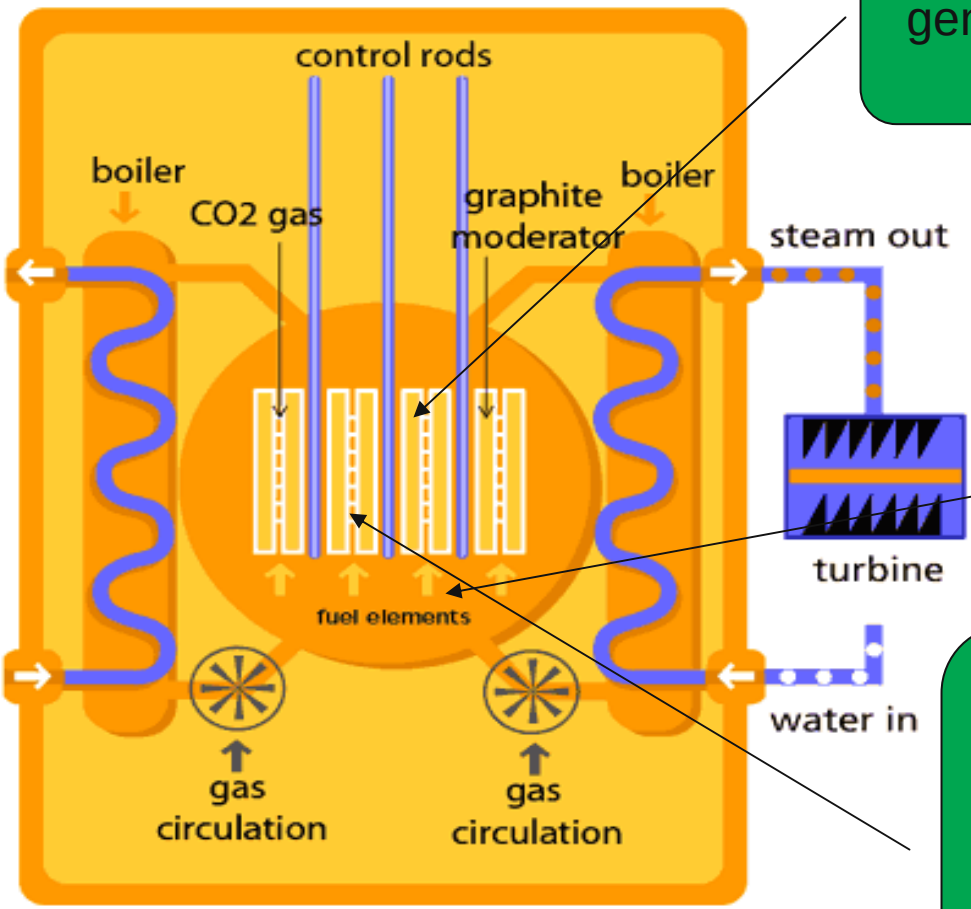
Fuel bundles





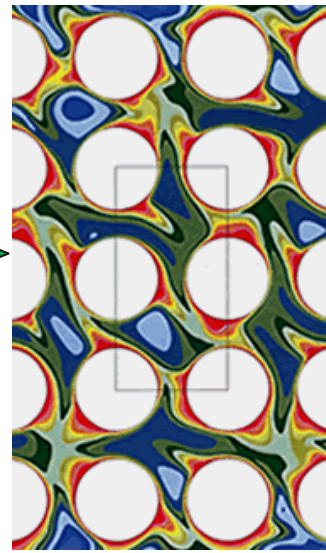
Control rods (o)

What is going on in a reactor core?



NEUTRONICS: Fission in fuel rods generates self-sustained, controlled neutron flux

THERMO-HYDRAULICS: Cooling agent (a fluid/ gas) extracts heat.



FUEL BEHAVIOR Nuclear reaction modifies the chemical composition of the fuel

The coupled multiphysics of nuclear reactors.

- Neutronics: Time scale: 10^(-21) s. 1 var 6 dimensions
- Thermohydraulics: Time scale 10^(-5s). 4 vars 3 dimensions.
- Fuel behavior: Time scales: 10^4 s. 100s of vars in 3 dimension.
- Most computationally intensive to date: Neutronics.

$$\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\hat{\Omega},E)+\Sigma_t(\vec{r},E)\psi(\vec{r},\hat{\Omega},E)$$
$$=\int\int\Sigma_s(\vec{r},\hat{\Omega}'\rightarrow\hat{\Omega},E'\rightarrow E)\psi(\vec{r},\hat{\Omega}',E')d\Omega'dE'$$
$$+\frac{1}{k}\chi(\vec{r},E)\int\int\nu(\vec{r},E')\Sigma_f(\vec{r},E')\psi(\vec{r},\hat{\Omega}',E')d\Omega'dE'$$

$$-\nabla\bullet D(E_i)\nabla\phi(r,E_i)+\Sigma_t\phi(r,E_i)$$
$$-\sum_{1=j\neq i}^{N_E}\Sigma^{E_j\rightarrow E_i}\phi(r,E_j)=\frac{\chi(E_i)}{K}\sum_{j=1}^{N_E}\nu(E_j)\Sigma_j^f\phi(r,E_j),$$

$$\rho C\left(\frac{dT}{dt}+u\bullet\nabla T\right)=\nabla\bullet\left(K\nabla T\right)+Q'''(r)$$

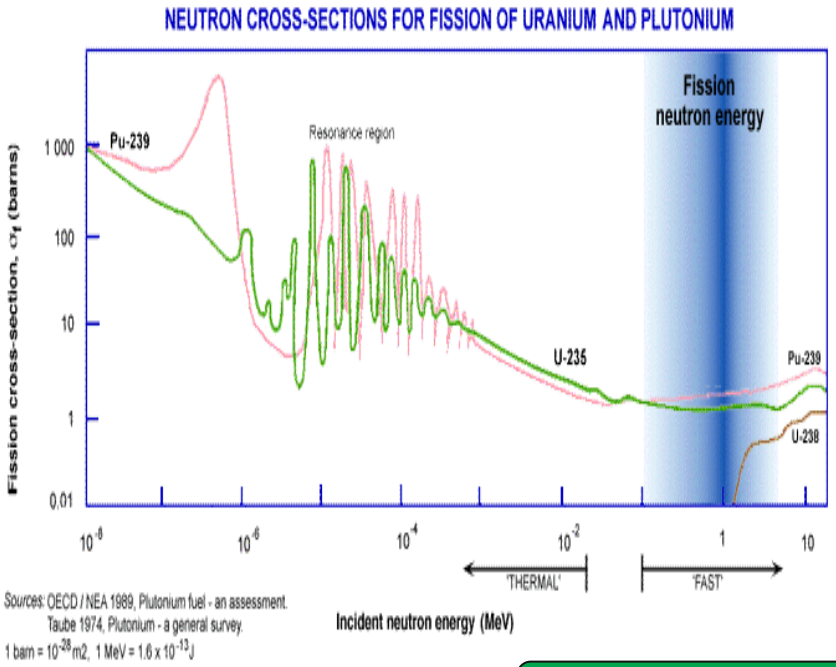
$$\frac{\partial u}{\partial t}+u\bullet\nabla u=-\frac{1}{\rho_c}\nabla p+\nu_c\nabla^2u,\nabla\bullet u=0$$

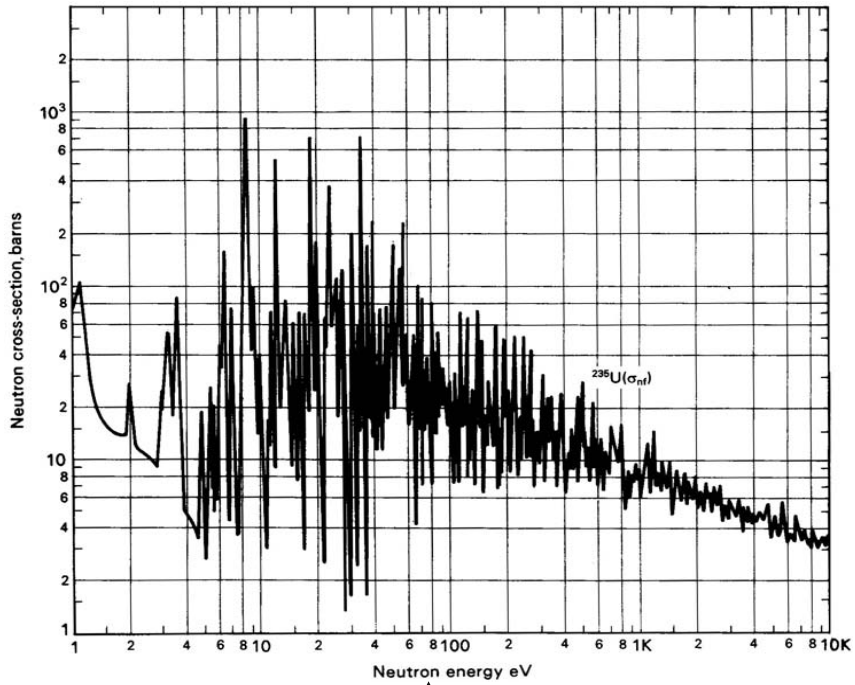
(Local) Isotopic depletion equations:

$$\frac{dN_A}{dt}=-\lambda_AN_A-\left[\sum_g\sigma_{a_g}^A\phi_g\right]N_A+\sum_{A'}\lambda^{A'\rightarrow A}N_{A'}+\sum_g\phi_g\sum_{A'}\sigma_{\gamma_g}^{A\rightarrow A'}N_A'$$

Can a 6-dimensional equation be so bad?...

- …Yes, because the 6th dimension is energy and the crossections (Σ) variations are astounding with respect to it.
- **We must accept (fairly large) uncertainty in the crossections !**





"inaccurately represented over 20ev"

Multiphysics-based design of nuclear reactors

- Must adress the parametric uncertainty.
- Of this, the most significant (by variation and number of parameters affected) is the error in the crossection since, even of the largest foreseeable architectures
  - We cannot resolve the resonancies (even tens of thousands of points will not do it for all elements in the spectrum).
  - We cannot resolve to sufficient resolution the time dependence of fuel composition, coupled with neutronics/thermo hydraulics by temperature
- We need *some form* of stochastic approach since
  - A pure error analysis approach is intractable, since even at small scales cross-section data is inaccurate.
  - We have decades of statistical data about crossections.
- We still must solve the coupled problem (eventually)

Now what?

- This will result in a huge stochastic optimization problem, unlikely to be solved in full generality in the foreseeable future.
- On the other hand we have access to a lot of high quality past research on how to construct reduced models for the physics.
- But “large uncertainty” calculations that go beyond linear perturbation have rarely been carried out, and this is one of the most promising and active conceptual areas.
- To carry out such calculations, we have started investigating stochastic finite element methods for use in nuclear reactor characterization – resulting in some interesting and challenging optimization problems.

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Uncertainty quantification (characterization?) of parametric equations

- Consider the parametric nonlinear equation

$$F(x,\omega) = 0, \quad x \in R^n,\ \omega \in \Omega \subset R^m,$$
$$F : R^n \times R^m \rightarrow R^n, \text{ a smooth function.}$$

- **Question:** How can I compute (or at least, efficiently approximate) the solution mapping $x(\omega)$ (and its distribution if ω has a PDF)?
- Sensitivity approach: Assume $F(x,\omega)$ is linear and ω Gaussian
- Monte Carlo answer:
  - Use parameter PDF and sample

$$\{\omega_i\},\ i = 1, 2, \ldots, M \Rightarrow \{\tilde{x}(\omega)_i = F^{-1}(0, \omega_i)\}$$

  - Followed by “histogram” or other post processing.
- Difficulties: Monte Carlo is slow and sensitivity approach is restrictive to relatively small uncertainty.

Discussion of Objectives

- **Can we derive an uncertainty characterization method that is more general than sensitivity and quicker than Monte Carlo?**
- There are several promising avenues (including combinations of them)
  - Randomized Quasi Monte Carlo?
  - Higher order sensitivity
  - Stochastic Finite Element
- In this work we investigate the promise of Stochastic Finite Element
- We concentrate on the parametric aspect alone (that is, approximating the mapping $x(\omega)$ and not its distribution (i.e. we look at the "hard" part, since with a good model, there is no need for further interaction with model)
- We discuss issues appearing in evaluating uncertainty in NR with respect to crossections and other parameters.
- Contributions: **Theoretical foundations for SFEM Galerkin approach and uncovered potential of collocation approach in nuclear reactor apps.**

Connection with other approaches.

- We truly have a problem of polynomial approximation – hardly new stuff.
- The “angle” here is that the mapping has large areas in which it is incredibly smooth, so it is worth investigating very high order approximations (e.g. order 30).
- The relation with (constrained) parametric optimization was never analyzed, to our knowledge.
- Clearly there is a relationship with other areas, (polynomial interpolation for derivative-free optimization, surface response methods) and we will investigate in the future the possibility of importing ideas and techniques.
- At the moment, we are interested in initial applications, attaching promising techniques to the appropriate type of problem and estimating how far it could take us.

Stochastic finite element in engineering application …

- 3-5 dimension fluid dynamics /reactive flow simulation (Ghanem and Najm, Gottlieb and Hesthaven).
- 50 dimensional PDEs with stochastic inputs (Liu and Hesthaven).
- 4 dimensions terrain uncertainty analysis for vehicle design (Sandu et al).
- Very active area of research, all the papers 2004-.
  - Google scholar “complementarity constraints” 252 (2004-)
  - Google scholar “stochastic finite element” 707 (2004-)

Stochastic Finite Element (SFEM) Notions and Notations

- The average operator

$$E_\omega[g(\omega)] = \int_\Omega W(\omega) g(\omega) d\omega. \text{ Here } W(\omega) \text{ may be PDF}$$

- The orthogonal polynomials

$$E_\omega \left[P_i(\omega) P_j(\omega) \right] = \delta_{ij}, \quad 0 \le i, j \le M_K$$
$$\omega = (\omega_1, \omega_2, \ldots, \omega_m),$$

- Typical multidimensional polynomial families are created by tensor products of Legendre, Laguerre, Chebyshev …
- The stochastic connection leads to the name of **polynomial chaos**
- Stochastic finite dimensional approximation space

$$\sum_{k=1}^{K} c_k P_k(\omega) = \tilde{x}(\omega) = \tilde{x}(\omega, \{c_k\}) \in \mathcal{V}_K$$

- **Note that PDF of outcome can be done now without using model!**

SFEM approximation procedures

- The model equation $F(x(\omega), \omega) = 0, \quad \omega \in \Omega$
- **The Galerkin (projection)** approach to approximate $x(\omega)$ enforces that the residual be orthogonal to the SFEM space $\mathcal{V}_K$

$$\left.\begin{array}{c} E_\omega \left[F(\tilde{x}(\omega, \{c_k\}) P_k(\omega) \right] = 0, \\ k = 1, 2, \ldots, K \end{array}\right\} \Rightarrow \{c_k\}_{k=1,2,\ldots,K}$$

- **The collocation approach (**which is a deterministic sampling, or response surface approach).
  - Choose sample points $\{\omega_i\} \; i = 1, 2, \ldots, K$ generally tensor product of “good” one-dimensional points (Chebyshev zeros, Gauss-Legendre nodes, etc..)
  - Compute the exact solution at these points $F(x(\omega_i), \omega_i) = 0$
  - Collocate the approximate solution at these points

$$\left.\begin{array}{c} \tilde{x}(\omega_i, \{c_k\}) = x(\omega_i), \\ k = 1, 2, \ldots, K \end{array}\right\} \Rightarrow \{c_k\}_{k=1,2,\ldots,K}$$

Comparison of the two approaches

- Galerkin:
  - Works even if the problem is discontinuous or nonsmooth.
  - Exponential convergence with increasing degree of polynomials if the problem is smooth, **BUT**
  - Needs to solve coupled nonlinear system of equations.
  - For complicated functions F, equations are hard to set up and need quadrature (since the averages cannot be exactly computed)
- Collocation:
  - The problems to be solved are decoupled
  - Easy to implement and setup, **BUT**
  - Its convergence properties are not understood for nonsmooth cases or incomplete tensor subset.

The weight function and scalar product

1. The weight function $W(\omega) : \mathbb{R}^m \to \mathbb{R}$ is nonnegative, that is, $W(\omega) \geq 0$, $\forall \omega \in \Omega$.

2. Any multivariable polynomial function $P(\omega)$ is integrable, that is,

$$\int_\Omega W(\omega)|P(\omega)|d\omega < \infty$$

Then, we define the scalar product and the norm

$$\langle g, h \rangle_W = \int_\Omega W(\omega) g(\omega)^T h(\omega) d\omega. \quad ||g||_W = \sqrt{\langle g, g \rangle}$$

where g, h are continuous functions from $\mathbb{R}^m$ to $\mathbb{R}^p$. Here $\Omega \in \mathbb{R}^m$ is an open set and $w(\omega)$ is a weight function.

Function Spaces

We define the square integrable space.

$$L^2_W[\mathbb{R}^m, \mathbb{R}^n] = \{f : \mathbb{R}^m \in \mathbb{R}^n | \, ||f||_W \leq \infty\}$$

We define the Sobolev space. $H^q_W[\mathbb{R}^m, \mathbb{R}^n]$ as the closure of $C^\infty[\mathbb{R}^m, \mathbb{R}^n]$ for the norm

$$||g||_{q,W} = \sum_{||i||_\infty \leq q} ||D^i g||_W$$

To point out stochastic connection, we use the notation

$$E_\omega[g(\omega)] = \int g(\omega) W(\omega) d\omega$$

Orthogonal polynomials

We can orthonormalize the set of polynomials in the variable ω and we obtain the orthogonal polynomials $P_i(\omega)$ that satisfy

- $\left\langle P_i, P_j \right\rangle = \delta_{ij}$, $0 \leq i, , j$. By convention, we always take P_0 to be the constant polynomial.
- The set $\{P_i\}_{i=0,1,2,\ldots}$ forms the basis of the complete space L^2_W.
- If $k_1 \leq k_2$, then deg $\left(P_{k_1}\right) \leq \left(P_{k_2}\right)$.

Example

For the case $m = 1$, $\Omega = [-1, 1]$, and $W(\omega) = \frac{1}{2}$, the orthonormal family are the normalized Legendre polynomial functions

$$P_k = \frac{1}{\sqrt{2}} \sqrt{\frac{2k+1}{2}} \frac{1}{2^k k!} \frac{d^k}{d\omega^k} \left(\omega^2 - 1\right)^k, \quad k = 1, 2, \ldots, K$$

Fourier Series

We can now define the Fourier coefficients as

$$c_k(f) = \langle f, P_k \rangle \in \mathbb{R}^p, \quad f \in L^2_W, \; k = 0, 1, \ldots$$

The projection operator: $f \in L^2_W$ on to the space of the polynomials of degree at most K

$$\Pi^W_K(f) = \sum_{k, \deg(P_k) \leq K} c_k(f) P_k(\omega)$$

All-important smoothness characterization

$$f \in H_W^q \Rightarrow \left\| f - \Pi_W^K(f) \right\|_W \leq C \frac{1}{K^{\epsilon q}} \tag{1}$$

When the function f is analytical q is unbounded and we obtain *exponential convergence*

In addition, a reciprocal also holds (Sobolev embedding), that is, there exists a parameter t such that, that depends only on $W(x)$ such that

$$\sum_{k \in \mathcal{N}} ||c_k(f)|| \deg(P_k)^t < \infty \Rightarrow f \in C^1(\Omega) \tag{2}$$

The exponential convergence leads to exponential convergence of the solution of (SO) to the solution of (O). in the W norm. The Sobolev embedding ensures that the solution is a strong solution: satisfies optimality condition for any ω.

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Galerkin approach for constrained optimization

$$(O) \qquad \min_{x \in R^n} f(x, \omega) \text{ subject to } g(x, \omega) = 0$$

$$(SO(K)) \qquad \begin{array}{ll} & \min_{c_1,\ldots,c_K} E_\omega \left[f(\tilde{x}(\omega, \{c_k\}), \omega) \right] \\ \text{subject to} & E_\omega [g(\tilde{x}(\omega, \{c_k\}), \omega) P_k(\omega)] = 0, \quad k = 1, 2, \ldots, M_K \end{array}$$

Optimization and approximation versus approximation and optimization.

- But wait, SFEM procedure recommends ...

$$\left.\begin{array}{rcl} \left\langle P_k(\omega)\left(\nabla_x f(\tilde{x}^K(\omega),\omega) + \right.\right. & & \\ \left.\left.\left(\tilde{\lambda}^K(\omega)\right)^T \nabla_x g(\tilde{x}^K(\omega),\omega)\right)\right\rangle & = & 0_n, \\ \left\langle P_k(\omega) g(\tilde{x}^K(\omega),\omega)\right\rangle & = & 0_p, \end{array}\right\} 0 \le k \le M_K.$$

Theorem If $\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{M_K}$ are a solution of (SO(K)) with multipliers $\hat{\lambda}_0, \hat{\lambda}_1, \ldots, \hat{\lambda}_{M_K}$. Then, $\hat{x}(\omega)$ and $\hat{\lambda}(\omega)$ satisfy the "SFEM equation ", if f and g have Lipschitz first derivatives.

$$\hat{x}^K(\omega) = \sum_{k=0,1,\ldots,M_K} \hat{x}_k P_k(\omega), \quad \hat{\lambda}^K(\omega) = \sum_{k=0,1,\ldots,M_K} \hat{\lambda}_k P_k(\omega).$$

- So we can find a Galerkin SFEM approximation of a parametric optimization problem as an optimization problem!

Is (SUO(K)) bounded below? Assumptions

A1 Uniformly bounded level sets assumption: There exist a function $\chi(\cdot)$ that is convex, nondecreasing, and that has bounded level sets, and a parameter $\gamma > 0$ such that

$$\chi\left(||x||^{\gamma}\right) \leq f(x,\omega), \quad ,\forall \omega \in \Omega. \qquad (1)$$

A2 Smoothness assumption: The function $f(x,\omega)$ is twice continuously differentiable in both arguments.

Result The objective function of the problem (SUO(K)) has bounded level sets.

Constraints

[A3] $\sigma_{\min}\left(\nabla_x g(\tilde{x}^*(\omega), \omega)\right) \geq \sigma_m, \forall \omega \in \Omega$.

[A4] The solution of the problem (O), $\tilde{x}^*(\omega)$ has Lipschitz continuous derivatives.

[A5] There exists $L > 0$ such that $||\nabla_x g(x_1, \omega) - \nabla_x g(x_2, \omega)|| \leq L\left(||x_1 - x_2||\right)$, $\forall x_1, x_2 \in \mathbb{R}^n$.

[A6] There exists a c such that $\left|\left|\left(\bar{J}^{K,Q}(\tilde{x}^*)\right)\right|\right| \leq c$, $\forall K, Q \in \mathbb{N}$.

[A7] $cC_G < \frac{1}{4}$. (small variation), where $C_G = \sup_{\omega \in \Omega} ||\nabla_x g(\tilde{x}^*(\omega), \omega)||$

Assumption Notations …

$$J_{ij}(\tilde{x}^K) = \left\langle \nabla_x g(\tilde{x}^k(\omega), \omega) P_i(\omega) P_j(\omega) \right\rangle \in \mathbb{R}^{p \times n},$$
$$i, , j = 0, 1, \ldots, K.$$

$$\bar{J}^{K,Q}(\tilde{x}) = \begin{bmatrix} \bar{J}_{0,K+1}(\tilde{x}) & \bar{J}_{0,K+2}(\tilde{x}) & \cdots & \bar{J}_{0,K+Q}(\tilde{x}) \\ \bar{J}_{1,K+1}(\tilde{x}) & \bar{J}_{1,K+2}(\tilde{x}) & \cdots & \bar{J}_{1,K+Q}(\tilde{x}) \\ \vdots & \vdots & \vdots & \vdots \\ \bar{J}_{K,K+1}(\tilde{x}) & \bar{J}_{K,K+2}(\tilde{x}) & \cdots & \bar{J}_{K,K+Q}(\tilde{x}) \end{bmatrix},$$

Inf-sup condition (smallest singular value)

The Jacobian at x^* of (SO(K)) defines the quadratic form.

$$G_2^K(\lambda, u) = \sum_{i,j=0}^{M_K} \lambda_i^T \left\langle P_i \nabla_x g(\tilde{x}^{*,K}(\omega), \omega) P_j \right\rangle u_j,$$

$$G^K = \inf_{\substack{\{\lambda_k \in \mathbb{R}^p\}_{k=0,1,\ldots,M_K} \\ \sum_{i=0}^{M_K} ||\lambda_k||^2 = 1}} \sup_{\substack{\{u_k \in \mathbb{R}^n\}_{k=0,1,\ldots,M_K} \\ \sum_{j=0}^{M_K} ||u_k||^2 = 1}} G_2^K(\lambda, u).$$

Lemma Define $\Gamma^K = A_0 - A_1 \left\| \tilde{x}^* - \tilde{x}^{*,K} \right\|_\infty - A_2 \left\| \tilde{x}^* - \tilde{x}^{*,K} \right\|_\infty^2$, where $A_0 = 1 - 4c^2 C_G^2$, $A_1 = 8c^2 C_G L$, $A_2 = 4c^2 L^2 + 2\frac{L^2}{\sigma_m^2}$. Then, if $\Gamma^K > 0$, it follows that $c\sigma_m < 1$ and

$$G^K \geq \sqrt{\frac{4\Gamma^K}{\frac{1}{\sigma_m^2} - c^2}}.$$

Convergence results

After quite a few technicalities, Kantorovich's theorem for non-square systems applies (need it since $\Pi_W^K(x^*)$ may not be feasible) to give.

Theorem Assume that $\tilde{x}^*(\omega)$ is smooth (infinitely differentiable). Then there exists K_0 such that (SO(K)) has a solution, $\forall K \geq K_0$.

Result If, in addition, the solution produced by (SO(K)), $\tilde{x}^K(\omega)$ is sufficiently smooth (its Fourier coefficients drop to 0 sufficiently fast), than it has a convergent subsequence, and any such subsequence satisfies the optimality conditions of (O).

Outline

1. New initiative in Nuclear Research and Development: GNEP to “close” the nuclear fuel cycle.
2. Economics of and coupled physical phenomena in nuclear reactors; sources of parameter uncertainty.
3. Stochastic Finite Element Methods (SFEM)
4. Application of SFEM to parametric optimization problems.
5. Numerical examples of SFEM application in one dimensional reactor models.

Optimization-Galerkin formulation of symmetric eigenvalue problems (one-group)

$$\left.\begin{array}{ll}\min & x^T Q(\omega) x \\ \text{s.t.} & x^T x = 1\end{array}\right\} \Rightarrow \left\{\begin{array}{ll}\min_{x_i, i=1,2,\ldots,K} & E_\omega\left[\left(\sum_{i=0}^{K} x_i P_i(\omega)\right)^T \left(Q+\omega D_Q\right)\left(\sum_{i=0}^{K} x_i P_i(\omega)\right)\right] \\ \text{s.t.} & E_\omega\left[\left(\sum_{i=0}^{K} x_i P_i(\omega)\right)^T \left(\sum_{i=0}^{K} x_i P_i(\omega)\right) P_k(\omega)\right] = E_\omega\left[P_k(\omega)\right] \\ & k = 1, 2, \ldots, K\end{array}\right.$$

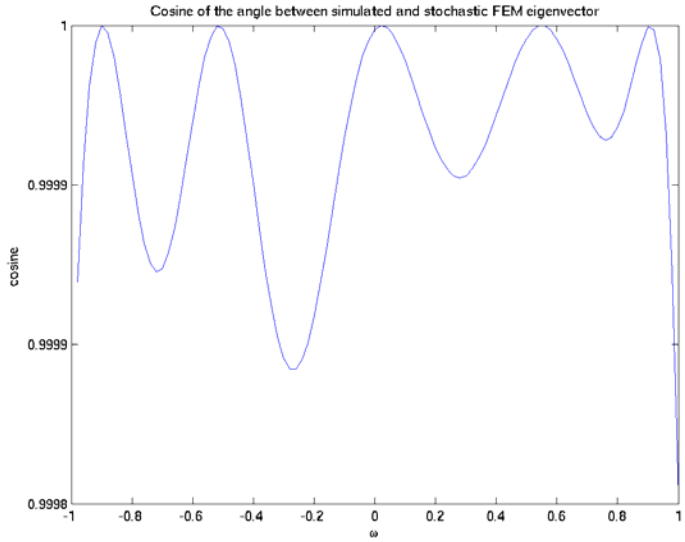
- Note that this problem can be *exactly* represented, even when multiple parameters are involved, modulo a series of quadratures, (if not, Galerkin is hard to formulate and may need quadrature)

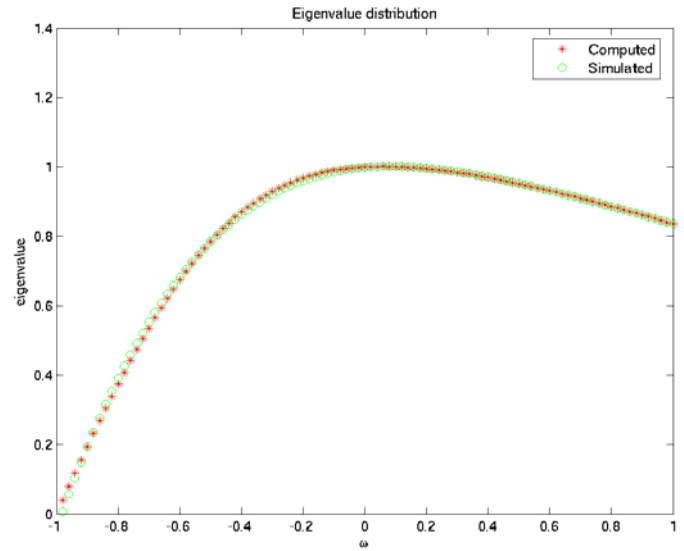
$$\begin{array}{ll}\min & \sum_{i=0}^{K} x_i^T Q x_i + \sum_{i=0}^{K}\sum_{j=0}^{K} x_i^T D_Q x_i E_\omega\left[P_i(\omega)(\omega) P_j(\omega)\right] \\ \text{s.t.} & \sum_{i=0}^{K}\sum_{j=0}^{K} x_i^T x_i E_\omega\left[P_i(\omega) P_k(\omega) P_j(\omega)\right] = E_\omega\left[P_k(\omega)\right] \quad k = 0,1,2,\ldots,K\end{array}$$

Numerical Example for n=2

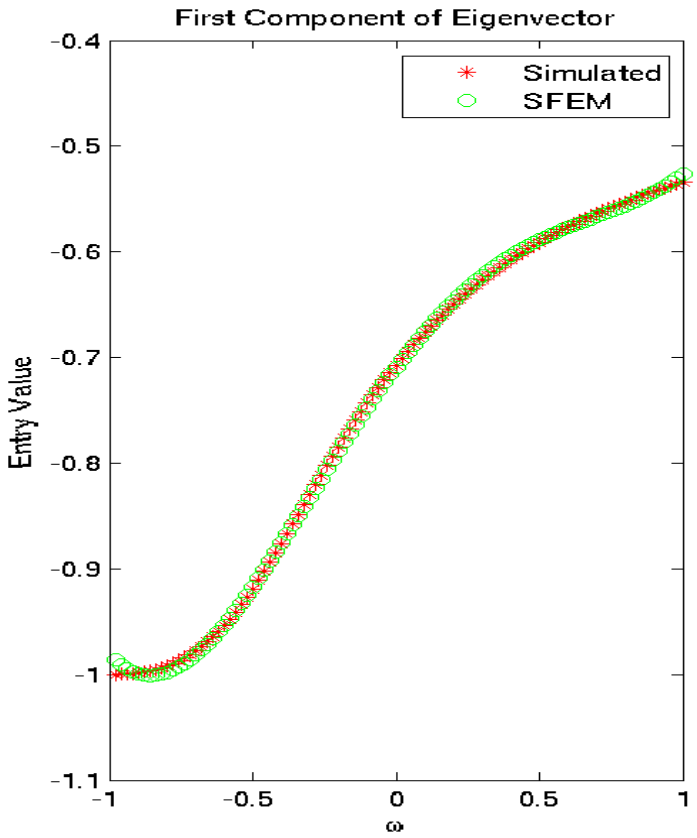
$$Q = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}; D_Q = \begin{bmatrix} 1 & 0.4 \\ 0.4 & 0.2 \end{bmatrix}$$

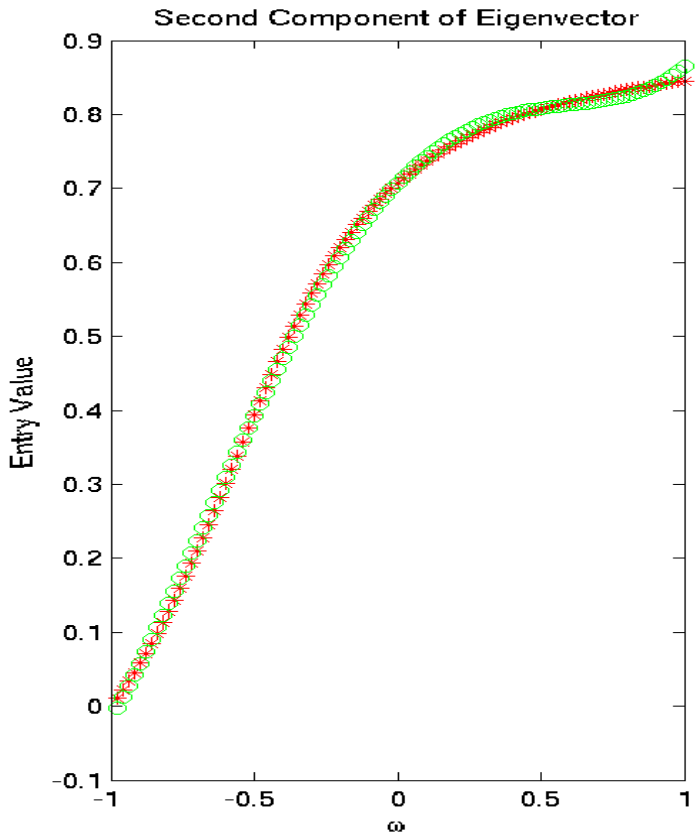
- Use Legendre polynomials with K=4.
- Note that the variations allowed are not small variations ! (though the matrix will stay positive definite).
- The error in the angle of the eigenvector is less than 1%.
- The eigenvalue distribution is excellent fit.





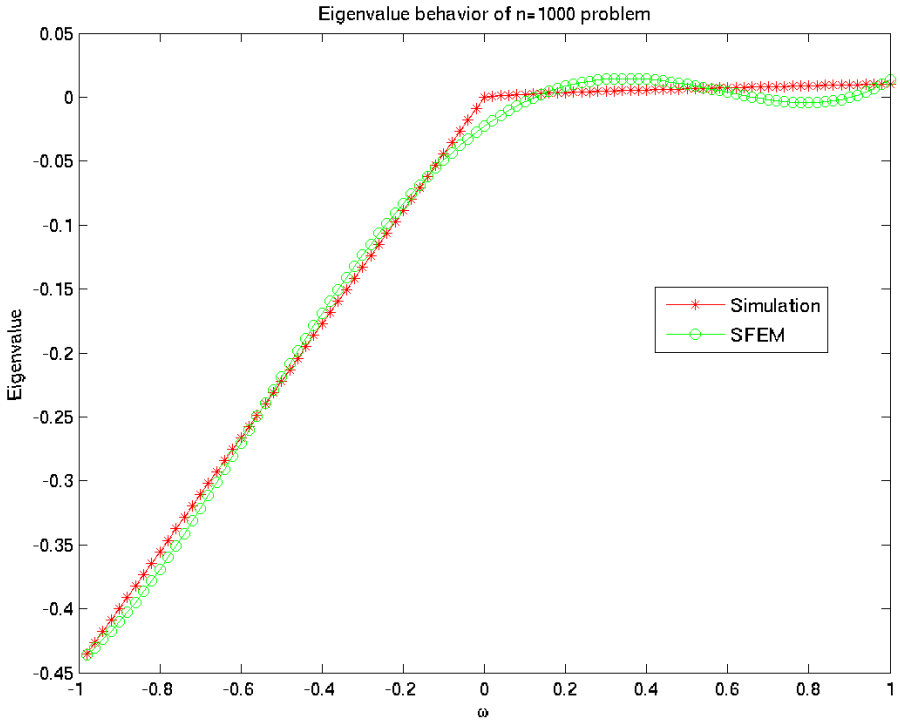
Example for n=2, eigenvector convergence





Galerkin Numerical Example for n=1000

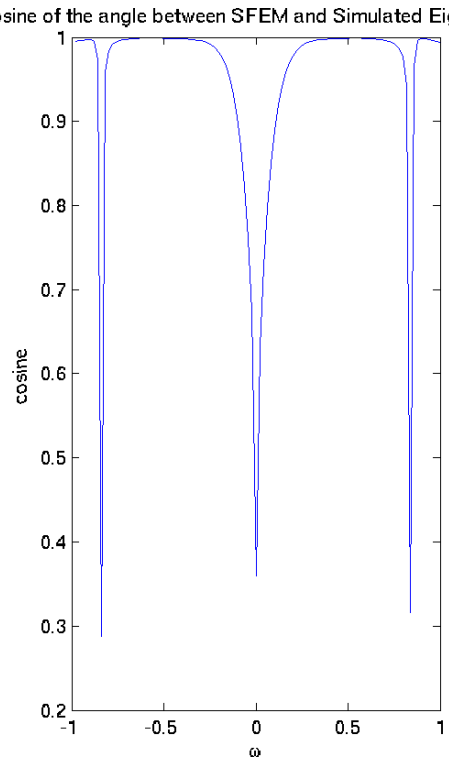
- Minimum eigenvalue problem for a one-dimensional diffusion equation, with uncertainty in absorption, a one dimensional neutronics problem.
- For K=4 The SCO formulation was solved in 7 seconds by KNITRO (one eig operation on same computer takes 13 seconds!)

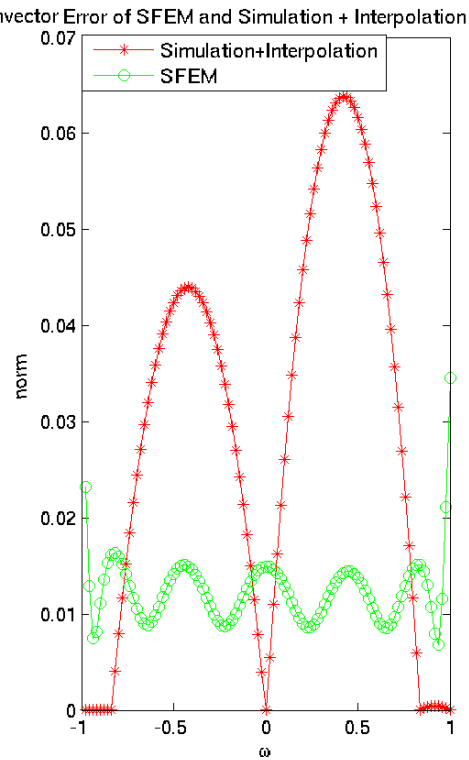


$$Q_{i,j}=\begin{cases}1 & i=j=1\\ 1 & i=j=n\\ -1 & |i-j|=1\\ 2 & 1<i=j<n\\ 0 & \text{otherwise}\end{cases},\quad D_{Qi,j}=\begin{cases}2\dfrac{i}{n}\dfrac{n-i}{n}\cos\left(\dfrac{i}{n}\right) & i=j\\ 0 & \text{otherwise}\end{cases}$$

Galerkin Numerical Example, eigenvector behavior

- At first sight, approximation is awful (left panel) but $\left\|\left(Q+\omega D_Q\right)\tilde{x}(\omega)-\tilde{\lambda}(\omega)\tilde{x}(\omega)\right\|$ has typical value of is 1%!
- The problem is the occasional degeneracy of the eigenvalue problem
- If we sample eigenvector at 5 (well-chosen ☺) points, and interpolate linearly, we get an error that is typically larger by a factor of 3-4.
- **This shows that black-box approaches (collocation, Monte Carlo,..), even enhanced with AD, may be sometimes unadvisable.**
- **Sensitivity approaches would not be applicable for such eigenvector uncertainty problems!**





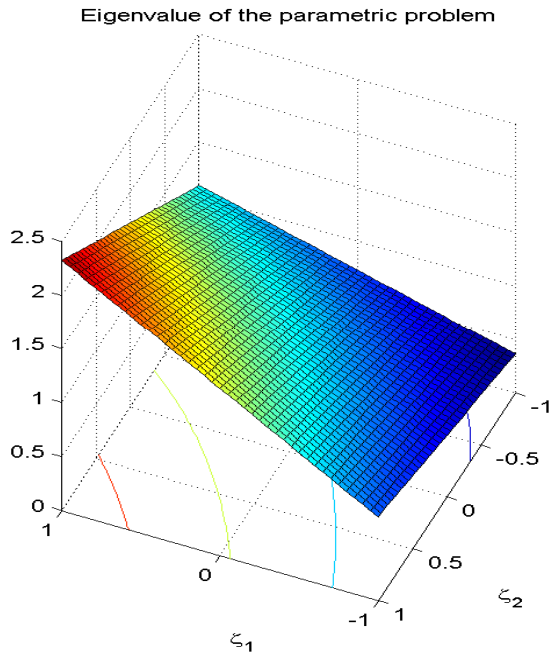
Galerkin formulation, generalized nonsymmetric eigenvalue problems for multigroup (diffusion and transport) models

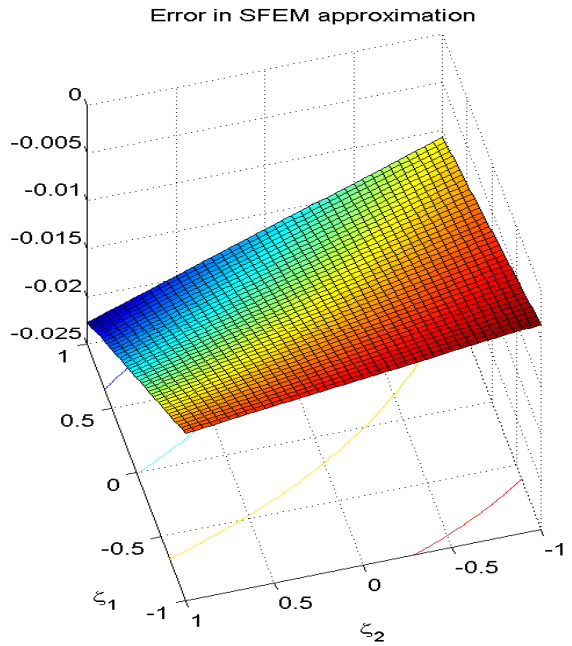
$$Q^1(\omega)x^1(\omega)+Q^2(\omega)x^2(\omega)=Q^3(\omega)x^3(\omega)$$
$$Q^5(\omega)x^2(\omega)=Q^4(\omega)x^1(\omega)$$
$$x^3(\omega)=\lambda(\omega)x^1(\omega)$$
$$x^1(\omega)^T\,x^1(\omega)=1$$

- Embed an optimization problem – allows us to use previous results and define a power-method-like iteration.

$$Q^1(\omega)x^1(\omega)+Q^2(\omega)x^2(\omega)=Q^3(\omega)x^3(\omega)$$
$$Q^5(\omega)x^2(\omega)=Q^4(\omega)x^1(\omega)$$
$$x^1(\omega)=\arg\min_{z,z(\omega)^T z(\omega)=1}\left(x^3(\omega)-z(\omega)\right)^T\left(x^3(\omega)-z(\omega)\right)$$

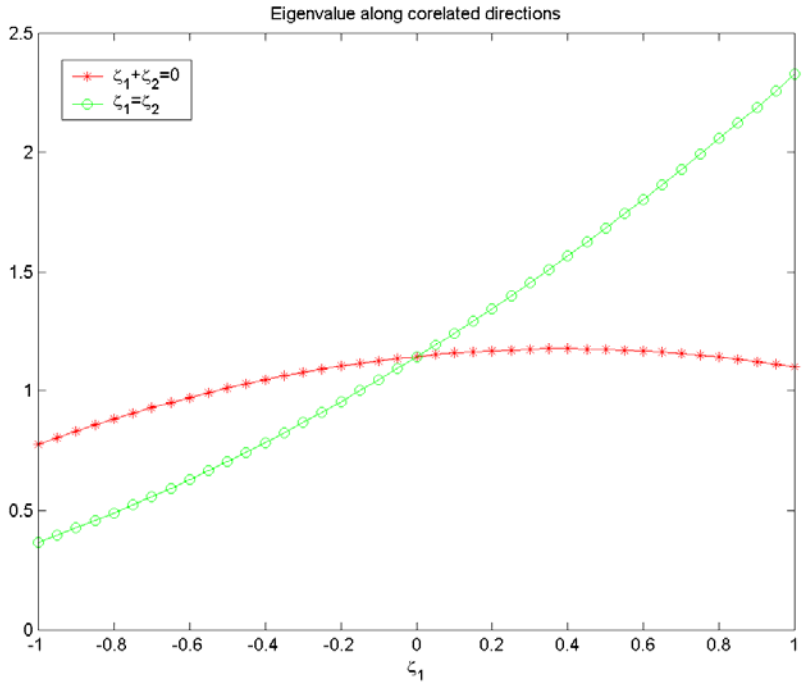
Results for keff for two-group 1D diffusion

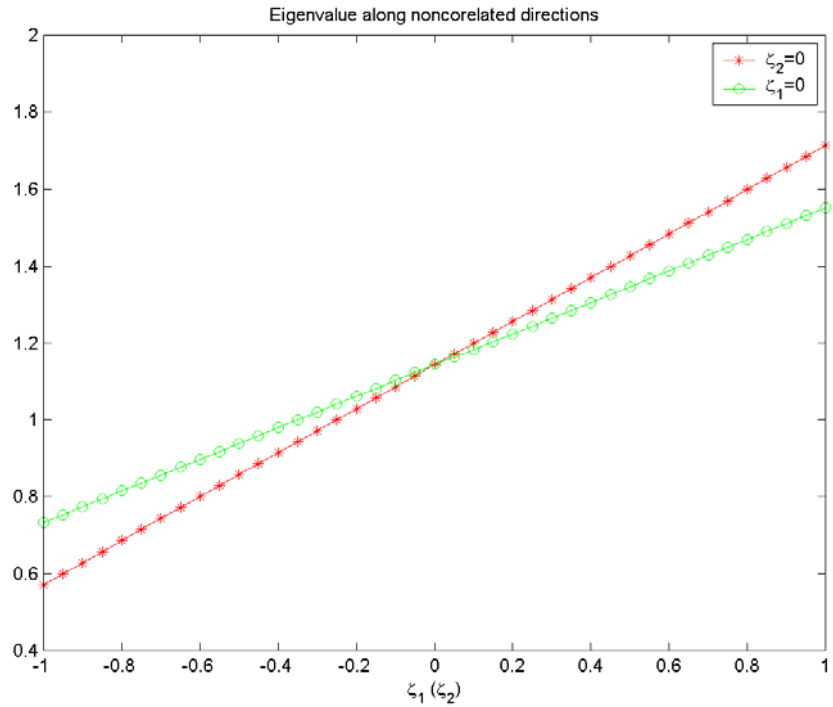




- Direct coupling only, correlated fission uncertainty and uncertainty in $\Sigma_{s,1\to 2}$
- Model takes 40s to compute; about the time to take 100 samples.
- If the goal is computation of distribution (for which 100 samples would be insufficient to compute distribution with such accuracy, and this is a *very* simple model), method more competitive than Monte Carlo.

Further (interesting) observation:





- Nonlinearity is invisible along the coordinate directions, but it is very significant along the correlated directions $\zeta_1 = \zeta_2,\ \zeta_2 = -\zeta_1$
- This shows that first-order derivative approximation may miss substantial information.
- This also shows that we have a lot of structure that we may exploit adaptively to reduce the size of the basis.

Keff for 4 group diffusion model--Collocation Approach

Method	Number of Parameters (Nr. Calibration Samples)	RMSE Error	Equivalent Monte Carlo Sample Reduction
Sensitivity	12	0.3352	1/1
Collocation degree 1	12	0.1320	1/6.5
Collocation degree 2	78	0.0301	6.5/121

- 11 crossections, direct transfer only.
- The error is estimated by averaging it over 100 random samples.
- The upshot is **not** that sensitivity is not useful, but that, **given a certain budget of information, we may be better off from including info from more than one point** (including sensitivity for higher order approaches)

How did we choose the collocation points and polynomials?

- Tensor Legendre polynomials of homogeneous degree up to d

$$\tilde{x}(\omega) = \tilde{x}(\omega_1, \omega_2, \ldots, \omega_m) = \sum_{i=0}^{d} \sum_{\substack{i_1+i_2\ldots+i_m=i \\ i_j \geq 0}} x_{i_1 i_2 \ldots i_m} \prod_{j=1}^{m} L_{i_j}(\omega_j)$$

- The collocation points are the simplex Chebyshev tensor roots

$$\omega^{i_1 i_2 \ldots i_m} = \left(\omega^{i_1}, \omega^{i_2}, \ldots, \omega^{i_m}\right); C_d\left(\omega^j\right) = 0,\ j = 1, 2, \ldots, m$$

- For large dimension m, one must prune the polynomials (cannot choose either simplex or full tensor), since it is subject to curse of dimensionality … though people have been doing 50 variables in SDEs with stochastic input.

Remaining challenges

- To approximate the parametric map in reprocessing and core design problems with SFEM when large-scale, coupled physics is present.
- To investigate adaptive techniques of selecting the polynomial basis, in conjunction with some form of sparse grids.
- Solve the coupled problems in large scale stochastic Galerkin.
- Determine well-posedness conditions for collocation with incomplete (non-tensor) bases.
- Refine convergence results for moderate smoothness.
- Define a mixed SFEM-sampling approach for 1000s of parameters.

Conclusions and future work

- Nuclear reactor application and reprocessing are the source of challenging uncertainty quantification problems, especially when trying to attain the GNEP aims.
- SFEM are promising approaches of generating quality approximations when uncertainty meets nonlinear.
- SFEM Galerkin models **are very robust** and work even in cases of nonsmooth problems where sampling-based or sensitivity methods would fail.
- **For smooth models, SFEM collocation models can be very competitive,** faster and more accurate than sensitivity approaches even for the same computational budget.
- Optimization issues appear at the lowest levels of uncertainty calculations for GNEP and this will likely continue and accelerate.

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- M. Anitescu, G. Palmiotti, Won-Sik Yang and Monika Neda. " STOCHASTIC FINITE-ELEMENT APPROXIMATION OF THE PARAMETRIC DEPENDENCE OF EIGENVALUE PROBLEM SOLUTION" Preprint ANL-MCS P1397-0307. To appear in Proceedings of the Mathematics, Computation and Supercomputing in Nuclear Applications, Monterey, 2007.

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