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Uncertainty Quantification in Reacting Flow

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Outline

1. Basics
2. Validation
3. Estimation of Uncertain Inputs
4. Challenges in Forward PC UQ
5. Closure

Overview of UQ Methods

Estimation of model/parametric uncertainty

- Expert opinion, data collection
- Regression analysis, fitting, parameter estimation
- Bayesian inference of uncertain models/parameters

Forward propagation of uncertainty in models

- Local sensitivity analysis (SA) and error propagation
- Fuzzy logic; Evidence theory — interval math
- Probabilistic framework — Global SA / stochastic UQ
  - Random sampling, statistical methods
  - Polynomial Chaos (PC) methods
    - Collocation methods — sampling — non-intrusive
    - Galerkin methods — direct — intrusive

Different Types of Uncertainty?

- Epistemic versus Aleatoric uncertainty
- Both *can* be handled equally well with probability theory
  - Bayesian versus Frequentist
  - Bayesian viewpoint encompasses both
  - Probabilistic math structure is self-consistent for both
- When interval methods are used in practical problems:
  - Challenges with blow up of interval ranges – Singer, SISC 2006
  - Resort to random sampling – Kreinovich, RC 2007
- Any quantity can be estimated
  - Expert opinion
  - Maximum Entropy
  - Bayes formula

Validation

- No model is “true"
- Validity is a statement of model utility for predicting a given observable under given conditions
- Inspection of model utility requires accounting for uncertainty
- Statistical tool-chest for model validation
  - Calibration based on a data subset and analysis of fit to its complement
  - Model comparison – Bayes Factors, Model Plausibility
  - Posterior predictive

Bayes formula for Parameter Inference

- Data Model (fit model + noise): $y = f(\lambda) + \epsilon$
- Bayes Formula:

$$p(\lambda, y) = p(\lambda|y)p(y) = p(y|\lambda)p(\lambda)$$

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}}\ \overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Prior: knowledge of λ prior to data
- Likelihood: forward model and measurement noise
- Posterior: combines information from prior and data
- Evidence: normalizing constant for present context

Exploring the Posterior

- Given any sample λ, the un-normalized posterior probability can be easily computed

$$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$

- Explore posterior w/ Markov Chain Monte Carlo (MCMC)
  - Metropolis-Hastings algorithm:
    - Random walk with proposal PDF & rejection rules
  - Computationally intensive, $\mathcal{O}(10^5)$ samples
  - Each sample: evaluation of the forward model
    - Surrogate models
- Evaluate moments/marginals from the MCMC statistics

Surrogate Models for Bayesian Inference

- Need an inexpensive response surface for
  - Observables of interest y
  - as functions of parameters of interest λ
- Fit a convenient polynomial to $y = f(\lambda)$
  - over the range of uncertainty in λ
  - Employ a number of samples (λ_i, y_i)
  - Fit with interpolants, regression, ... global/local
  - With uncertain λ :
    - Construct polynomial chaos response surface

Polynomial Chaos Methods for UQ

- Model uncertain quantities as random variables (RVs)
- Any RV with finite variance can be represented as a Polynomial Chaos expansion (PCE)

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

  - $u_k(\mathbf{x},t)$ are mode strengths
  - $\boldsymbol{\xi}(\omega) = \{\xi_1,\cdots,\xi_n\}$ is a vector of standard RVs
  - $\Psi_k()$ are functions orthogonal w.r.t. the density of $\boldsymbol{\xi}$

- with dimension n and order p:

$$P+1 = \frac{(n+p)!}{n!p!}$$

Orthogonality

By construction, the functions $\Psi_k()$ are orthogonal with respect to the density of the basis/*germ* ξ

$$u_k(\mathbf{x},t) = \frac{\langle u\Psi_k\rangle}{\langle \Psi_k^2\rangle} = \frac{1}{\langle \Psi_k^2\rangle}\int u(\mathbf{x},t;\lambda(\boldsymbol{\xi}))\,\Psi_k(\boldsymbol{\xi})p_{\boldsymbol{\xi}}(\boldsymbol{\xi})d\boldsymbol{\xi}$$

Examples:

- Hermite polynomials with Gaussian basis
- Legendre polynomials with Uniform basis, ...
- Global versus Local PC methods
  - Adaptive domain decomposition of the stochastic support of u

Intrusive PC UQ: A direct *non-sampling* method

- Given model equations: $\mathcal{M}(u(\mathbf{x},t);\lambda) = 0$
- Express uncertain parameters/variables using PCEs

$$u = \sum_{k=0}^{P} u_k \Psi_k; \quad \lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$$

- Substitute in model equations; apply Galerkin projection
- New set of equations: $\mathcal{G}(U(\mathbf{x},t),\Lambda) = 0$
  - with $U = [u_0,\ldots,u_P]^T$, $\Lambda = [\lambda_0,\ldots,\lambda_P]^T$
- Solving this system *once* provides the full specification of uncertain model ouputs

Non-intrusive Spectral Projection (NISP) PC UQ

- *Sampling*-based
- Relies on black-box utilization of the computational model
- Evaluate projection integrals *numerically*
- For any model output of interest $\phi(\boldsymbol{x}, t; \lambda)$:

$$\phi_k(\boldsymbol{x}, t) = \frac{1}{\langle \Psi_k^2 \rangle} \int \phi(\boldsymbol{x}, t; \lambda(\boldsymbol{\xi}))\, \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad k = 0, \ldots, P$$

- Integrals can be evaluated using
  - A variety of (Quasi) Monte Carlo methods
  - Quadrature/Sparse-Quadrature methods

PC Surrogate

$$\lambda(\boldsymbol{\xi}) = \sum_{k=0}^{P} \lambda_k \Psi_k(\boldsymbol{\xi})$$

$$u = f(\lambda(\boldsymbol{\xi})) \qquad u = \sum_{k=0}^{P} u_k \Psi_k(\boldsymbol{\xi})$$

- Surrogate can be constructed with any presumed $p_\lambda(\lambda)$
  - Convenient linear option: $\lambda = \lambda_0 + \lambda_1 \xi$
- PDF(ξ) controls local accuracy of the surrogate over λ
  - A uniform ξ implies uniform weighting of the error residual over λ
- Any forward-UQ method of choice can be used to construct the surrogate

PC Surrogate Construction for Noisy Functions

- Quadrature formulae presume a degree of smoothness
  - No convergence for a noisy function

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

- Sparse-Quadrature formulae are *ill-conditioned* and highly-sensitive to noise
  - No convergence with order
  - Error grows with increased dimensionality
- Options in the presence of noise:
  - RMS fitting for PC coefficients
  - Bayesian inference of PC coefficients

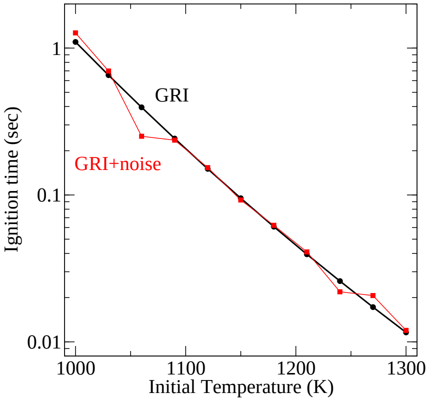
Parameter Estimation in Chemical Systems

- Forward UQ requires the joint PDF on the input space
  - Published data is frequently inadequate
- Bayesian inference can provide the joint PDF
  - Requires raw data ... which is not available
- At best: nominal parameter values and error bars
- Fitting hypothesized PDFs to each parameter nominals/bounds independently is not a good answer
  - Correlations and joint PDF structure can be crucial to uncertainty in predictions

Generate ignition "data" using a detailed model+noise

- Ignition using a detailed chemical model for methane-air chemistry
- Ignition time versus Initial Temperature
- Multiplicative noise error model
- 11 data points:

$$d_i = t_{\text{ig},i}^{\text{GRI}}(1 + \sigma\epsilon_i)$$
$$\epsilon \sim N(0, 1)$$



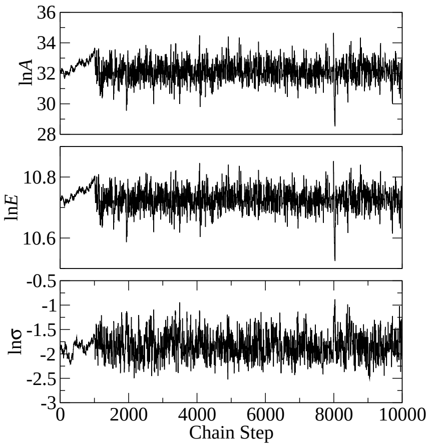
Fitting with a simple chemical model

- Fit a global single-step irreversible chemical model

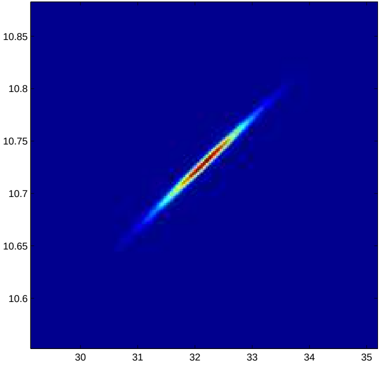
$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$\begin{aligned} \mathfrak{R} &= [CH_4][O_2]k_f \\ k_f &= A\exp(-E/R^oT) \end{aligned}$$

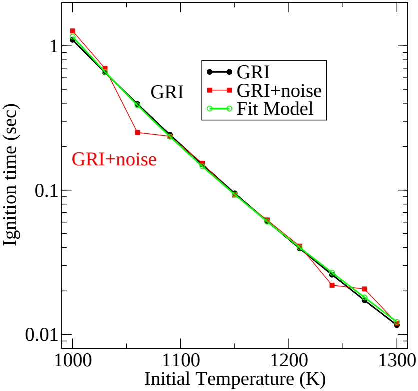
- Infer 3-D parameter vector $(\ln A, \ln E, \ln \sigma)$
- Good mixing with adaptive MCMC when start at MLE



Bayesian Inference Posterior and Nominal Prediction

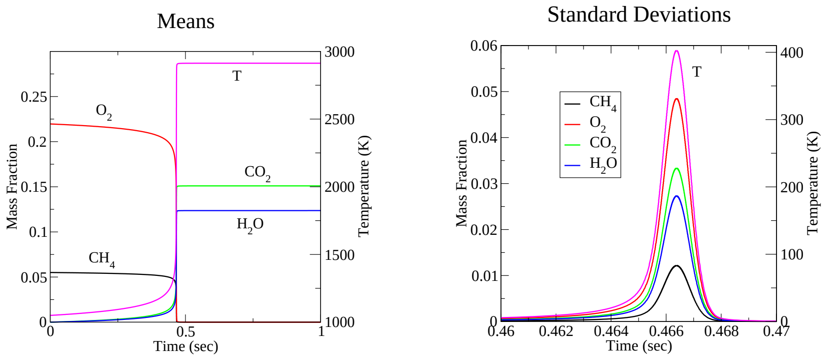


Marginal joint posterior on $(\ln A, \ln E)$ exhibits strong correlation



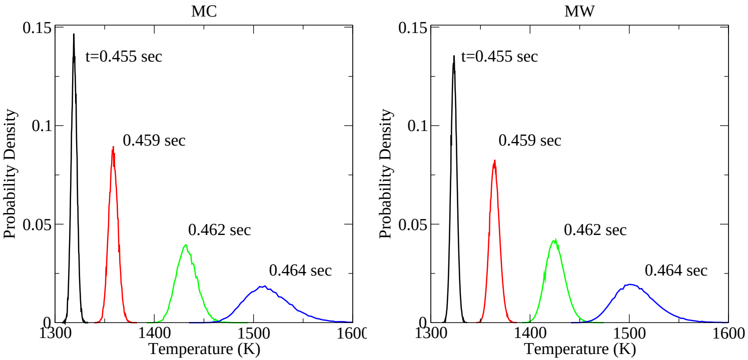
Nominal fit model is consistent with the true model

Correlation Slope χ and Chemical Ignition



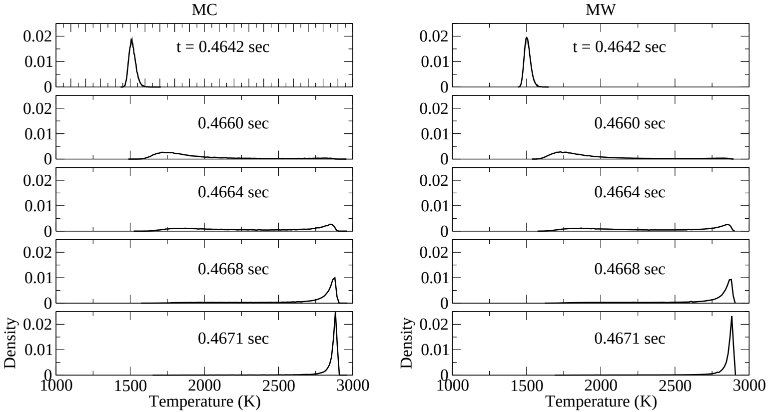
- 4^{th} Order Multiwavelet PC, Multiblock, Adaptive
- $\sigma_{T,\max} \sim$ 400 K during ignition transient, $\chi \sim 0.03$

Time evolution of Temperature PDFs in preheat stage



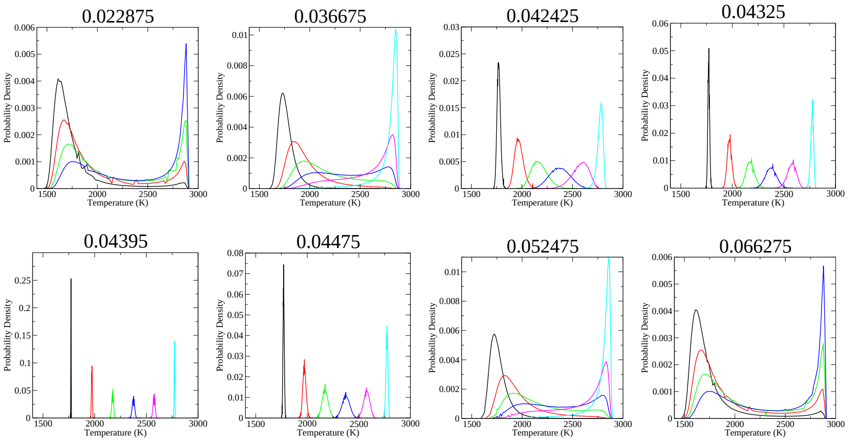
- Similar results from MC (20K samples) and MW PC
- Increased uncertainty, and long high–T PDF tails, in time

Evolution of Temp. PDF – Fast Ignition Transient



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

Time evolution of Temperature PDFs for different χ



- Bimodal solution PDFs for high uncertainty growth
- Unimodal for low uncertainty growth, with $\chi \approx 0.044$

Central Challenge for UQ in Chemical Kinetic Models

- Need joint PDF on model parameters for forward UQ
- Joint PDF structure is crucial
- Joint PDF not available for chemical kinetic parameters
- At best, have
  - Nominal parameter values
  - Bounds, *e.g.* marginal 5%, 95% quantiles
- PDF ***can*** be constructed by repeating experiments or access to original raw data
  - Neither is feasible
- Is there a way to construct an approximate PDF ***without*** access to raw data?
  - Yes!

Data Free Inference (DFI)

(Berry *et al.*, JCP, in review)

- Intuition: In the absence of data, the structure of the fit model, combined with the nominals and bounds, implicitly inform the correlation between the parameters
- Goal: Make this information *explicit* in the joint PDF
- DFI: discover a consensus joint PDF on the parameters consistent with given information:
  - Nominal parameter values
  - Bounds
  - The fit model
  - The data range
  - ... potentially other/different constraints

Data Free Inference Challenge

Discarding initial data, reconstruct marginal $(\ln A, \ln E)$ posterior using the following information

- Form of fit model
- Range of initial temperature
- Nominal fit parameter values of $\ln A$ and $\ln E$
- Marginal 5% and 95% quantiles on $\ln A$ and $\ln E$

Further, for now, presume

- Multiplicative Gaussian errors
- $N = 8$ data points

DFI Algorithm Structure

Basic idea:

- Explore the space of hypothetical data sets
  - MCMC chain on the data
  - Each state defines a data set
- For each data set:
  - MCMC chain on the parameters
  - Evaluate statistics on resulting posterior
  - Accept data set if posterior is consistent with given information
- Evaluate pooled posterior from all acceptable posteriors

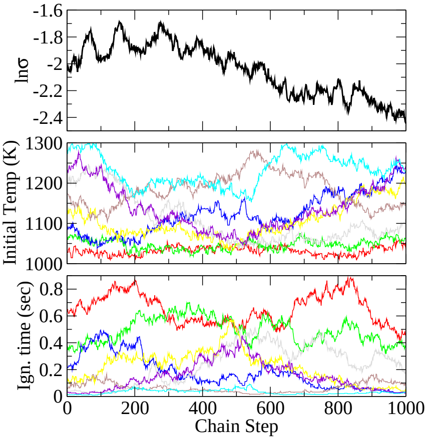
  Logarithmic pooling:

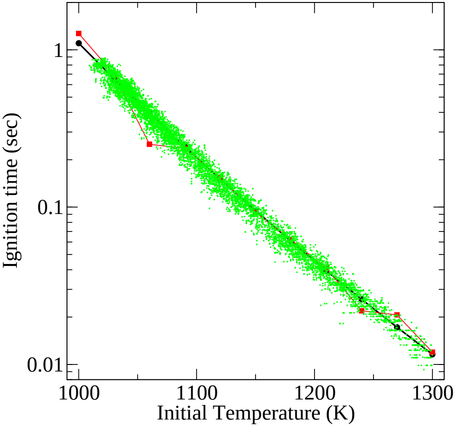
$$p(\lambda|y) = \left[\prod_{i=1}^{K} p(\lambda|y_i)\right]^{1/K}$$

DFI Uses two nested MCMC chains

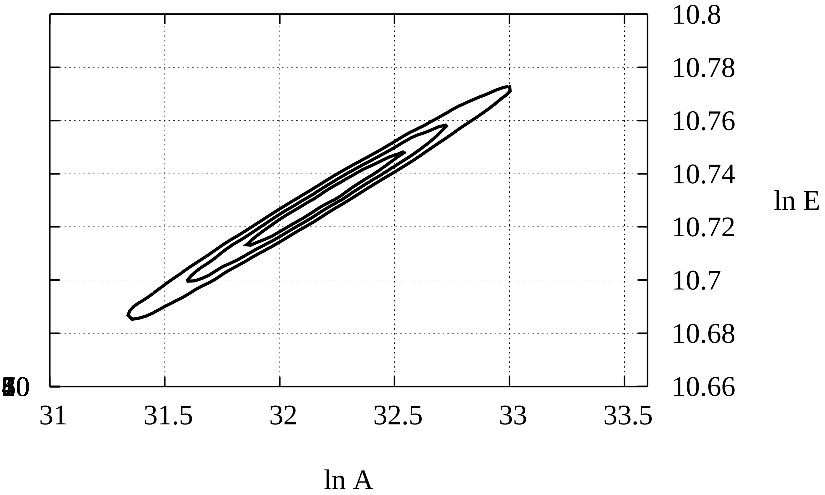
- An outer chain on the data, $(2N+1)$–dimensional
  - Generally high-dimensional
  - N data points (x_i, y_i) + σ
  - Likelihood function captures constraints on parameter nominals+bounds
- An inner chain on the model parameters
  - Conventional MCMC for parameter estimation
  - Likelihood based on fit-model
  - parameter vector $(\ln A, \ln E, \ln \sigma)$
- Computationally challenging
  - Single-site update on outer chain
  - Adaptive MCMC on inner chain
  - Run multiple outer chains in parallel, and aggregate resulting acceptable data sets

Short sample from outer/data chain

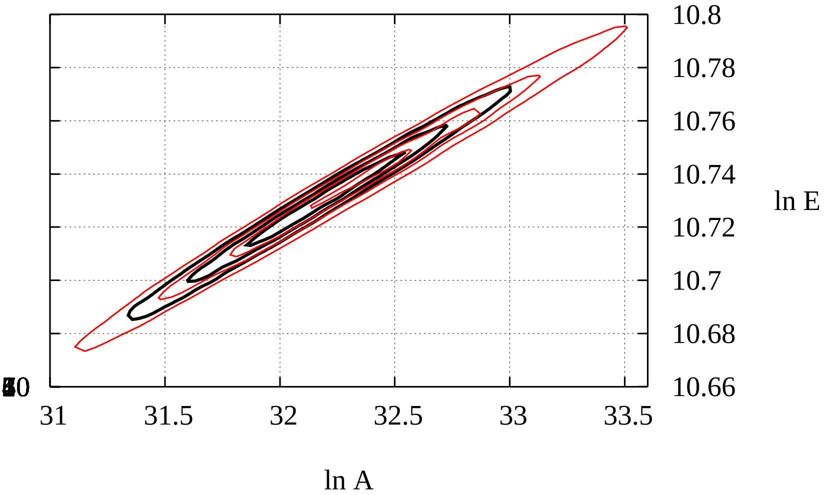




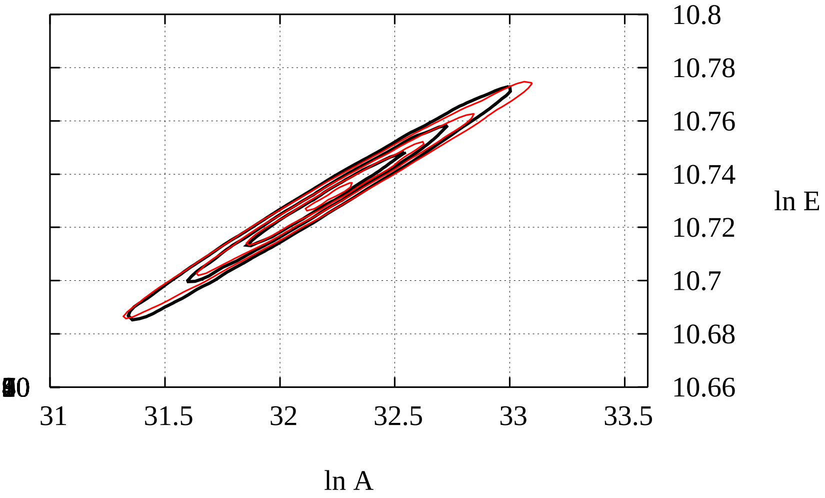
Reference Posterior – based on actual data



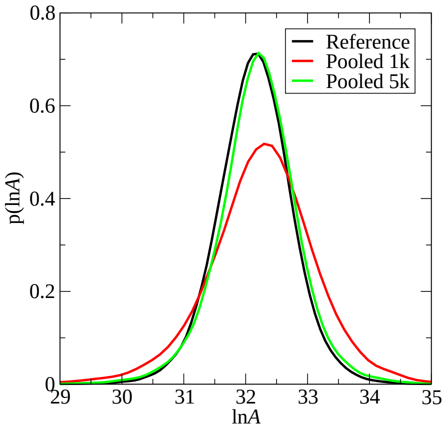
Ref + DFI posterior based on a 1000-long data chain

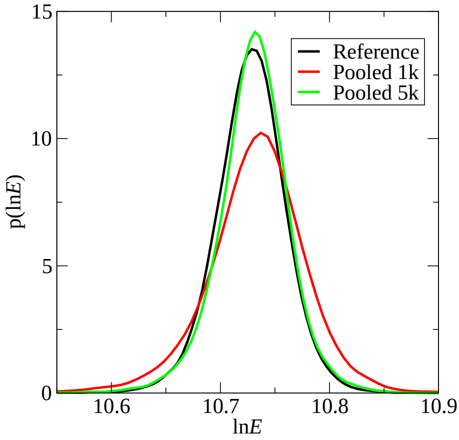


Ref + DFI posterior based on a 5000-long data chain



Marginal Pooled DFI Posteriors on $\ln A$ and $\ln E$





Challenges in Forward PC UQ – High-Dimensionality

- Dimensionality n of the PC basis: $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_n\}$
  - number of degrees of freedom
  - $P + 1 = (n + p)!/n!p!$ grows fast with n
- Impacts:
  - Size of intrusive system
  - # non-intrusive (sparse) quadrature samples
- Generally $n \approx$ number of uncertain parameters
- Reduction of n:
  - Sensitivity analysis
  - Dependencies/correlations among parameters
  - Identification of dominant modes in random fields
    Karhunen-Loéve, PCA, ...

Challenges in Forward PC UQ – Non-Linearity

- Bifurcative response at critical parameter values
  - Rayleigh-Bénard convection
  - Transition to turbulence
  - Chemical ignition
- Discontinuous $u(\lambda(\boldsymbol{\xi}))$
  - Failure of global PCEs in terms of smooth $\Psi_k()$
  - $\Leftrightarrow$ failure of Fourier series in representing a step function
- Local PC methods
  - Subdivide support of $\lambda(\boldsymbol{\xi})$ into regions of smooth $u \circ \lambda(\boldsymbol{\xi})$
  - Employ PC with compact support basis on each region
  - A spectral-element vs. spectral construction

Challenges in Forward PC UQ – Time Dynamics

- Systems with limit-cycle or chaotic dynamics
- Large amplification of phase errors over long time horizon
- PC order needs to be increased in time to retain accuracy
- Remedies
  - Time shifting/scaling
  - Choose smooth observables
- Futile to attempt representation of detailed turbulent velocity field $\boldsymbol{v}(\boldsymbol{x}, t; \lambda(\boldsymbol{\xi}))$ as a PCE
  - Fast loss of correlation due to energy cascade
  - Problem studied in 60's and 70's
- Focus on flow statistics, *e.g.* Mean/RMS quantities
  - Well behaved
  - $\Rightarrow$ Use non-intrusive methods with DNS/LES of turbulence

Closure

- UQ is increasingly important in computational modeling
- Probabilistic UQ framework
  - PC representation of random variables
  - Utility in forward UQ
    - Intrusive PC methods
    - Non-intrusive methods
  - Utility in inverse problems – surrogates
    - Bayesian inference
    - Model validation
- Need for probabilistic characterization of uncertain inputs
  - Correlations important for uncertainty in predictions
  - DFI $\Rightarrow$ joint PDF consistent with available information