

Lecture 2

- Intrusive PC UQ
 - Basic ODE implementation
 - Pseudo-spectral construction
 - convection-diffusion equation
 - Navier-Stokes equations
 - chemical ignition
- Non-intrusive PC UQ
 - Random sampling
 - Non-Intrusive Spectral Projection (NISP)
 - Stochastic Sensitivity coefficients
 - Deterministic sampling: quadrature, cubature

Intrusive Spectral Stochastic UQ Formulation: ODE Example

- Sample ODE with parameter λ :

$$\frac{du}{dt} = \lambda u$$

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

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

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

Galerkin Projection on $\Psi_i(\xi)$

$$\frac{d}{dt} \left(\sum_{k=0}^P u_k(t) \Psi_k(\xi) \right) = \left(\sum_{p=0}^P \lambda_p \Psi_p(\xi) \right) \left(\sum_{q=0}^P u_q(t) \Psi_q(\xi) \right)$$

$$\sum_{k=0}^P \frac{du_k(t)}{dt} \Psi_k(\xi) = \sum_{p=0}^P \sum_{q=0}^P \lambda_p u_q(t) \Psi_p(\xi) \Psi_q(\xi)$$

$$\left\langle \sum_{k=0}^P \frac{du_k(t)}{dt} \Psi_k(\xi) \Psi_i(\xi) \right\rangle = \left\langle \sum_{p=0}^P \sum_{q=0}^P \lambda_p u_q(t) \Psi_p(\xi) \Psi_q(\xi) \Psi_i(\xi) \right\rangle$$

$$\sum_{k=0}^P \frac{du_k(t)}{dt} \langle \Psi_k(\xi) \Psi_i(\xi) \rangle = \sum_{p=0}^P \sum_{q=0}^P \lambda_p u_q(t) \langle \Psi_p(\xi) \Psi_q(\xi) \Psi_i(\xi) \rangle$$

$$\frac{du_i}{dt} \langle \Psi_i^2 \rangle = \sum_{p=0}^P \sum_{q=0}^P \lambda_p u_q \langle \Psi_p \Psi_q \Psi_i \rangle$$

Resulting Spectral ODE system

- $(P + 1)$ -dimensional ODE system

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

where $C_{pqi} = \langle \Psi_p \Psi_q \Psi_i \rangle / \langle \Psi_i^2 \rangle$

- The tensor C_{pqi} can be evaluated once and stored for any given PC order and dimension

1D 4th-Order C_{ijk} Example

$\langle \Psi_i \Psi_j \Psi_k \rangle$	value
$\langle \Psi_0 \Psi_0 \Psi_0 \rangle$	1
$\langle \Psi_0 \Psi_1 \Psi_1 \rangle$	1
$\langle \Psi_0 \Psi_2 \Psi_2 \rangle$	2
$\langle \Psi_0 \Psi_3 \Psi_3 \rangle$	6
$\langle \Psi_0 \Psi_4 \Psi_4 \rangle$	24
$\langle \Psi_1 \Psi_1 \Psi_2 \rangle$	2
$\langle \Psi_1 \Psi_2 \Psi_3 \rangle$	6
$\langle \Psi_1 \Psi_3 \Psi_4 \rangle$	24
$\langle \Psi_2 \Psi_2 \Psi_2 \rangle$	8
$\langle \Psi_2 \Psi_2 \Psi_4 \rangle$	24
$\langle \Psi_2 \Psi_3 \Psi_3 \rangle$	36
$\langle \Psi_2 \Psi_4 \Psi_4 \rangle$	192
$\langle \Psi_3 \Psi_3 \Psi_4 \rangle$	216
$\langle \Psi_4 \Psi_4 \Psi_4 \rangle$	1728

k	$\langle \Psi_k^2 \rangle$
0	1
1	1
2	2
3	6
4	24

- $C_{ijk} = \langle \Psi_i \Psi_j \Psi_k \rangle / \langle \Psi_k^2 \rangle$
- and,

$$\begin{aligned} \langle \Psi_i \Psi_j \Psi_k \rangle &= \langle \Psi_i \Psi_k \Psi_j \rangle = \\ \langle \Psi_j \Psi_i \Psi_k \rangle &= \langle \Psi_j \Psi_k \Psi_i \rangle = \\ \langle \Psi_k \Psi_i \Psi_j \rangle &= \langle \Psi_k \Psi_j \Psi_i \rangle \end{aligned}$$

- with other not-reported $\langle \Psi_i \Psi_j \Psi_k \rangle$ zero

Pseudo-Spectral Construction-1

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

Spectral:

$$\begin{aligned} w_i &= \left\langle \lambda u^2 v \right\rangle_i \\ &= \sum_{j=0}^P \sum_{k=0}^P \sum_{l=0}^P \sum_{m=0}^P \lambda_j u_k u_l v_m \left\langle \Psi_j \Psi_k \Psi_l \Psi_m \right\rangle_i, \quad i = 0, \dots, P \end{aligned}$$

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

Pseudo-Spectral Construction–2

$$\tilde{w} = uv : \tilde{w}_i = \langle uv \rangle_i = \sum_{j=0}^P \sum_{k=0}^P u_k v_j \langle \Psi_k \Psi_j \rangle_i, \quad i = 0, \dots, P$$

$$\hat{w} = u\tilde{w} : \hat{w}_i = \langle u\tilde{w} \rangle_i = \sum_{j=0}^P \sum_{k=0}^P u_k \tilde{w}_j \langle \Psi_k \Psi_j \rangle_i, \quad i = 0, \dots, P$$

$$w = \lambda\hat{w} : w_i = \langle \lambda\hat{w} \rangle_i = \sum_{j=0}^P \sum_{k=0}^P \lambda_k \hat{w}_j \langle \Psi_k \Psi_j \rangle_i, \quad i = 0, \dots, P$$

- Aliasing errors
- Efficiency, and convenience

Debusschere et al., *SIAM J. Sci. Comp.*, 2004.

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 ? ...
 - Fragile
 - convergence issues
 - high-order PC multiplications
 - instabilities

Integration approach for non-polynomial functions

- Consider the ODE $\frac{du}{dx} = u$, with solution $u = e^x$
- e^x can be obtained from

$$du = u dx \quad \Rightarrow \quad e^x - e^{x_0} = \int_{x_0}^x u \, dx$$

- Similarly for e^{-x^2} , and $\ln(x)$

$$e^{-x^2} - e^{-x_0^2} = \int_{x_0}^x -2xu \, dx, \quad \ln(x) - \ln(x_0) = \int_{x_0}^x \frac{dx}{x}$$

- Agrees well with directly sampled pdf if PC order is high enough to resolve pdf of solution

A More General Integration approach for irrational functions

- To evaluate $u(x)$, $x = \sum_{k=0}^P x_k \Psi_k$, $u = \sum_{k=0}^P u_k \Psi_k$,
 - use a deterministic IC x_a such that $u(x_a)$ is known
 - express $\dot{u} = du/dx = f(u, x)$;
 - ... **require:** f is a rational function
 - ... ensures that $(\dot{u})_k$ are found from the u_k and x_k coeffs
 - evaluate the integral:

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

- 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 $\dot{u} = u \cos x$
- CPU-intensive, only slightly more robust than Taylor series

Inversion and division can be done without Taylor series.

- Assume three stochastic variables u , v , and w

$$w = \frac{u}{v} \Rightarrow vw = u$$

- Mode k of the stochastic product

$$\langle vw \rangle_k = \sum_{m=0}^P \sum_{l=0}^P C_{klm} v_l \cdot w_m = u_k$$

- System of $P + 1$ linear algebraic equations in w_m with known u_k and v_l ,

$$V_{km} = \sum_{l=0}^P C_{klm} v_l, \quad \mathbf{V}\mathbf{w} = \mathbf{u}$$

- More robust than Taylor series expansion for $1/u$
- What about the condition number of \mathbf{V} ?

Pseudo-Spectral Construction - UQ library

- Construction allows for a general representation using a new pseudo-spectral (PS) overloaded multiplication operation '*'

$$w = \lambda * u * u * v$$

where each deterministic function multiplication is transformed into a corresponding polynomial chaos product

- Prototype library of pseudo-spectral utilities:
 - uq_prod2: returns the PS-product of two input chaos polynomials ($u * v$)
 - uq_ipow: returns an integer exponentiation of a chaos pol. ($u^n = u * u * \dots * u$)
 - uq_inv: returns $1/u$
 - etc ...
- Potential meta-code: take a general deterministic code function $F(u)$, produce a pseudo-spectral stochastic function $\tilde{F}(\tilde{u})$
- Possibility of transforming legacy deterministic code into corresponding pseudo-spectral stochastic code.

Spectral UQ: Incompressible Flow - Stochastic Projection Method

- $(P + 1)$ Galerkin-Projected Mom./Cont. Eqns, $q = 0, \dots, P$:

$$\frac{\partial \mathbf{v}_q}{\partial t} + \nabla \cdot \langle \mathbf{v}\mathbf{v} \rangle_q = -\nabla p_q + \frac{1}{\text{Re}} \nabla \cdot \left\langle \mu [(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T] \right\rangle_q$$
$$\nabla \cdot \mathbf{v}_q = 0$$

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

$$\frac{\tilde{\mathbf{v}}_q - \mathbf{v}_q^n}{\Delta t} = C_q^n + D_q^n$$
$$\nabla^2 p_q = -\frac{1}{\Delta t} \nabla \cdot \tilde{\mathbf{v}}_q$$
$$\frac{\mathbf{v}_q^{n+1} - \tilde{\mathbf{v}}_q}{\Delta t} = -\nabla p_q$$

- $P + 1$ *decoupled* Poisson Eqns for the pressure modes

Le Maître et al., *J. Comp. Phys.*, 2001.

Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Gaussian viscosity PDF

$$-\nu = \nu_0 + \nu_1 \xi$$

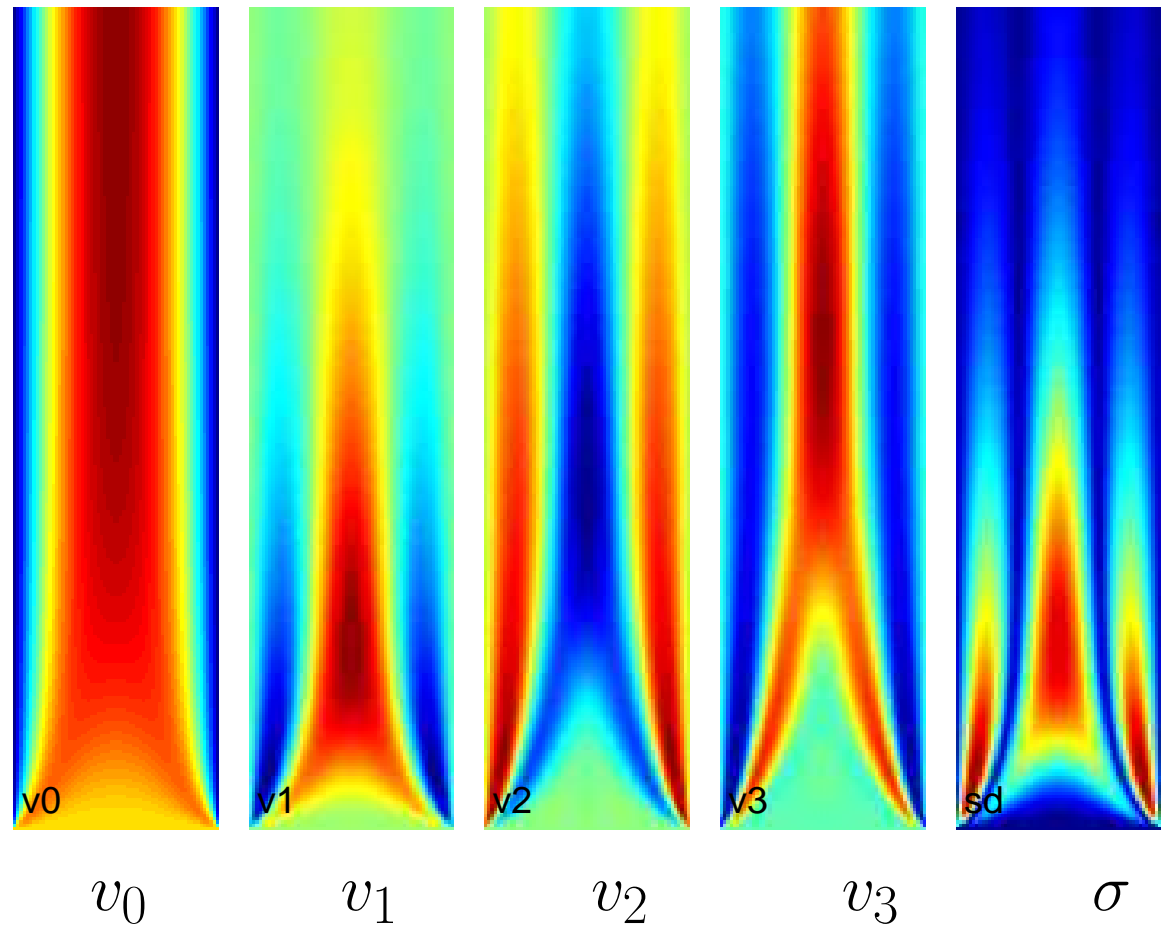
- Streamwise velocity

$$-v = \sum_{i=0}^P v_i \Psi_i$$

– v_0 : mean

– v_i : i -th order mode

$$-\sigma^2 = \sum_{i=1}^P v_i^2 \langle \Psi_i^2 \rangle$$



UQ in Convective Vortical Flows

- What about UQ In turbulent/unsteady-vortical flow?
- Spectral PC representation of turbulence limited by growth in phase errors
 - Demonstrated in 60's-70's
- Problem shows up, say, in describing evolution of a pendulum with uncertain initial conditions
- Sampling-based averaging also presents difficulties.
 - Smearred “average” of flow structure due to a number of realizations does not resemble *any* of them.
- Must address statistics of select flow observables
 - where such quantities are meaningful

Governing Dimensionless Low Mach Number Equations

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

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

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

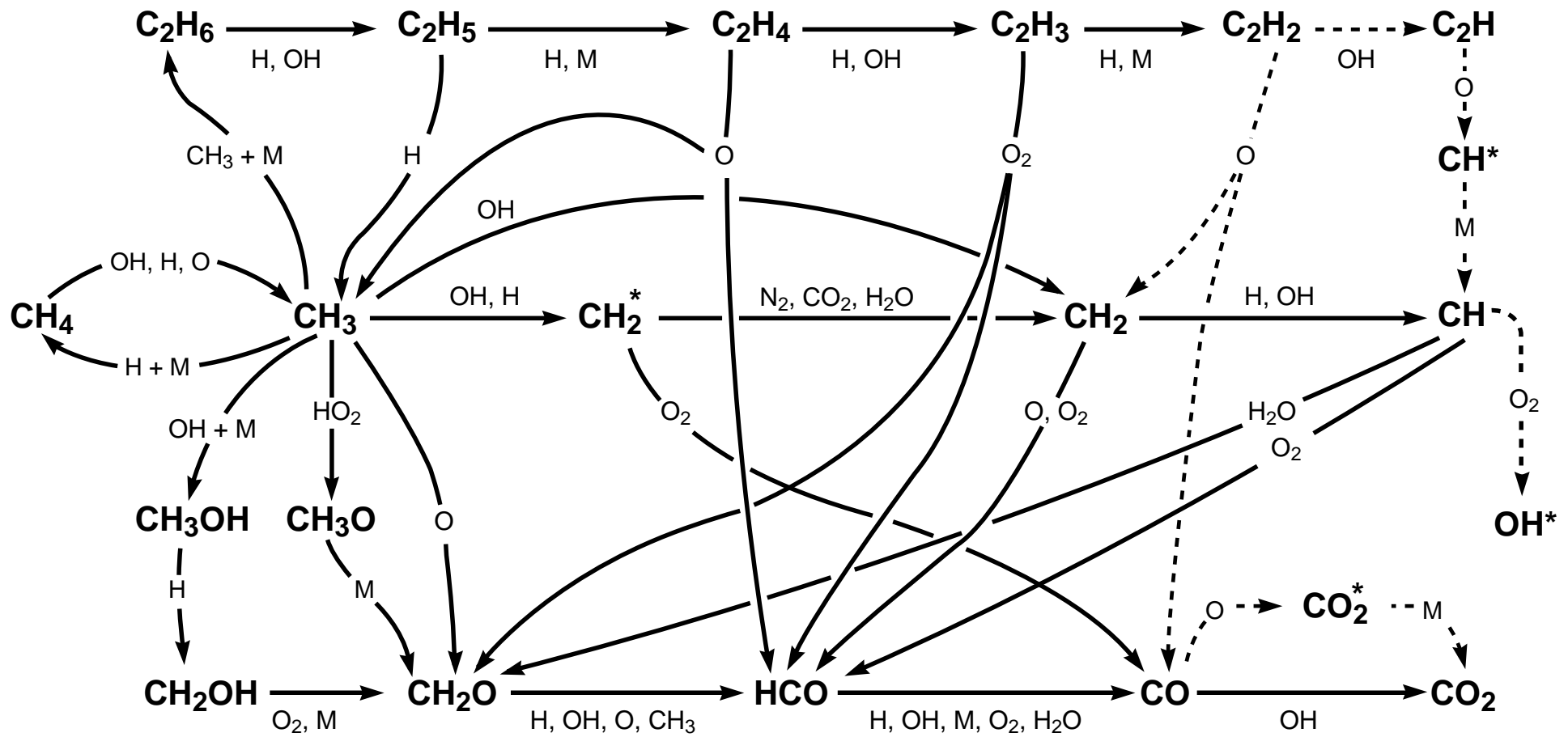
$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) = -\frac{1}{\text{ReSc}} \nabla \cdot (\rho Y_i \mathbf{V}_i) + \text{Da} w_i \quad i = 1, \dots, N$$

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

-
- Low Mach No., no body forces, bulk viscosity, or radiation
 - Neglect Soret and Dufour effects

\mathbf{U} is the unit tensor

Dominant Reaction Pathways, Atm. $\text{CH}_4 + \text{Air}$



H.N. Najm *et al.*, *Comb. Flame*, 1998.

Spectral UQ Formulation: low M 2D Reacting Flow Equations

$$\frac{\partial \rho_q}{\partial t} + \nabla \cdot \langle \rho \mathbf{v} \rangle_q = 0$$

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

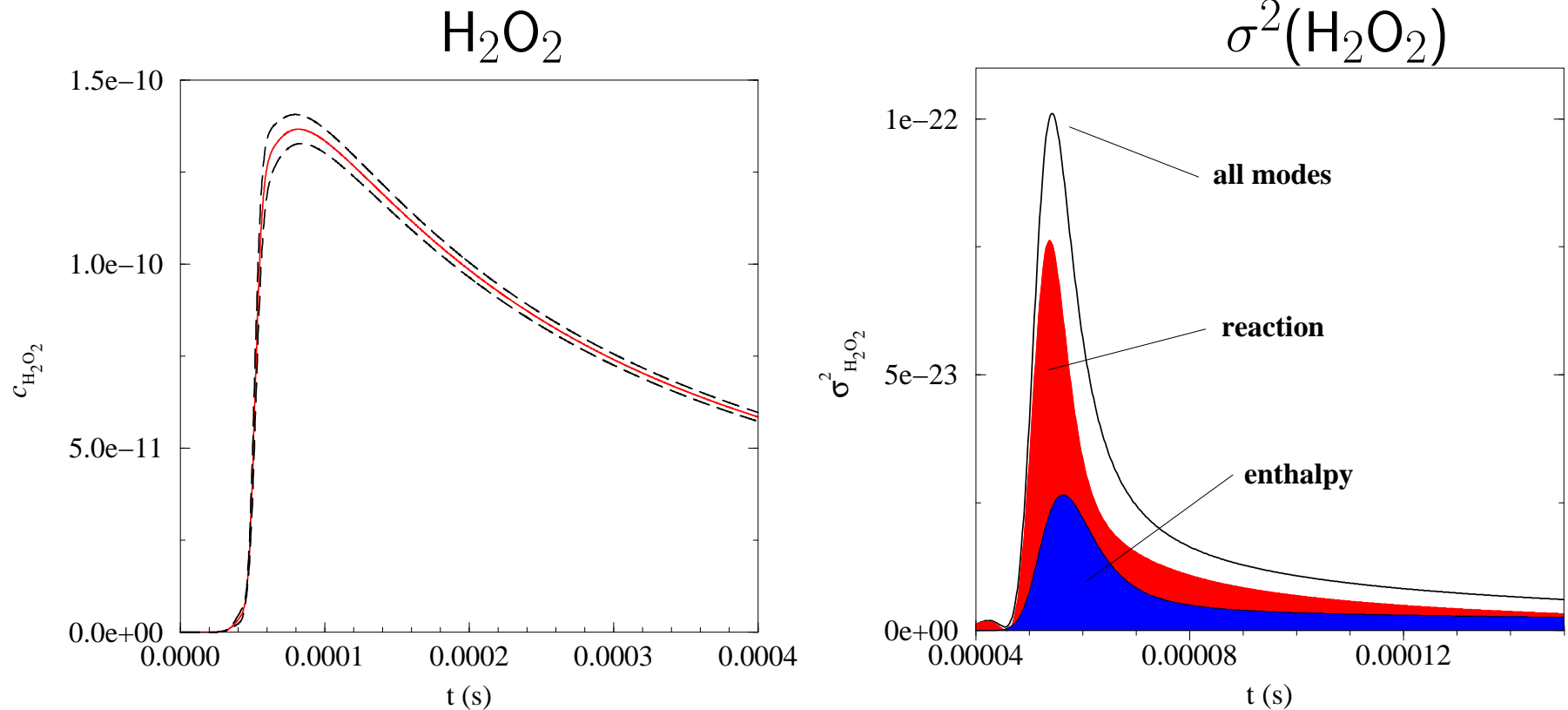
$$\begin{aligned} \frac{\partial T_q}{\partial t} + \langle \mathbf{v} \cdot \nabla T \rangle_q &= \left\langle \frac{(\gamma - 1) dp_o}{\gamma \rho c_p dt} \right\rangle_q + \frac{1}{RePr} \left\langle \frac{\nabla \cdot (\lambda \nabla T)}{\rho c_p} \right\rangle_q - \frac{1}{ReSc} \left\langle \sum_{i=1}^N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

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

- 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

0D Intrusive H₂-Air Ignition : Uncertainty in [H₂O₂]

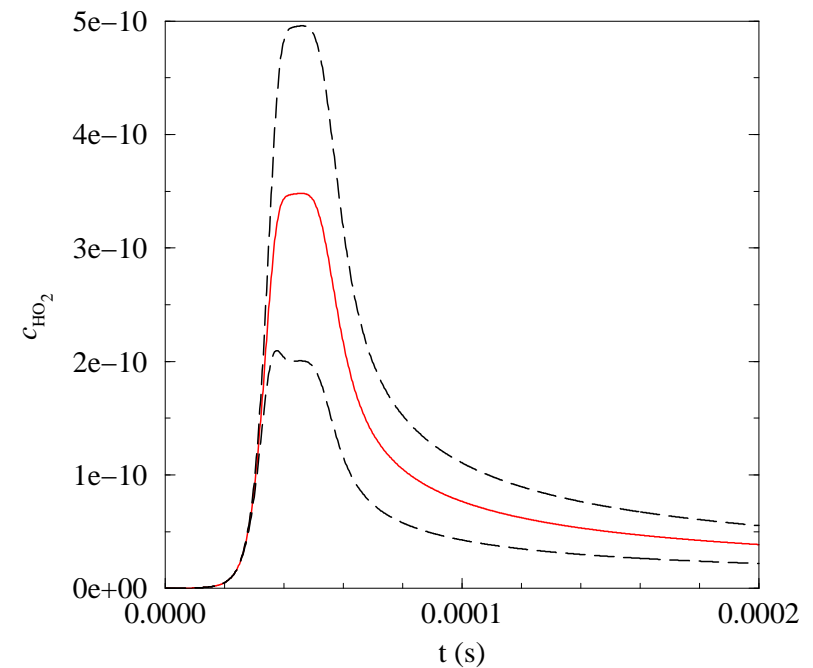


- 3rd-order PC, 2 uncertain parameters
- Fast rise in the mean [H₂O₂], little amplification in its uncertainty
- Rxn rate uncertainty has negligible consequence as equilibrium is approached

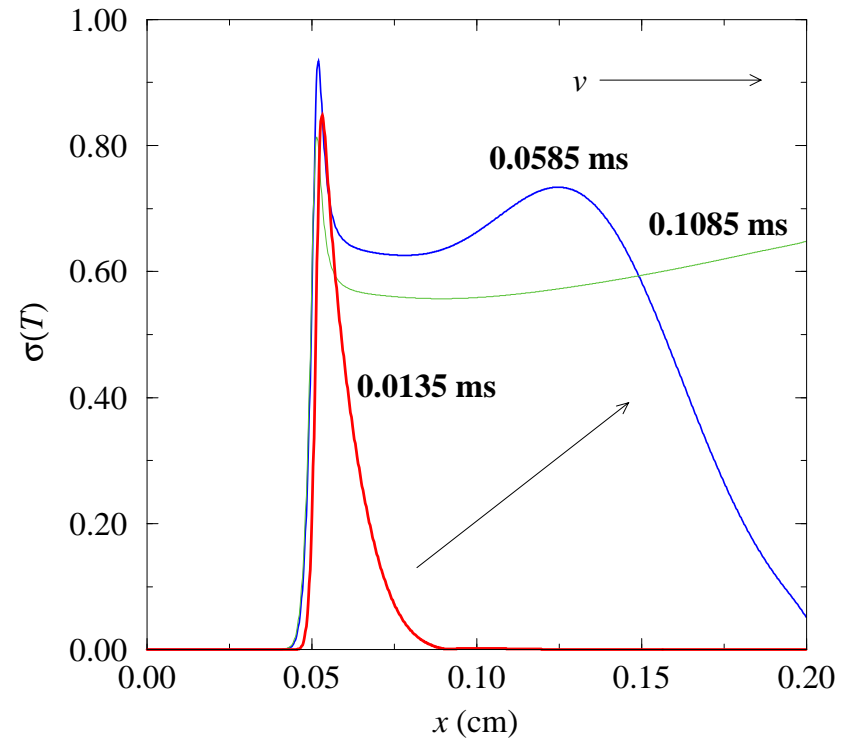
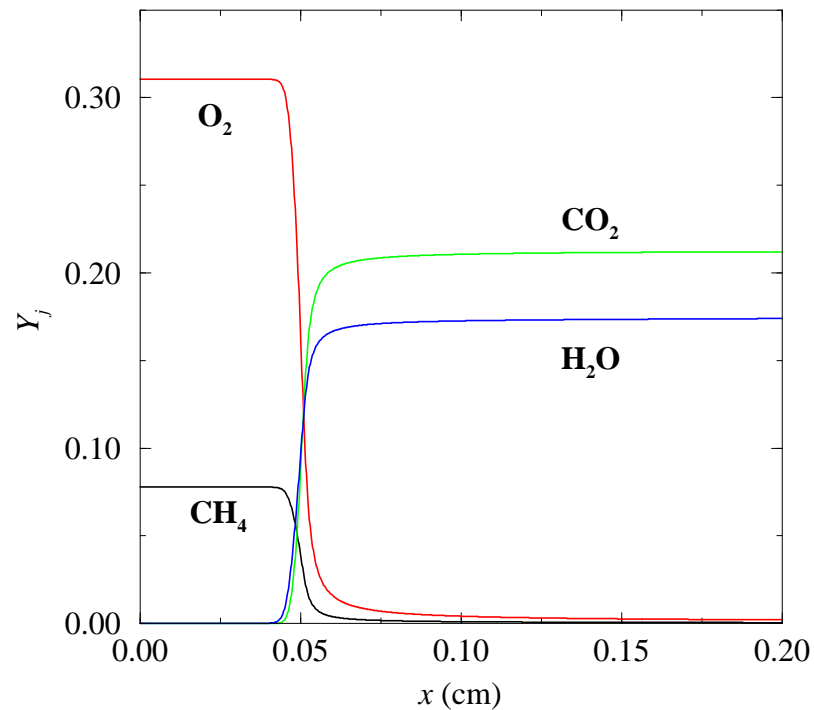
M.T. Reagan *et al.*, *Comb. Theo. Mod.*, 2004.

0D Intrusive H₂-Air Ignition : Uncertainty in [HO₂]

- Very fast rate of growth of the mean [HO₂]
- Followed by a similarly fast rise in the standard deviation
- Much larger uncertainty than H₂O₂
- COV of HO₂ is about 40%
 - persists near equilibrium
 - Amplification of enthalpy uncertainty



1D CH₄-Air Flame: Intrusive UQ



- Single-step global mechanism
- 3rd-order PC, 1 uncertain parameter: $h_{\text{CO}_2}^o : \sigma = 0.1\%$
- Numerical stability challenges – to be further visited later

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

- Sample parameters using Monte Carlo
- Compute realizations of the model outputs
- Project MC statistics on the spectral mode strengths $u_k(t)$

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

– Evaluate integrals numerically (MC, quadrature, cubature)

- Uncertain model output

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

Sampling Issues in NISP 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

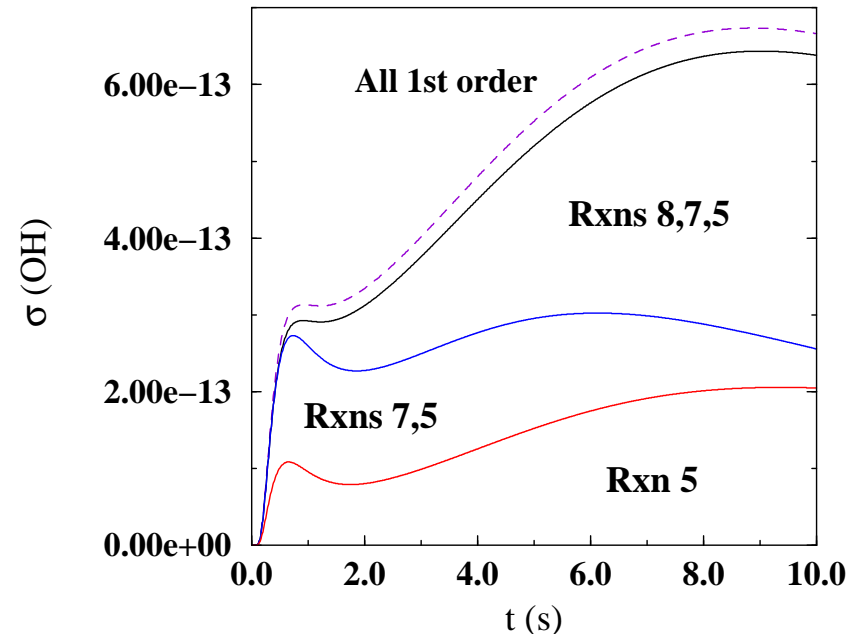
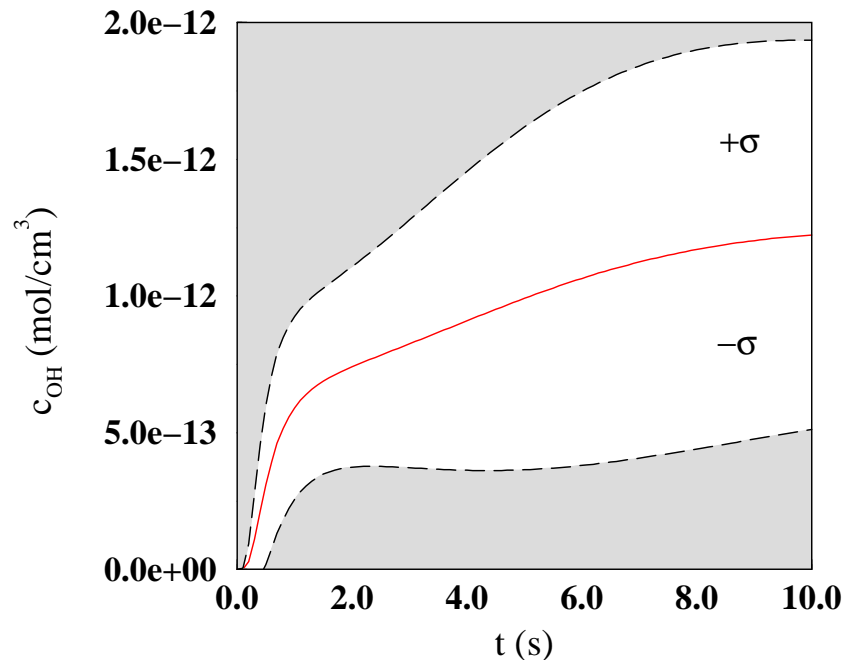
NISP UQ Application: Premixed H₂-O₂ Chemistry at Super-Critical Water Oxidation (SCWO) Conditions

- 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 ↔ H ₂ O	1.620E+14	0	75	3.16
2. H ₂ + OH ↔ H ₂ O + H	1.024E+08	1.6	1660	1.26
3. H + O ₂ ↔ HO ₂	1.481E+12	0.6	0	1.58
4. HO ₂ + HO ₂ ↔ H ₂ O ₂ + O ₂	1.867E+12	0	775	1.41
5. H ₂ O ₂ + OH ↔ H ₂ O + HO ₂	7.829E+12	0	670	1.58
6. H ₂ O ₂ + H ↔ HO ₂ + H ₂	1.686E+12	0	1890	2.00
7. H ₂ O ₂ ↔ OH + OH	3.0000E+14	0	24400	3.16
8. OH + HO ₂ ↔ H ₂ O + O ₂	2.891E+13	0	-250	3.16

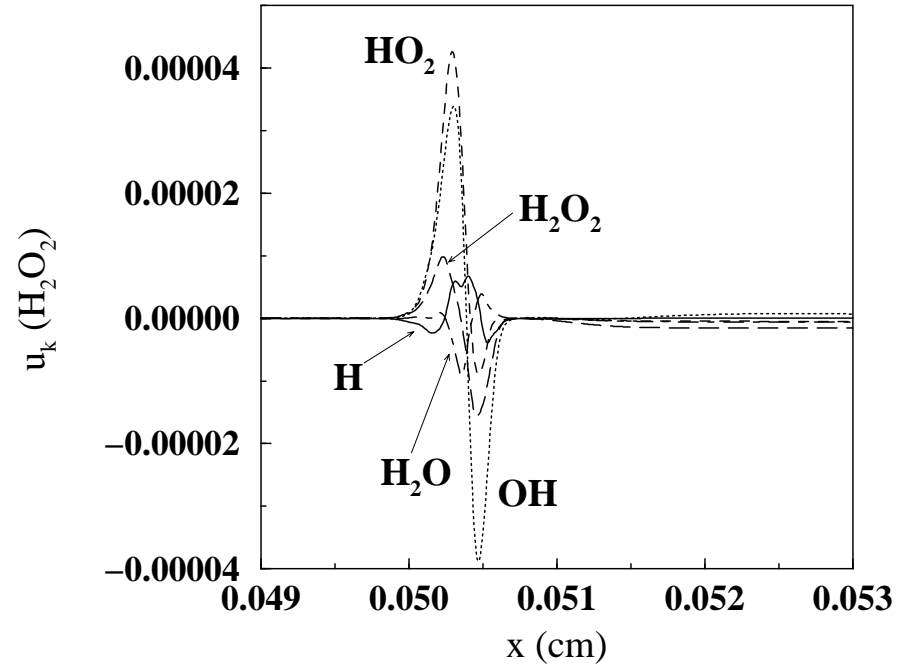
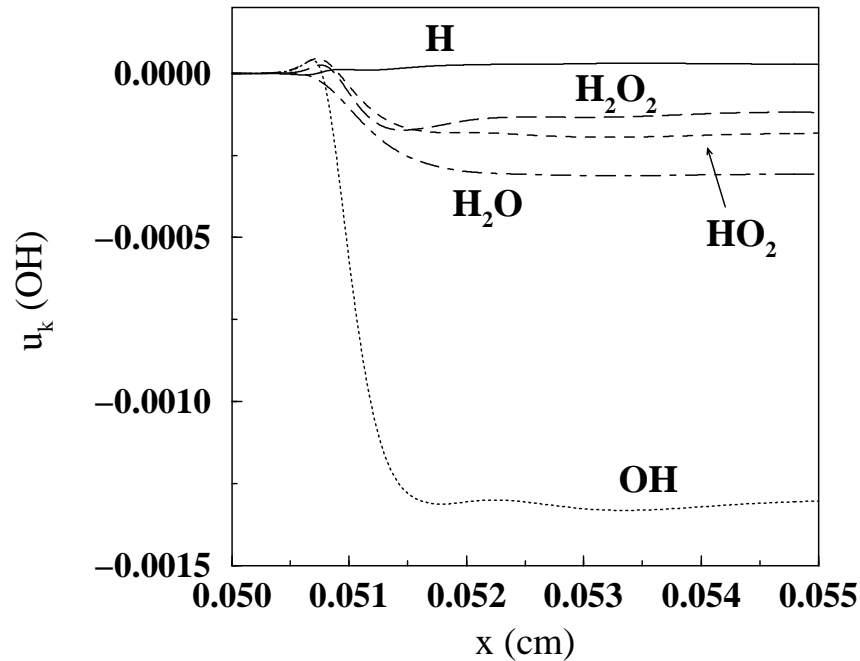
Species	μ_0	2σ
H	52.10	0.01
OH	9.3	0.2
H ₂ O	-57.80	0.01
H ₂ O ₂	-32.53	0.07
HO ₂	3.0	0.5

0D H₂-O₂ Isothermal Isobaric SCWO Ignition



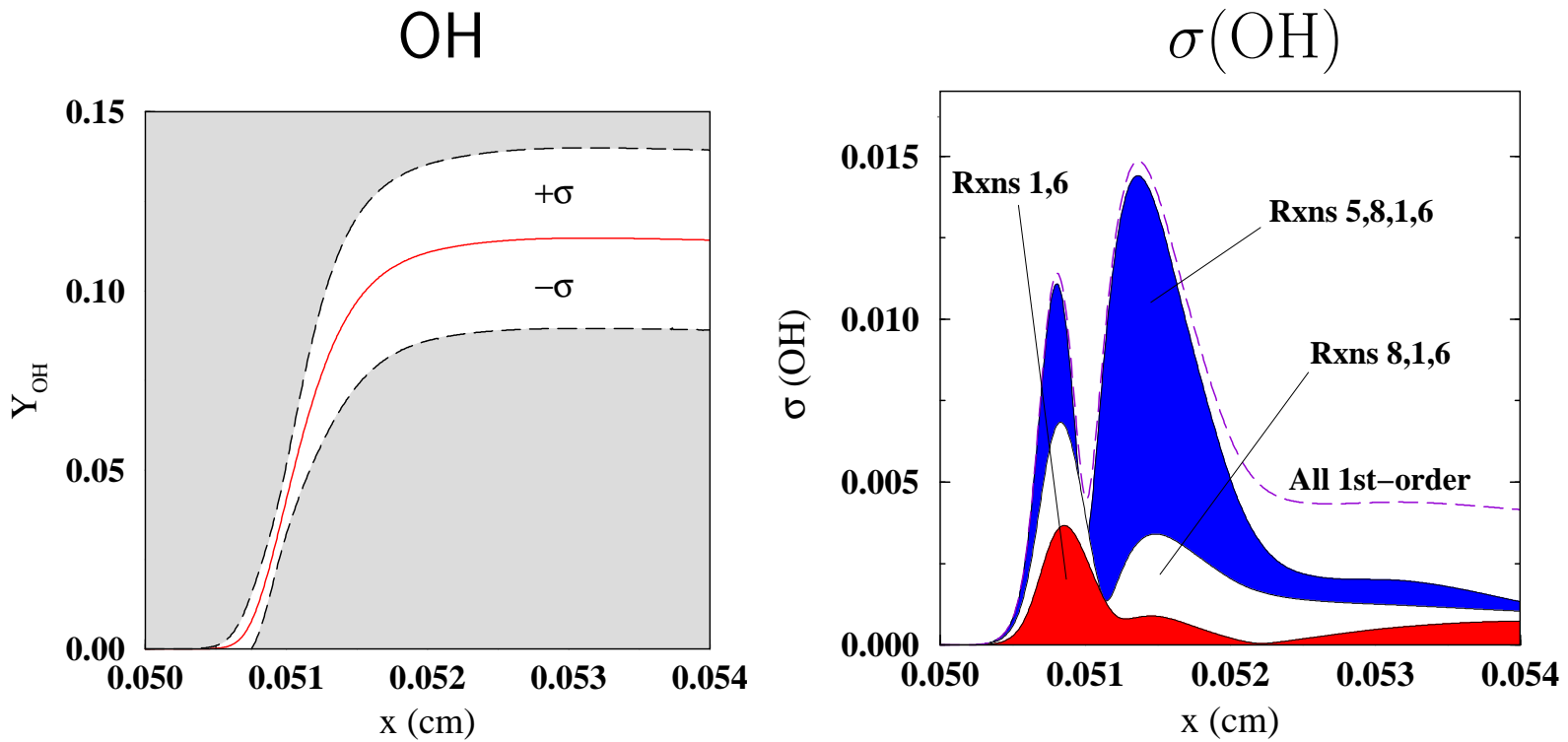
- Mean and standard deviation predictions validated against published data
- Initial fast growth in uncertainty followed by a slower approach to a steady-state with *large* OH uncertainty
- Reactions 7 & 8 have dominant roles in the OH uncertainty

Relative Roles of Uncertainties in Enthalpies (1D SCWO Flame)



- Enthalpy uncertainty plays a smaller role than reaction rates in the uncertainty of predicted OH and H_2O_2
- Dominant roles for OH and HO_2 enthalpies

1D H₂-O₂ SCWO Flame NISP UQ/Chemkin-Premix

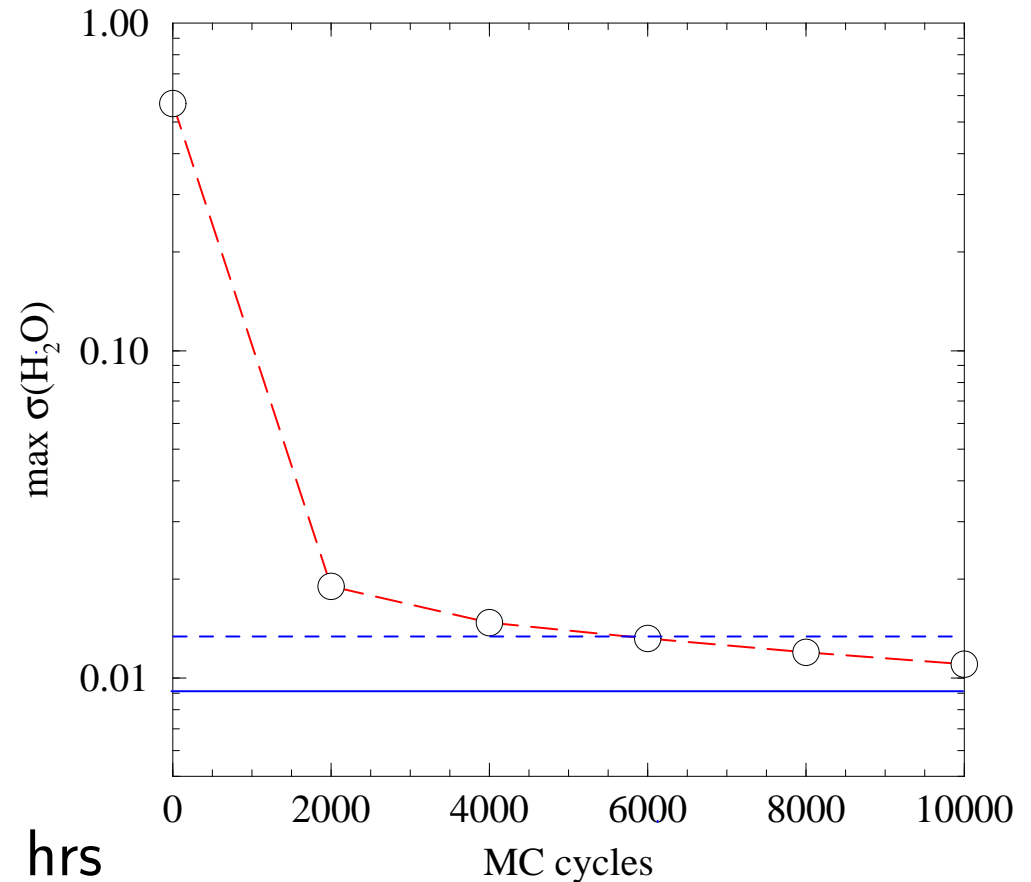


- Fast growth in OH uncertainty in the primary reaction zone
- Constant uncertainty and mean of OH in post-flame region
- Uncertainty in pre-exponential of Rxn.5 ($H_2O_2 + OH = H_2O + HO_2$) has largest contribution to uncertainty in predicted OH

M.T. Reagan *et al.*, *Comb. Flame*, 2003.

CPU-time Savings with Intrusive Spectral Strategy

- 0D H₂-O₂ 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



Sensitivity Analysis

For an ODE system:

$$\frac{dX}{dt} = w(X, t; A)$$

where $X = \{X_i\}$ is the solution vector, and $A = \{A_k\}$ is the vector of model parameters, the first order sensitivity coefficients,

$$\zeta_{ik} = \frac{\partial X_i}{\partial A_k}$$

are integrated in time using the ODE system

$$\frac{d\zeta_{ik}}{dt} = \frac{\partial w_i}{\partial A_k} + \sum_j \frac{\partial w_i}{\partial X_j} \zeta_{jk}$$

obtained by differentiation of dX_i/dt w.r.t. A_k .

The normalized sensitivity coefficients are given by:

$$S_{ik} = \frac{\partial \ln X_i}{\partial \ln A_k} = \frac{A_k}{X_i} \zeta_{ik}$$

Error Propagation

Let the standard deviation in each $\ln A_k$ be σ_k , then the total contribution of each reaction k to the variance in the mole fraction of species i is

$$z_{ki}^2 = \left(A_k \frac{\partial X_i}{\partial A_k} \right)^2 \sigma_k^2$$

Variances are additive, and the total variance in the mole fraction of each species i , is the sum of the N reaction contributions:

$$[\sigma(X_i)]^2 = \sum_{k=1}^N z_{ki}^2$$

- Linear ... no higher order information or coupling bet params
- Intrusive ... involves recoding
- Concerns about overprediction of output uncertainties

First-Order Sensitivity Information in a PC Expansion

- Conventional sensitivity

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

- Sensitivity in a stochastic UQ context

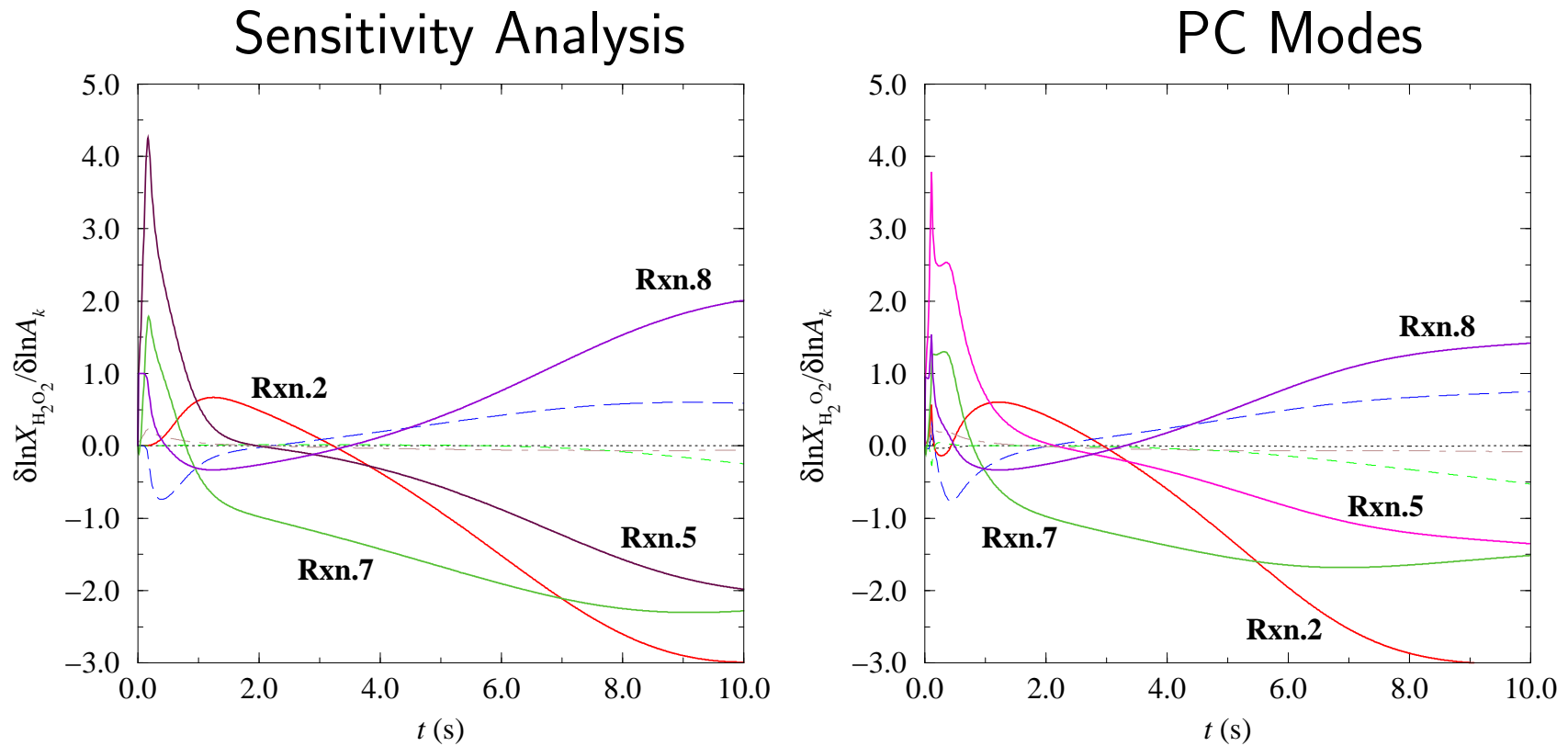
$$\lambda = \sum_{k=0}^P \lambda_k \Psi_k(\xi), \quad u = \sum_{k=0}^P u_k \Psi_k(\xi)$$

- 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

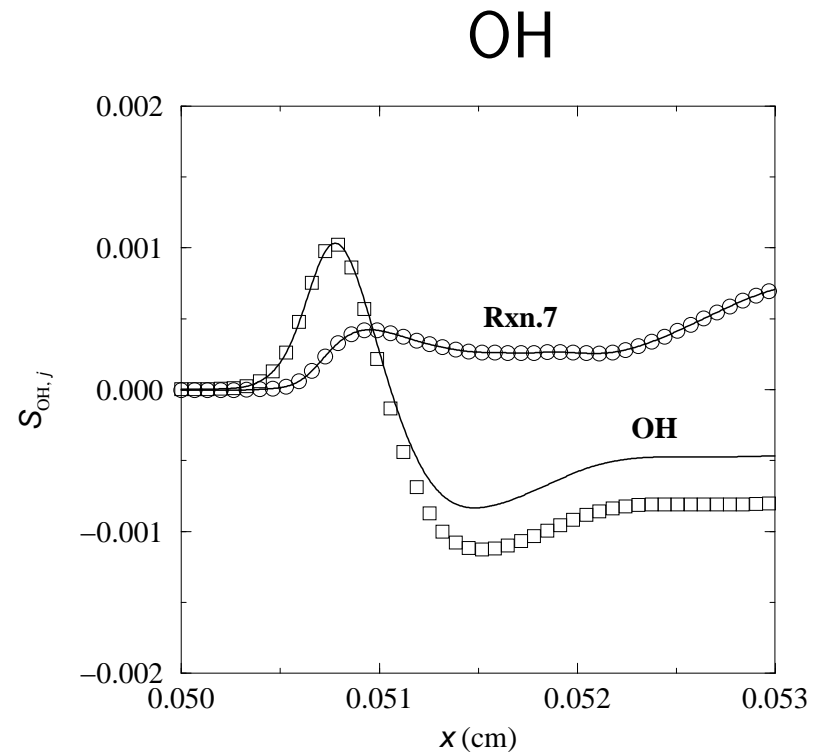
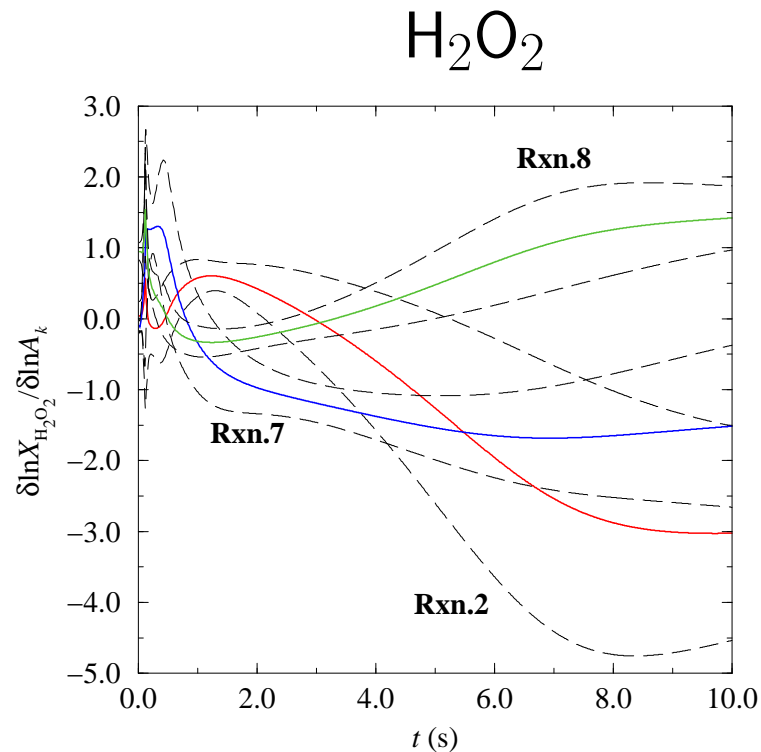
0D H₂-O₂ SCWO Isoth. Isob. Ignition : First Order Sensitivities



- H₂O₂ first-order sensitivity coefficients predicted from both conventional sensitivity analysis and first-order PC expansions are in overall agreement

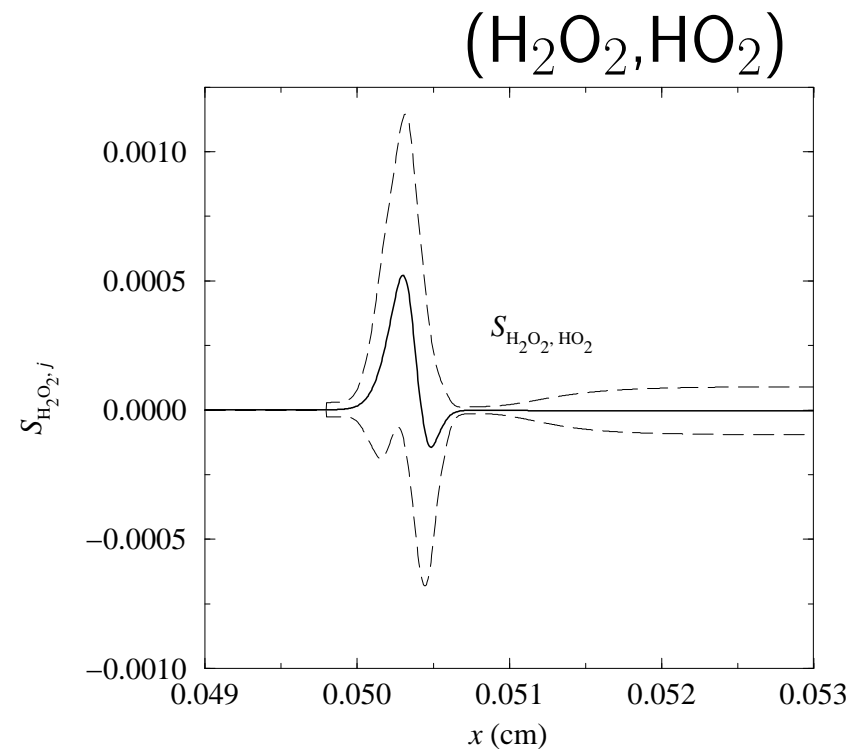
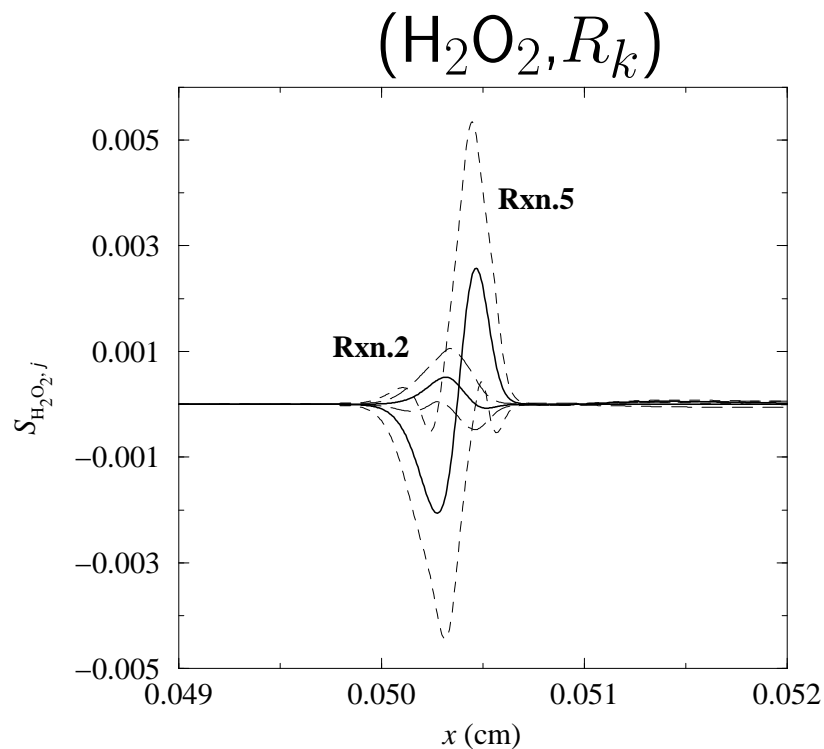
M.T. Reagan *et al.*, *Int. J. Chem. Kin.*, 2005.

SCWO Stochastic Sensitivities – Means and 1- σ Envelopes



- H₂O₂ stochastic sensitivity coefficients in 0D system
 - 1- σ uncertainty bounds
- Mean OH stochastic sensitivity coefficients (1D flame)
 - Means can differ from first-order results due to high-order information

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

Closure — Lecture 2

- Covered
 - Use of PCEs for propagating uncertainty
 - Intrusive and non-intrusive approaches
 - Pseudo-spectral implementation
 - Non-intrusive spectral projection
 - Applications to NS eqns, and chemically reacting flow
 - Uncertain sensitivity information
- Next
 - Challenges with non-linearities and constraints
 - Multiwavelet construction
 - Oscillatory systems