Uncertainty Quantification in Low Mach Number Reacting Flow Computations

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Acknowledgement:

US Dept. of Energy, Div. of Chemical Sciences, Biosciences, and Geosciences
Sandia National Labs, LDRD Program

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

Numerical Integration of Atmospheric Premixed CH_4-Air Flames

- H Diffusivity, $D_{\mathrm{H,N_2,1900K}} \simeq 0.003\,\mathrm{m}^2/\mathrm{s}$
- Flame thermal thickness, $\delta_f \simeq 0.7\,\mathrm{mm}$
- CH-radical profile FWHM in the reaction zone, $\delta_{\mathrm{CH}} \simeq 100\ \mu\mathrm{m}$
  - Necessary spatial resolution, $\Delta x \simeq 15\mu\mathrm{m}$

- Convective CFL restriction

$$\frac{U_{\max}\Delta t}{\Delta x} < 1 \qquad \Rightarrow \Delta t < 1.5\,\mu\mathrm{s} \qquad (U = 10\ \mathrm{m/s})$$

- Explicit diffusion stability constraint in 2D

$$\frac{D_{\max}\Delta t}{\Delta x^2} < \frac{1}{4} \quad \Rightarrow \Delta t < 20\,\mathrm{ns}$$

- Chemical Stiffness, GRImech1.2 : $\Rightarrow \Delta t \leq 2\,\mathrm{ns}$ (Explicit)

Low Mach Number Approximation

- Expand flow quantities in terms of $\epsilon = \gamma M^2$

$$p = p_0 + \epsilon p_1 + \epsilon^2 p_2 + \cdots$$

- Take the limit as $M \longrightarrow 0$, retain lowest order terms
- Generally accepted for $M < 0.3$, i.e. $M^2 < 0.1$
- Consequences
  - Neglects elastic compressibility of the fluid
  - The zeroth-order (in ϵ) momentum equations reduce to $\nabla p_0 = 0$
  - The dynamic pressure $p_1 = p_1(\boldsymbol{x}, t)$ survives in the $(\mathcal{O}(\epsilon))$ mom. eqs
  - The stagnation pressure $p_0 = p_0(t)$ survives in the state equation
  - The state equation couples ρ and p_0
  - Coupling of $\boldsymbol{v}$ and ρ through the momentum equations and p is lost
  - Requires **both** low M^2 **and** fast acoustic time scales, vis. singing flames

Governing 2D Dimensionless Low Mach Number Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = -\frac{\partial p}{\partial x} + \frac{1}{Re}\left[\frac{4}{3}\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right) - \frac{2}{3}\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial x}\right)\right]$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho v u)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} = -\frac{\partial p}{\partial y} + \frac{1}{Re}\Phi_y$$

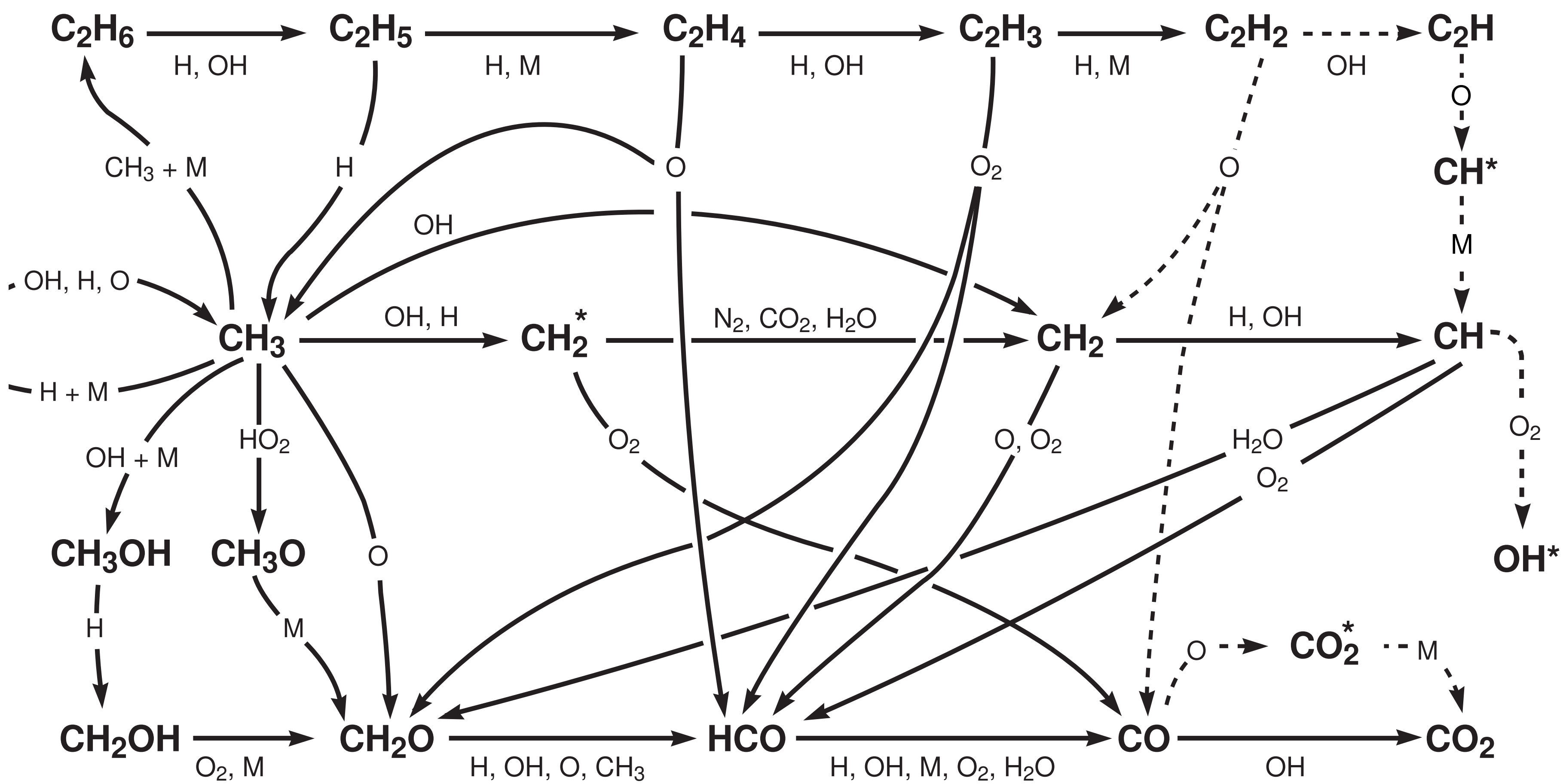
$$\rho c_p \frac{DT}{Dt} = \frac{(\gamma - 1)}{\gamma}\frac{dp_o}{dt} + \frac{1}{RePr}\nabla \cdot (\lambda \nabla T) - \frac{\rho}{ReSc}\sum_{i=1}^{N} c_{p,i}\mathbf{V}_i \cdot \nabla T - Da \sum_{i=1}^{N} h_i w_i$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) = -\frac{1}{ReSc}\nabla \cdot (\rho Y_i \mathbf{V}_i) + Da\ w_i \qquad i = 1, \cdots, N$$

$$p_o = \frac{\rho T}{\overline{\overline{W}}}$$

- 2D, Low Mach No., no body forces, no radiation.
- Neglect Soret and Dufour effects

Dominant Reaction Pathways, GRImech1.2, Atm. CH_4+Air



Intrusive Spectral Stochastic UQ Formulation

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

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

- 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

Intrusive Spectral Stochastic UQ Formulation: ODE Example

- Sample ODE with parameter λ:

$$\frac{du}{dt} = \lambda u, \qquad u(0) = u_0$$

- 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 Hermite polynomials $\quad < \Psi_i \Psi_j > = < \Psi_i^2 > \delta_{ij}$

- Substitute PC expansions for λ and u in the ODE, and reformulate:

$$\frac{du_i}{dt} = \sum_{p=0}^{P} \sum_{q=0}^{P} \lambda_p u_q C_{pqi}, \quad i = 0, 1, \cdots, P$$

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

Pros & Cons

- This intrusive spectral construction is potentially very efficient
  - N-dimensional **linear**: $du/dt = f(u)$, with M-gaussian parameters
    - requires one solution of a $2N$-dimensional linear system
  - Non-linearities and non-gaussian behaviour ... no general answer
- It allows the identification of individual contributions of model parameters to uncertainty in predictions
  - Highlights parameters where additional experimental measurements would have the greatest impact on improving the quality of predictions
- Significant complexity, model & numerics reformulation, code rewrite
- Non-linear chemical source terms may require high-order expansions
- Stability issues related to finite probabilities of negative concentrations
  - Hermite-polynomials and Normal ξ OK for weak nonlinearity
  - Need (non-Gaussian) ξ-basis with positive-support for chemistry
  - Laguerre-polynomials and Gamma-distributions may do well in flames

Chemical Source Term

- Complex and Expensive *Spectral* representation
  - Arrhenius rate expressions, thermodynamic properties, forward and reverse rates, third-body and pressure corrections
  - *Many*-dimensional expectation coefficients and summations
- Alternative *Pseudo-Spectral* technique
  - Simpler, Modular, Efficient
  - Projection of pair-wise products of n-order polynomials onto an n-order polynomial

Pseudo-Spectral Construction - 1

$$w = \lambda u^2 v, \qquad u = \sum_{k=0}^{P} u_k \Psi_k, \qquad \text{similarly for } \lambda \;\&\; v$$

Spectral : $$w_i = \sum_{j=0}^{P}\sum_{k=0}^{P}\sum_{l=0}^{P}\sum_{m=0}^{P} \lambda_j u_k u_l v_m \frac{\langle \Psi_j \Psi_k \Psi_l \Psi_m \Psi_i \rangle}{\langle \Psi_i^2 \rangle}, \quad i = 0, \ldots, P$$

Pseudo-Spectral: Project each product onto a $(P+1)$-polynomial before proceeding further

$$\tilde{w} = uv \quad \Rightarrow \quad \tilde{w}_i = \sum_{j=0}^{P}\sum_{k=0}^{P} u_k v_j \frac{\langle \Psi_k \Psi_j \Psi_i \rangle}{\langle \Psi_i^2 \rangle}, \quad i = 0, \ldots, P$$

$$\hat{w} = u\tilde{w} \quad \Rightarrow \quad \hat{w}_i = \sum_{j=0}^{P}\sum_{k=0}^{P} u_k \tilde{w}_j \frac{\langle \Psi_k \Psi_j \Psi_i \rangle}{\langle \Psi_i^2 \rangle}, \quad i = 0, \ldots, P$$

$$w = \lambda\hat{w} \quad \Rightarrow \quad w_i = \sum_{j=0}^{P}\sum_{k=0}^{P} \lambda_k \hat{w}_j \frac{\langle \Psi_k \Psi_j \Psi_i \rangle}{\langle \Psi_i^2 \rangle}, \quad i = 0, \ldots, P$$

Pseudo-Spectral Construction for Non-Polynomial Functions

- How to propagate PC expansions ($\{u_k\} \Rightarrow \{v_k\}$) through functions like

$$v = \frac{1}{u}, \quad v = \ln\, u, \quad \text{or} \quad v = e^{u}$$

- Use local polynomial approximations, e.g. Taylor series ? ... NO
  - Fragile
  - convergence issues
  - high-order PC multiplications
  - instabilities

Inversion and division can be done without Taylor series.

- Assume three stochastic variables a, b, and c

$$c = \frac{a}{b} \Rightarrow \qquad b \cdot c = a$$

- Mode k of stochastic product $a = b \cdot c$

$$\sum_{m=0}^{P} \sum_{l=0}^{P} C_{klm} b_l \cdot c_m = a_k$$

- System of $P + 1$ linear algebraic equations in c_m with known a_k and b_l,

$$B_{km} = \sum_{l=0}^{P} C_{klm} b_l, \quad \mathbf{Bc} = \mathbf{a}$$

- Solve using GMRES, or your favorite linear solver
- More robust than Taylor series expansion for $1/u$
- What about the condition number of $\mathbf{B}$?

Integration approach for non-polynomial functions —- (1)

- Require: $u = u(x)$ with $\dot{u} = \mathrm{d}u/\mathrm{d}x$ being a rational function of u and/or x
- For $x \in \mathbb{R}$, $u \in \mathbb{R}^{\mathbb{R}}$, u is the solution of the ODE : $\mathrm{d}u/\mathrm{d}x = \dot{u}$

$$\mathrm{d}u = \dot{u}\mathrm{d}x$$

$$u(x_b) - u(x_a) = \int_{x_a}^{x_b} \dot{u}\, \mathrm{d}x$$

- Then, let x,u, and $v = \dot{u}$ be given by their PC expansions,

$$x(s,\theta) = \sum_{i=0}^{P} x_i(s)\Psi_i(\theta), \quad u(s,\theta) = \sum_{i=0}^{P} u_i(s)\Psi_i(\theta), \quad v(s,\theta) = \sum_{i=0}^{P} v_i(s)\Psi_i(\theta)$$

where s parameterizes the evolution of the spectral mode strengths along a path in the x-space from x_a to x_b.

Integration approach for non-polynomial functions — (2)

Then

$$\left.\frac{\partial u}{\partial s}\right|_\theta = v\left.\frac{\partial x}{\partial s}\right|_\theta, \qquad \text{and} \qquad \int_{s_a}^{s_b} \left.\frac{\partial u}{\partial s}\right|_\theta \mathrm{d}s = \int_{s_a}^{s_b} v\left.\frac{\partial x}{\partial s}\right|_\theta \mathrm{d}s$$

where

$$\left.\frac{\partial u}{\partial s}\right|_\theta = \sum_{i=0}^{P} \frac{\mathrm{d}u_i}{\mathrm{d}s}\Psi_i$$

$$\left.\frac{\partial x}{\partial s}\right|_\theta = \sum_{i=0}^{P} \frac{\mathrm{d}x_i}{\mathrm{d}s}\Psi_i$$

and, substituting above

$$\sum_{i=0}^{P} \Psi_i \int_{s_a}^{s_b} \frac{\mathrm{d}u_i}{\mathrm{d}s}\mathrm{d}s = \int_{s_a}^{s_b} (\sum_{i=0}^{P} v_i\Psi_i)(\sum_{j=0}^{P} \frac{\mathrm{d}x_j}{\mathrm{d}s}\Psi_j)\,\mathrm{d}s$$

or

$$\sum_{i=0}^{P} \Psi_i(u_i(s_b) - u_i(s_a)) = \sum_{j=0}^{P} \int_{s_a}^{s_b} \sum_{i=0}^{P} \Psi_i\Psi_j v_i \frac{\mathrm{d}x_j}{\mathrm{d}s}\,\mathrm{d}s$$

Integration approach for non-polynomial functions — (3)

Then, apply Galerkin projection on the k-th mode,

$$u_k(s_b) - u_k(s_a) = \sum_{j=0}^{P} \int_{s_a}^{s_b} \sum_{i=0}^{P} C_{ijk} v_i \frac{\mathrm{d}x_j}{\mathrm{d}s} \,\mathrm{d}s$$

Consider the integral :

$$I_{jk} = \int_{s_a}^{s_b} \sum_{i=0}^{P} C_{ijk} v_i \frac{\mathrm{d}x_j}{\mathrm{d}s} \,\mathrm{d}s$$

Since $v = v(u(x), x)$, then $v_i = v_i(x) = v_i(x_0, x_1, \cdots, x_P)$. In the evaluation of I_{jk}, only one x-coefficient, x_j is varied, while $x_{r \neq j}$ are constant. Thus, in this context, $v_i = v_i(x_j; x_{r \neq j}) = v_i(x_j)$, such that

$$I_{jk} = \int_{x_j(s_a)}^{x_j(s_b)} \sum_{i=0}^{P} C_{ijk} v_i \mathrm{d}x_j$$

and

$$u_k(s_b) - u_k(s_a) = \sum_{j=0}^{P} \int_{x_j(s_a)}^{x_j(s_b)} \sum_{i=0}^{P} C_{ijk} v_i \mathrm{d}x_j$$

Integration approach for non-polynomial functions — (4)

Thus

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

- To evaluate $u(x)$, $x = \sum_{k=0}^{P} x_k \Psi_k$, $u = \sum_{k=0}^{P} u_k \Psi_k$,
  - use an initial condition x_a such that $u(x_a)$ is known
    ... e.g. $x_a = x_0 \in \mathbb{R}$, and $u(x_a) = u(x_0) = u_0 \in \mathbb{R}$, $u_{k>0}(x_a) = 0$
  - express $\dot{u} = \mathrm{d}u/\mathrm{d}x = f(u, x)$, where f is a rational function
    ... ensures that $(\dot{u})_k$ are readily found from the known u_k and x_k coeffs at each integration step
- ok for e^x, e^{x^2}, and $\ln(x)$, with $\dot{u} = u$, $2xu$, and $1/x$ resp.
  - but not for $e^{\sin(x)}$, with $\dot{u} = u \cos(x)$
- Increased accuracy and robustness compared to Taylor series expansions
- Agrees well with directly-sampled PDFs
  - if PC order is high enough to accurately describe solution statistics

Spectral UQ Formulation: Incompressible Flow – Stochastic Projection Method

- Formulation:

$$\frac{\partial u_q}{\partial t} + \sum_{j,k=0}^{P} \mathcal{C}_{jk} C_{jkq} = -\frac{\partial p_q}{\partial x} + \frac{1}{Re} \sum_{i,j=0}^{P} \mathcal{D}_{ij} C_{ijq}, \qquad (1D)$$

$$\frac{\partial \mathrm{v}_q}{\partial t} = C_q - \nabla p_q + D_q, \qquad 2D : \mathrm{v} = (u, v)$$

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

$$\frac{\tilde{\mathrm{v}}_q - \mathrm{v}_q^n}{\Delta t} = C_q^n + D_q^n$$

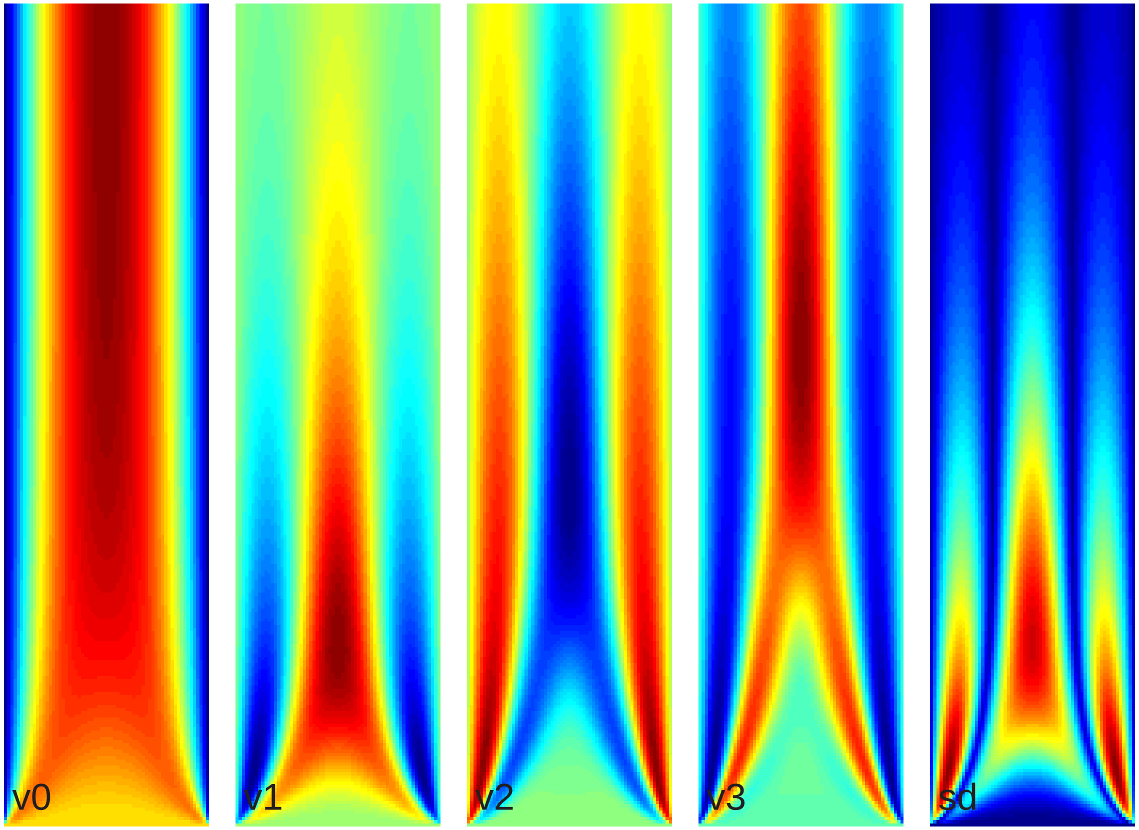
$$\nabla^2 p_q = \frac{-1}{\Delta t} \nabla \cdot \tilde{\mathrm{v}}_q$$

$$\frac{\mathrm{v}_q^{n+1} - \tilde{\mathrm{v}}_q}{\Delta t} = -\nabla p_q$$

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

Laminar 2D Channel Flow with Stochastic 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
  - $\sigma = \sqrt{\sum_{i=1}^{P} v_i^2 < \Psi_i^2 >}$



v_0 v_1 v_2 v_3 σ

Spectral UQ Formulation: low M 2D Momentum Equations

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = -\frac{\partial p}{\partial x} +$$

$$\frac{1}{Re}\left[\frac{4}{3}\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right) - \frac{2}{3}\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial x}\right)\right]$$

$$u = \sum_{k=0}^{P} u_k \Psi_k, \quad v = \sum_{k=0}^{P} v_k \Psi_k, \quad \rho = \sum_{k=0}^{P} \rho_k \Psi_k, \quad p = \sum_{k=0}^{P} p_k \Psi_k, \quad \mu = \sum_{k=0}^{P} \mu_k \Psi_k$$

$$U = \rho u = \sum_{k=0}^{P} U_k \Psi_k, \quad C_{ijkq} = \frac{\langle \Psi_i \Psi_j \Psi_k \Psi_q \rangle}{\langle \Psi_q^2 \rangle}, \quad C_{ijq} = \frac{\langle \Psi_i \Psi_j \Psi_q \rangle}{\langle \Psi_q^2 \rangle}$$

$$\frac{\partial U_q}{\partial t} + \sum_{i,j,k=0}^{P}\left[\frac{\partial(\rho_i u_j u_k)}{\partial x} + \frac{\partial(\rho_i u_j v_k)}{\partial y}\right] C_{ijkq} = -\frac{\partial p_q}{\partial x} +$$

$$\frac{1}{Re}\sum_{i,j=0}^{P}\left[\frac{4}{3}\frac{\partial}{\partial x}\left(\mu_i\frac{\partial u_j}{\partial x}\right) - \frac{2}{3}\frac{\partial}{\partial x}\left(\mu_i\frac{\partial v_j}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu_i\frac{\partial u_j}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu_i\frac{\partial v_j}{\partial x}\right)\right] C_{ij}$$

Spectral UQ Formulation: Species Conservation Equation

$$\frac{\partial(\rho Y_i)}{\partial t} = -\nabla\cdot(\rho \mathrm{v} Y_i) + \frac{1}{Re\ Sc}\nabla\cdot(\rho D_i \nabla Y_i) + Da\ w_i, \qquad i = 1,\ldots,N$$

$$\rho = \sum_{k=0}^{P}\rho_k\Psi_k, \quad Y_i = \sum_{k=0}^{P}\rho_k\Psi_k, \quad \mathrm{v} = \sum_{k=0}^{P}\mathrm{v}_k\Psi_k, \quad D_i = \sum_{k=0}^{P}D_{i,k}\Psi_k, \quad w_i = \sum_{k=0}^{P}w_{i,k}\Psi_k$$

$$R_i = \rho Y_i = \sum_{k=0}^{P}R_{i,q}\Psi_q$$

$$\frac{\partial R_{i,q}}{\partial t} = -\sum_{j,k,p=0}^{P}\left[\nabla\cdot(\rho_j \mathrm{v}_k Y_{i,p}) + \frac{1}{Re\ Sc}\nabla\cdot(\rho_j D_{i,k}\nabla Y_{i,p})\right] C_{jkpq} + Da\ w_{i,q}$$

$$(q = 0,\ldots,P. \quad i = 1,\ldots,N)$$

- Explicit Operator-Split transport terms integration
- Implicit chemical source term integration: $N(P+1)$ coupled ODEs

Non-intrusive Spectral (NIS) UQ Formulation

- Construct spectral stochastic descriptions of uncertain parameters λ
- Sample parameter space and compute Monte-Carlo (MC) realizations of the deterministic model $u^i(t)$, $i = 1, \ldots, N$
- Project MC statistics on the spectral mode strengths $u_k(t)$

$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

- Sacrifices efficiency for reduced complexity *and* stability
  - May require excessively large number of samples to converge
- Retains spectral sensitivity information
- Allows designing UQ wrappers around legacy code

Sampling Issues in Non-Intrusive Spectral (NIS) Uncertainty Quantification (UQ)

- Need to minimize the number of samples required for evaluating spectral mode strengths
- Collocation techniques (DEMM, SRSM)
  - Minimize errors at sample points
  - High efficiency : number of samples $\sim$ number of unknowns
- Galerkin projection (NISP)
  - Minimize RMS error
  - Less efficient but potentially more robust to nonlinearities
  - Projection is a Quadrature operation - samples are quadrature points
    * Latin Hypercube Sampling
    * Gauss-Hermite Quadrature
    * Sparse Quadrature / Cubature

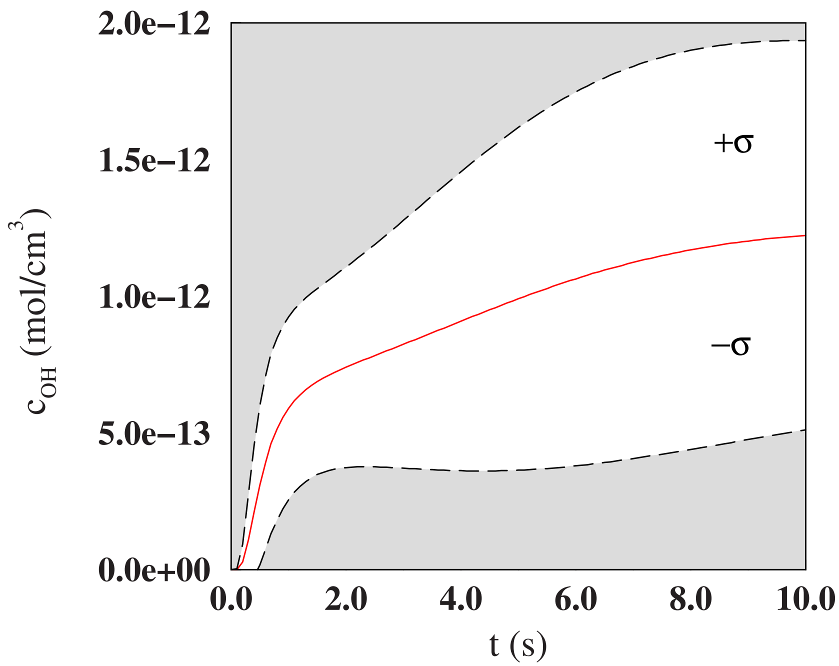
NISP UQ Application: 0D/1D Premixed H_2-O_2 at Super-Critical Water Oxidation (SCWO) Conditions

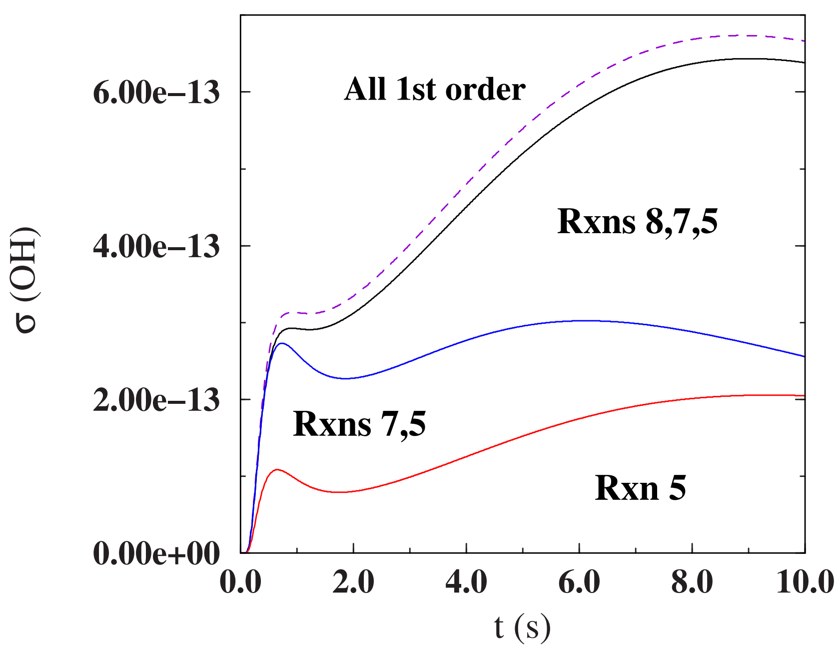
- Allow uncertainties in reaction rate constants and thermodynamic properties, per published experimental data
- Wrap NIS processing around a deterministic reacting flow code
- Using 8-step simplified SCWO Hydrogen mechanism (McRae)

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

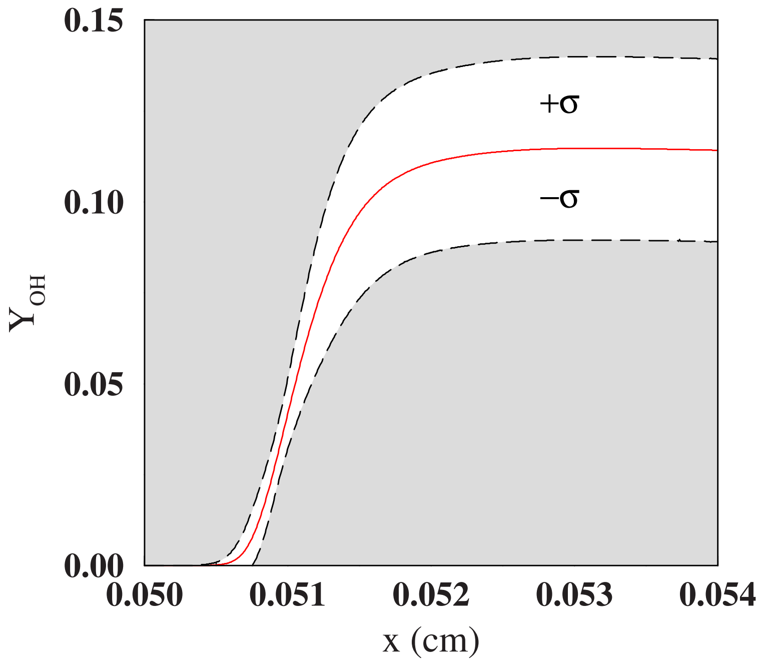
0D H_2-O_2 SCWO Ignition

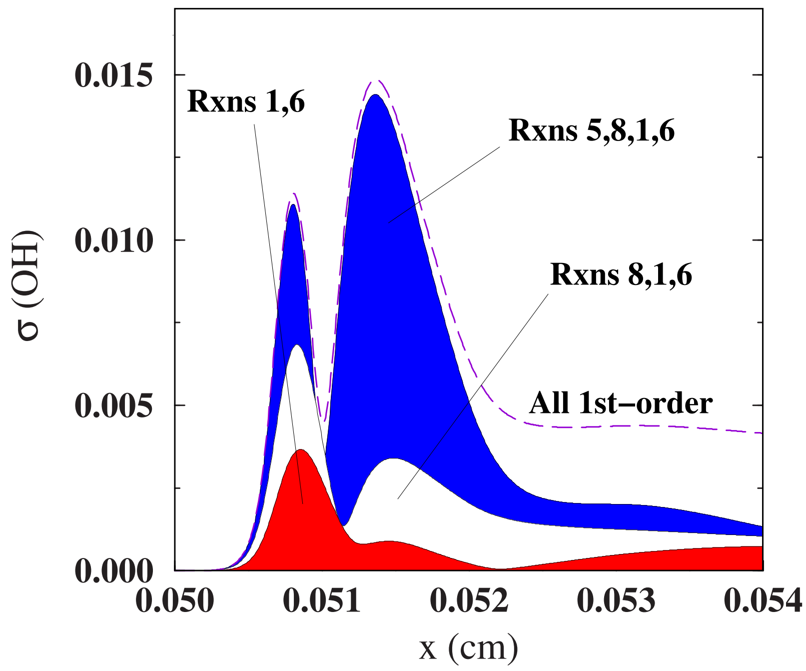




- Mean and standard deviation predictions validated against published data
- Initial fast growth in uncertainty followed by a slower approach to a steady-state with *large* OH uncertainty
- Reactions 7 & 8 have dominant roles in the OH uncertainty

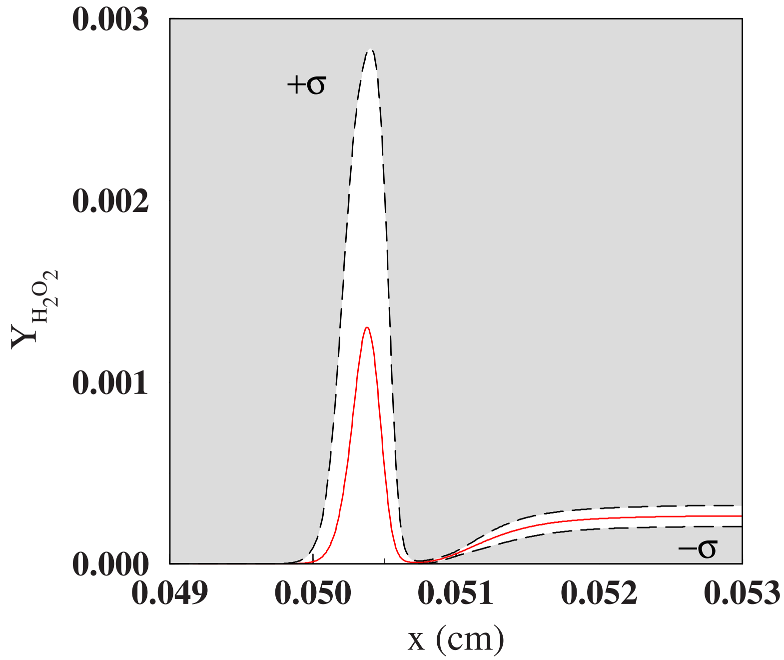
1D H_2-O_2 SCWO Flame NISP UQ/Chemkin-Premix

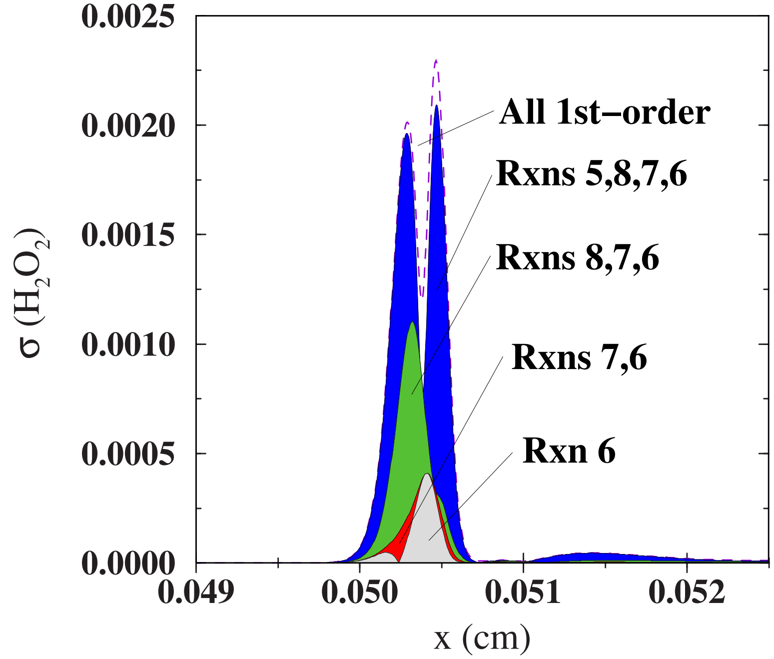




- 1D freely propagating H_2-O_2 flame at SCWO conditions
- Fast growth in OH uncertainty in the primary reaction zone
- Steady level of uncertainty and mean of OH in the post-flame region
- Uncertainty in pre-exponential of Rxn.5 (H_2O_2+OH=H_2O+HO_2) has largest contribution to uncertainty in the predicted OH field

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

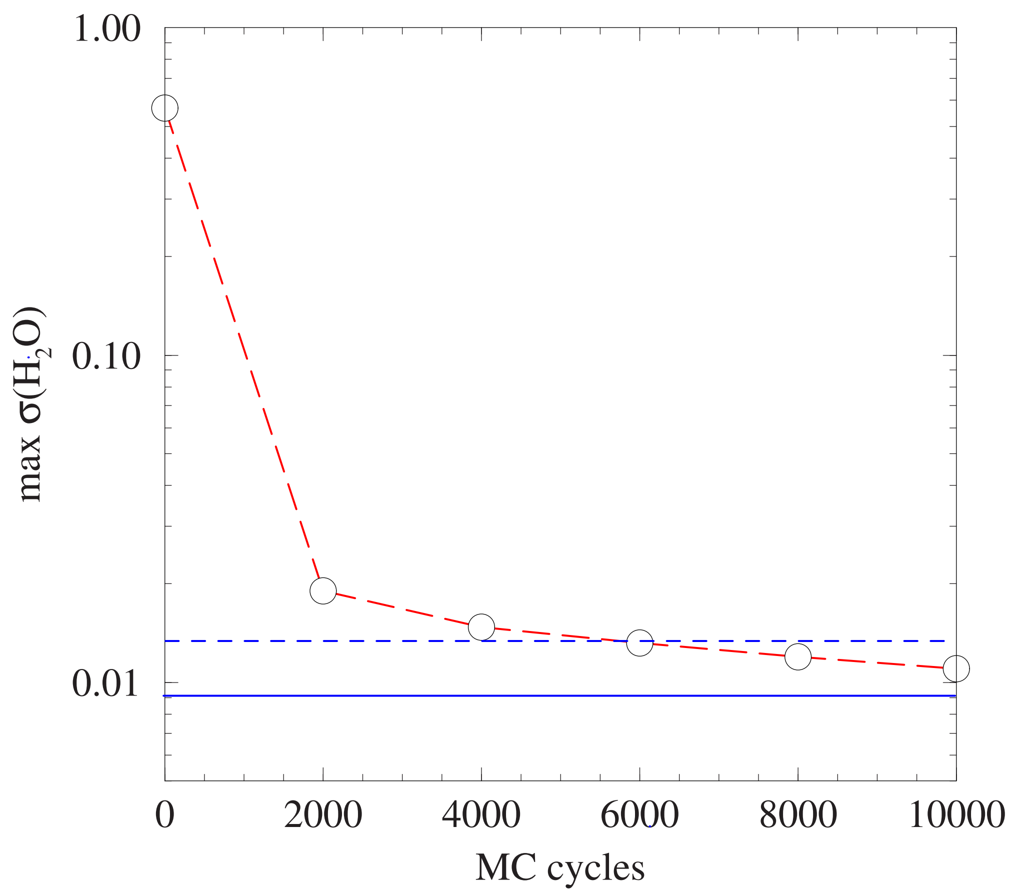




- Very large uncertainty in H_2O_2 prediction, COV=σ/μ=100% !!
- Dominant source is again Rxn.5 (H_2O_2+OH=H_2O+HO_2)
- Not a robust model for predicting H_2O_2 under SCWO conditions
- Results highlight the utility of additional experimental measurements of A_5

CPU-time Savings with Intrusive Spectral Strategy

- 0D H_2-O_2 SCWO ignition
- NISP standard deviation tends to that from the intrusive construction
- NISP comes to within 50% of the intrusive value after 6000 Latin-Hypercube realizations
- 6000 sample runs $\sim$ 48 CPU hrs
- 1 intrusive run $\sim$ 2 hrs



Experience with Instabilities

- When integrating a chemical system, e.g. ignition or 1D flame, 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
- Resulting fast rate of growth leads to failure due to finite arithmetic precision
- Adaptive stiff integrator (e.g. DVODE) unable to keep up the integration
- Typically occurs when the standard deviation increases significantly, becoming a sizeable fraction of the mean.
- Increasing PC order does not help much

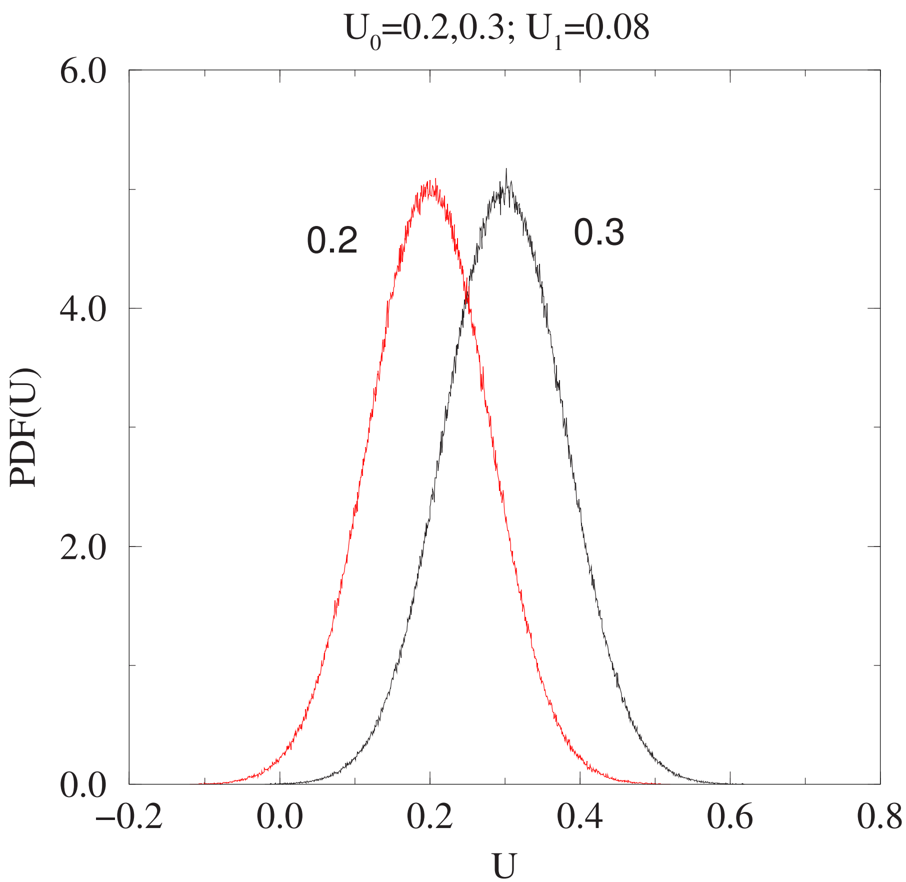
A Study of *Intrusive* UQ Instabilities using a Model Problem

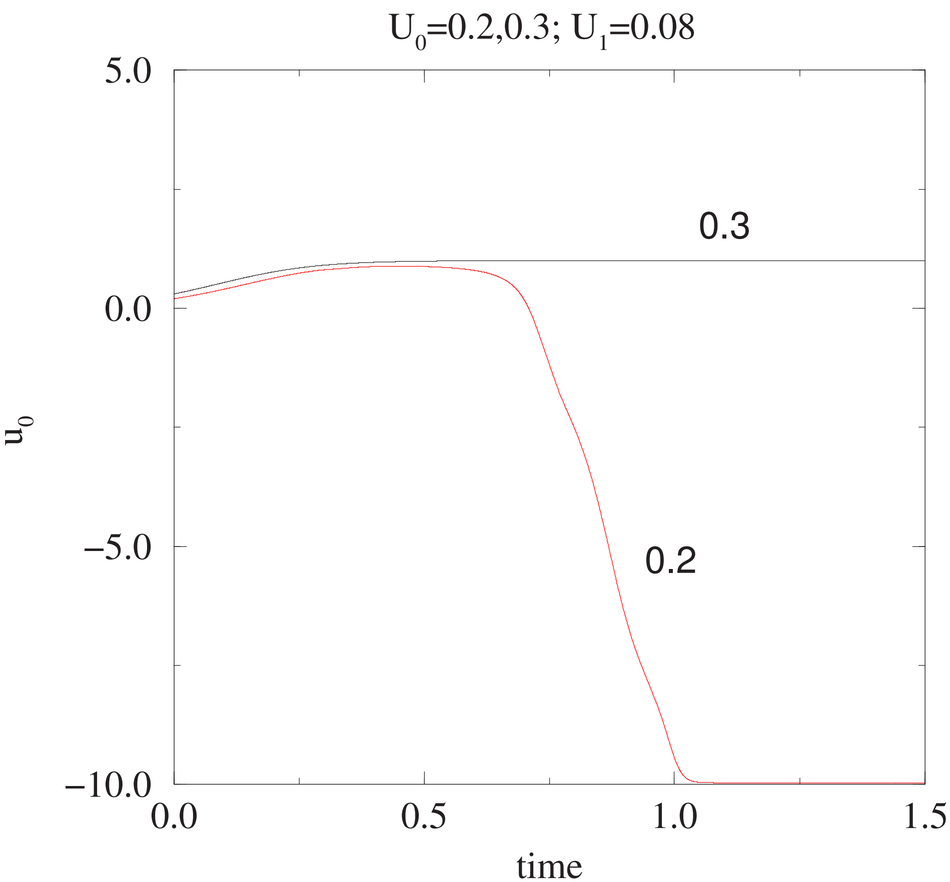
- Does the truncation of the PC expansion at P, and the resulting truncation error, lead to numerical instabilities akin to aliasing of unresolved high wavenumber energy in finite difference discretizations, and corruption of low wavenumber modes?
- Is a minimum spectral mode strength decay rate necessary for stability?
- Consider a model problem

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

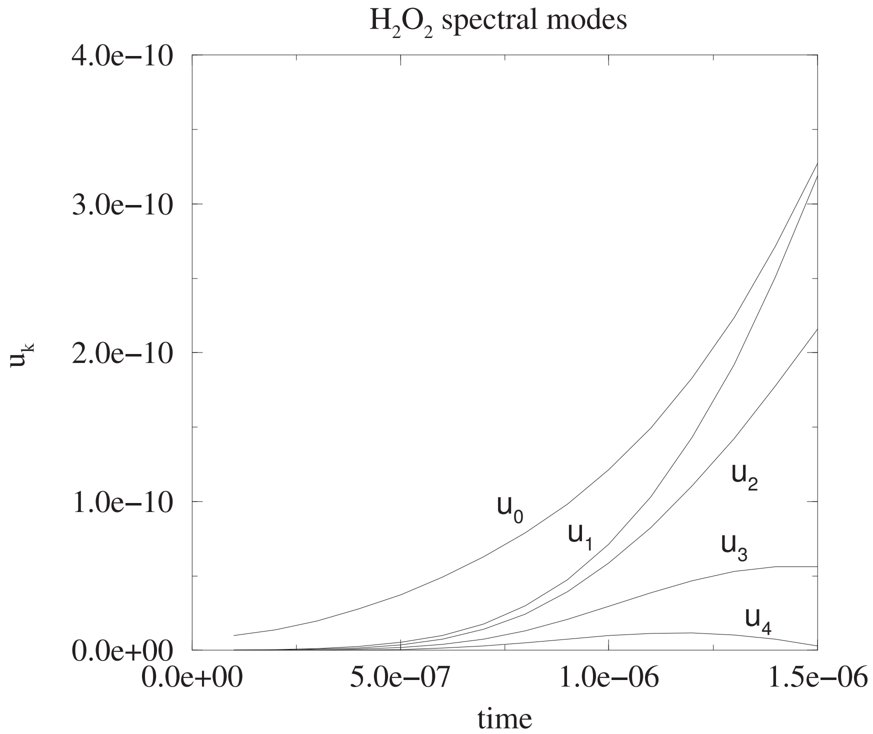
  Attractors at $u = -10$, $u = 1$, and a repulsive fixed point at $u = 0$.
- Let the initial condition $u(t = 0) = U$ be stochastic, $U = \sum_{k=0}^{P} U_k \Psi_k$.
- Integrate the reformulated chaos system for the time evolution of u_k, $k = 0, \ldots, P$, using DVODE

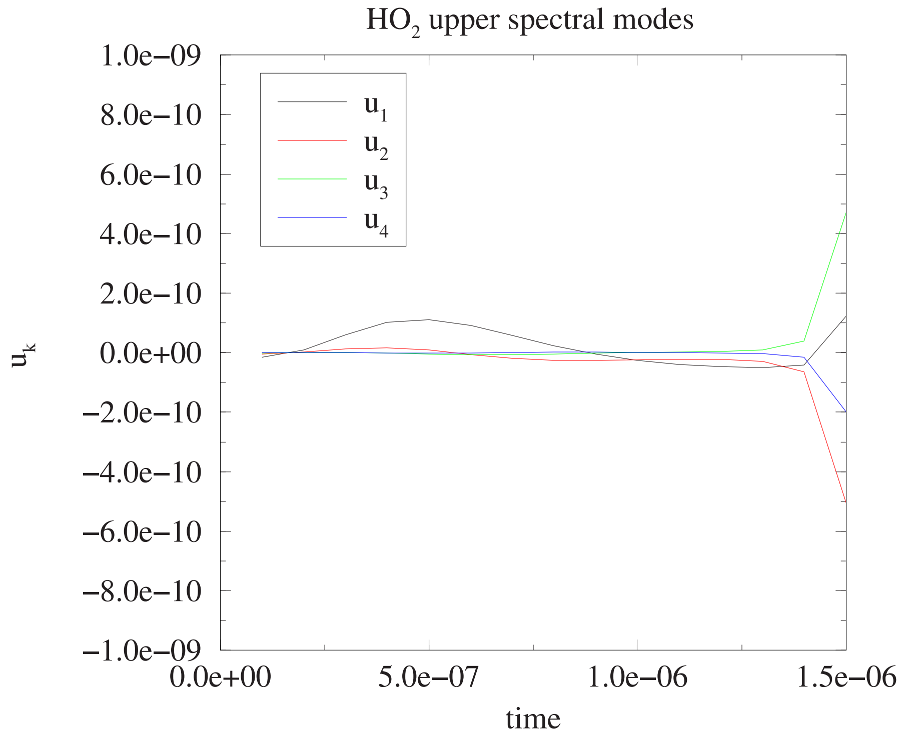
Model Problem: Two Finite Attractors: Consequence of Initial PDF tail zero crossing





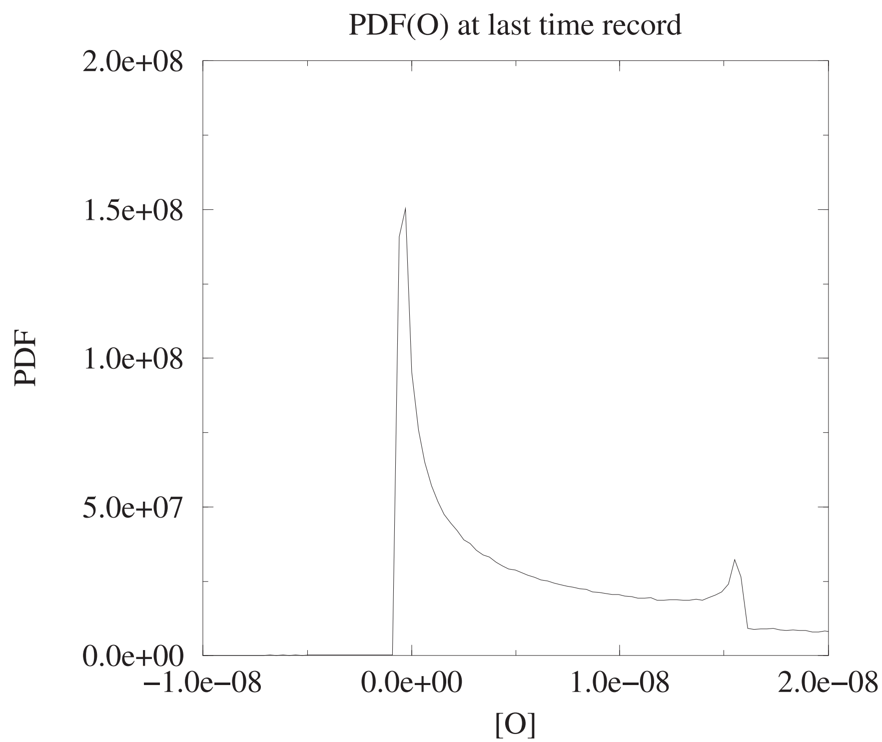
Ignition Instability — (1)





- Blowup occurs as u_1 approaches u_0.
- Large rates of change observed in higher order modes.
- Problem is typically observed when the computed PC expansions of physical quantities (e.g. ρ, T, Y_i) correspond to PDFs with significant probability of negative values.

Ignition Instability — (2)



- PDF of [O] exhibits significant probability of non-physical negative values
- Finite probability of zero values of ρ would lead to ill-conditioned stochastic inversion matrices for $T = 1/\rho$

Summary

- UQ analysis is necessary for validation and improved understanding of the robustness and reliability of reacting flow models
- Spectral stochastic techniques offer significant efficient analysis capabilities allowing a detailed understanding of the role of each uncertain parameter in the model
- These techniques have been demonstrated in non-reacting and reacting 0D/1D/2D low Mach number flows
- Intrusive/non-intrusive versions provide requisite sensitivity information
  - Intrusive construction was found to be *much* more efficient than the non-intrusive MC-based approach, for 0D ignition
- Non-linearities of chemical source terms offers challenges as regards the growth of uncertainty, bifurcation, etc, for *large* uncertainties in parameters
- Investigate alternative bases, e.g. Laguerre-Gamma