Uncertainty Quantification in Reacting Flow Computations

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The Validation Challenge

- Validation of a computational model :
  - Establish ”agreement” between predictions and empirical observations
- Establishing model validity requires ”error bars” on computational predictions
  - Disagreement without error bars cannot be used to conclude that a particular model is not valid
  - Disagreement within the range of uncertainty of the results can be due to parametric uncertainty

The Case for Uncertainty Quantification

- UQ is needed for :
  - validation of scientific models
  - validation of predictive codes
  - engineering design optimization
  - assessment of confidence in computational predictions
  - enabling decision-making strategies based on predictive models
  - assimilation of observational data and model construction in noisy environments
  - multiscale/multiphysics modeling

Sources of Uncertainty

- model structure
  - participating physical processes
  - governing equations
  - constitutive relations
- model parameters
  - transport properties
  - thermodynamic properties
  - constitutive relations
  - rate coefficients
- initial and boundary conditions
- geometry

Focus on parametric UQ

Elements of a UQ strategy

- Estimation of model/parametric uncertainties based on data
  - Deterministic framework
    - Regresssion analysis, fitting, parameter estimation
  - Probabilistic framework
    - Bayesian inference of uncertain models/parameters
- Forward propagation of uncertainty in computational models
  - Deterministic framework
    - Local Sensitivity analysis (SA); Error propagation
    - Interval math
  - Probabilistic framework – Global SA / stochastic UQ
    - Sampling based — non-intrusive
    - Direct — intrusive

Stochastic Framework

- Laplacian/Bayesian conception of probability
  - Probability $\equiv$ degree of knowledge
  - Uncertain quantity $\equiv$ random variable
  - Contrast with Frequentist framework

- Inference with Bayes theorem

$$p(m|d)p(d) = p(d|m)p(m)$$

  A formal framework for

  - representation of knowledge
  - learning from data
  - incorporation of prior knowledge
  - construction of uncertain models
  - avoidance of overfitting

Issues with Least Squares (LS) Parameter Estimation

- Choice of optimal number of fit parameters (p)
  - $\chi_R^2 = \chi^2/(\mathcal{D} - p)$ decreases with increased p
  - Versus Ockham's razor principle in Bayesian analysis
- LS best fit is the Maximum Likelihood Estimate (MLE) assuming gaussian noise in the data
- LS Estimation of Uncertainty in inferred parameter values relies on assumed linearity of the model in the parameters
- No general means of handling nuisance parameters

Role of Bayes Formula in Parameter Inference

- Bayes Formula:

$$p(\lambda, y) = p(\lambda|y)p(y) = p(y|\lambda)p(\lambda)$$

or:

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}} \;\; \overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Infer PDF of λ rather than the least-squares estimate of λ
- Posterior contains all information about λ
  - including both prior information and data
- Evidence is a normalizing constant – ignore

The Posterior — towards parametric uncertainties

Parameter λ_k marginal probability:

$$p(\lambda_k|y) = \int p(\lambda|y)\, \mathrm{d}\lambda_{1:k-1}\mathrm{d}\lambda_{k+1:\mathcal{M}}$$

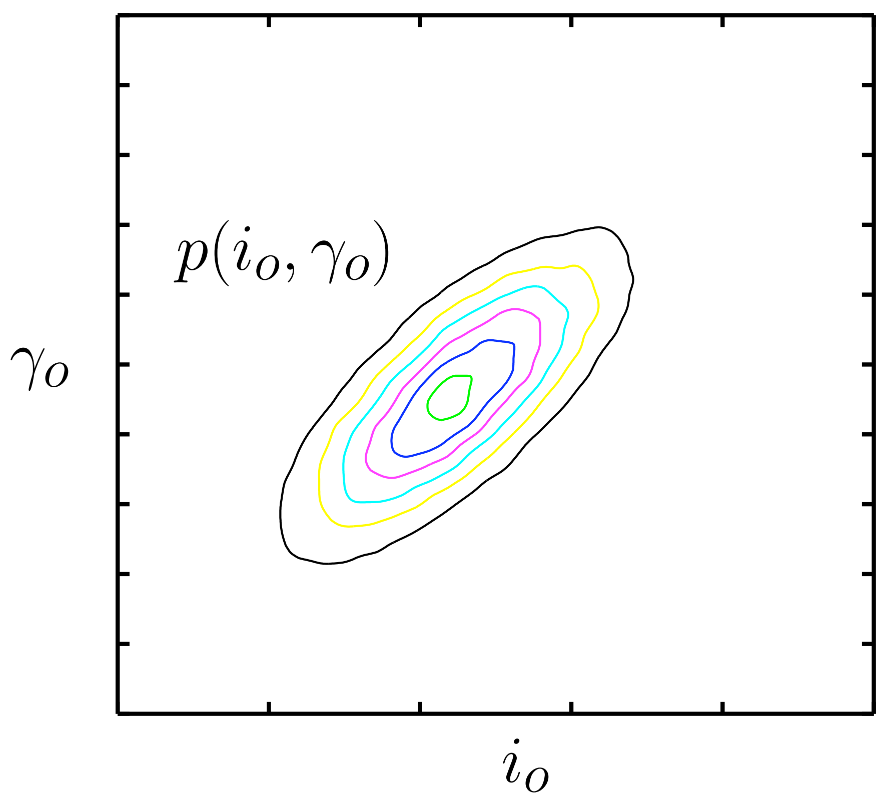
- Given any sample $\{\lambda\}$, the un-normalized posterior probability can be easily computed

$$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$

- Explore the posterior using Markov Chain Monte Carlo (MCMC)
- Can use uninformed priors
- Evaluate marginals from the MCMC statistics

Construction Allows Exploration of Correlations among Parameters

- Available naturally from the MCMC procedure
- Useful for understanding interplay between data and model
- Needed for subsequent UQ



Computational Cost of Bayesian Solution of Inverse Problems

- MCMC procedures typically require $\mathcal{O}(10^5)$ samples of the forward model
  - A barrier to the utilization of Bayesian methods when the forward model is computationally expensive
- This sampling is analogous to that used in forward UQ
- Use intrusive Polynomial Chaos UQ methods to construct an inexpensive surrogate for the forward model
  - Orders of magnitude speedup in MCMC

Marzouk, Najm, and Rahn *J. Comp. Phys.*, (2007)

Spectral Stochastic UQ Formulation — Polynomial Chaos

- An L_2 random variable $u(\boldsymbol{x}, t, \theta)$ can be described by a Polynomial Chaos (PC) expansion in terms of:
  - Hermite polynomials Ψ_k, $k = 1, \ldots, \infty$;
  - the associated infinite-dimensional Gaussian basis $\{\xi_i(\theta)\}_{i=1}^{\infty}$;
  - spectral mode strengths $u_k(\boldsymbol{x}, t)$, $k = 1, \ldots, \infty$.

- Truncated to finite dimension n and order p, the PC expansion for u is written as

$$u(\boldsymbol{x}, t, \theta) \simeq \sum_{k=0}^{P} u_k(\boldsymbol{x}, t) \Psi_k(\underline{\xi}(\theta))$$

where $\underline{\xi}(\theta) = \{\xi_1(\theta), \cdots, \xi_n(\theta)\}$.

Non-intrusive – Sampling-Based – Spectral Projection (NISP) UQ

- Express uncertain model parameters/output as PC expansions
- Sample parameter distributions
- Compute realizations of the model output u
- Project on the PC mode strengths of model output

$$u_k = \frac{\langle u\Psi_k\rangle}{\langle\Psi_k^2\rangle} = \frac{1}{\langle\Psi_k^2\rangle}\int u\Psi_k(\xi)\rho(\xi)d\xi, \quad k = 0,\ldots,P$$

  – Evaluate integrals numerically (MC, quadrature, cubature)

- Construct uncertain model output

$$u(x,t;\theta) = \sum_{k=0}^{P} u_k(x,t)\Psi_k(\xi(\theta))$$

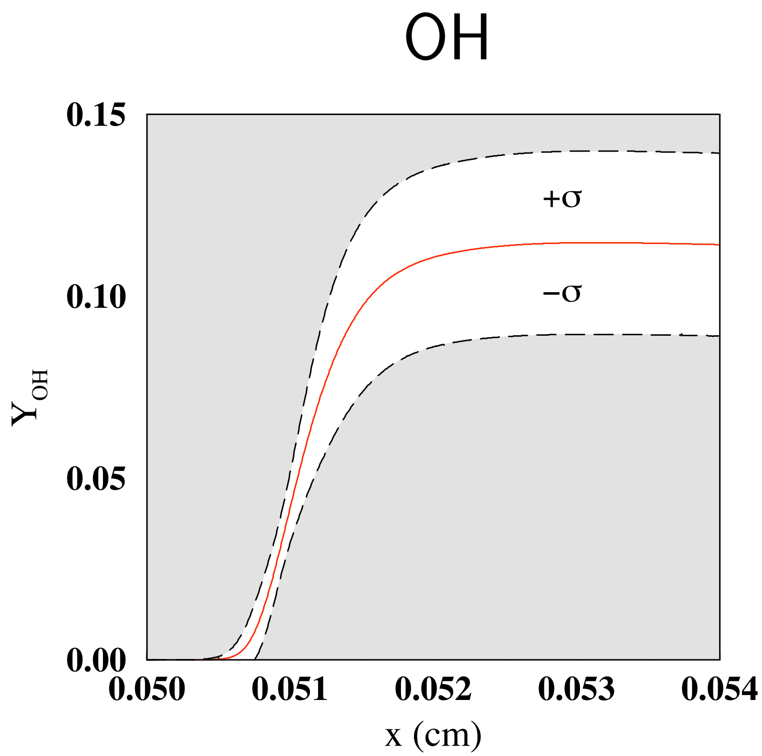
NISP UQ Application: Premixed H_2-O_2 Chemistry at Super-Critical Water Oxidation (SCWO) Conditions

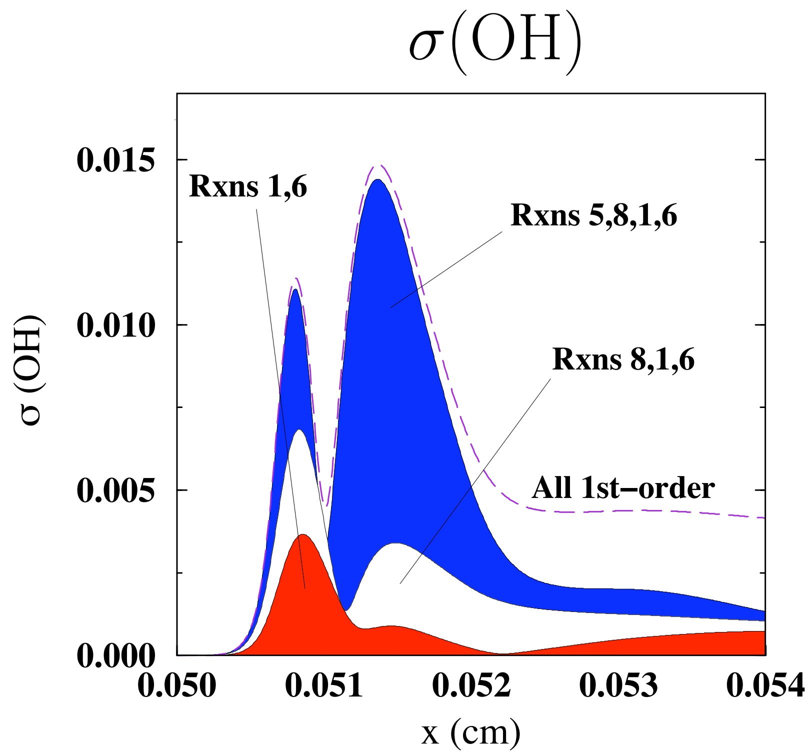
- Allow uncertainties in reaction rate constants and thermodynamic properties, per published experimental data
- Wrap NISP processing around a deterministic reacting flow code
- Using 8-step simplified SCWO Hydrogen mechanism (McRae)

Reaction			A	n	E_a/R	UF
1. OH + H	$\leftrightarrow$	H_2O	1.620E+14	0	75	3.16
2. H_2 + OH	$\leftrightarrow$	H_2O + H	1.024E+08	1.6	1660	1.26
3. H + O_2	$\leftrightarrow$	HO_2	1.481E+12	0.6	0	1.58
4. HO_2 + HO_2	$\leftrightarrow$	H_2O_2 + O_2	1.867E+12	0	775	1.41
5. H_2O_2 + OH	$\leftrightarrow$	H_2O + HO_2	7.829E+12	0	670	1.58
6. H_2O_2 + H	$\leftrightarrow$	HO_2 + H_2	1.686E+12	0	1890	2.00
7. H_2O_2	$\leftrightarrow$	OH + OH	3.0000E+14	0	24400	3.16
8. OH + HO_2	$\leftrightarrow$	H_2O + O_2	2.891E+13	0	-250	3.16

Species	μ_0	2σ
H	52.10	0.01
OH	9.3	0.2
H_2O	-57.80	0.01
H_2O_2	-32.53	0.07
HO_2	3.0	0.5

1D H_2-O_2 SCWO Flame NISP UQ/Chemkin-Premix





- Fast growth in OH uncertainty in the primary reaction zone
- Constant uncertainty and mean of OH in post-flame region
- Uncertainty in pre-exponential of Rxn.5 (H_2O_2+OH=H_2O+HO_2) has largest contribution to uncertainty in predicted OH

First-Order Sensitivity Information in a PC Expansion

- Conventional sensitivity

$$u = u(x, t; \lambda): \qquad S = \left.\frac{\partial u}{\partial \lambda}\right|_{\lambda_0} \sim \left.\frac{\delta u}{\delta \lambda}\right|_{\lambda_0}$$

- Sensitivity in a stochastic UQ context

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \qquad u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$$

- For Hermite Ψ_k:

$$S = \frac{\partial u}{\partial \lambda} = \frac{\partial u / \partial \xi}{\partial \lambda / \partial \xi} = \frac{\sum_{k=0}^{P-1} (k+1) u_{k+1} \Psi_k}{\sum_{k=0}^{P-1} (k+1) \lambda_{k+1} \Psi_k} = \sum_{k=0}^{P} S_k \Psi_k$$

- Extends to multi-D case with independent parameters

Intrusive Spectral Stochastic UQ Formulation: ODE Example

- Sample ODE with parameter λ:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \lambda u$$

- Let λ be uncertain; introduce $\xi \sim \mathcal{N}(0,1)$.
  Express λ and u using PCEs in ξ:

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k, \qquad u = \sum_{k=0}^{P} u_k \Psi_k$$

- Substitute in ODE and apply a Galerkin projection on $\Psi_i(\xi)$,

$$\frac{du_i}{dt} = \sum_{p=0}^{P} \sum_{q=0}^{P} \lambda_p u_q C_{pqi}, \quad i = 0, \ldots, P$$

where the $C_{pqi} = \left\langle \Psi_p \Psi_q \Psi_i \right\rangle / \left\langle \Psi_i^2 \right\rangle$ are known coefficients

Pseudo-Spectral Implementation

Spectral Product : $w = uv$

$$w = u * v \quad \Rightarrow \quad w_i = \langle uv \rangle_i \,, \quad i = 0, \cdots, P$$

Psuedo-spectral higher-order polynomial terms :

$$w = \lambda u^2 v \quad \Rightarrow \quad w = \lambda * (u * (u * v))$$

Division :

$$w = \frac{u}{v} \quad \Rightarrow \quad \langle vw \rangle_k = u_k, \quad \text{solve linear equation system for } w_k$$

Arbitrary functions $u = f(x)$ where $\dot{u} = \frac{\mathrm{d}f}{\mathrm{d}x}$ is a rational function of x & u :

$$u_k(x_b) - u_k(x_a) = \sum_{j=0}^{P} \int_{(x_a)_j}^{(x_b)_j} \sum_{i=0}^{P} C_{ijk} (\dot{u})_i \mathrm{d}x_j$$

Spectral UQ: Incompressible Flow - Stochastic Projection Method

- $(P+1)$ Galerkin-Projected Momentum equations, $q = 0, \ldots, P$:

$$\frac{\partial \boldsymbol{v}_q}{\partial t} + \nabla \cdot \langle \boldsymbol{v}\boldsymbol{v} \rangle_q = -\nabla p_q + \frac{1}{\mathrm{Re}} \nabla \cdot \left\langle \mu [(\nabla \boldsymbol{v}) + (\nabla \boldsymbol{v})^T] \right\rangle_q$$

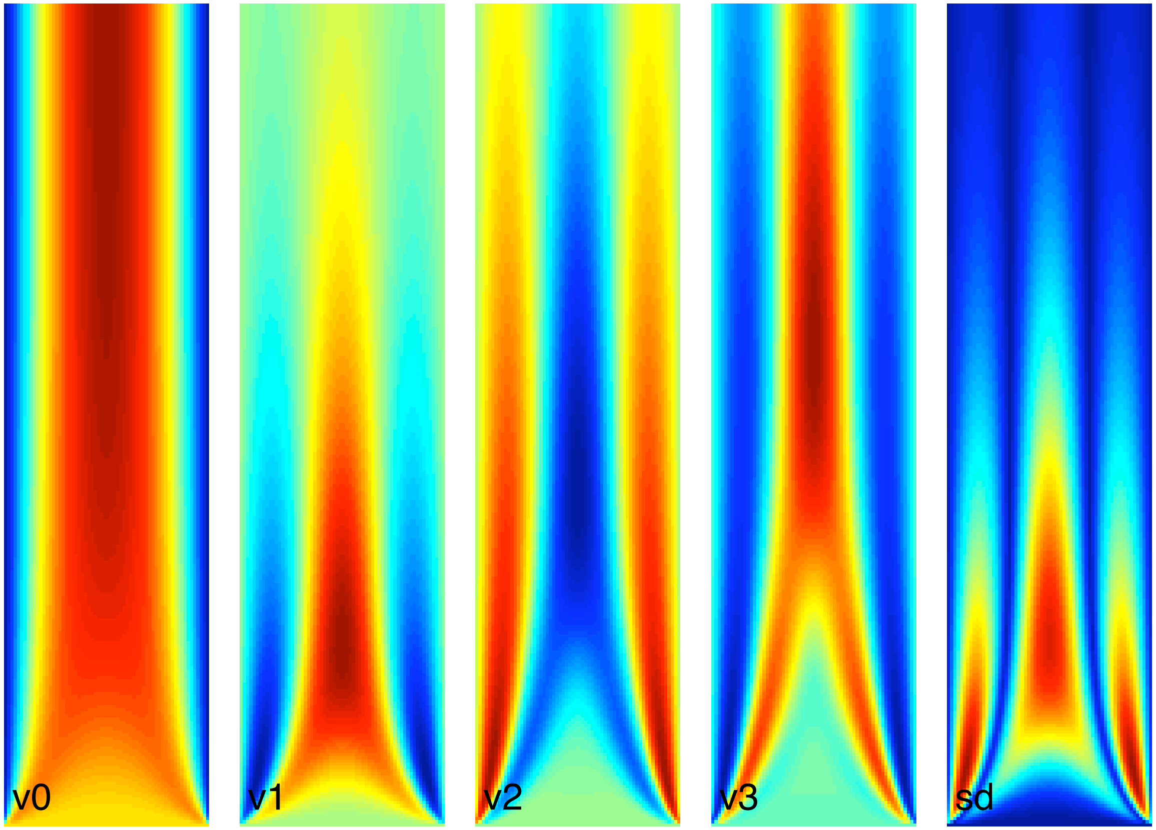
- Projection: for $q = 0, \ldots, P$:

$$\begin{aligned} \frac{\tilde{\boldsymbol{v}}_q - \boldsymbol{v}_q^n}{\Delta t} &= C_q^n + D_q^n \\ \nabla^2 p_q &= -\frac{1}{\Delta t} \nabla \cdot \tilde{\boldsymbol{v}}_q \\ \frac{\boldsymbol{v}_q^{n+1} - \tilde{\boldsymbol{v}}_q}{\Delta t} &= -\nabla p_q \end{aligned}$$

- $P + 1$ *decoupled* Poisson Equation solutions for the pressure modes.

Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Gaussian viscosity PDF
  - $\nu = \nu_0 + \nu_1 \xi$
- Streamwise velocity
  - $v = \sum_{i=0}^{P} v_i \Psi_i$
  - v_0: mean
  - v_i: i-th order mode
  - $\sigma^2 = \sum_{i=1}^{P} v_i^2 \left\langle \Psi_i^2 \right\rangle$



v_0 $\quad v_1$ $\quad v_2$ $\quad v_3$ $\quad \sigma$

Spectral UQ Formulation: low M 2D Reacting Flow Equations

$$
\begin{aligned}
\frac{\partial \rho_q}{\partial t} + \nabla \cdot \langle \rho \boldsymbol{v} \rangle_q &= 0 \\
\frac{\partial \langle \rho \boldsymbol{v} \rangle_q}{\partial t} + \nabla \cdot \langle \rho \boldsymbol{v} \boldsymbol{v} \rangle_q &= -\nabla p_q + \frac{1}{\mathrm{Re}} \nabla \cdot \left\langle \mu [(\nabla \boldsymbol{v}) + (\nabla \boldsymbol{v})^T] - \frac{2}{3} \mu (\nabla \cdot \boldsymbol{v}) \mathbf{U} \right\rangle_q
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial T_q}{\partial t} + \langle \boldsymbol{v} \cdot \nabla T \rangle_q = \left\langle \frac{(\gamma - 1)}{\gamma \rho c_p} \frac{dp_o}{dt} \right\rangle_q + \frac{1}{RePr} \left\langle \frac{\nabla \cdot (\lambda \nabla T)}{\rho c_p} \right\rangle_q - \frac{1}{ReSc} \left\langle \sum_{i=1}^{N} \frac{c_{p,i}}{c_p} \boldsymbol{V}_i \cdot \nabla T \right\rangle_q \\
- \ Da \left\langle \frac{1}{\rho c_p} \sum_{i=1}^{N} h_i w_i \right\rangle_q
\end{aligned}
$$

$$
\frac{\partial \langle \rho Y_i \rangle_q}{\partial t} + \nabla \cdot \langle \rho \boldsymbol{v} Y_i \rangle_q = -\frac{1}{ReSc} \nabla \cdot \langle \rho Y_i \boldsymbol{V}_i \rangle_q + Da \ \langle w_i \rangle_q \qquad i = 1, \ldots, N
$$

- Time Integration:
  - Operator-Split reaction-diffusion integration of $(P+1)(N+1)$ species and energy eqns
  - Stochastic Projection Method integration of $(P+1)$ momentum equations

UQ in constant-pressure ignition

N-species, with mass fractions Y_i:

$$\frac{\mathrm{d}Y_i}{\mathrm{d}t} = \frac{w_i}{\rho}, \quad i = 1, \cdots, N$$
$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{w_T}{\rho c_p}$$

with $w_T = -\sum_{i=1}^{N} w_i$ and $w_i = \sum_{k=1}^{M} \nu_{ik}\mathcal{R}_k$

Example: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Stoichiometric coefficients : $\nu_{ik} = \{1, 2, 1, 2\}$

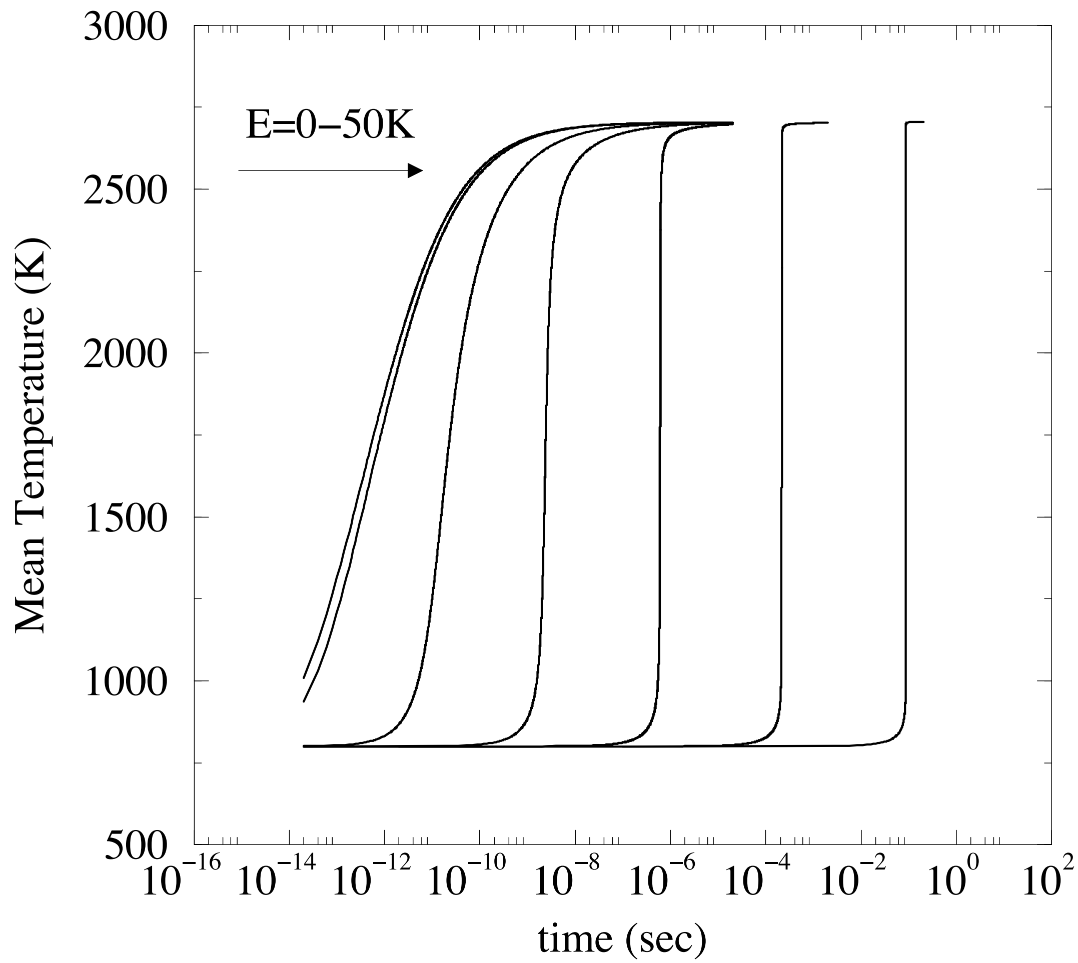
Reaction rate of progress : $\mathcal{R}_k = [CH_4][O_2]^2 \, A_k T^{n_k} e^{-E_k/T}$

- Quantify reaction-rate pre-exponential (A_k) uncertainty with multiplicative factor F_k :

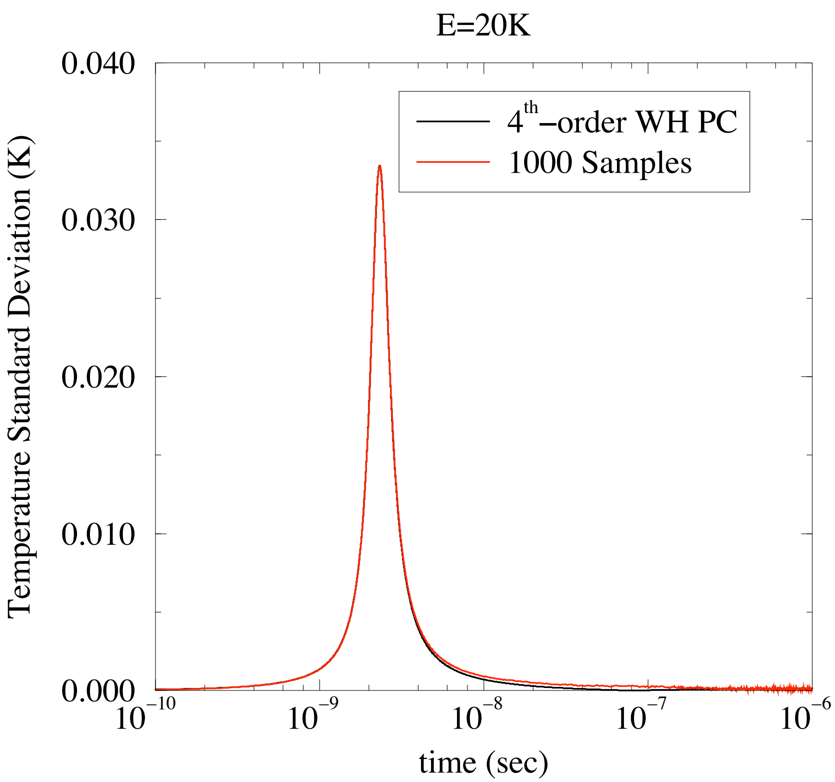
$$P\left(\frac{A_k}{F_k} < A_k < F_k A_k\right) = 0.95$$

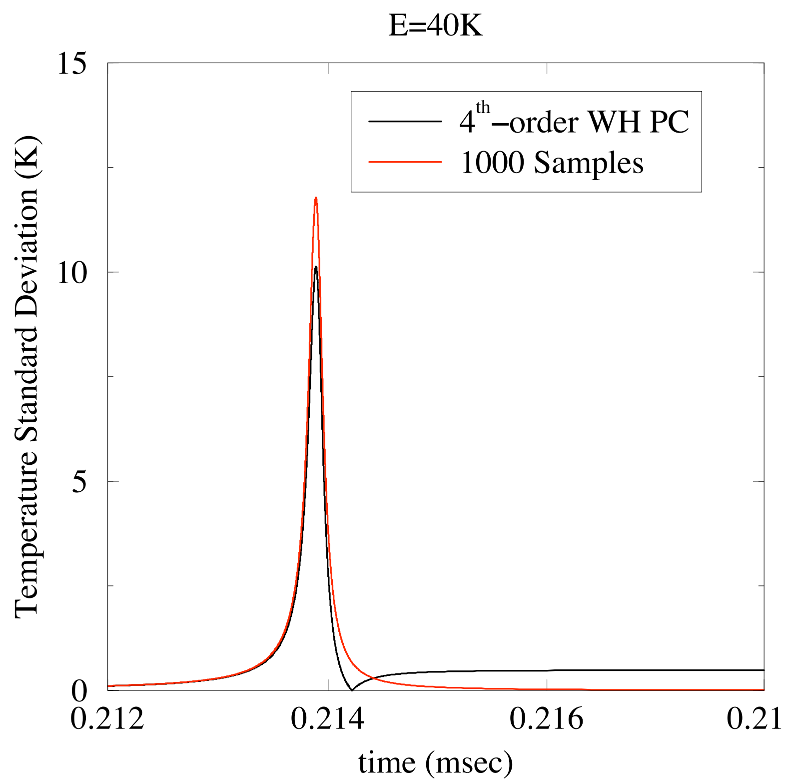
Large activation energy (E_k) exponentials lead to very fast changes in species concentrations and temperature

- Methane-air ignition — Global single-step irreversible mechanism
- Initial $T = 800K$
- Stoichiometric
- $p = 1$ atm (constant)



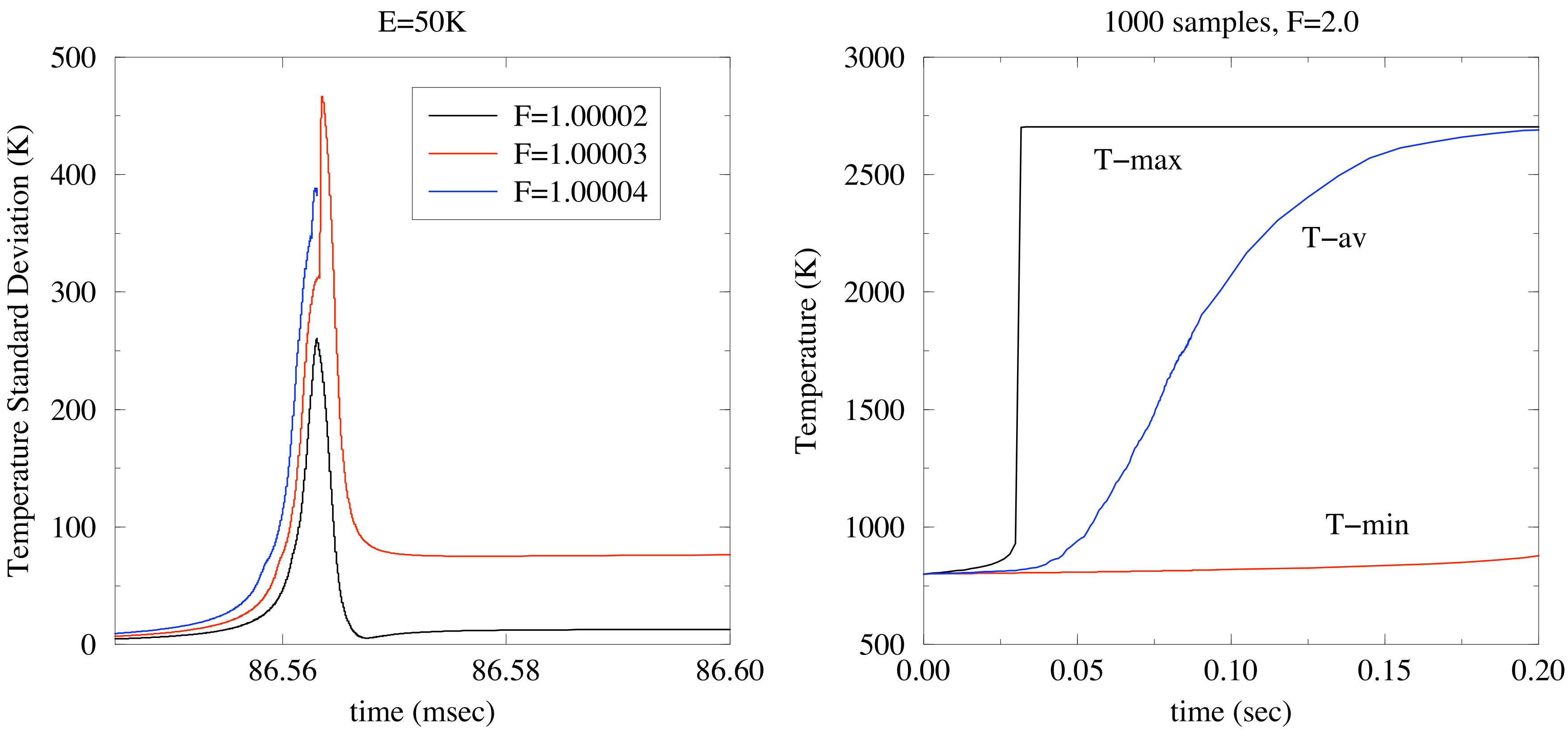
Increased E_k leads to higher peak dT/dt and higher consequence of small uncertainties in reaction rate constants





- $A_k = A_k(\xi)$, 1-D Wiener-Hermite
- PC UQ captures sampled stochastic behavior at low E_k
  - with miniscule uncertainty in A_k ($F = 1.00002$, COV$=10^{-5}$).
- Unphysical effects observed at high activation energy

Increasing A_k COV towards minimally-practical levels leads to failed time integration

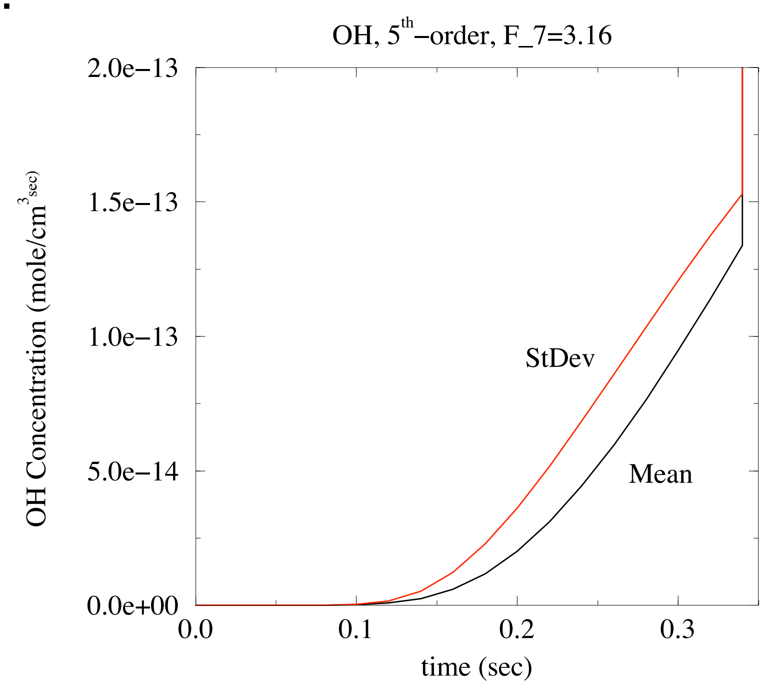


- Unrealistic to expect a WH PC expansion in 1D to capture expected PDFs at realistic reaction-rate parametric uncertainties
- Need increased dimensionality of the PCEs, using multiple ξ's for each uncertain parameter, for increased accuracy and stability

UQ in constant-pressure isothermal ignition – H_2-O_2 SCWO system

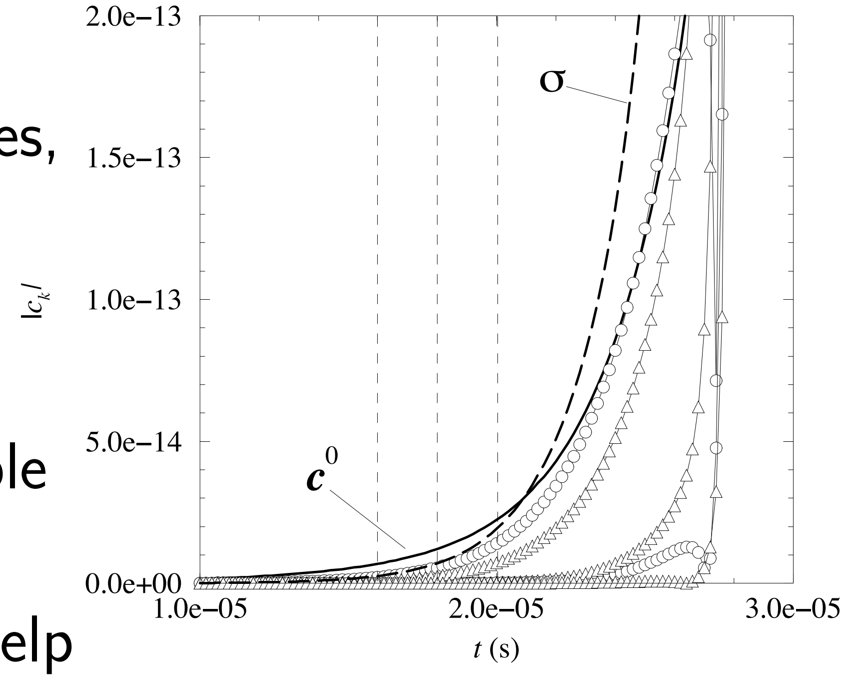
- Using 1D Wiener-Hermite PC, with order P
- Computations stable for small reaction-rate uncertainty
- SCWO with only Rxn-7 uncertain :
  - $P = 1$: stable*
  - $P = 2$: fails for $UF_k \geq 2.55$
  - $P = 3$: stable*
  - $P = 4, 5$: fails for $UF_k \geq 2.23$

*(up to empirical $UF_k = 3.16$)



Experience with Instabilities and Intrusive PC UQ

- Regions of explosive mode growth can lead to instabilities.
- Fast growth of high-order modes, and fast drift of the solution towards unphysical values
- Standard deviation increases significantly, becoming a sizeable fraction of the mean.
- Increasing PC order does not help
- NB. all with fixed PC dimension



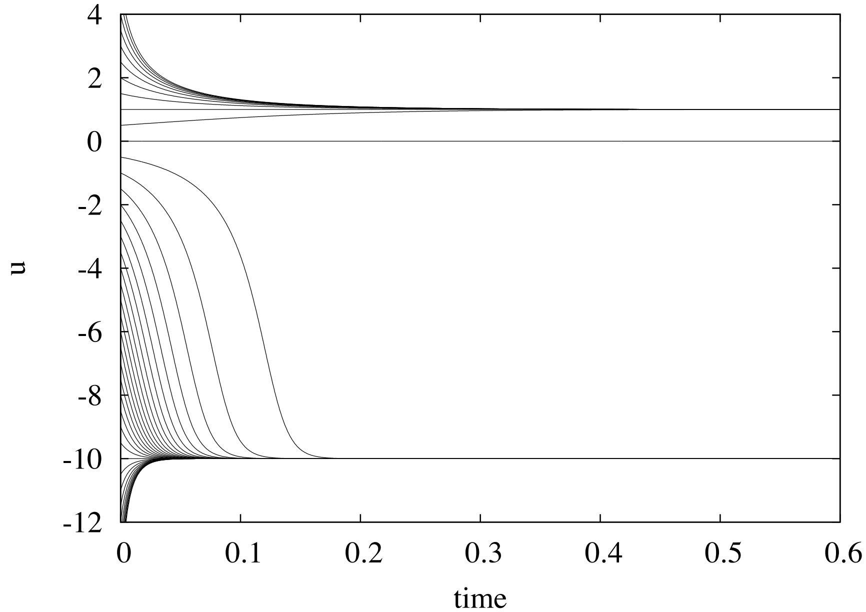
Reagan, Najm, Debusschere, Le Maître, Knio, and Ghanem, *CTM*, 2004;

Causes of instability in Chemical Systems

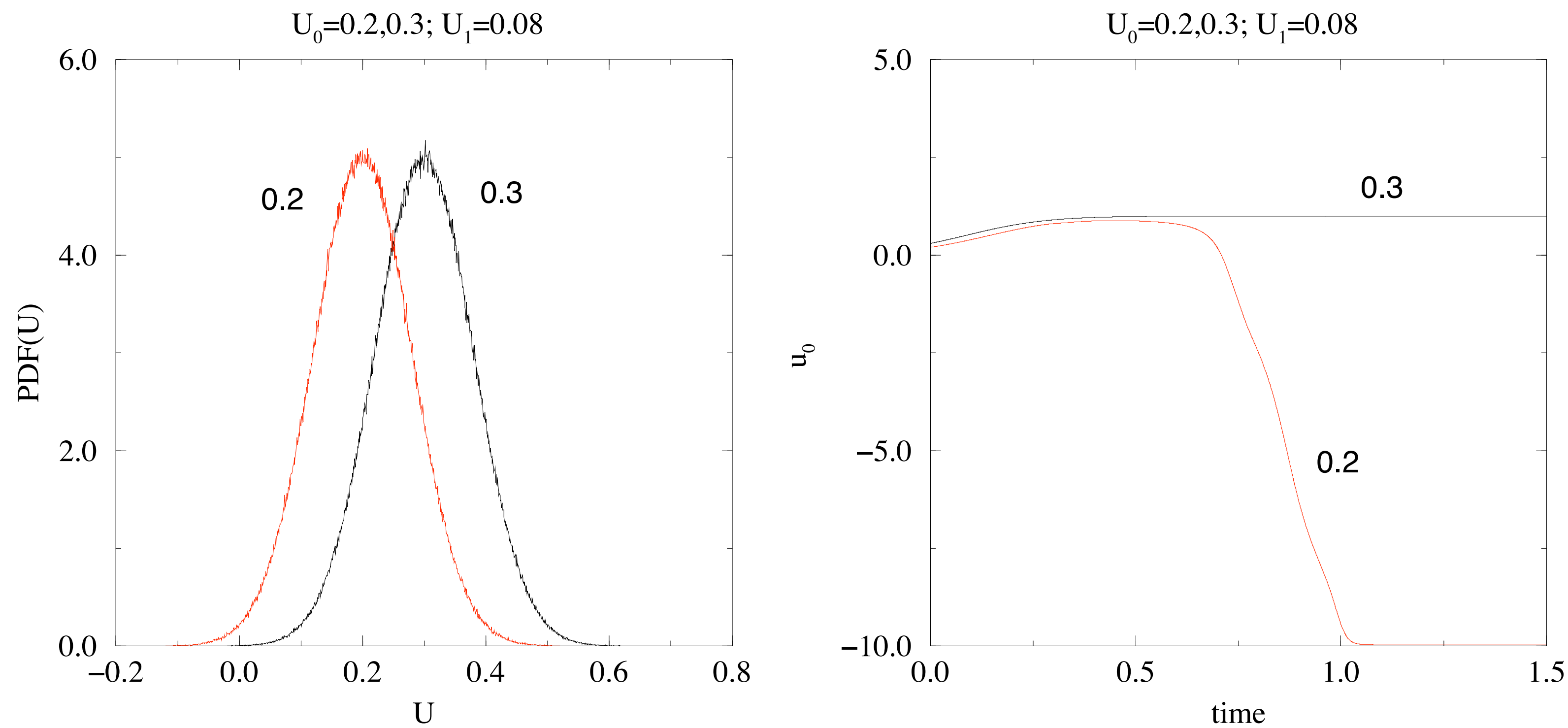
- Gaussian has infinite support
- Finite probability of negative concentrations
  - Cannot satisfy strict positivity
  - Result of finite PC order and fixed PC dimension
- Fails in chemical systems

Model Problem: Bifurcations and Intrusive PC UQ

- Consider a model problem : $\frac{du}{dt} = u(u+10)(1-u)$
- Fixed points: attractive: $u = -10, 1$; repulsive: $u = 0$
- Initial condition stochastic: $U = \sum_{k=0}^{P} U_k \Psi_k$.
- Integrate for $u_k(t)$, $k = 0, \dots, P$



Model Problem: Consequence of Initial PDF tail zero crossing



- $\sigma_U/U_0 >\approx$30% attracts u_0 towards negative region
- Even for low σ_U, increasing PC order leads to similar drift
- Similar behavior for Gaussian or Lognormal initial condition
- Similarly with Laguerre polynomial/Gamma distribution basis

Challenges with the use of a Global PC Basis for Intrusive UQ

- Global PC expansion with N-th order polynomial will have N roots/zero-crossings in general
- Representing a RV with a global PC expansion (over all ξ)
  - with fixed dimensionality and order
  - will 'sample' both positive and negative u-realizations
  - irrespective of PDF(u)
- Fails when strict positivity is necessary for stability
  - e.g. reaction rate constants, concentrations, temp
- Possible remedies with appropriate filtering strategies
- Eval local low order basis vs. the global high order approach
  - Wavelets, Multi-Resolution Analysis

Le Maître *et al.*, *J. Comp. Phys.*, 197, 28-57, 2004
Le Maître *et al.*, *J. Comp. Phys.*, 197, 502-531, 2004

Uncertainty Quantification with Multiwavelets

- An uncertain field quantity $u(\mathbf{x}, t, \theta)$ is expressed using PC

$$u = \sum_{k=0}^{P} u_k(\mathbf{x}, t)\Psi_k(\xi_1, \ldots, \xi_N), \qquad \xi_i \sim N(0,1)$$

- Introduce $\zeta_i = p(\xi_i)$: CDF of ξ_i, where $\zeta_i \sim U(0,1)$

$$u = g(\xi_1, \ldots, \xi_N) = f(\zeta_1, \ldots, \zeta_N)$$

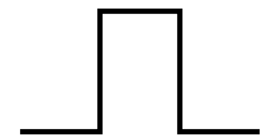
- Represent $f(\boldsymbol{\zeta})$ using N-D multiwavelets (Alpert, 1993)

$$u = \sum_{\lambda=0}^{Q} \tilde{u}_\lambda(\mathbf{x}, t)\, \mathcal{W}_\lambda(\zeta_1, \ldots, \zeta_N)$$

Le Maître, Ghanem, Knio, and Najm, *J. Comp. Phys.*, 197:28-57 (2004)
Le Maître, Najm, Ghanem, and Knio, *J. Comp. Phys.*, 197:502-531 (2004)

Haar scaling functions

$$\phi^w(y) = \begin{cases} 1, & 0 \le y < 1 \\ 0 & \text{otherwise} \end{cases}$$

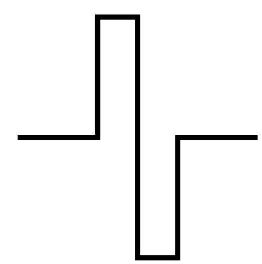


Scaled Haar functions, scaling factor j, and sliding factor k,

$$\phi^w_{jk}(y) = 2^{j/2}\phi^w(2^j y - k)$$

Haar function (mother wavelet)

$$\psi^w(y) \equiv \frac{1}{\sqrt{2}}\phi^w_{1,0}(y) - \frac{1}{\sqrt{2}}\phi^w_{1,1}(y) = \begin{cases} 1, & 0 \le y < \frac{1}{2}, \\ -1, & \frac{1}{2} \le y < 1, \\ 0, & \text{otherwise.} \end{cases}$$



Wavelet family

$$\psi^w_{j,k}(y) = 2^{j/2}\psi^w(2^j y - k), \quad j = 0, 1, \ldots \text{ and } k = 0, \ldots, 2^j - 1$$

Wiener-Haar Construction

The set of $\psi^w_{j,k}(y)$ is an orthonormal system

Any function $f \in L^2([0,1])$ can be arbitrarily well approximated by the sum of its mean and a finite linear combination of the $\psi^w_{j,k}(y)$.

The wavelet set $W_{j,k}(\xi(\theta)) \equiv \psi^w_{j,k}(p(\xi))$ forms a basis for the space of L^2 random processes.

$$X(\xi(\theta)) = X_o + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} X^w_{j,k} \psi^w_{j,k}(p(\xi)) = \sum_{\lambda} X_\lambda W_\lambda(\xi(\theta))$$

Multidimensional $\{\xi_1, \xi_2, \dots, \xi_N\}$,

$$\mathcal{W} = \prod_{k=1}^{N} W_{\lambda_k}(\xi_k)$$

Multidimensional Multiwavelet Construction

- Wiener-Haar PC able to represent uncertainty in systems exhibiting bifurcations depending on parameter values
- Poor convergence relative to PC constructions with smooth global bases on smooth functions
- Use multiwavelet construction (Alpert, 1993) employing higher order polynomials instead of the Haar-functions
- For efficient multidimensional construction, use
  - Block-decomposition of the stochastic space
  - A local MW construction on each block employing
    - Scaled Legendre polynomials
    - First level Multiwavelet details
  - Adaptive resolution in each dimension on each block

Multi-Wavelets on $[0, 1]$

Multiwavelet family:

$$\psi_{jl}^{k}(x) = 2^{k/2}\psi_j(2^k x - l), \qquad j = 0, \ldots, N_o,\ l = 0, \ldots, 2^k$$

where the $\psi_j(x)$, $j = 0, 1, \ldots, N_o$, are piecewise polynomial functions of degree less or equal to N_o, satisfying orthonormality conditions, and having $N_o + 1$ vanishing first moments.

Rescaled Legendre Polynomials:

$$\phi_i(x) = \frac{L_i(2x - 1)}{l_i}$$

where l_i is a normalization factor ensuring orthonormality.

Polynomial Family:

$$\phi_{il}^{k}(x) = 2^{k/2}\phi_i(2^k x - l), \qquad i = 0, \ldots, N_o,\ l = 0, \ldots, 2^k - 1$$

Multi-Wavelet Expansion

Full MW expansion of $f(x)$, $x \sim U(0,1)$:

$$f^{N_o,N_r}(x) = F^{N_o,0} + \sum_{k=0}^{N_r-1} \sum_{l=0}^{2^k-1} \left(\sum_{i=0}^{N_o} \mathrm{d}f_{il}^k \psi_{il}^k(x) \right)$$

where

$$F^{N_o,N_r}(x) = \sum_{l=0}^{2^{N_r}-1} \sum_{i=0}^{N_o} F_{il}^{N_r} \phi_{il}^{N_r}(x)$$

and

$$F_{il}^{N_r} = \left\langle \phi_{il}^{N_r}(x), f(x) \right\rangle$$

$$\mathrm{d}f_{il}^k = \left\langle \{F^{N_o,k+1}(x) - F^{N_o,k}(x)\}, \psi_{il}^k(x) \right\rangle$$

Optimal Adaptive MW Construction

Multiblock decomposition of the N-dimensional stochastic space.
1D 2-block decomposition example :

$$[f(x)]_{x\sim U(0,1)} \quad \Rightarrow \quad \begin{cases} [f_1(x_1)]_{x_1\sim U(0,1/2)} \\ [f_2(x_2)]_{x_2\sim U(1/2,1)} \end{cases}$$

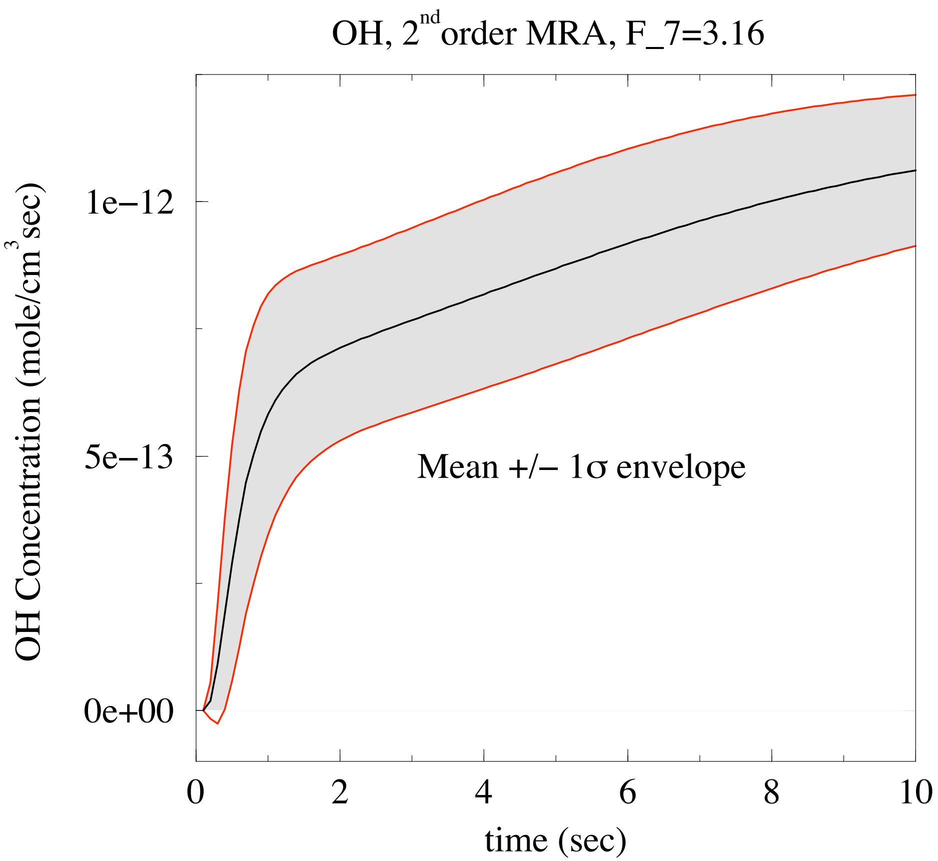
On each block :
Use Legendre Polynomials + *only* 1^{st}-level wavelet details :

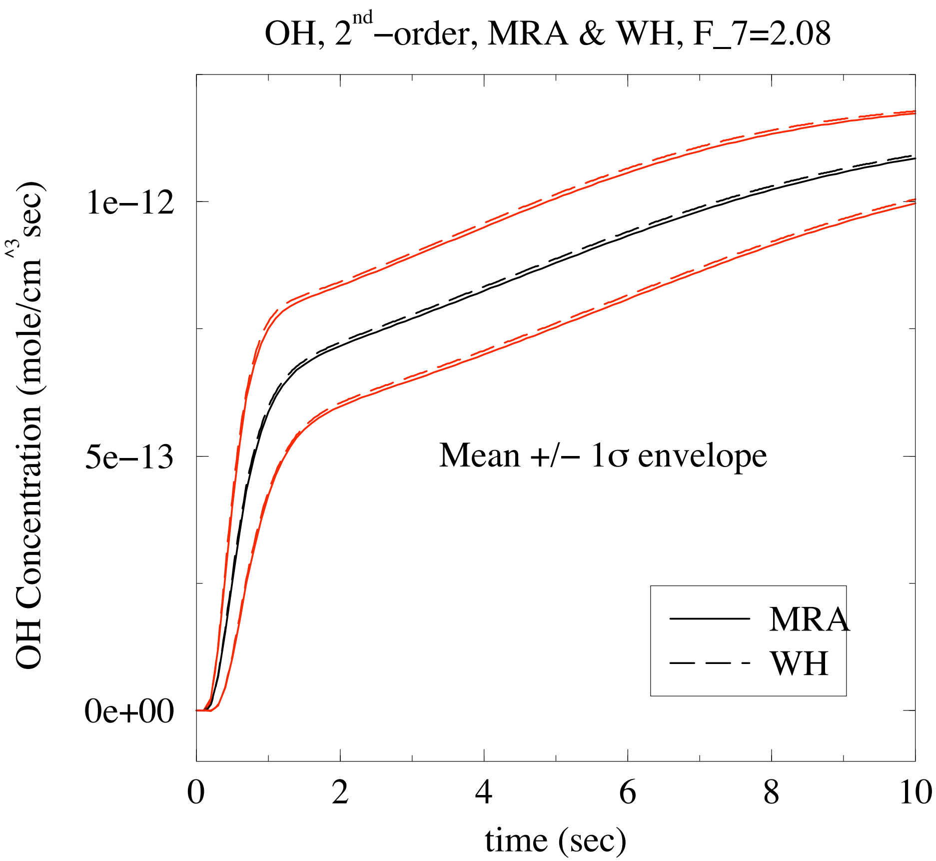
$$f^{N_o,1}(x) = \sum_{i=0}^{N_o} F_{i0}^{0}\phi_i(x) + \sum_{i=0}^{N_o} df_{i0}^{0}\psi_i(x)$$

Independent intrusive PC UQ problem on each block.
Adaptively choose block decomposition in each dimension, and the expansion order N_o within each block.

UQ in constant-pressure isothermal ignition — MRA

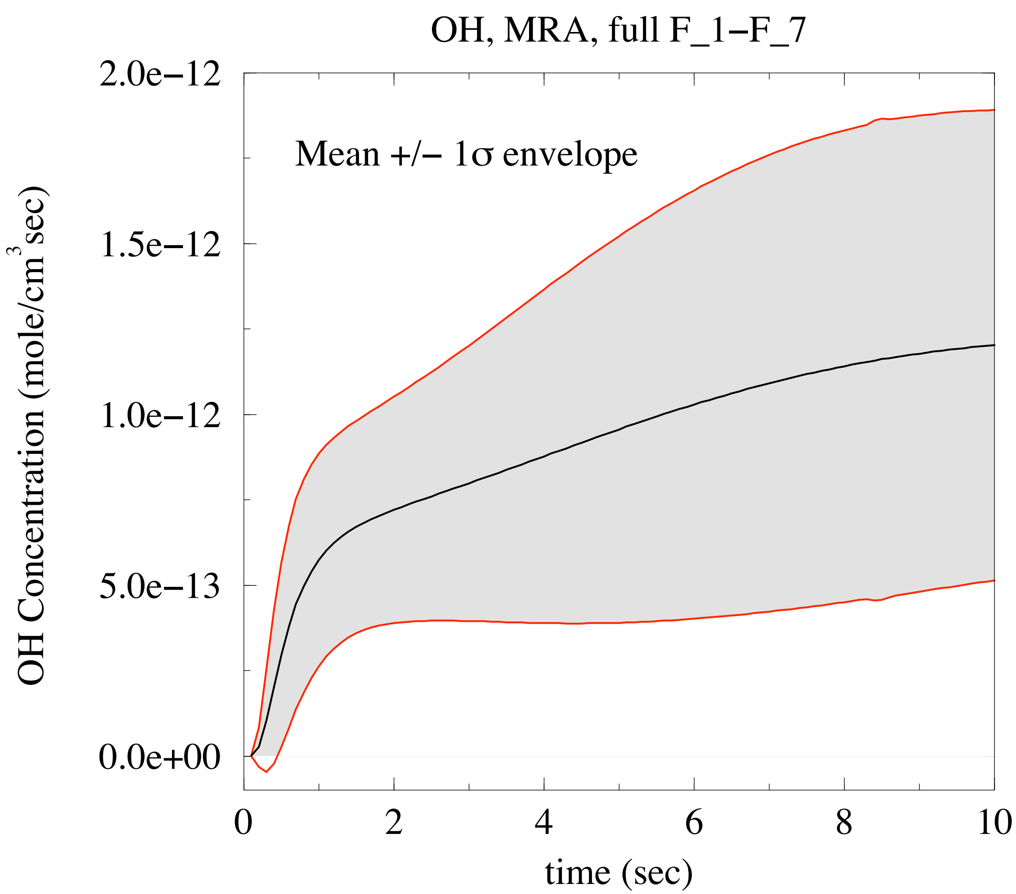
- H_2-O_2 SCWO with only Rxn-7 uncertain $(F_7 = 3.16)$





UQ in constant-pressure isothermal ignition — MRA

- H_2-O_2 supercritical water oxidation model
- Empirically-based uncertainty in all 7 reactions
- Adaptive refinement of MW block decomposition in each dimension



Le Maître, Najm, Pébay, Ghanem, and Knio, *SIAM J. Sci. Comp.*, 22(2):864-889, 2007

Conclusions

- Non-intrusive Spectral UQ
  - PC-construction enables extraction of sensitivities
  - Quadrature and cubature to reduce no. of samples
- Intrusive Spectral UQ in reacting flow
  - Global basis OK for weakly non-linear systems
  - Potential utility of multiple ξ's per uncertain parameter
  - Adaptive multiwavelet MRA construction
    - Accuracy, robustness, and efficiency demonstrated on a number of model problems
    - Resolves global PC difficulties
    - Demonstration in exothermic ignition and flames in progress

Prospects

- Cubature methods for efficient evaluation of high dimensional integrals
- Adaptive general multiwavelet solution of non-linear systems
- Challenges
  - Convection
  - Limit-cycle and chaotic systems
  - Dimensionality