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Uncertainty Quantification: Enabling Predictive Simulations

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Overview

- Introduction
- Basic methods for uncertainty quantification
- Application to chemical kinetics
- Advanced uncertainty quantification topics

Overview

- Introduction
  - Predictive simulation
  - Sources of uncertainty
  - Uncertainty quantification objectives
- Basic methods for uncertainty quantification
- Application to chemical kinetics
- Advanced uncertainty quantification topics

Predictive simulations enable science based design

- Empirical design is inefficient and costly
  - Trial and error does not work well for complex systems
- Experiments not always feasible or permissible
  - Reliability of nuclear weapons
  - Climate change mitigation approaches
- Predictive simulations provide insight into the underlying physics that drive complex systems
  - Identification of key mechanisms
  - Allows for rigorous optimization strategies

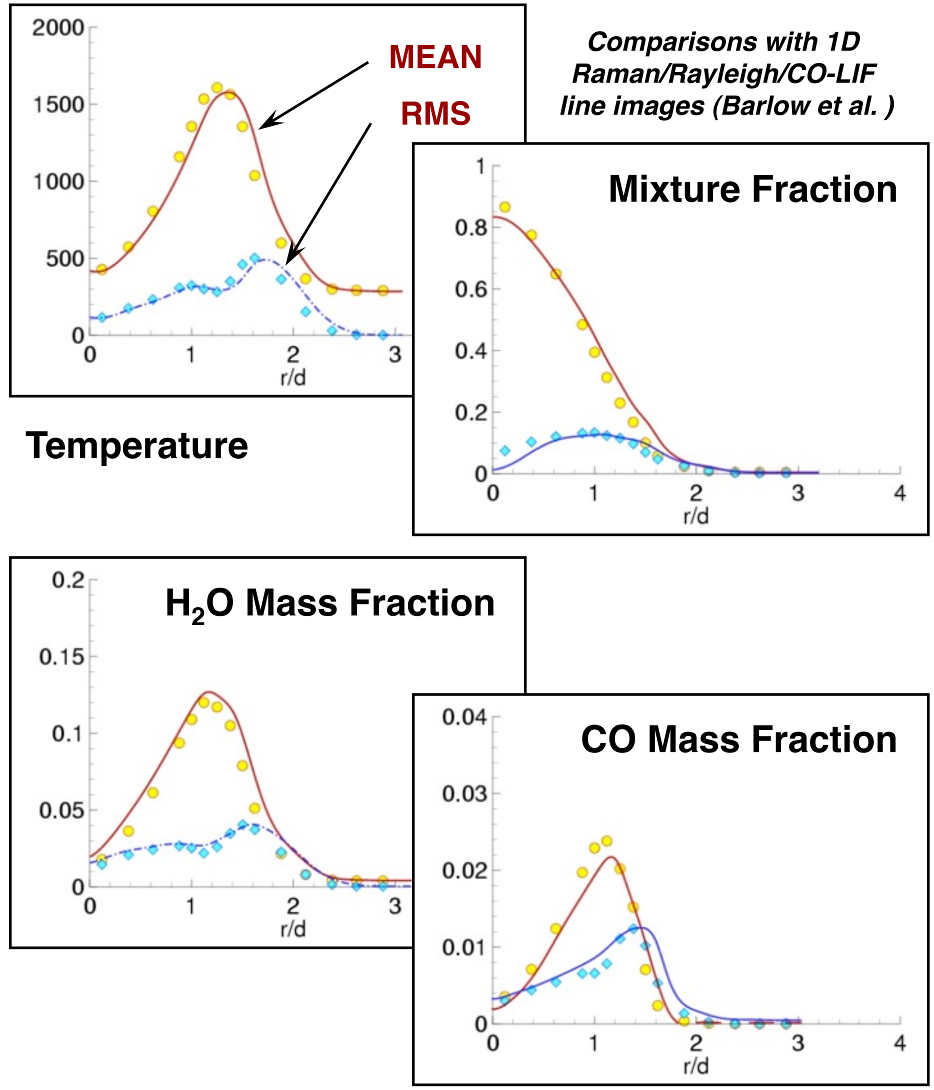
Model validation requires targeted experiments

DLR-A Flame: Re_d = 15,200

Fuel: 22.1% CH_4, 33.2% H_2, 44.7% N_2

Coflow: 99.2% Air, 0.8% H_2O

Detailed Chemistry and Transport: 12-Step Mechanism (J.-Y. Chen, UC Berkeley)



Predictive simulation requires careful assessment of all sources of error and uncertainty

- Numerical errors
  - Grid resolution
  - Time step size
  - Time integration order
  - Spatial derivative order
- Epistemic uncertainty
  - Initial and boundary conditions
  - Model parameters
  - Model equations
- Aleatory uncertainty / intrinsic variability
  - Stochastic processes
  - Sampling noise

Governing equations

- Mass:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}) + \nabla\cdot(\theta\overline{\rho}\tilde{\mathbf{u}}) = \overline{\dot{\rho}}_s$$

- Momentum:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{\mathbf{u}}) + \nabla\cdot\left[\theta\left(\overline{\rho}\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}} + \frac{\mathcal{P}}{M^2}\mathbf{I}\right)\right] = \nabla\cdot(\theta\vec{\vec{\mathcal{T}}}) + \overline{\dot{\mathbf{F}}}_s$$

- Total Energy:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{e}_t) + \nabla\cdot[\theta(\overline{\rho}\tilde{e}_t + \mathcal{P})\tilde{\mathbf{u}}] = \nabla\cdot\left[\theta\left(\vec{\mathcal{Q}}_e + M^2(\vec{\vec{\mathcal{T}}}\cdot\tilde{\mathbf{u}})\right)\right] + \theta\overline{\dot{Q}}_e + \overline{\dot{Q}}_s$$

- Species:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\mathcal{S}}_i) + \theta\overline{\dot{\omega}}_i + \overline{\dot{\omega}}_{s_i}$$

• Spray Source Terms • Composite Stresses/Fluxes • Chemical Source Terms

Smagorinsky sub-grid scale model

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla \cdot \tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] - \overline{\rho}\left(\tilde{\mathbf{u}} \mathbin{\widetilde{\otimes}} \tilde{\mathbf{u}} - \tilde{\tilde{\mathbf{u}}} \otimes \tilde{\tilde{\mathbf{u}}}\right)$$

Dynamic modeling and reacting flows involve additional complexity

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

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- Energy Flux:

$$\vec{\mathcal{Q}}_e = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr}\right)\frac{C_p}{Re}\nabla\tilde{T} + \sum_{i=1}^{N}\tilde{h}_i\vec{\mathcal{S}}_i \; - \; \overline{\rho}C_p\left(\widetilde{\tilde{T}\tilde{\mathbf{u}}} - \tilde{\tilde{T}}\tilde{\tilde{\mathbf{u}}}\right)$$

- Mass Flux:

$$\vec{\mathcal{S}}_i = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i}\right)\frac{1}{Re}\nabla\tilde{Y}_i \; - \; \overline{\rho}\left(\widetilde{\tilde{Y}_i\tilde{\mathbf{u}}} - \tilde{\tilde{Y}}_i\tilde{\tilde{\mathbf{u}}}\right)$$

Coefficients C_R, Pr_t, and Sc_{t_i} Evaluated Dynamically as Functions of Space and Time

UQ assesses confidence in model predictions and allows resource allocation for fidelity improvements

- Parameter inference
  - Determine parameters from data
  - Characterize uncertainty in inferred parameters
- Propagate input uncertainties through computational model
  - Account for uncertainty from all sources
  - Resolve coupling between sources
- Analysis
  - Sensitivity analysis
  - Attribution
- Enables model calibration, validation, selection, averaging

Overview

- Introduction
- Basic methods for uncertainty quantification
  - Representation of random variables
  - Forward propagation
  - Parameter inference
- Application to chemical kinetics
- Advanced uncertainty quantification topics

Polynomial Chaos expansions offer compact representations of random variables

- Random variables are represented as (truncated) Polynomial Chaos (PC) expansions

$$\lambda(\theta) \approx \sum_{k=0}^{P} \lambda_k \Psi_k\left(\xi_1, \xi_2, \cdots, \xi_{N_{\dim}}\right) \qquad P+1 = \frac{\left(N_{\dim} + N_{ord}\right)!}{\left(N_{\dim}! N_{ord}!\right)} \qquad \xi_i = N(0,1)$$

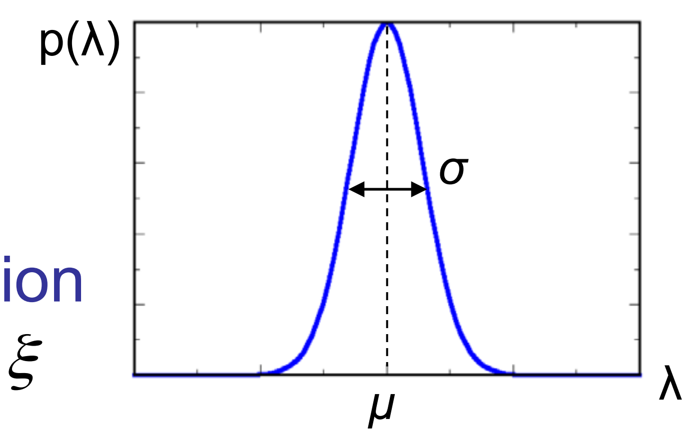
- One-dimensional Gauss-Hermite PC

$$\Psi_0(\xi) = 1$$
$$\Psi_1(\xi) = \xi$$
$$\Psi_2(\xi) = \xi^2 - 1$$
$$\Psi_3(\xi) = \xi^3 - 3\xi$$
$$\Psi_4(\xi) = \xi^4 - 6\xi^2 + 3$$

$$\lambda_k = \frac{\langle \lambda \Psi_k \rangle}{\langle \Psi_k^2 \rangle} \qquad \langle \lambda \Psi_k \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \lambda \Psi_k e^{-\xi^2/2} d\xi$$

- Parameter with Gaussian distribution

$$\lambda = \mu + \sigma \xi$$



Propagation of uncertainty

- Consider example ODE with uncertain parameter λ

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

- Represent both u and λ with PC expansions

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k \qquad\qquad \lambda_k \text{ known}$$

$$\mathrm{u}(\mathrm{t}) = \sum_{k=0}^{P} u_k(t) \Psi_k \qquad\qquad u_k(t) \text{ unknown}$$

- Additional uncertain parameters introduce new stochastic dimensions
- Intrusive and non-intrusive approaches for determining the PC coefficients u_k

Spectral intrusive propagation of uncertainty

- Substitute PC expansions for u and λ in the governing equation
- Perform Galerkin projection onto the PC basis functions
  - System of equations for the PC coefficients $u_k(t)$
  - (P+1) coupled deterministic equations

Substituting PC expansions into the governing equation yields deterministic equations for PC coefficients

- Example ODE with uncertain parameter λ

$$\frac{du}{dt} = \lambda u^2 \qquad \lambda = \sum_{i=0}^{P} \lambda_i \Psi_i \qquad u(t) = \sum_{j=0}^{P} u_j(t) \Psi_j$$

- Substitute PC expansions in the ODE

$$\frac{d}{dt} \sum_{j=0}^{P} u_j(t) \Psi_j = \left(\sum_{l=0}^{P} \lambda_l \Psi_l \right) \left(\sum_{m=0}^{P} u_m(t) \Psi_m \right) \left(\sum_{n=0}^{P} u_n(t) \Psi_n \right)$$

$$\sum_{j=0}^{P} \frac{du_j(t)}{dt} \Psi_j = \sum_{l=0}^{P} \sum_{m=0}^{P} \sum_{n=0}^{P} \lambda_l u_m(t) u_n(t) \Psi_l \Psi_m \Psi_n$$

- Multiply by Ψ_k, take expectation and use orthogonality

$$\left\langle \Psi_k \sum_{j=0}^{P} \frac{du_j(t)}{dt} \Psi_j \right\rangle = \left\langle \Psi_k \sum_{l=0}^{P} \sum_{m=0}^{P} \sum_{n=0}^{P} \lambda_l u_m(t) u_n(t) \Psi_l \Psi_m \Psi_n \right\rangle$$

$$\frac{du_k(t)}{dt} = \sum_{l=0}^{P} \sum_{m=0}^{P} \sum_{n=0}^{P} \lambda_l u_m(t) u_n(t) C_{klmn} \qquad C_{klmn} = \frac{\langle \Psi_k \Psi_l \Psi_m \Psi_n \rangle}{\langle \Psi_k^2 \rangle}$$

Spectral intrusive propagation in practice

- Pros
  - Elegant
  - One time solution of system of equations for the PC coefficients fully characterizes uncertainty in all variables at all times
  - Tailored solvers can (potentially) take advantage of new hardware developments
- Cons
  - Often requires re-write of the original code
  - Reformulated system is factor (P+1) larger than the original system and can be challenging to solve
- Many efforts in the community to automate intrusive UQ
  - UQToolkit http://www.sandia.gov/UQToolkit/
  - Sundance http://www.math.ttu.edu/~klong/Sundance/html/
  - Stokhos http://trilinos.sandia.gov/packages/stokhos/
  - …

Non-intrusive or sampling-based propagation of uncertainty

- Do not require changes to the original solver code
  - Used as black box to generate samples
- Two main categories
  - Galerkin projection approaches
  - Collocation approaches

Non-intrusive spectral projection (NISP) for uncertainty propagation

- Obtain u_k by direct projection onto PC basis

$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u\,\Psi_k e^{-\xi^2/2} d\xi \Big/ \langle \Psi_k^2 \rangle$$

- Random sampling approach: $\int_{-\infty}^{\infty} f(\xi) e^{-\xi^2} dx \cong \frac{1}{N} \sum_{i=1}^{N} f(\xi_i)$
  - Monte Carlo (MC), Latin Hypercube Sampling (LHS), …
  - Convergence as $1/\sqrt{N}$
- Quadrature approach: $\int_{-\infty}^{\infty} f(\xi) e^{-\xi^2} dx \cong \sum_{i=1}^{N_{qp}} w_i f(\xi_i)$
  - Gauss-Hermite quadrature for u_k exact with N_{qp} = P+1 if u is a polynomial of order P (one-dimensional)
  - Evaluate u at N_{qp} quadrature points corresponding to different values of $\lambda(\xi_i)$

Collocation approaches rely on interpolation

- Do not perform projection onto the basis functions
- Consider $u = g(\lambda)$
- Sample parameter space

$$\lambda_i = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi_i)$$

- Solve a system of equations for u_k

$$\mathrm{u}_i = g(\lambda_i) = \sum_{k=0}^{P} u_k \Psi_k(\xi_i)$$

- Many variants depending on location and number of sample points
  - Generally more samples than PC coefficients

Sampling-based approaches in practice

- Pros
  - Easy to use as wrappers around existing codes
  - Embarrassingly parallel
- Cons
  - Most methods suffer severely from curse of dimensionality

$$N = n^d$$

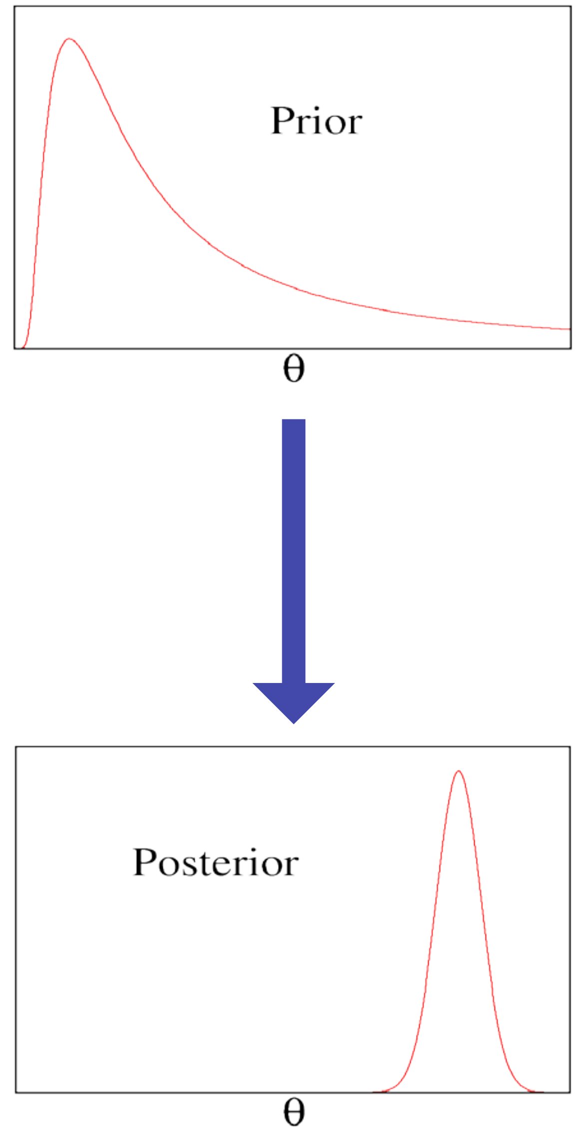
    - (Adaptive) sparse quadrature/collocation methods
- Sampling methods have found very, very widespread use in the community
  - DAKOTA http://dakota.sandia.gov/

Bayesian methods provide probabilistic framework for parameter inference

- Bayes rule

$$\overbrace{P\left(\theta \mid D, M\right)}^{\text{posterior}} = \frac{\overbrace{P\left(D \mid \theta, M\right)}^{\text{likelihood}} \overbrace{P\left(\theta \mid M\right)}^{\text{prior}}}{\underbrace{P\left(D \mid M\right)}_{\text{evidence}}}$$

- Probabilistic framework
  - Naturally handles uncertainties
  - Posterior width indicates confidence in inferred information
  - Can handle heterogeneous data sources
  - Lends itself well to model comparison (Bayes factors)



Likelihood measures goodness-of-fit

$$L(\theta) \propto \prod_{i=1}^{N} e^{-dist[d_i, m(\theta)]/s_i^2}$$

Compare experimental data $D = \{d_i\}_{i=1}^{N}$

with computational model output $m(\theta)$

via *measurement* model $\text{Measured Quantity} = f_i(\text{Modeled Quantity})$

and instrument noise s_i

e.g., Gaussian assumption,

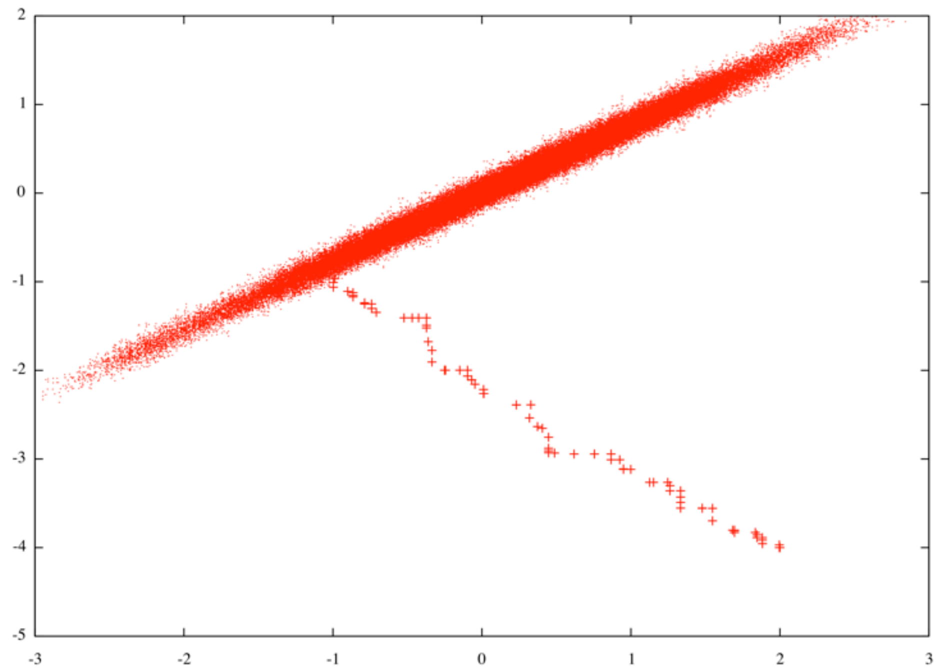
$$dist[d_i, m(\theta)] = [d_i - f_i(m(\theta))]^2$$

- Instrument noise and measurement model details often inferred as *hyperparameters.*

Posterior distribution generally sampled with Markov Chain Monte Carlo (MCMC)

- Basic Metropolis-Hastings algorithm
  - Generate new sample θ^2 from Gaussian proposal distribution centered at current state θ^1
    - Proposal distribution width determines mixing
  - Compute

$$\alpha = \min\left(1, \frac{p\left(\theta^2 \middle| D, M\right)}{p\left(\theta^1 \middle| D, M\right)}\right)$$



  - Accept new sample with probability α
- Many variations / enhancements exist

Overview

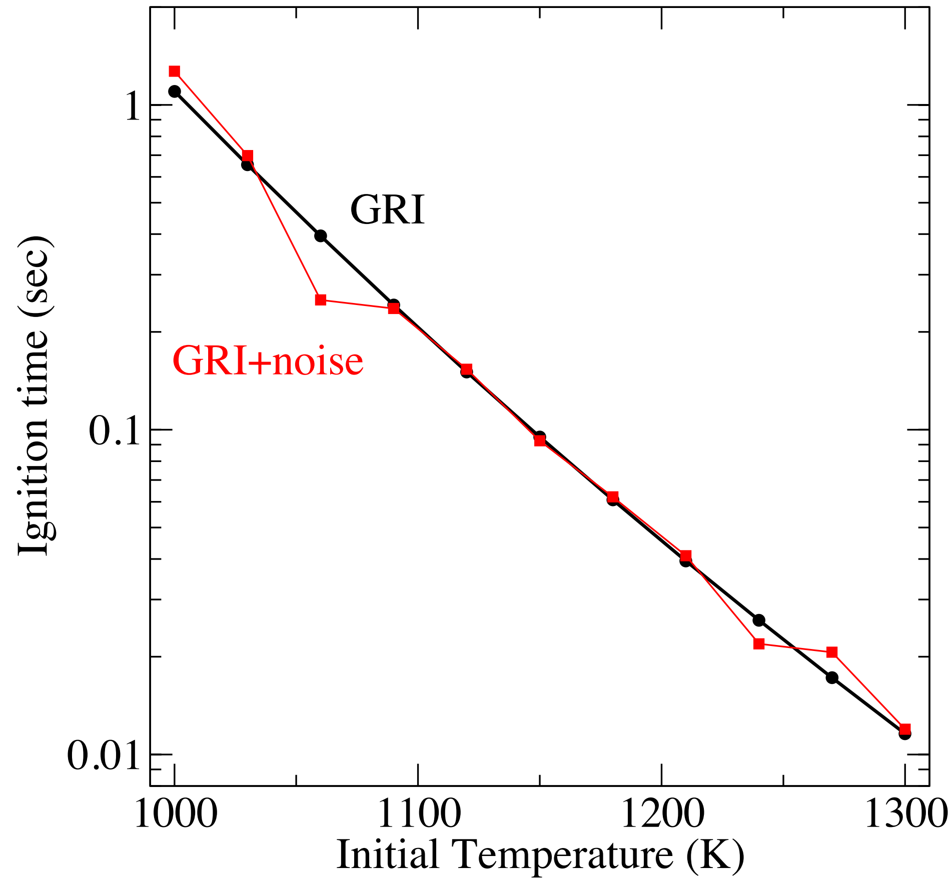
- Introduction
- Basic methods for uncertainty quantification
- Application to chemical kinetics
  - Inference and propagation of reaction kinetics uncertainty
  - Effect of correlation between inferred parameters
- Advanced uncertainty quantification topics

Synthetic "experimental ignition data" generated from detailed chemistry model with added noise

- GRI 3.0 model for methane-air chemistry
- Ignition time versus initial temperature
- Multiplicative noise added

$$d_i = t_{\mathrm{ig},i}^{\mathrm{GRI}} \left(1 + \sigma \varepsilon_i\right)$$

$$\varepsilon_i \sim \mathcal{N}\left(0,1\right)$$



Global single-step irreversible chemical model is fitted to ignition data

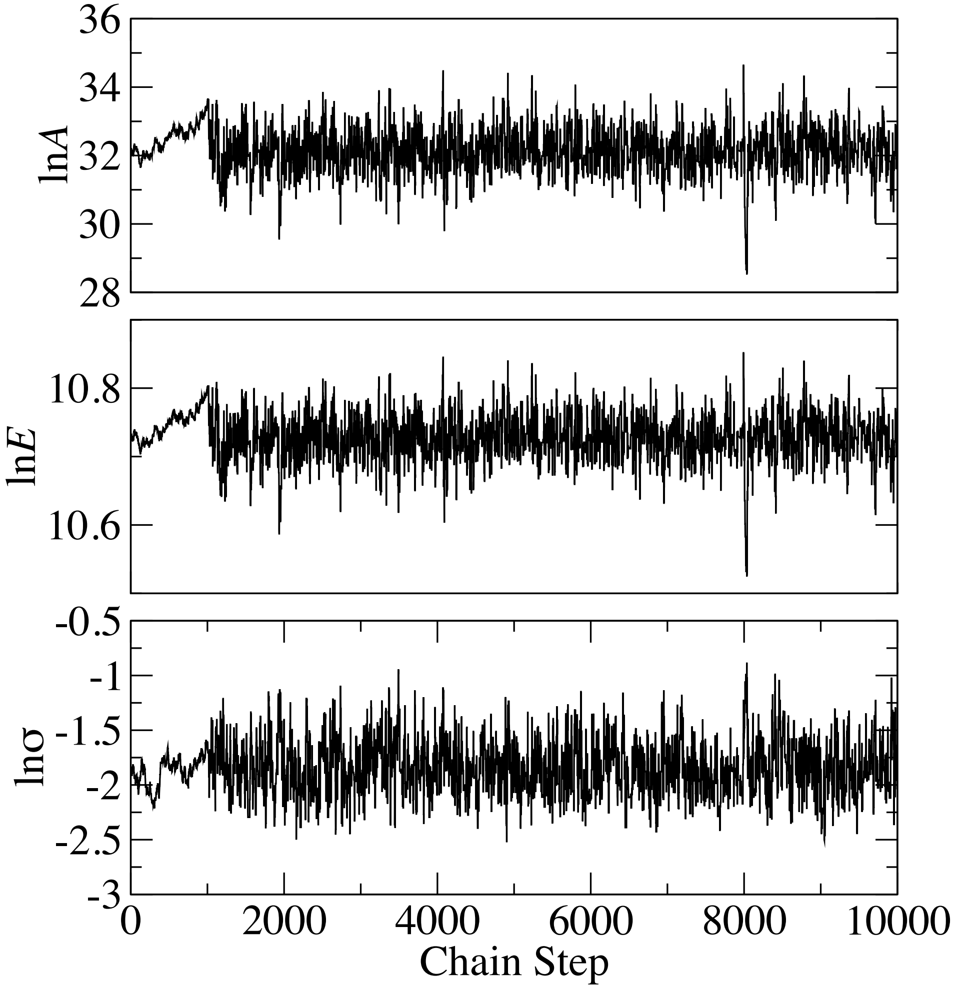
- Model equations

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

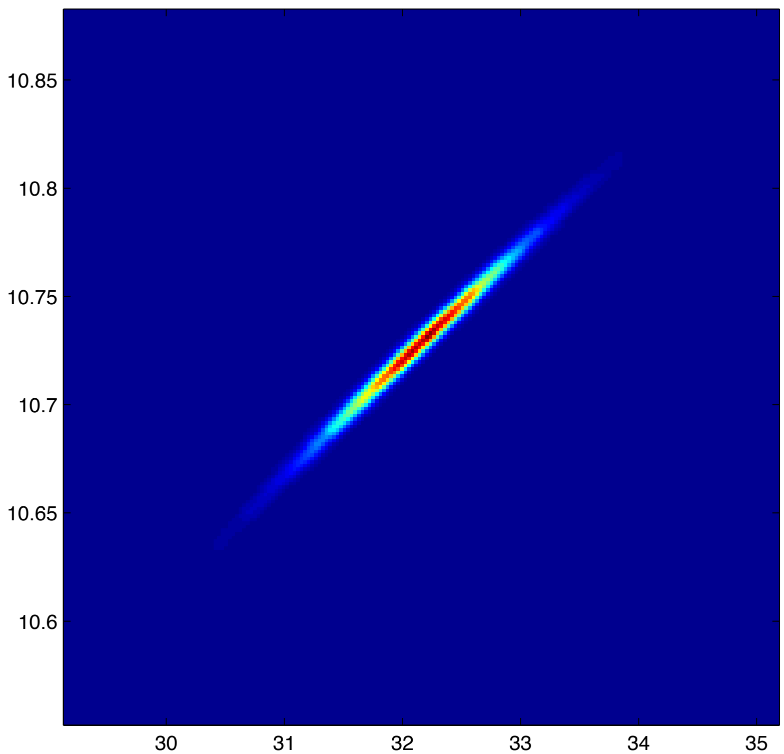
$$\mathcal{R} = [CH_4][O_2]k_f$$

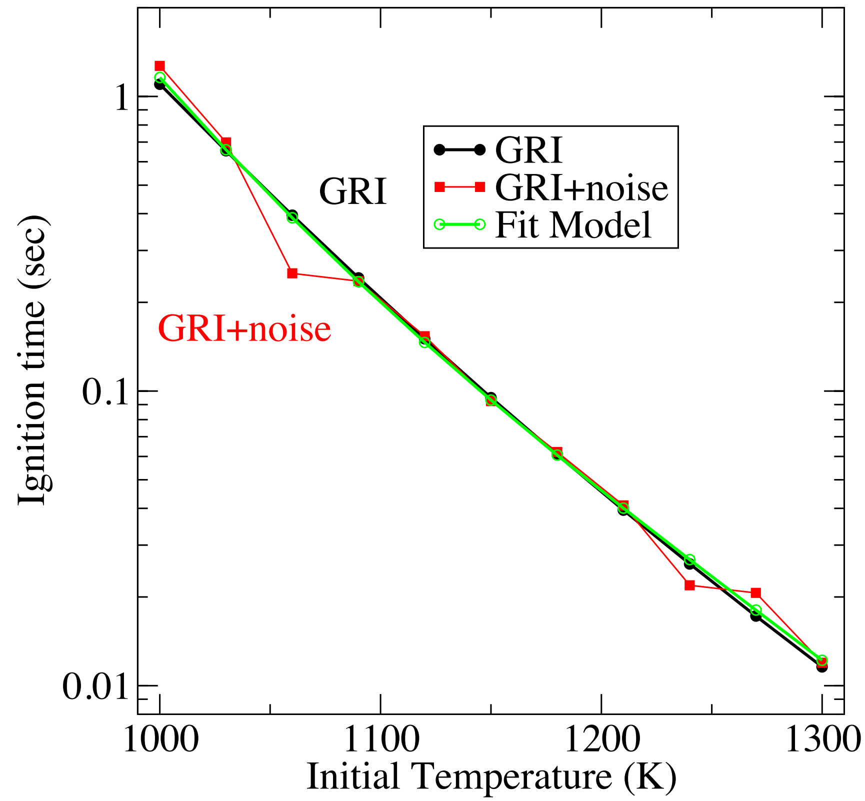
$$k_f = A\exp\left(-E/R^0T\right)$$

- Infer 3-D parameter vector ($\ln A$, $\ln E$, $\ln \sigma$)
- Good mixing with adaptive MCMC when starting at Maximum Likelihood Estimate (MLE)



Calibrated global model fits the data well



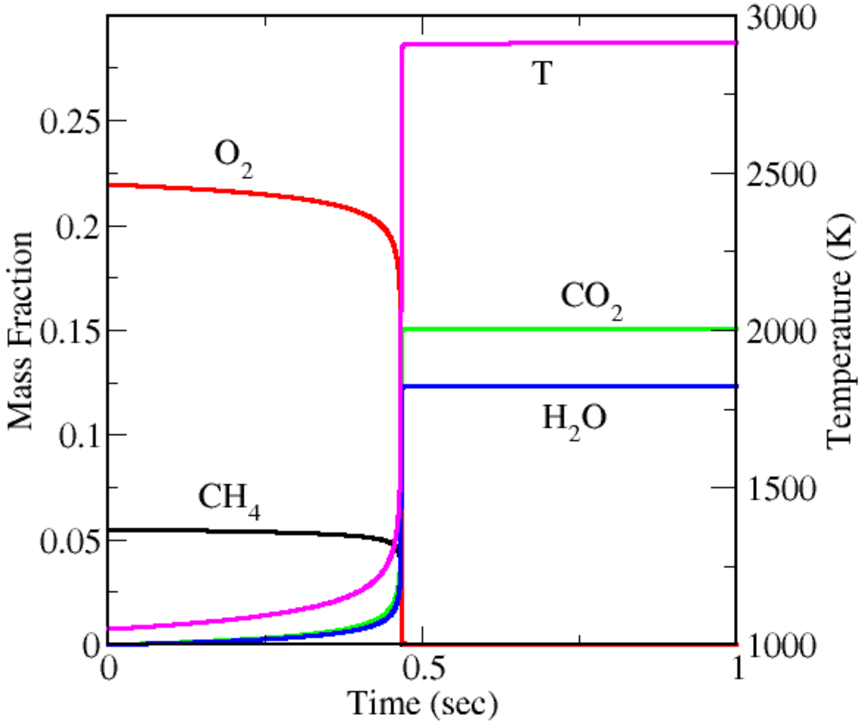


- Marginal posterior (ln *A*, ln *E*) shows strong correlation between the inferred parameters
- Model both with one Gaussian random variable

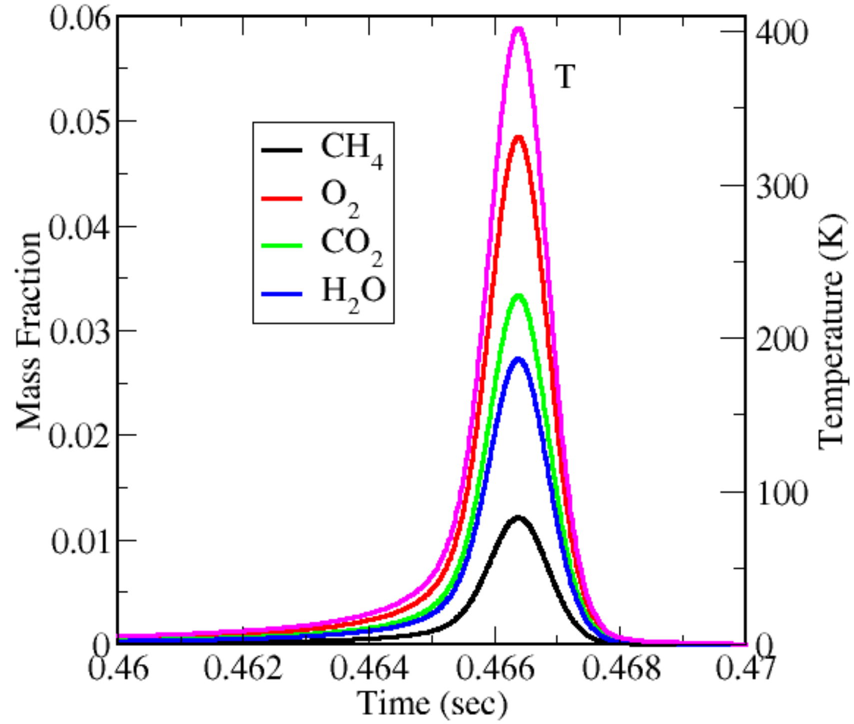
$$\chi = \frac{\sigma_{\ln E}}{\sigma_{\ln A}}$$

Uncertainty in forward model predictions

Means

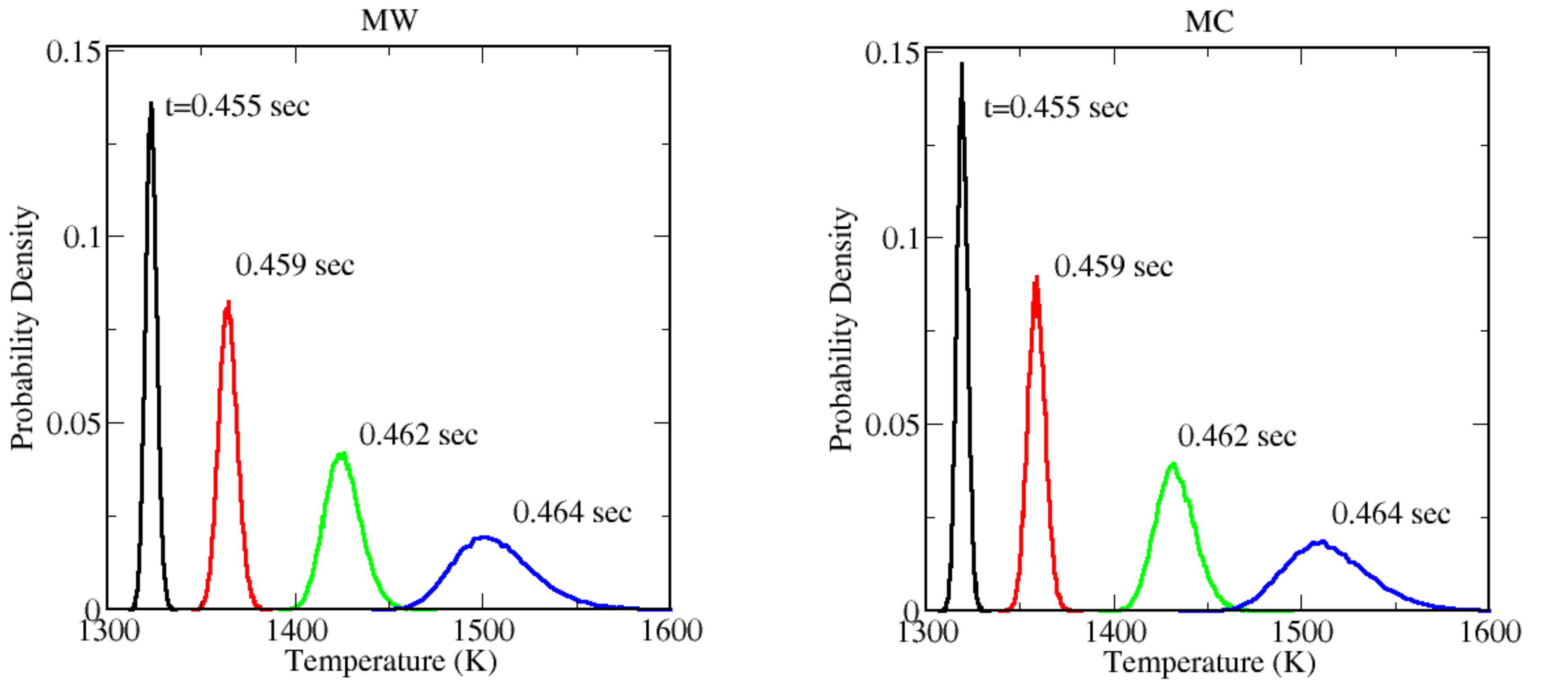


Standard Deviations



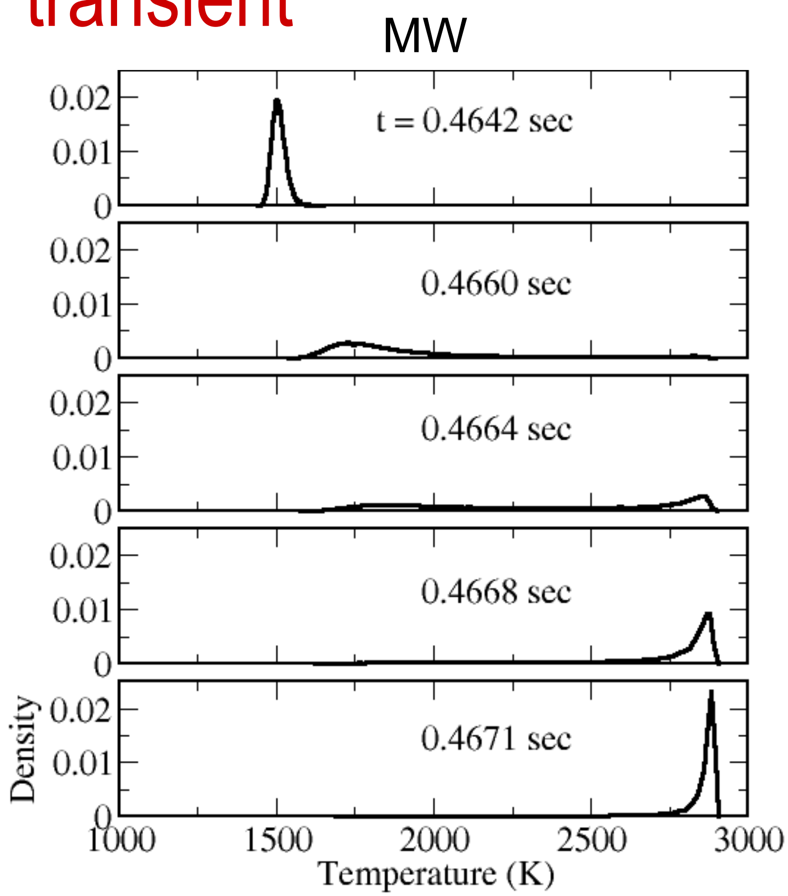
- 4^{th} order multiwavelet PC, multiblock adaptive
- Max standard deviation in T about 400K for χ = 0.03

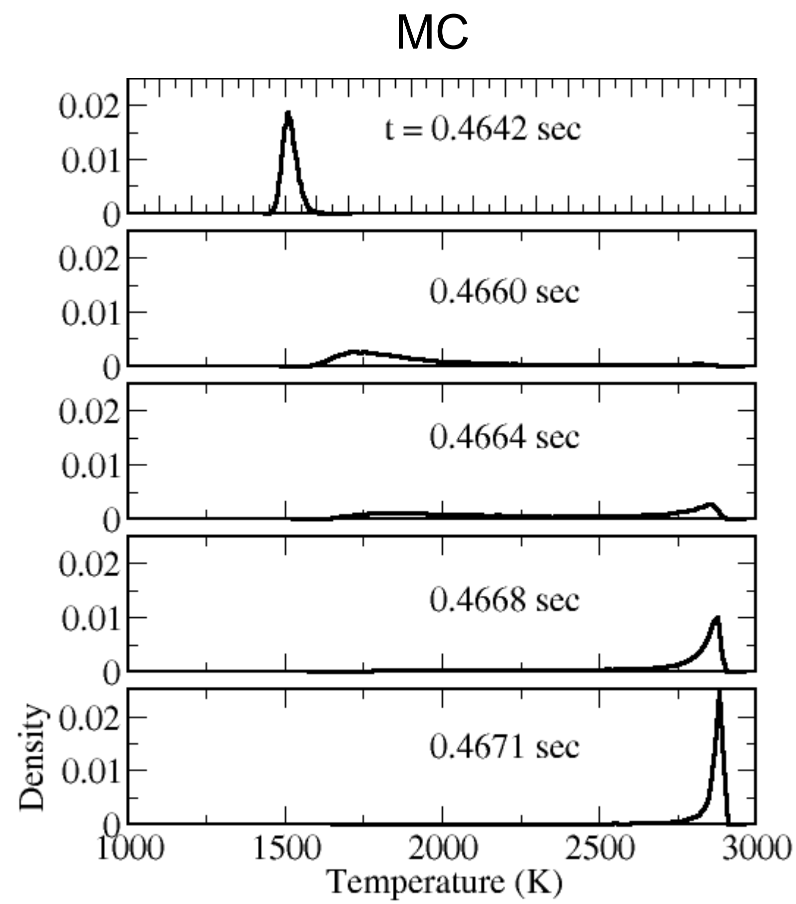
Evolution of temperature PDFs during preheat phase



- Similar results from Monte Carlo (20K samples) as intrusive PC
- With time, uncertainty increases and high-*T* tails get longer

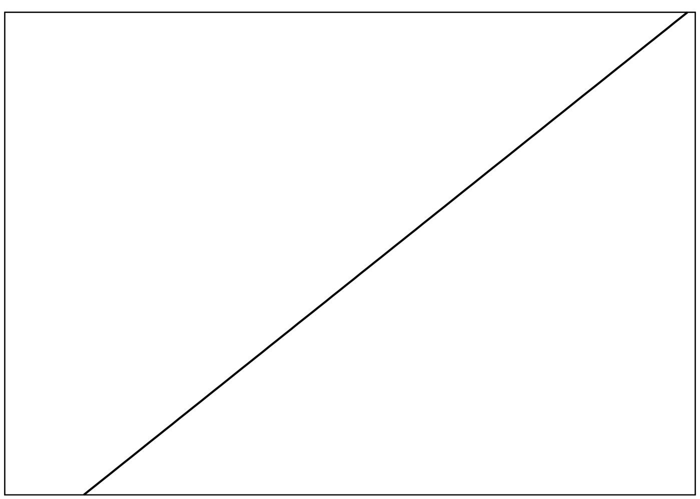
Evolution of temperature PDFs during ignition transient

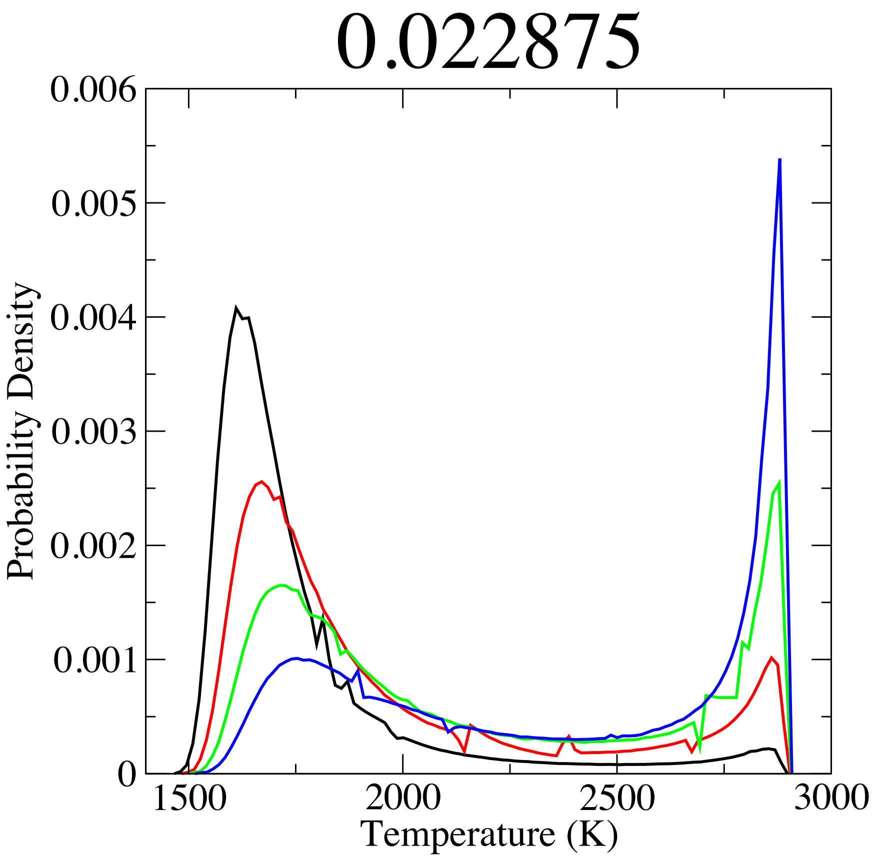




- Transition from unimodal to bimodal pdfs
- Leakage of probability mass from pre-heat PDF high–*T* tail

Correlation slope between uncertain parameters has a strong effect on predicted ignition transient uncertainty





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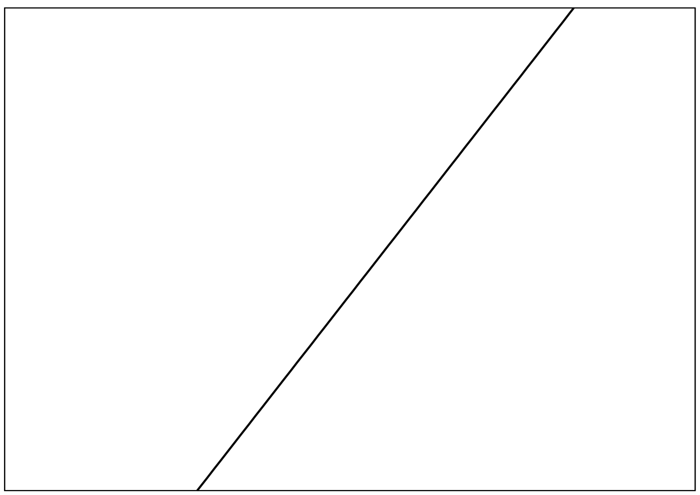

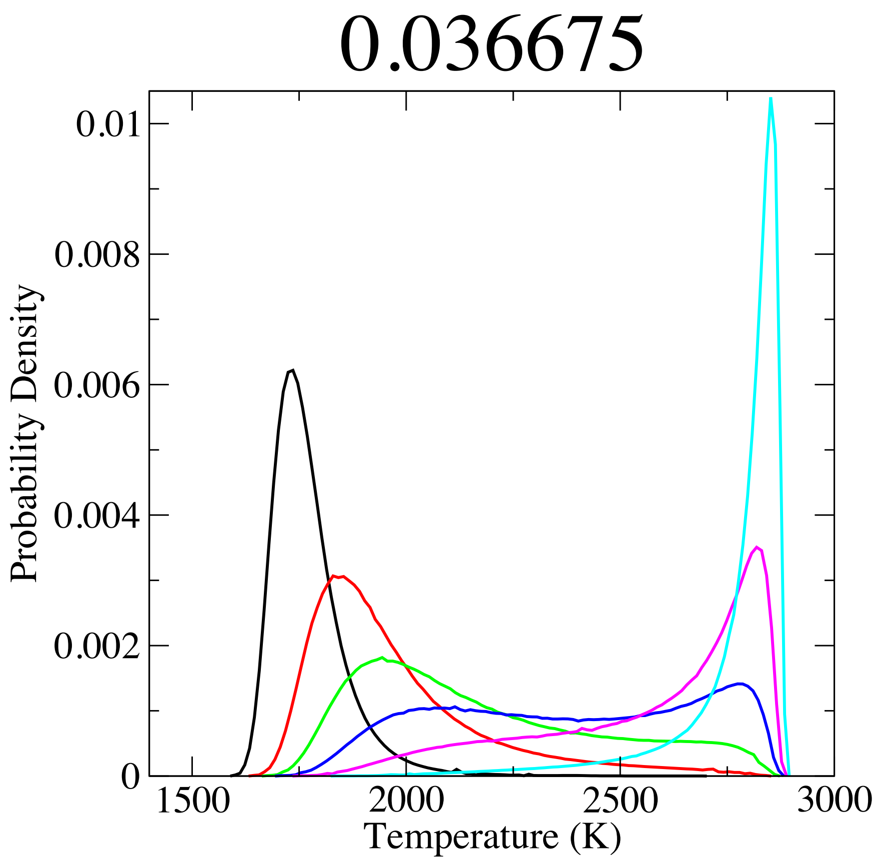

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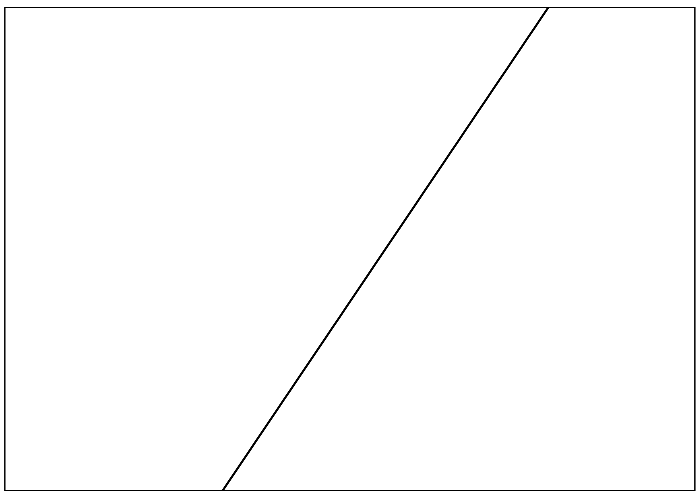

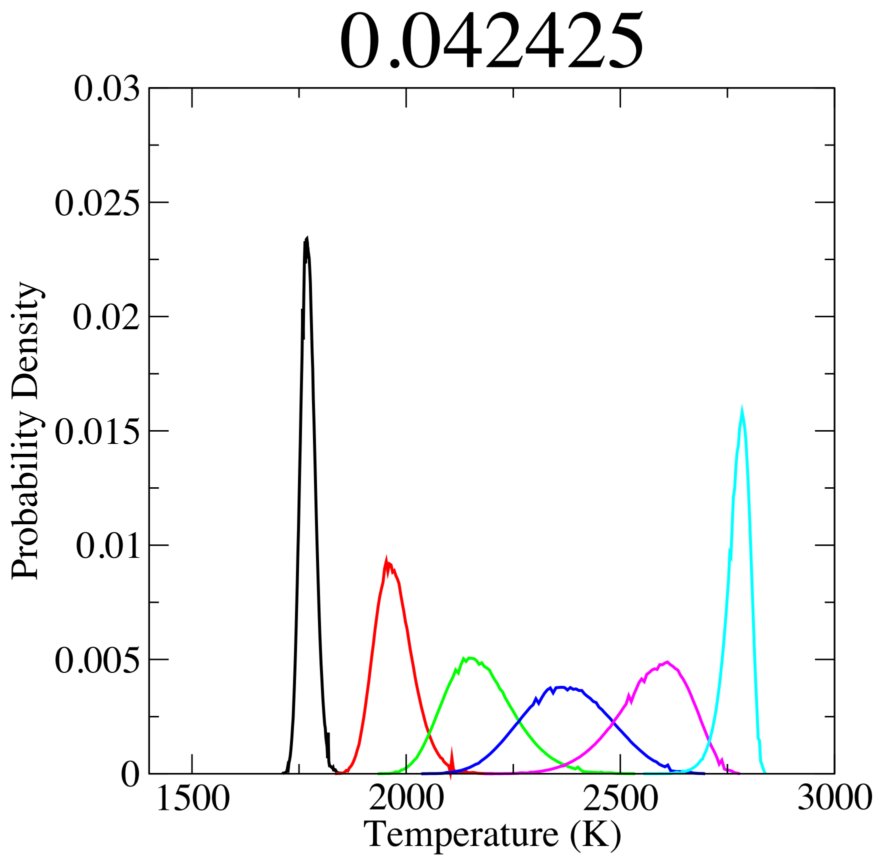

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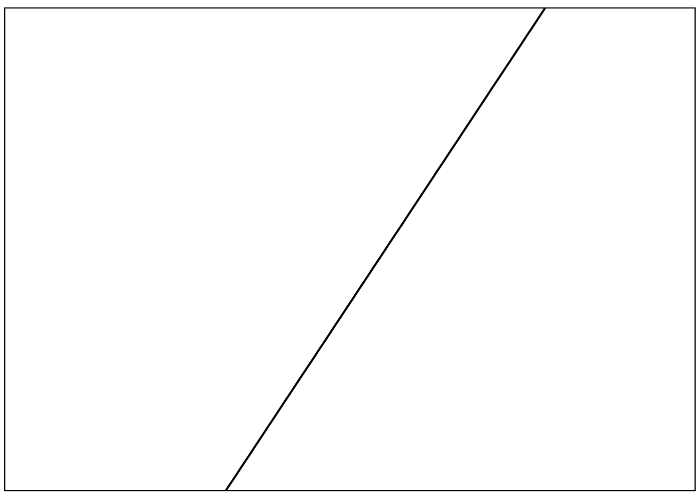

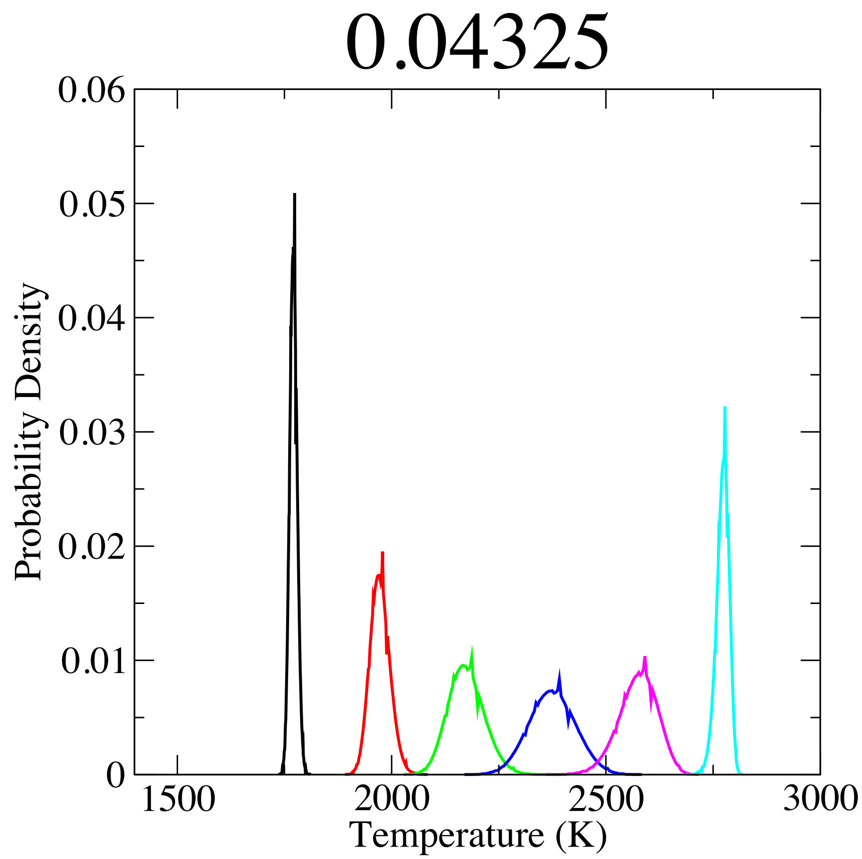

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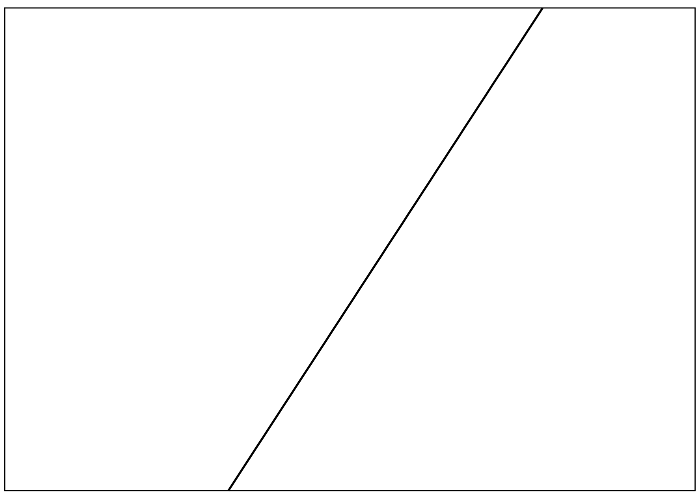

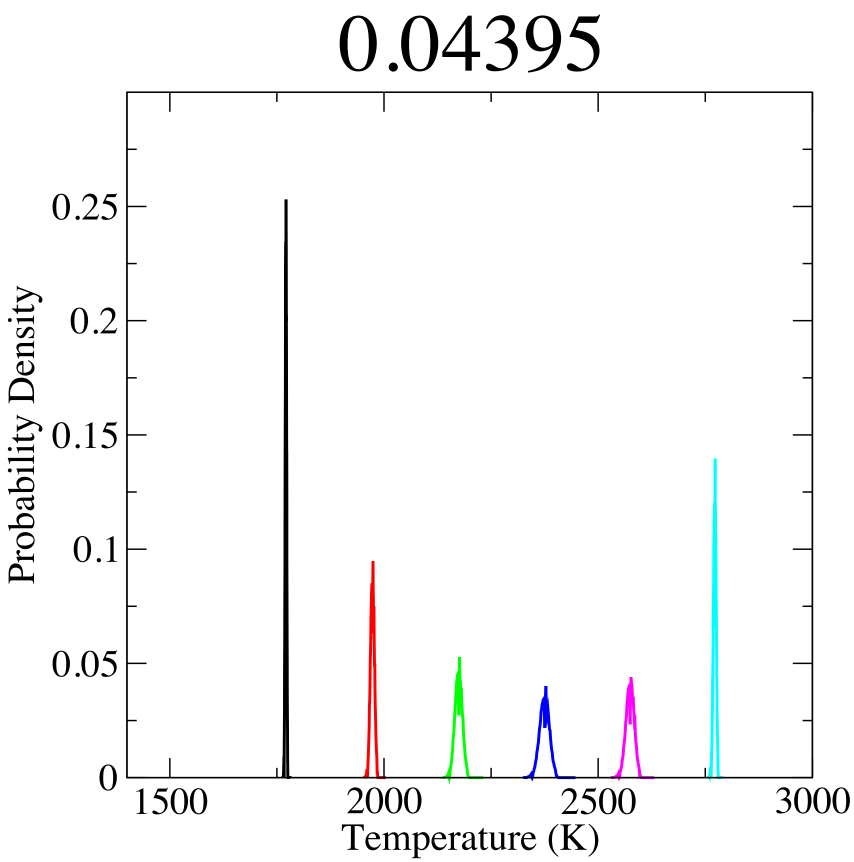

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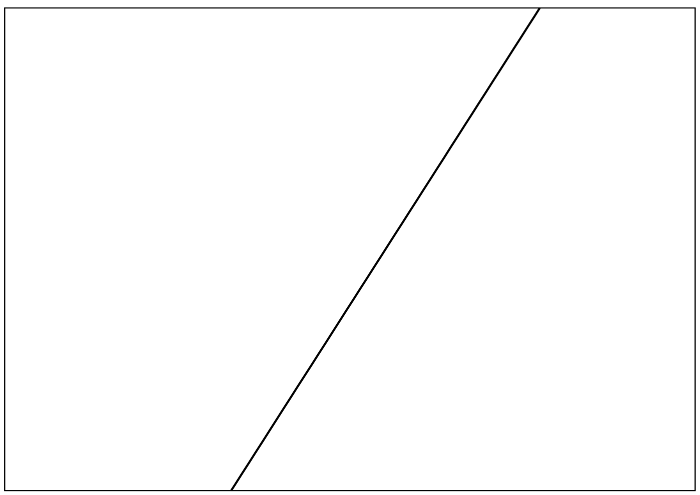

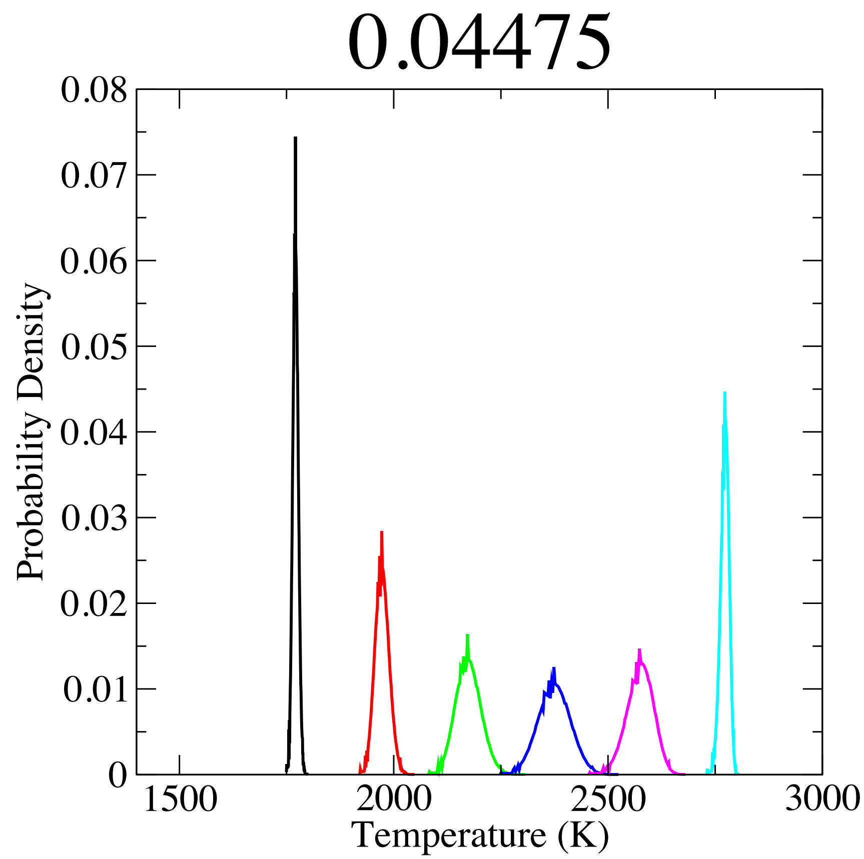

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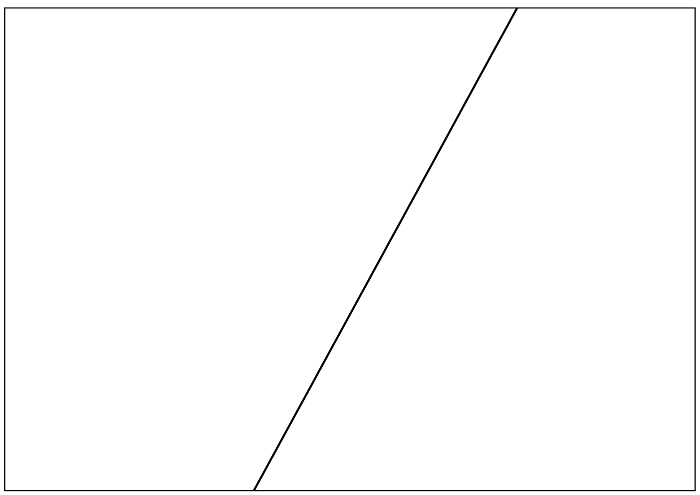

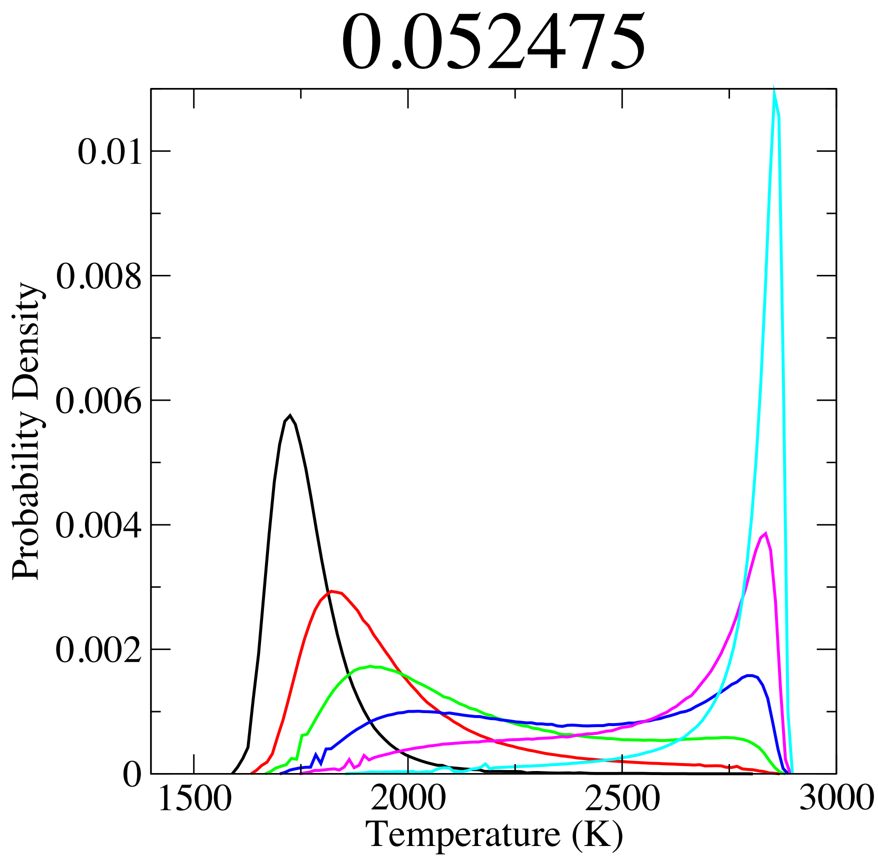

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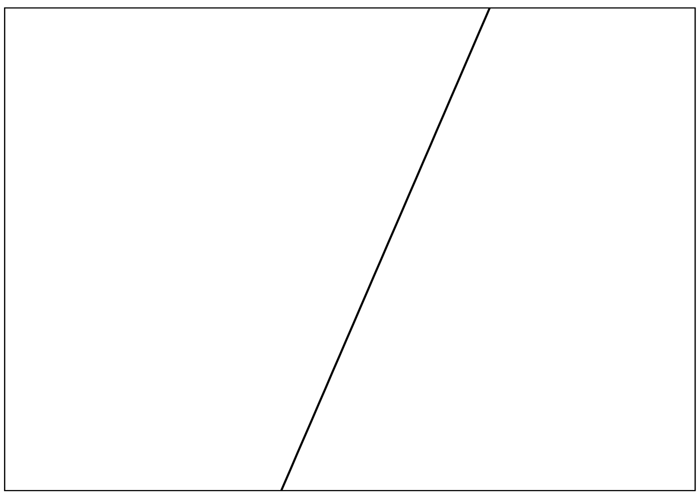
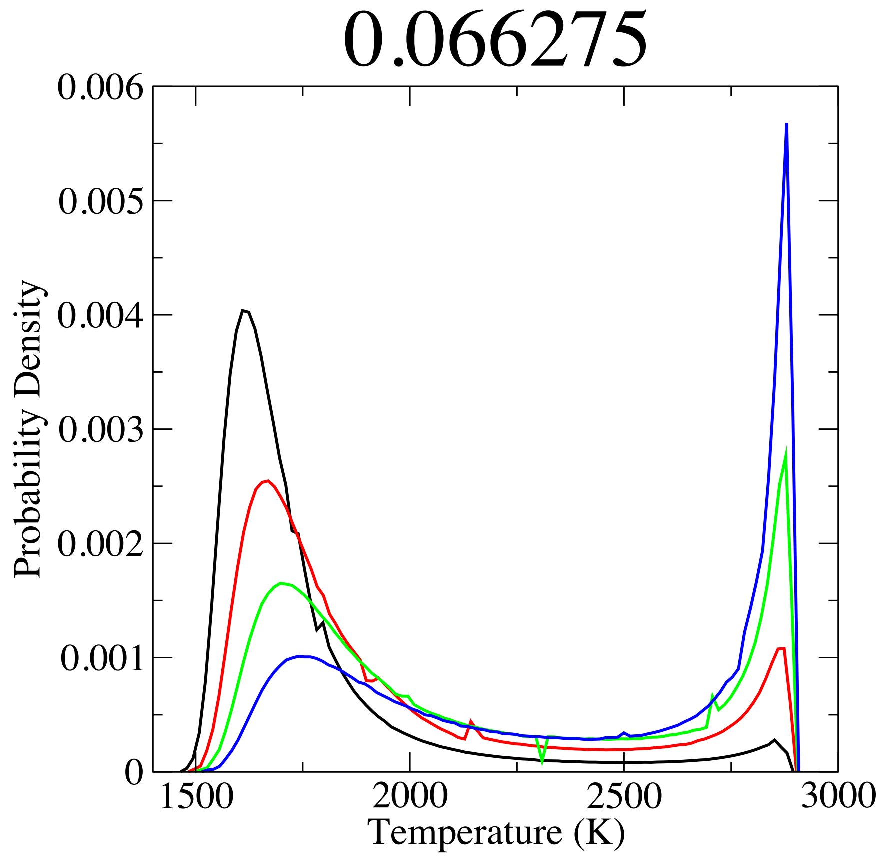




Overview

- Introduction
- Basic methods for uncertainty quantification
- Application to chemical kinetics
- Advanced uncertainty quantification topics
  - Model validation
  - Surrogate models
  - High-dimensional systems
  - Discontinuities / non-linearities
  - Data free inference

Model validation approaches

- *Model sanity checks:*
  - Posterior predictive check

$$P\left(d \middle| D, M\right) = \int P\left(d \middle| \theta, D, M\right) P\left(\theta \middle| D, M\right) d\theta$$

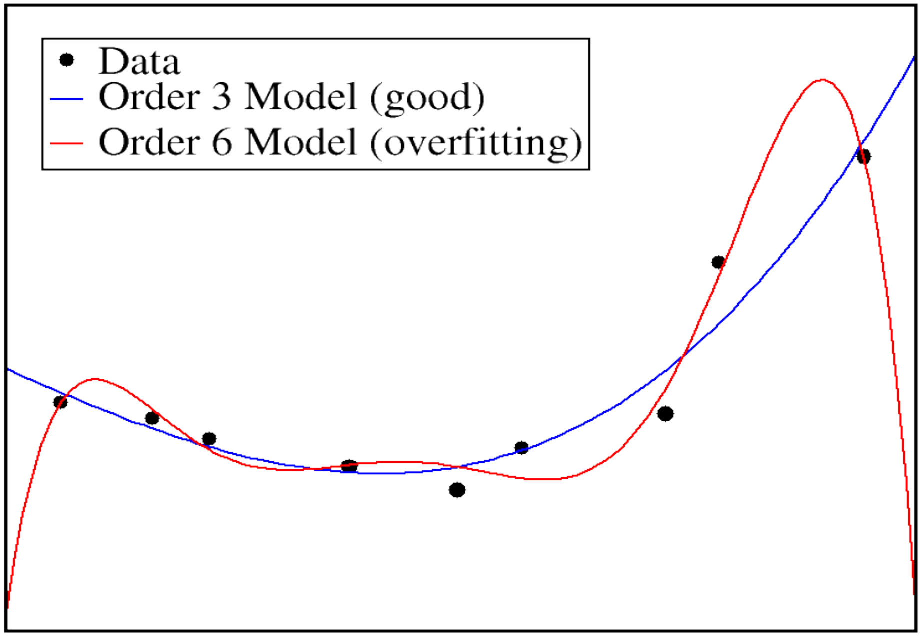
    - Compare posterior predictions of quantities of interest versus existing/new data sets
    - Perform cross-validation
  - Model discrepancy terms

$$d_i = f_i\left(m(\theta) + \delta_m(\theta)\right) + \sigma_i \varepsilon$$

    - Discover structural deficiencies in forward model
    - Enrich model until model discrepancy term small enough
- *Model comparison and plausibility*
  - How adequate is the model for the given dataset, irrespective of model parameters?

Model evidence term combines goodness-of-fit and model complexity

- Likelihood marginalized over all parameters
- Represents Ockham's razor



$$P(D|M) = \int P(D|\theta, M)\, P(\theta|M)\, d\theta$$

$$\log P(D|M) = \overbrace{\int P(\theta|D,M) \log P(D|\theta,M) d\theta}^{\text{average posterior fit}} - \overbrace{\int P(\theta|D,M) \log \frac{P(\theta|D,M)}{P(\theta|M)} d\theta}^{\text{model complexity penalty}}$$

Relative entropy or information gain between prior and posterior

Model comparison is based on model evidence term

- Model Selection: evidence ratio (Bayes Factor)

$$BF = \frac{P(D \mid M_1)}{P(D \mid M_2)}$$

- Model Averaging: based on plausibility for robust predictions

$$M = \{M_i\ , i = 1, \ldots, N_M\}$$

$$P(M_i \mid D) \propto P(D \mid M_i) P(M_i)$$

$$P(q \mid D, M) = \sum_{i=1}^{N_M} P(q \mid D, M_i) P(M_i \mid D)$$

Beck and Yuen (2004), Cheung *et al* (2011).

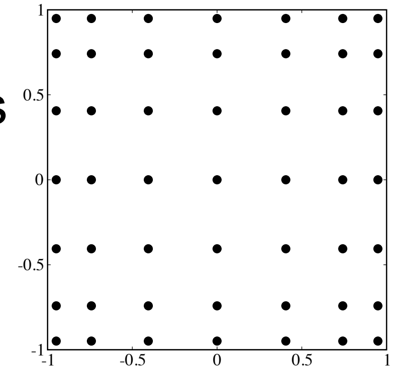
Polynomial Chaos (PC) as a cheap surrogate model

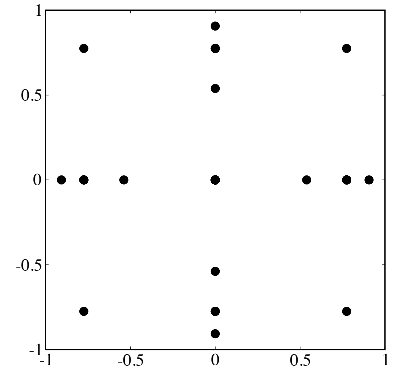
- Input parameter $\theta = \theta_0 + \theta_1 \xi \quad \xi \in [-1, 1]$
- Model output $m(\theta) \approx \sum_k m_k \Psi_k(\xi)$

$\Psi_k(\xi)$ are, *e.g.*, Legendre orthogonal polynomials

- PC modes m_k can be found by
  - orthogonal projection
    - simulate the model at specific parameter values (quadrature)
    - fails for noisy model outputs
  - Bayesian inference
    - works with any set of model simulations
    - robust with respect to noisy outputs
    - leads to random PC modes, i.e. stochastic surrogate model
    - BUT, good accuracy may require prohibitively many simulations

Some outstanding challenges in UQ





- High-dimensional systems
  - (Adaptive) sparse quadrature rules
  - Dimensionality reduction methods
- Discontinuities or strong non-linearities
  - Make global PC expansions fail
  - Domain or data decomposition
  - Infer parameterization of discontinuity and represent smooth function on both sides
- Data to infer full probabilistic description of model inputs often not available
  - Mean and standard deviation may be only thing known
  - Use Data-Free-Inference (DFI) to determine full distribution

Summary

- UQ is an essential component of predictive simulations
  - Assess confidence in model predictions
  - Resource allocation for fidelity improvement
- Many mature approaches available for propagating uncertainties through computational models
- Accurate characterization of the input uncertainties is essential
  - Joint distribution between inputs needed
- Model comparison approaches are emerging
- Many challenges remain

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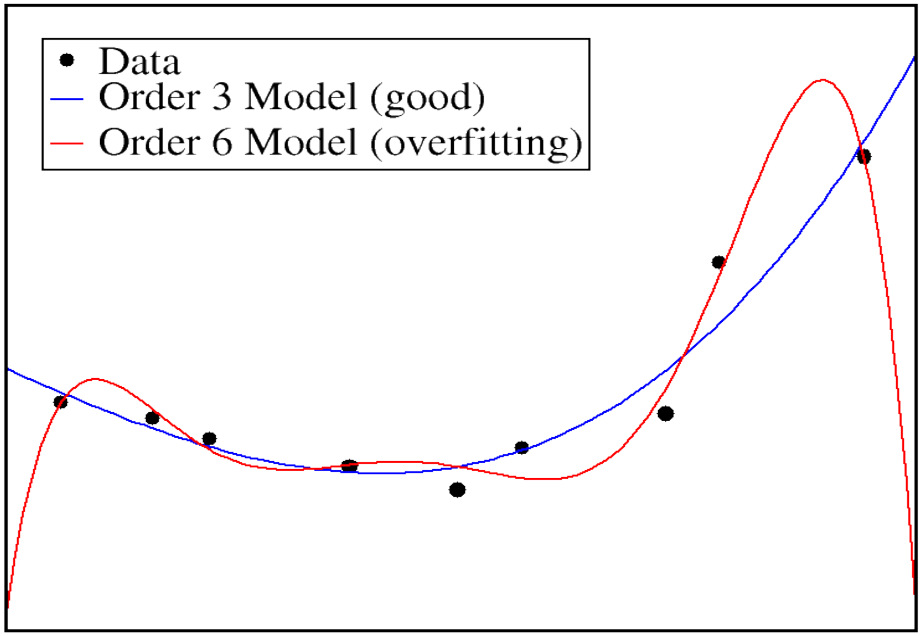
  - At other institutions
    - Omar Knio (JHU), Youssef Marzouk (MIT), Roger Ghanem (USC), Olivier Le Maître (LIMSI), Kevin Long (TTU)
- Key sponsors
  - DOE Advanced Scientific Computing Research
  - SNL Lab Directed Research and Development program

References

Supplementary Material

Ockham's Razor



Relative entropy
or
information gain between
prior and posterior

$$\log P(D|M) = \overbrace{\int P(\theta|D,M)\log P(D|\theta,M)d\theta}^{\text{average posterior fit}} - \overbrace{\int P(\theta|D,M)\log\frac{P(\theta|D,M)}{P(\theta|M)}d\theta}^{\text{model complexity penalty}}$$

Model Evidence balances data fit and model complexity,
i.e. penalizes against overfitting

Non-intrusive spectral projection (NISP) to obtain Polynomial Chaos representation for observables

- Observable is statistical property y = <f(**X**(**λ**))>
- (Truncated) Polynomial Chaos (PC) expansions spectrally represent dependence on uncertain inputs **λ**

$$y(\theta) \approx \sum_{k=0}^{P} c_k \Psi_k \left(\eta_1, \eta_2, \cdots, \eta_{N_{\dim}}\right) \qquad P+1 = \frac{\left(N_{\dim} + N_{ord}\right)!}{\left(N_{\dim}! N_{ord}!\right)}$$

- Basis functions **Ψ** are orthogonal polynomials in standard random variables **η** allowing Galerkin projections

$$c_k = \frac{\left\langle y(\boldsymbol{\lambda}(\boldsymbol{\eta}))\Psi_k(\boldsymbol{\eta})\right\rangle}{\left\langle \Psi_k^2 \right\rangle} = \frac{\int y(\boldsymbol{\lambda}(\boldsymbol{\eta}))\Psi_k(\boldsymbol{\eta}) p(\boldsymbol{\eta}) d\boldsymbol{\eta}}{\left\langle \Psi_k^2 \right\rangle} = \frac{\sum_i w_i \, y(\boldsymbol{\lambda}(\boldsymbol{\eta}_i))\Psi_k(\boldsymbol{\eta}_i)}{\left\langle \Psi_k^2 \right\rangle}$$

- Sparse quadrature needed for high-dimensional systems

Bayesian methods offer a probabilistic framework well suited to infer PC coefficients from noisy data

$$\underbrace{p(\mathbf{c}|D)}_{\text{Posterior}} \propto \underbrace{p(D|\mathbf{c})}_{\text{Likelihood}} \underbrace{p(\mathbf{c})}_{\text{Prior}} \qquad D = \{y_i\}_{i=1}^{N}$$

- Assume uniformly distributed priors
- Gaussian likelihood
  - With σ estimated from Central Limit Theorem or inferred
- Posterior is explored using Markov Chain Monte Carlo sampling
  - Maximum a posteriori (MAP) parameter estimate used

$$\mathbf{c}^{\mathrm{MAP}} = \mathrm{argmax}_{\mathbf{c}}\, p(\mathbf{c}|D)$$

  - Width of posterior shows confidence in inferred parameters for given amount of data
- Generate data by sampling system at locations of sparse quadrature points

Karhunen-Loève (KL) decomposition expands X in terms of the eigenfunctions of its covariance function

$$C(t_1,t_2) = \left\langle \left(X(t_1,\boldsymbol{\theta}) - \overline{X}(t_1)\right)\left(X(t_2,\boldsymbol{\theta}) - \overline{X}(t_2)\right)\right\rangle$$

$$= \sum_{k=1}^{\infty} \lambda_k X_k(t_1) X_k(t_2)$$

$$\int_{T_0}^{T_1} C(t_1,t_2) X_k(t_1)\,dt_1 = \lambda_k X_k(t_2)$$

$$X(t,\boldsymbol{\theta}) = \overline{X}(t) + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\, X_k(t)\,\xi_k \qquad t \in [T_0, T_1]$$

- $X_k(t)$: orthonormal eigenfunctions of the covariance function
- λ_k : corresponding eigenvalues
- ξ_k : uncorrelated, zero-mean, unit-variance random variables
- Covariance function obtained from sampled system trajectories

Uncertain and stochastic dynamical systems

- Two types of uncertainty
  - Reducible (epistemic): can be reduced by additional or better measurements
  - Irreducible (aleatory): due to inherent stochasticity in the system
- Some examples
  - Reaction rate constants in combustion mechanism
  - Physical property values in a solid mechanics problem
  - Turbulent eddies around an airplane wing
  - Small scale variabilities (weather) in a global circulation model
  - Chemical reactions between a small number of molecules
- Uncertainty Quantification (UQ) propagates characterized uncertainties through system model
- Sensitivity analysis determines influence of each parameter on the observables of interest

Stochastic processes can be represented in PC form using a Karhunen-Loève decomposition

- For example: random variability in a temperature boundary condition
- Model random variability as: $T = T_0 \times \left[1 + g(x,\theta)\right]$
- Assume stochastic process has autocorrelation function

$$C\left(\left|x_1 - x_2\right|\right) = \sigma_g^2 \exp\left(-\left|x_1 - x_2\right| / L_c\right)$$

- $g(x,\theta)$ is written in terms of the eigenfunctions $C_k(x)$ of the autocorrelation function C using a Karhunen-Loève decomposition

$$g\left(x,\theta\right) = \left\langle g \right\rangle + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\, C_k(x) \xi_k \Rightarrow g\left(x,\theta\right) \approx \sum_{k=0}^{N_{KL}} g_k(x) \Psi_k(\theta)$$