Stochastic Methods for Uncertainty Quantification in Reacting Flow Modeling

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Motivation for Uncertainty Quantification (UQ)

- Rational model validation with respect to experimental measurements requires estimates of ranges of *error* in each set of data
- Experimental error-bars are (usually) available
- How large are the error bars on the computational results?
- Sources of error/uncertainty in the prediction
  - Model uncertainty
  - Parametric uncertainty
  - Numerical discretization errors
- Determining that numerical and experimental error bars do not overlap enables a decision on the efficacy of the *model* as distinct from the role of the *parameters*
- Focus on quantification of parameteric uncertainty (UQ)
  - in chemically reacting flow computations

General Approach for Parametric UQ

- Define the physical model and associated parameters
- Determine which parameters are uncertain, and by how much
- Model uncertain parameters as stochastic quantities with known PDFs
- Propagate the uncertainty through the model
  - Monte-Carlo approach
  - Spectral approach
  - Error propagation/sensitivity analysis
  - other
- Evaluate PDFs of model outputs and determine their stochastic behaviour

Spectral Stochastic UQ Formulation

- Model uncertain parameters as random variables
- A stochastic process $u(x,t,\theta)$ can be described by :
  a Polynomial Chaos (PC) expansion in terms of Hermite polynomials Ψ_k,
  their associated Gaussian basis $\xi(\theta)$,
  and spectral mode strengths $u_k(x,t)$

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

- Literature:

  Wiener : 1938 : Homog. Chaos – span of Hermite pol. functionals of a Gaussian process

  Cameron & Martin : 1947 : L^2 Convergence for any L^2 stochastic process

  Ghanem & Spanos : 1991 : Application to UQ in Stochastic Finite Element Method

  Le Maître *et al.* : 2001,2002 : Application to Fluid Flow

  Xiu & Karniadakis : 2002 : Conv. rate for Gaussian/non-Gaussian processes

  Debusschere *et al.* : 2003 : Application to electrochemistry in microfluid flow

  Reagan *et al.* : 2003 : Application to reacting thermofluid flow

  J. Comp. Phys. 2001,2002; Phys. Fluids 2003; Comb. Flame 2003

Non-intrusive Spectral Projection (NISP) UQ Formulation

- Model problem : $du/dt = f(u,\lambda) \ldots \lambda$: parameter
- Let λ be uncertain : Represent it as a stochastic quantity
  - Introduce a new dimension ξ, where ξ is a Normal random variable
  - Use P-th order Polynomial Chaos (PC) expansions:

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

  - The Ψ_k's are orthogonal $\quad <\Psi_i \Psi_j> = <\Psi_i^2> \delta_{ij}$
- Sample ξ-space and compute realizations of the deterministic model
- Project MC statistics on the spectral mode strengths $u_k(t)$

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

  - Evaluate integrals numerically

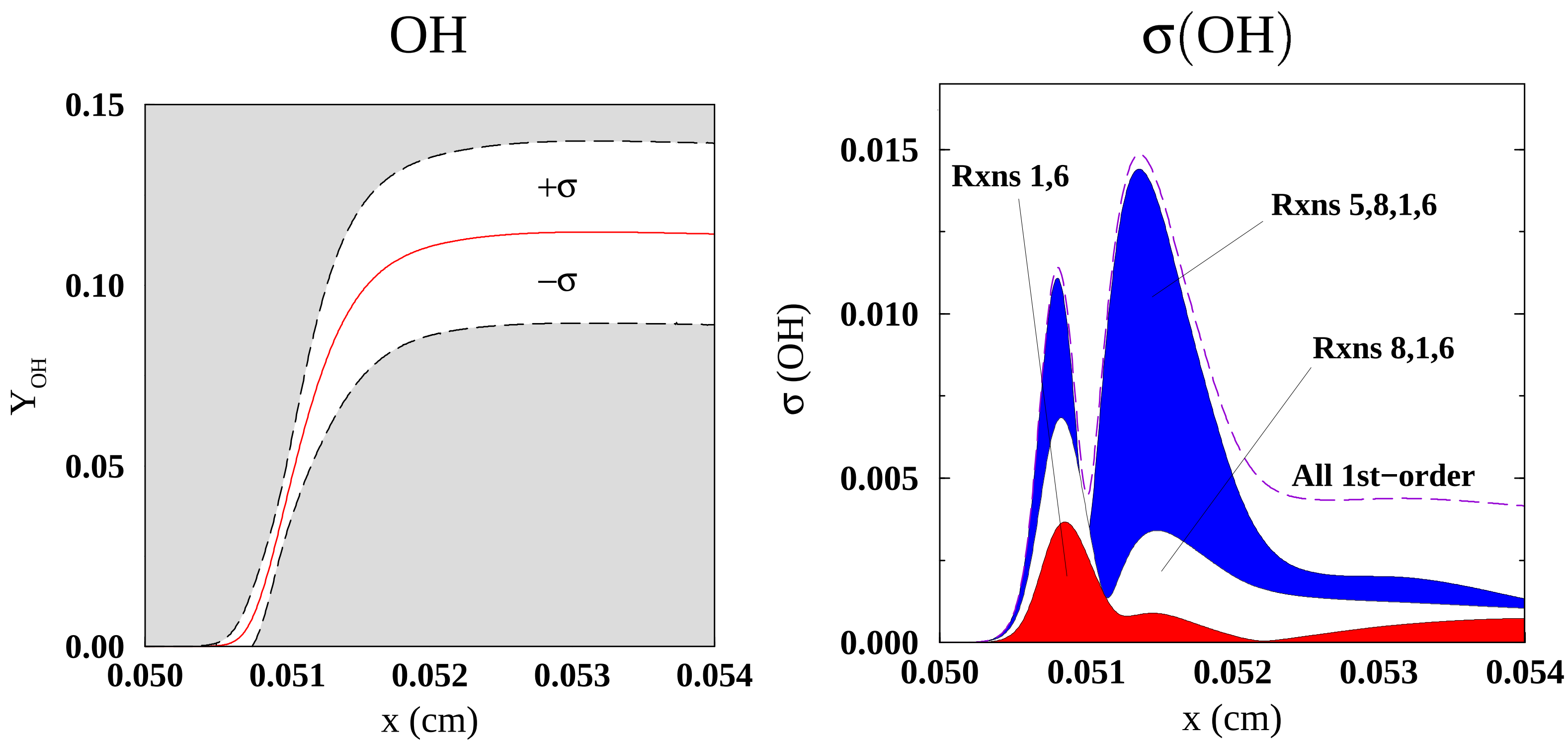
NISP UQ Application: Premixed H_2-O_2 Chemistry at Super-Critical Water Oxidation (SCWO) Conditions

- 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

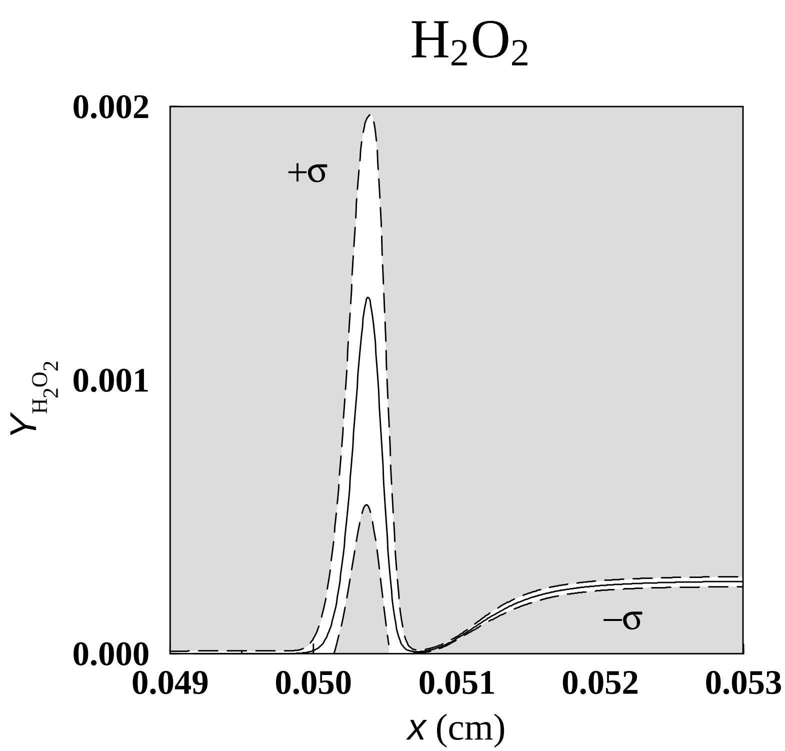
Species	μ_0	2σ
H	52.10	0.01
OH	9.3	0.2
H_2O	-57.80	0.01
H_2O_2	-32.53	0.07
HO_2	3.0	0.5

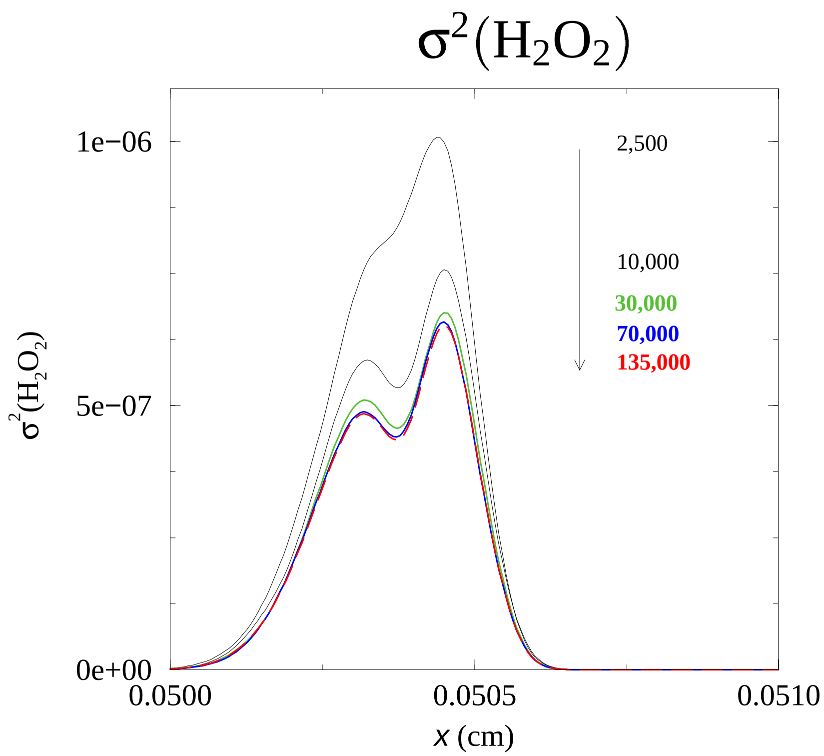
1D H_2-O_2 SCWO Flame NISP UQ/Chemkin-Premix



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

1D H_2-O_2 SCWO Flame NISP UQ/Chemkin-Premix
3^{rd} order PC





- Large uncertainty in H_2O_2 prediction
- Variance converges after 30,000 LHS samples

First-Order Sensitivity Information in a PC Expansion

- Conventional sensitivity

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

- Sensitivity in a stochastic UQ context

$$\lambda = \sum_0^P \lambda_k \Psi_k(\xi), \qquad u = \sum_0^P u_k \Psi_k(\xi), \qquad p(u) = f(x,t,p(\lambda))$$

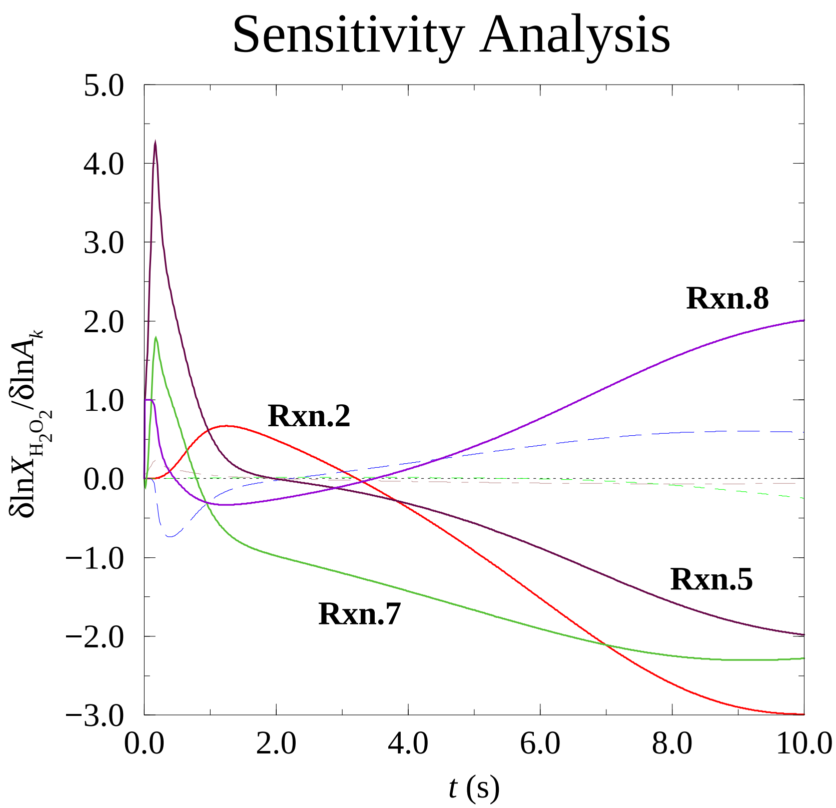
  – treat ξ as a continuous & differentiable independent variable
    * evaluate $\partial u/\partial\lambda$ over range of values of λ

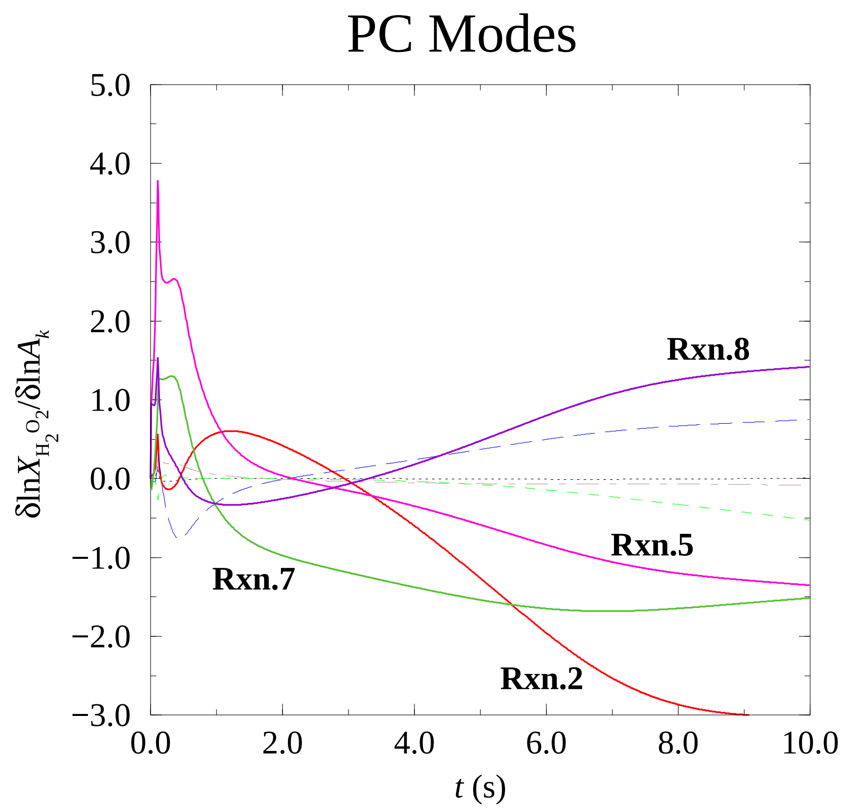
$$S = \frac{\partial u}{\partial \lambda} = \frac{\partial u/\partial \xi}{\partial \lambda/\partial \xi} = \frac{\sum_{k=0}^{P-1}(k+1)u_{k+1}\Psi_k}{\sum_{k=0}^{P-1}(k+1)\lambda_{k+1}\Psi_k} \qquad \text{(for Hermite } \Psi_{\mathrm{k}})$$

  – evaluate PC expansion for the *stochastic* sensitivity coefficient

$$S = \sum_{k=0}^{P} S_k \Psi_k, \qquad p(S) = F(x,t,p(\lambda),p(u))$$

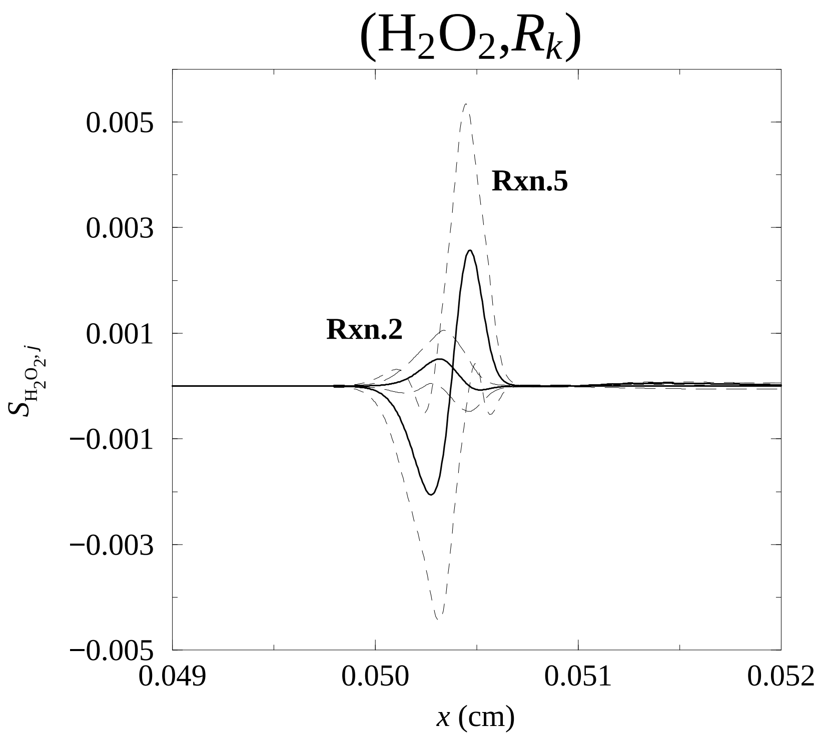
0D H_2-O_2 SCWO Isoth. Isob. Ignition : First Order Sensitivities

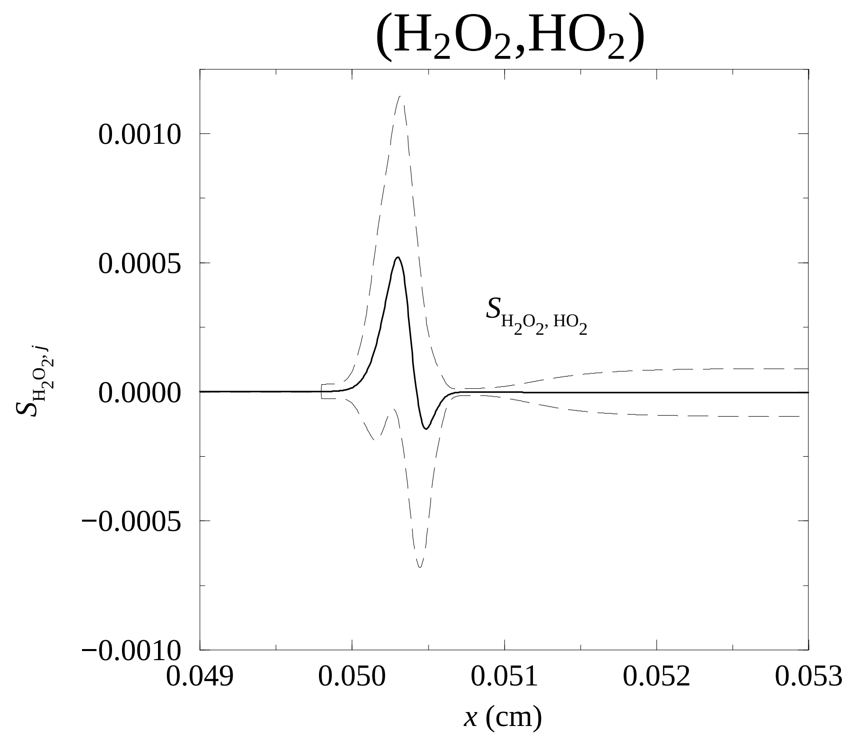




- H_2O_2 first-order sensitivity coefficients predicted from both conventional sensitivity analysis and first-order PC expansions are in overall agreement

SCWO Stochastic Sensitivities – Means and 1-σ Envelopes





- Uncertainty bounds in sensitivity coefficients provide for confidence intervals in sensitivity information
  - Can alter qualitative statements about system response

Intrusive Spectral Stochastic UQ Formulation: ODE Example

- Sample ODE with parameter λ: $\quad \dfrac{du}{dt} = \lambda u, \qquad u(0) = u_0$
- Let λ be uncertain : Represent it as a stochastic quantity
  - Introduce a new dimension ξ, where ξ is a Normal random variable
  - Use P-th order Polynomial Chaos (PC) expansions:

$$\lambda \; = \; \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \quad u = \sum_{k=0}^{P} u_k \Psi_k(\xi), \qquad (\lambda_k \text{ known, } u_k(t) \text{ unknown})$$

  - The Ψ_k's are orthogonal $\quad < \Psi_i \Psi_j > = < \Psi_i^2 > \delta_{ij}$
- Substitute PC expansions in the ODE, and apply Galerkin projection:

$$\frac{du_i}{dt} = \frac{\langle \lambda u \Psi_i \rangle}{\langle \Psi_i^2 \rangle} \; \equiv \; \langle \lambda u \rangle_i = \sum_{p=0}^{P} \sum_{q=0}^{P} \lambda_p u_q C_{pqi}, \quad i = 0, \cdots, P$$

where the $C_{pqi} = \langle \Psi_p \Psi_q \rangle_i$ 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 :

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

Governing Dimensionless Low Mach Number Equations

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

$$
\rho c_p \frac{DT}{Dt} = \frac{(\gamma - 1)}{\gamma} \frac{d p_o}{dt} + \frac{1}{RePr} \nabla \cdot (\lambda \nabla T) - \frac{\rho}{ReSc} \sum_{i=1}^{N} c_{p,i} \mathbf{V}_i \cdot \nabla T - Da \sum_{i=1}^{N} h_i w_i
$$

$$
\begin{aligned}
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho v Y_i) &= -\frac{1}{ReSc} \nabla \cdot (\rho Y_i \mathbf{V}_i) + Da\, w_i \qquad i = 1, \cdots, N \\
p_o &= \frac{\rho T}{\overline{\overline{W}}}
\end{aligned}
$$

- Low Mach No., no body forces, no radiation, mixture-averaged transport
- Neglect Soret and Dufour effects

Spectral UQ: Incompressible Flow - Stochastic Projection Method

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

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

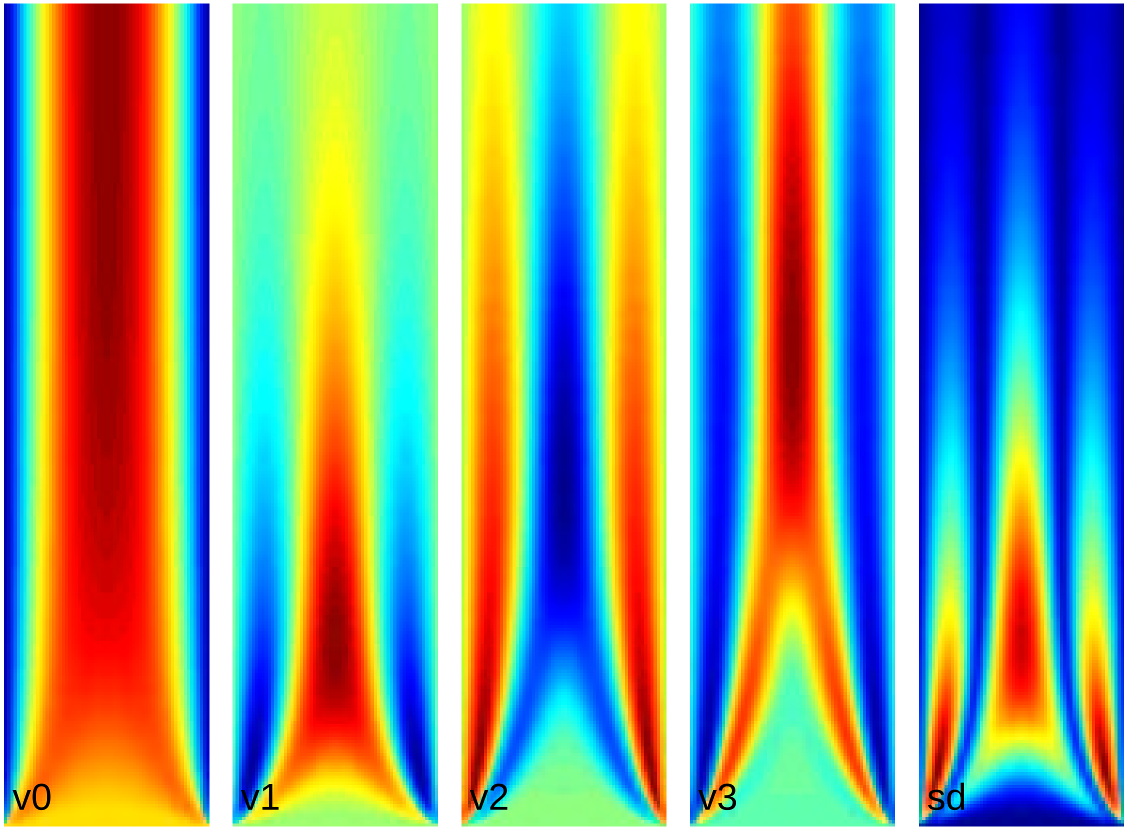
- Projection: for $q = 0, \ldots, P$:

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

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

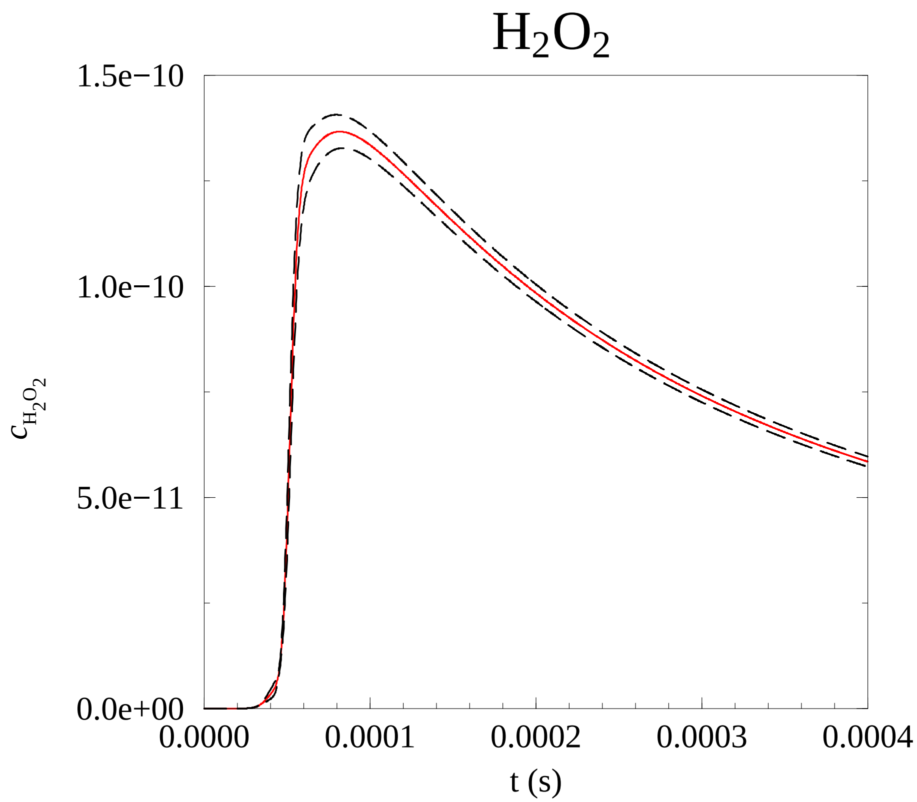
Laminar 2D Channel Flow with Uncertain Viscosity

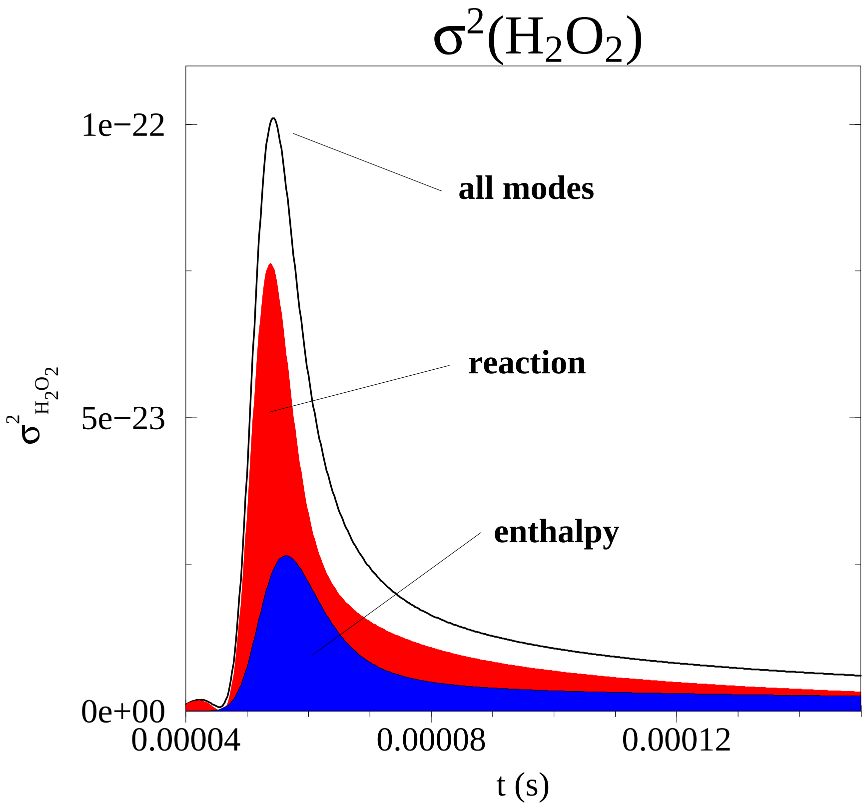
- Incompressible flow
- Gaussian viscosity PDF
  - $\nu = \nu_0 + \nu_1 \xi$
- Streamwise velocity
  - $v = \sum_{i=0}^{P} v_i \Psi_i$
  - v_0: mean
  - v_i: i-th order mode
  - $\sigma^2 = \sum_{i=1}^{P} v_i^2 \left\langle \Psi_i^2 \right\rangle$



v_0 v_1 v_2 v_3 σ

0D Intrusive H_2-Air Ignition : Uncertainty in $[H_2O_2]$

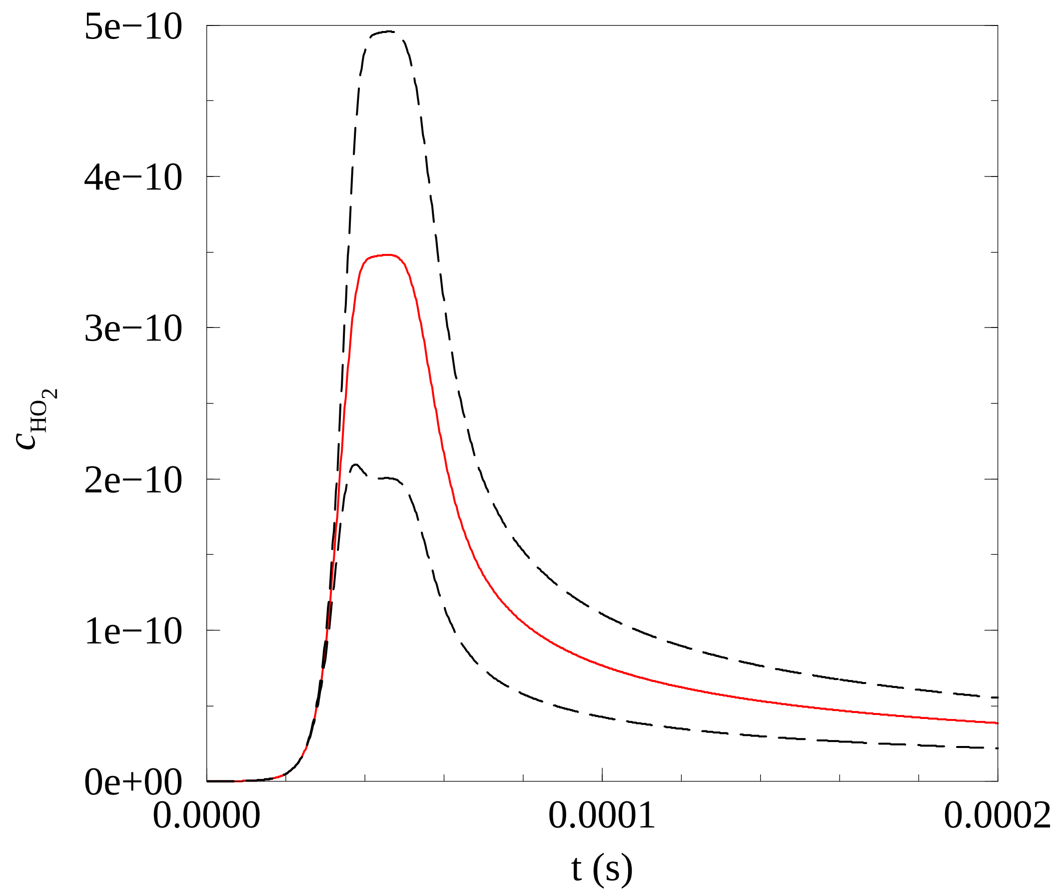




- 3^{rd}-order PC, 2 uncertain parameters
- Fast rise in the mean $[H_2O_2]$, little amplification in its uncertainty
- Rxn rate uncertainty has negligible consequence as equilibrium is approached

0D Intrusive H_2-Air Ignition : Uncertainty in $[HO_2]$

- Very fast rate of growth of the mean $[HO_2]$
- Followed by a similarly fast rise in the standard deviation
- Much larger uncertainty than H_2O_2
- COV of HO_2 is about 40%
  - persists near equilibrium
  - Amplification of enthalpy uncertainty



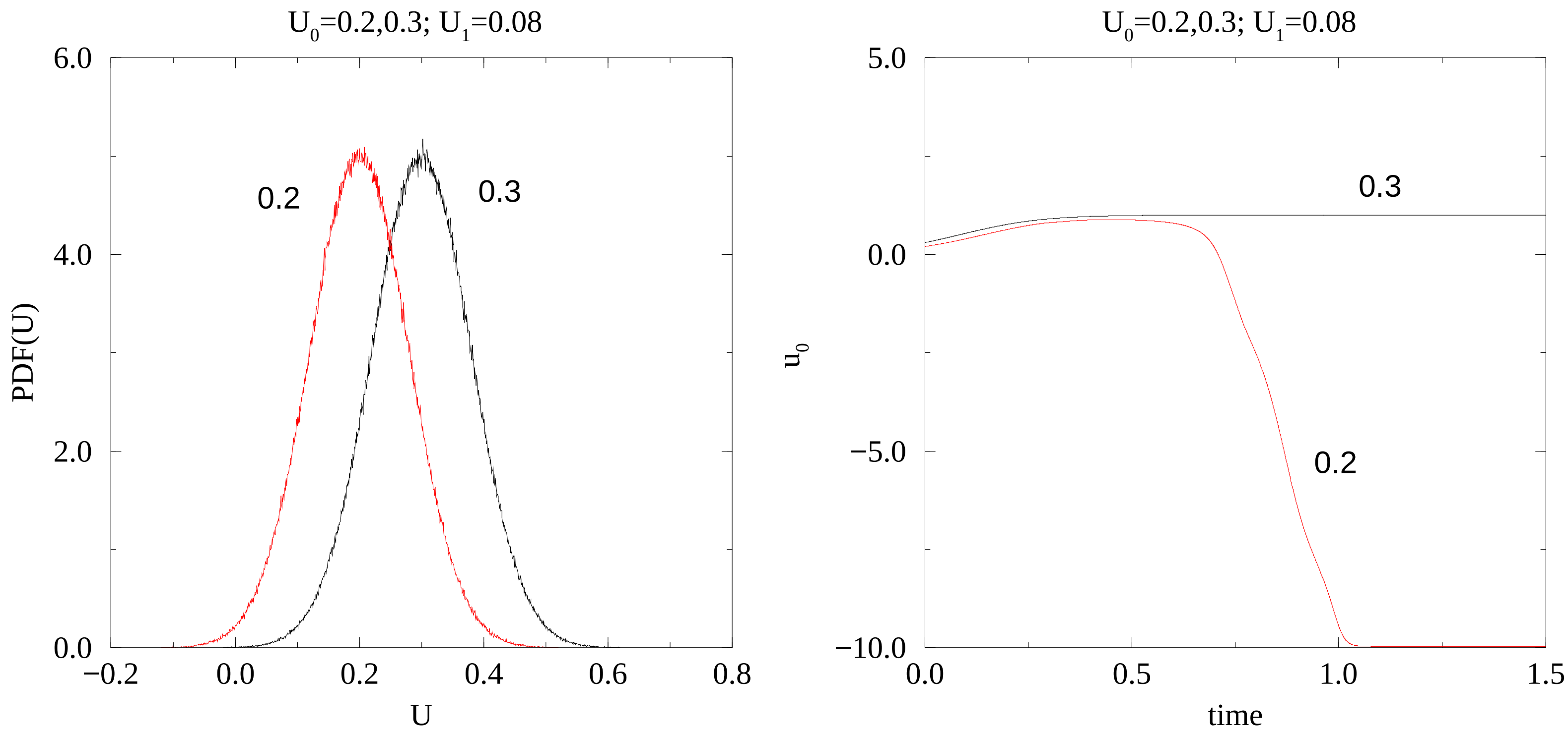
Experience with Instabilities and Intrusive PC UQ

- When integrating a chemical system, e.g. ignition, regions of explosive mode growth (positive eigenvalues) can lead to instabilities.
- Instability manifested in the fast growth of higher order modes, and fast drift of the solution towards unphysical values
- Typically occurs when the standard deviation increases significantly, becoming a sizeable fraction of the mean.
- Consider a model problem

$$\frac{du}{dt} = u(u+10)(1-u)$$

  Attractors at $u=-10$, $u=1$, and a repulsive fixed point at $u=0$.
- Let the initial condition $u(t=0)=U$ be stochastic, $U=\sum_{k=0}^{P} U_k \Psi_k$.
- Integrate the reformulated chaos system for the time evolution of u_k, $k=0,\ldots,P$

Model Problem: Consequence of Initial PDF tail zero crossing



- Given an initial condition U with a positive mean U_0
  - increasing σ_U/U_0 above $\approx$30% attracts u_0 towards negative territory
- Even for small σ_U, increasing the PC order leads to similar drift
- Similar behavior for Gaussian or Lognormal initial condition
- Similar behavior with the Laguerre polynomial/Gamma distribution basis

Conclusions

- Spectral stochastic UQ techniques offer significant analysis capabilities for chemical models
- Large predicted uncertainty in specific model outputs highlights the need for careful choice of flame observable for experimental validation
- Large numbers of LHS samples required for convergence of NISP
  - Particularly as PC order is increased
  - Pursue sparse-quadrature/cubature for high-dimensional integrals
- First-order PC UQ results agree with first-order sensitivity analysis
- Full-order PC, first-order sensitivity analysis
  - Quantify mean and distribution of sensitivity coefficient
- Intrusive PC UQ highly efficient for mildly nonlinear smooth problems
- Intrusive UQ with global PC expansions not robust for dynamical systems with potential bifurcations
  - Pursue local functional representation