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Uncertainty Quantification in Chemical Systems using Polynomial Chaos Constructions

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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
  - 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 (prior info $+$ data)
- Prior encapsulates all prior information
- Likelihood function: fit model and measurement noise
- Evidence is a normalizing constant – ignore

Bayesian Inference of Uncertain Rate Coefficients

$\mathrm{CH_4} + 2\mathrm{O_2} \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}$

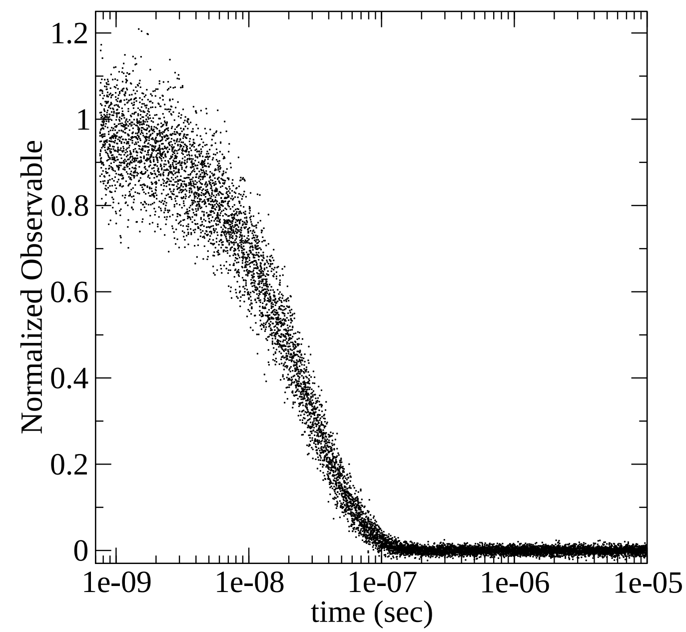
$\mathcal{R} = [\mathrm{CH_4}]\,[\mathrm{O_2}]^2\,k(T)$

$k(T) = A\,T^n\,e^{-E/R^oT}$

Presume a $[\mathrm{CH_4}]$ observable:

$I(T,t) = e^{-[\mathrm{O_2}]^2 k(T) t}$

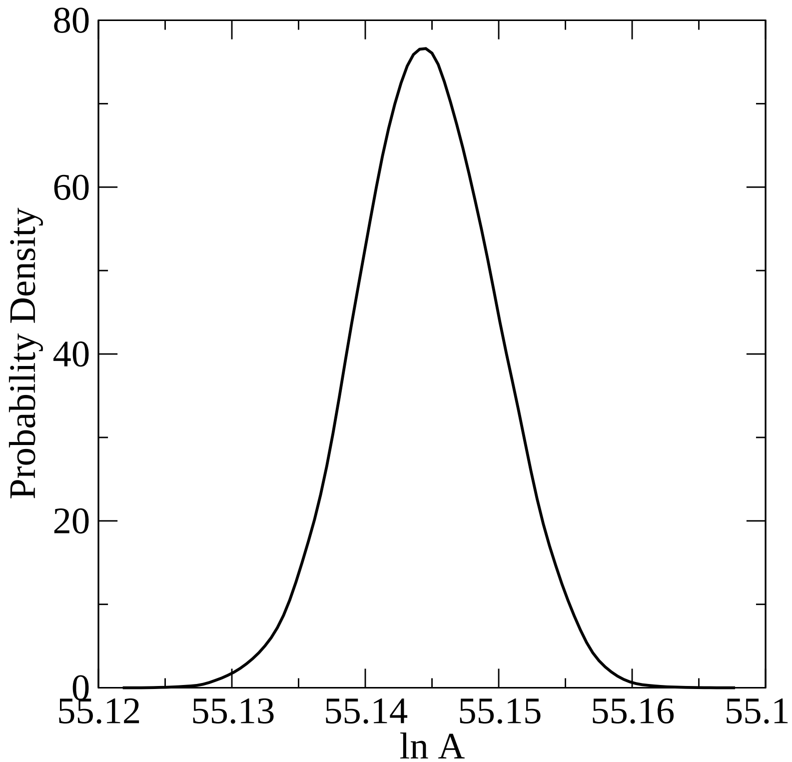
where $[\mathrm{O_2}]$ is $\sim$ constant
for trace $[\mathrm{CH_4}]$

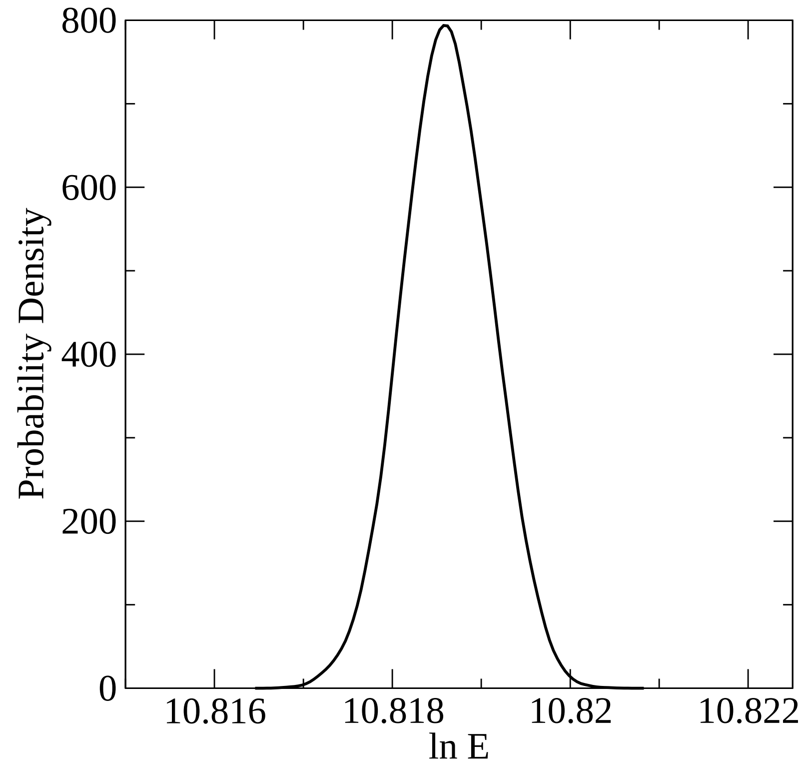


Presume noisy $I(T,t)$ exponential decay data generated using $A = 9.0e23$, $n = 0$, $E = 5.0e4$ with added Gaussian noise

Infer PDFs for A and E using Bayesian inference

Marginal PDFs for A and E

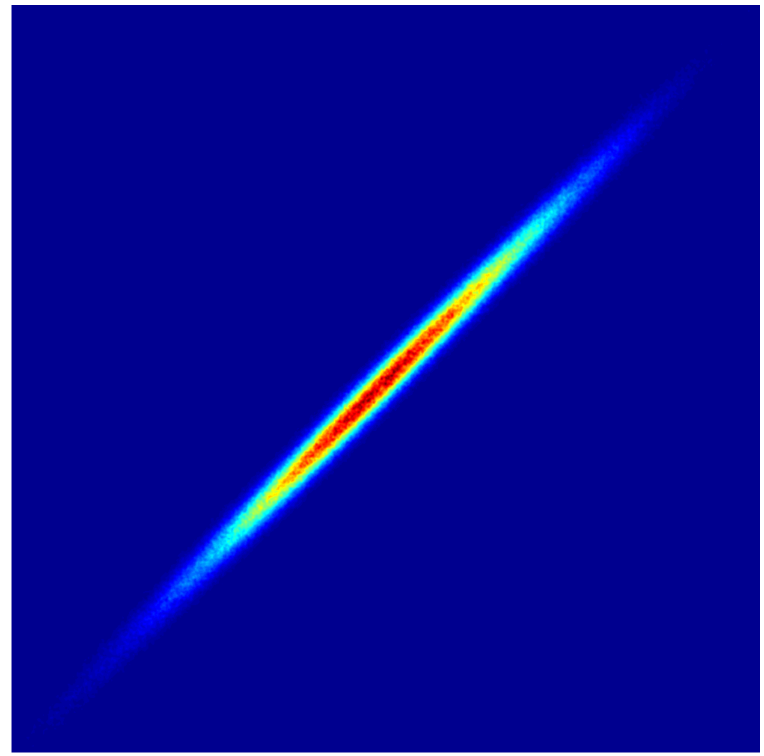




Marginal posterior PDFs for $\ln A$ and $\ln E$, evaluated using Markov Chain Monte Carlo (MCMC)

Joint PDF of A and E

- Evidence of very strong correlation
- Natural result of fitting the Arrhenius expression
- A single stochastic degree of freedom (dimension) can model uncertainty in both variables
- Correlation needs to be built into the forward UQ problem



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

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

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 $\Psi_i(\xi)$,

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

where the $C_{pqi} = \langle \Psi_p \Psi_q \Psi_i \rangle / \langle \Psi_i^2 \rangle$ 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 Formulation: low M 2D Reacting Flow Equations

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

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

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

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

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

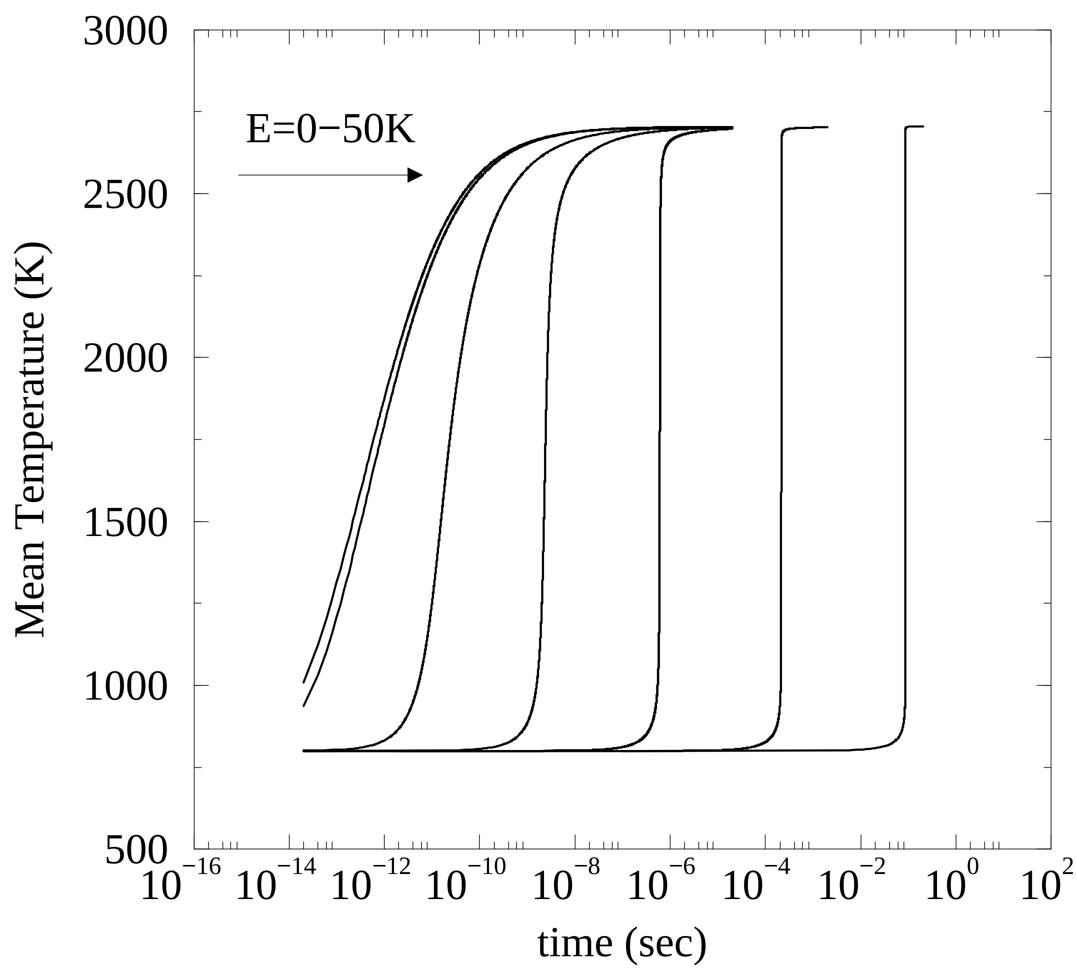
Example: $\mathrm{CH_4} + 2\mathrm{O_2} \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}$

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

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

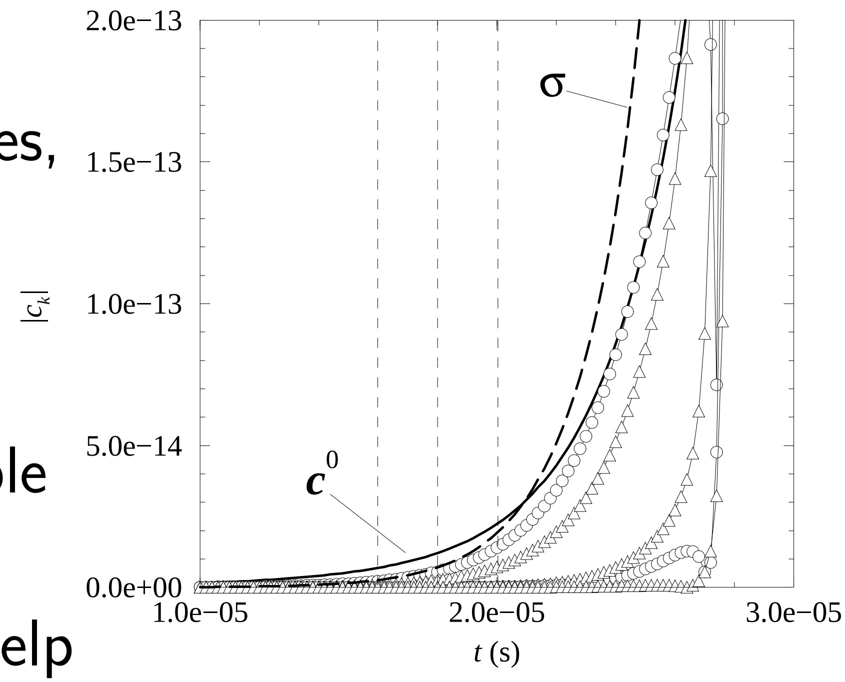
Large activation energy (E_k) exponentials lead to very fast changes in species concentrations and temperature

- Methane-air ignition — Global single-step irreversible mechanism
- Initial $T = 800K$
- Stoichiometric
- $p = 1$ atm (constant)
- WH PC fails at realistic E with even miniscule uncertainty



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;

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-Wavelet, Multi-Resolution Analysis

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)

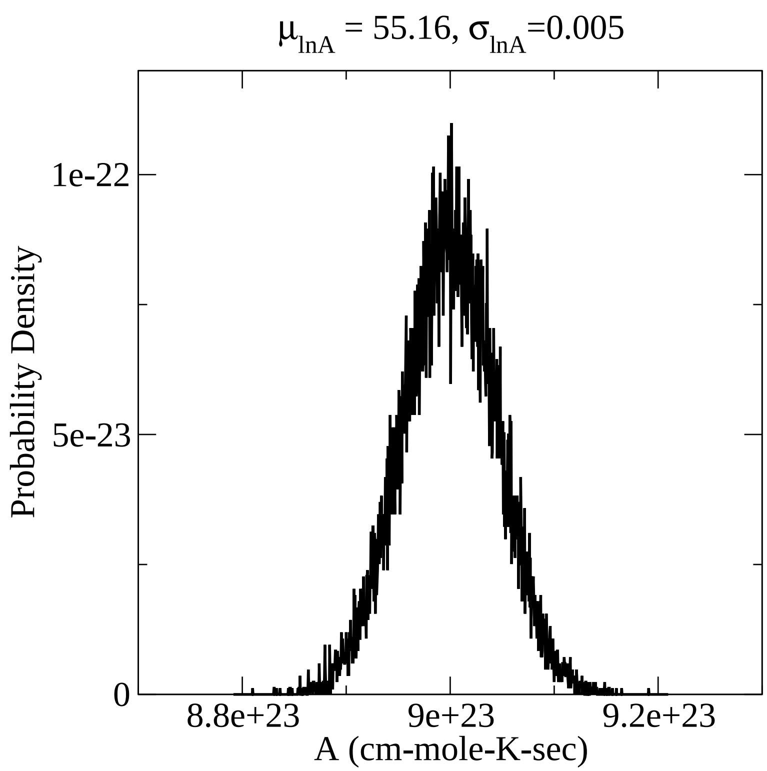
$$u = \sum_{\lambda=0}^{Q} \tilde{u}_\lambda(\mathbf{x}, t)\, \mathcal{W}_\lambda(\zeta_1, \ldots, \zeta_N)$$

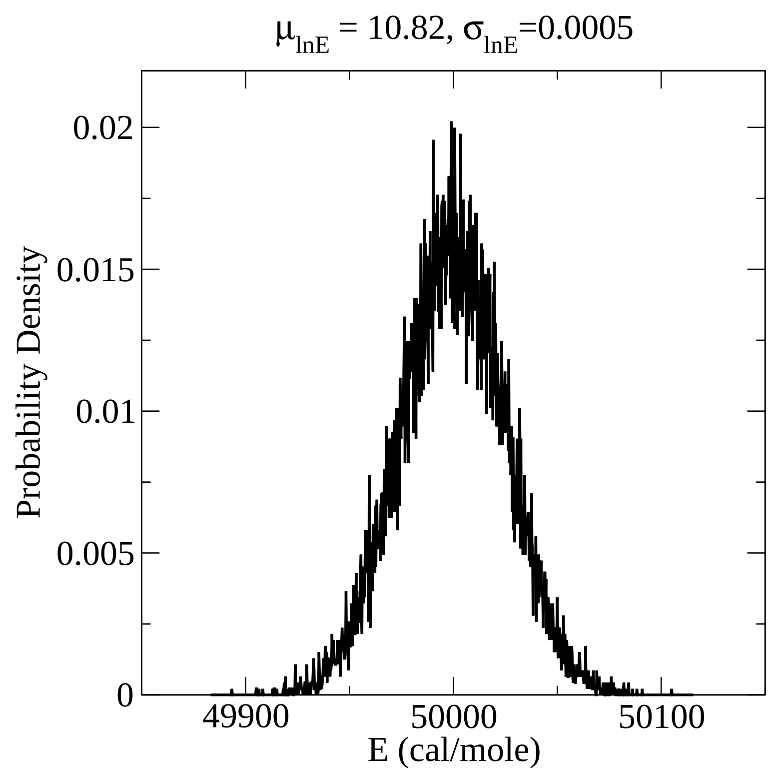
Le Maître, Ghanem, Knio, and Najm, *J. Comp. Phys.*, 197:28-57 (2004)
Le Maître, Najm, Ghanem, and Knio, *J. Comp. Phys.*, 197:502-531 (2004)

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

Using MW PC for homogeneous Methane-Air ignition

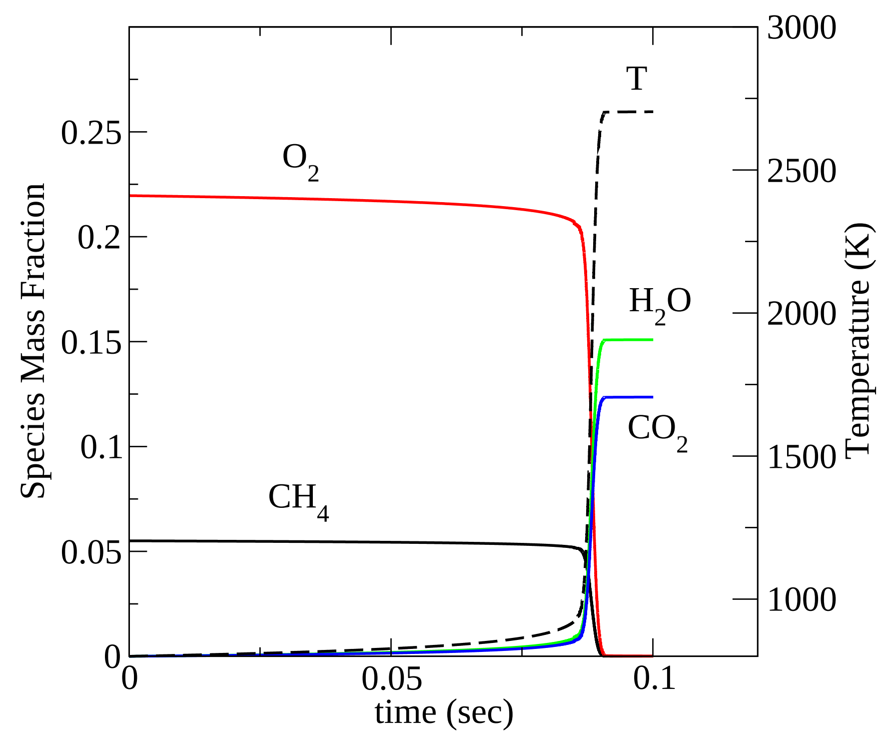




- Global methane air
- Uncertain (A, E) with perfect correlation
  - $\ln A$: $\mu = \ln(9.0e23)$, $\sigma = 0.005$
  - $\ln E$: $\mu = \ln(5.0e4)$, $\sigma = 0.0005$

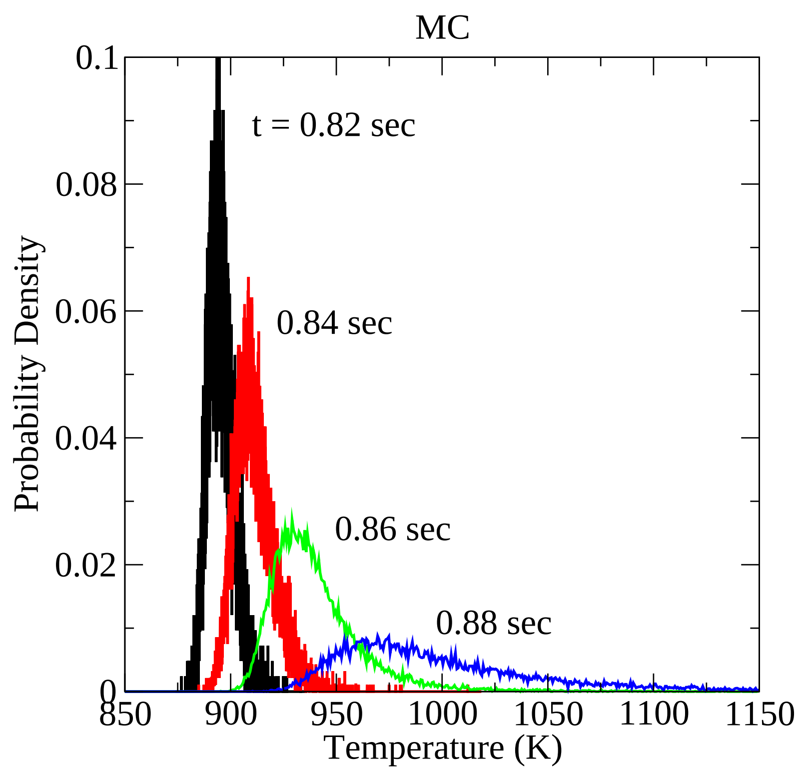
Using MW PC for homogeneous Methane-Air ignition

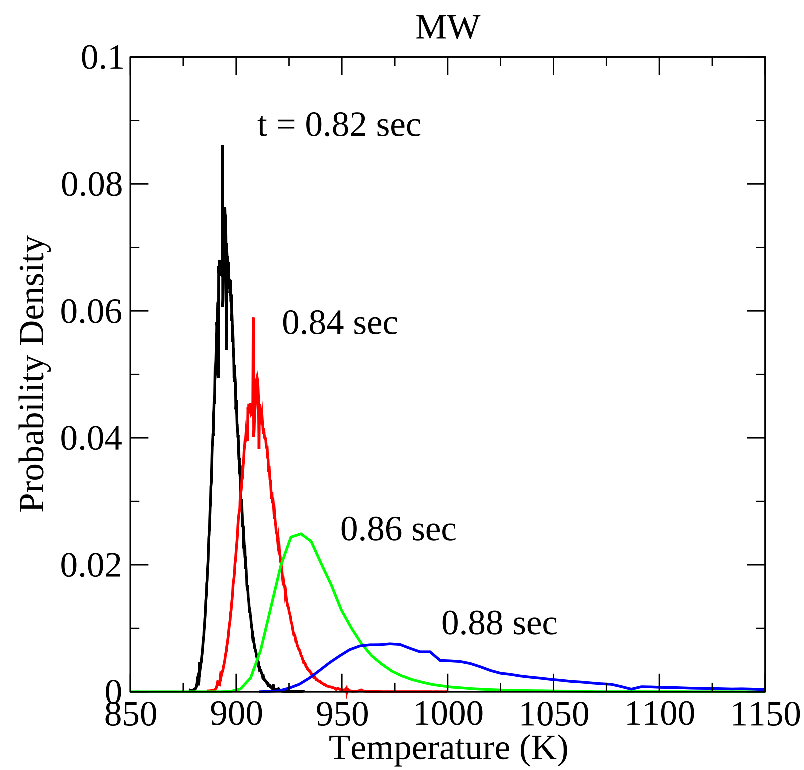
- Constant pressure
  - 1 atm
- Deterministic IC
  - Stoichiometric
  - $T_o = 800$ K
- 4^{th} Order MW PC
- Adaptive time stepping
  - Each step:
    call DVODE with
    internal implicit Adams
    time integrator



Time evolution of mean species mass fractions and temperature

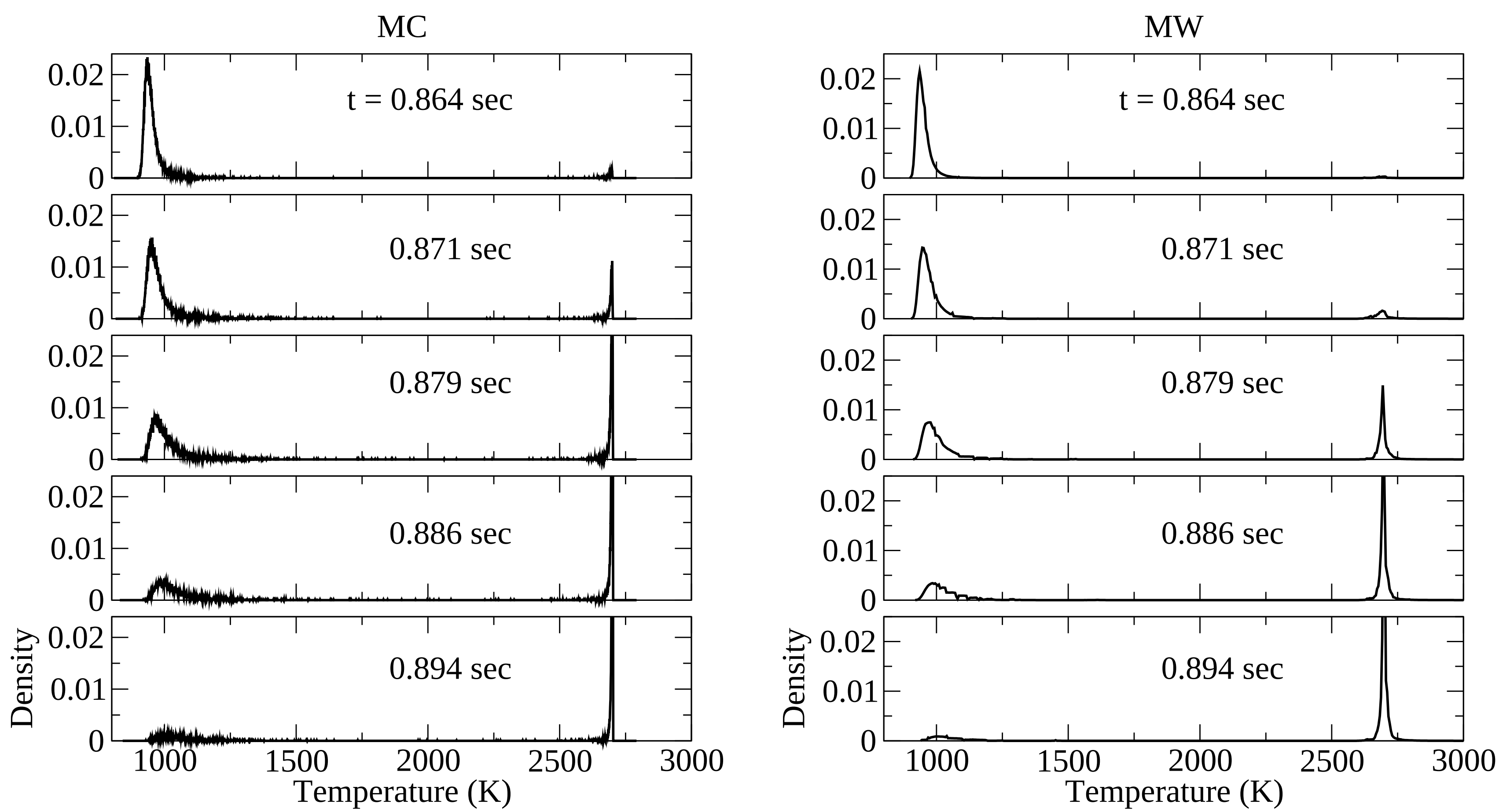
Time evolution of Temperature PDFs in preheat stage





- Similar results from MC (20K samples) and MW computations
- Increased uncertainty, and long high–T PDF tails, in time

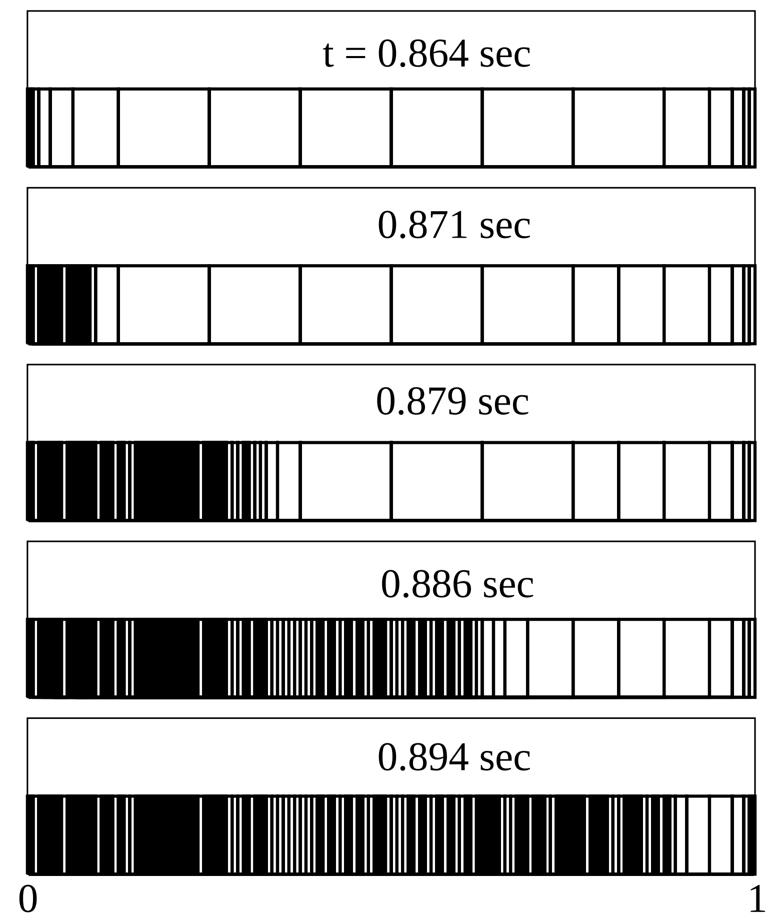
Time evolution of Temperature PDFs during fast ignition transient



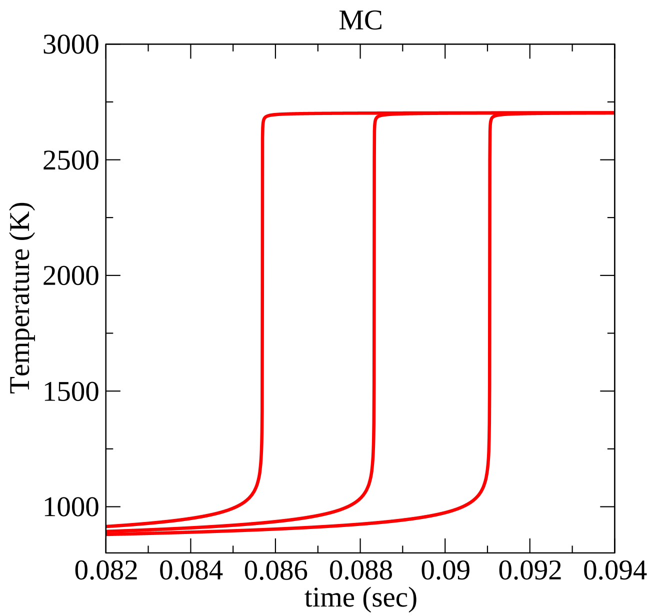
- Transition from unimodal to bimodal PDFs
- "Leakage" of probability mass from pre-heat PDF high–T tail

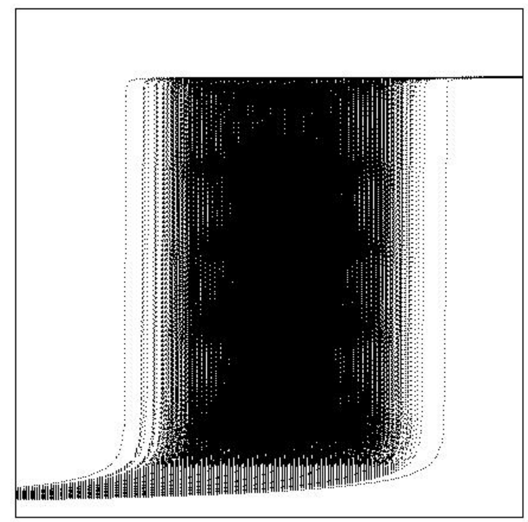
Adaptively refined block decomposition in 1D stochastic space

- Low/high (A, E) values ignite earlier/later in time
- Block decomposition refinement proceeds to higher ζ values in time
- Refinement retains specified maximum degree of uncertainty per block



Computational Challenges with intrusive MW PC for ignition





- Reformulated MW PC ODE system:
  - Fast active time scales : $\mathcal{O}(1)$ ns
  - Outer DVODE time step : $\mathcal{O}(1)$ μs
  - Time span during which fast time scales are active: $\mathcal{O}(10)$ ms

Conclusions

- Intrusive Spectral UQ in reacting flow
  - Global basis OK for weakly non-linear systems
  - Adaptive multiwavelet construction
    - Resolves many global PC difficulties
    - Robust time integration for high activation energy and large parametric uncertainty still requires significant time integration customization
    - Demonstration in exothermic ignition illustrates computational challenges with the observation of long time periods during which fast time scales are active

Contributors

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