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Uncertainty Quantification in Computational Models of Large Scale Physical Systems

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Seminar

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Outline

1. Introduction
2. PC Smoothing
3. Sparse Regression
4. Multilevel Multifidelity
5. Scramjet Application
6. Closure

Definition of Uncertainty Quantification (UQ)

UQ is the end-to-end estimation and analysis of uncertainty in:

models and their parameters

- assimilation of experimental/observational data
- model fitting and parameter estimation

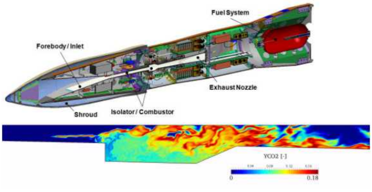
model predictions

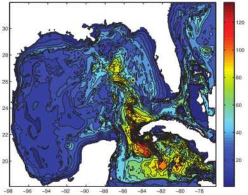
- forward propagation of parametric uncertainty to model outputs
- Analysis, comparison and selection among alternate plausible models

The Case for Uncertainty Quantification

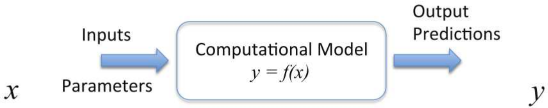
UQ is needed in:

- Assessment of confidence in computational predictions
- Validation and comparison of scientific/engineering models
- Robust design optimization under uncertainty
- Use of computational predictions for decision-support
- Assimilation of observational data and model construction
- Multiscale and multiphysics model coupling



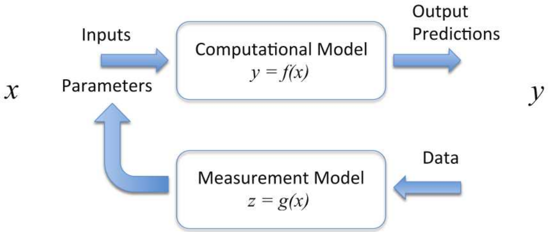


Uncertainty Quantification and Computational Science



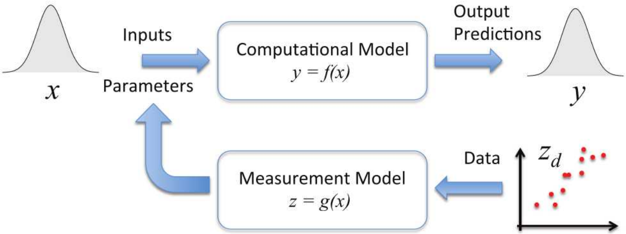
Forward problem

Uncertainty Quantification and Computational Science



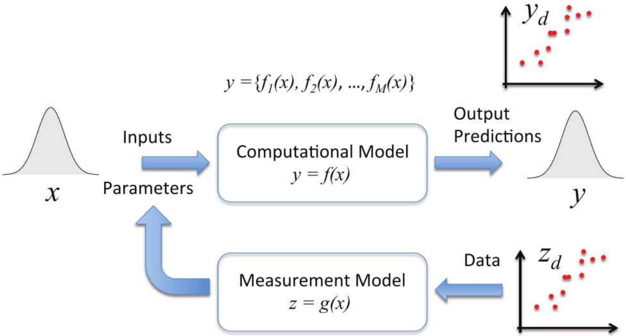
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

Probabilistic Forward UQ – $y = f(x)$

Represent uncertain quantities using probability theory

Random sampling, Monte Carlo

- Generate random samples $\{x^i\}_{i=1}^N$ from the PDF of x, $p(x)$
- Bin the corresponding $\{y^i\}$ to construct $p(y)$
- Not feasible for computationally expensive $f(x)$
  - slow convergence of MC/QMC methods
    $\Rightarrow$ very large N required for reliable estimates

Build a cheap surrogate for $f(x)$, then use Monte Carlo/others

- Collocation – interpolants
- Regression – fitting
- Galerkin methods
  - Polynomial Chaos (PC) methods

Polynomial Chaos Expansion (PCE)

- Model uncertain quantities as random variables (RVs)
- Given a *germ* $\boldsymbol{\xi}(\omega) = \{\xi_1, \cdots, \xi_n\}$ – a set of *i.i.d.* RVs
  - where $p(\boldsymbol{\xi})$ is uniquely determined by its moments

Any RV in $L^2(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$ can be written as a PCE:

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

- $u_k(\boldsymbol{x}, t)$ are mode strengths
- $\Psi_k()$ are multivariate functions orthogonal w.r.t. $p(\boldsymbol{\xi})$

Essential Use of Polynomial Chaos Expansions in UQ

Strategy:

- Represent model parameters/solution as random variables
- Construct PCEs for uncertain parameters
- Evaluate PCEs for model outputs

Advantages:

- Computational efficiency
- Utility
  - Moments: $\mathrm{E}(u) = u_0$, $\mathrm{var}(u) = \sum_{k=1}^{P} u_k^2 \langle \Psi_k^2 \rangle$, ...
  - Global Sensitivities – fractional variances, Sobol' indices
  - Surrogate for forward model

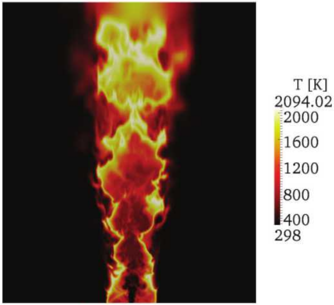
Requirement:

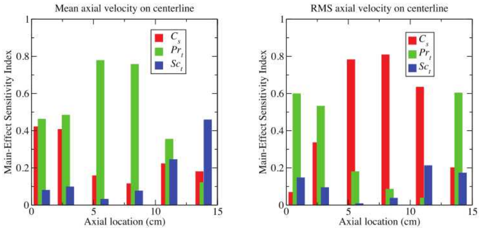
- RVs in L^2, *i.e.* with finite variance, on $(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$

UQ in LES computations: turbulent bluff-body flame

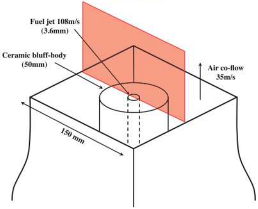
with M. Khalil, G. Lacaze, & J. Oefelein, Sandia Nat. Labs

- CH_4-H_2 jet, air coflow, 3D flow
- Re=9500, LES subgrid modeling
- 12×10^6 mesh cells, 1024 cores
- 3 days run time, 2×10^5 time steps
- 3 uncertain parameters (C_s, Pr_t, Sc_t)
- 2^{nd}-order PC, 25 sparse-quad. pts





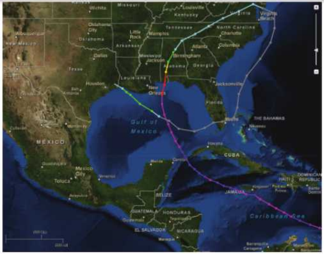
Main-Effect Sensitivity Indices

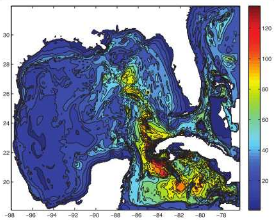


J. Oefelein & G. Lacaze, SNL

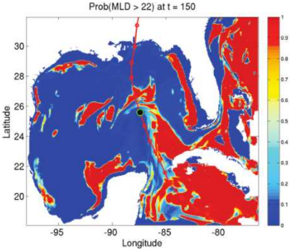
UQ in Ocean Modeling – Gulf of Mexico

A. Alexanderian, J. Winokur, I. Sraj, O.M. Knio, Duke Univ.
A. Srinivasan, M. Iskandarani, Univ. Miami; W.C. Thacker, NOAA





- Hurricane Ivan, Sep. 2004
- HYCOM ocean model (hycom.org)
- Predicted Mixed Layer Depth (MLD)
- Four uncertain parameters, *i.i.d.* U
  - subgrid mixing & wind drag params
- 385 sparse quadrature samples



(Alexanderian *et al.*, Winokur *et. al.*, *Comput. Geosci.*, 2012, 2013)

High dimensionality is a major challenge in forward UQ

- High dimensionality is the result of
  - Large number of uncertain parameters/inputs
  - Large number of degrees of freedom in random field inputs
- PCE sparse-quadrature requires an unfeasible number of model evaluations for very high dimensional systems
- MC requires similarly large number of samples when the number of important dimensions is very high
- Typically, physical model output quantities of interest are *smooth*
  - Only a small number of inputs are important
- In this case, the way out is:
  - Use global sensitivity analysis (GSA) with MC to identify important parameters
  - Use PCE sparse-quadrature on the reduced dimensional space for accurate forward UQ

Global Sensitivity Analysis (GSA)

- Random sampling-based
  - Define parametric PDFs
  - Sample them
    - Monte Carlo (MC) sampling
    - Quasi-Monte Carlo (QMC) methods
      e.g. Latin Hypercube sampling (LHS) ...
  - Run forward model for each sample
  - Evaluate statistics/PDFs of output observables
  - Sensitivity information
    - Scatter plots; Correlation measures; Regression
    - Importance Measures; Sobol' sensitivity indices
- Response surface construction based on samples
  - followed by sensitivity and/or UQ
- Analysis of Variance (ANOVA)
  - High Dimensional Model Representation (HDMR)

Hi-dimension with large-scale computational models

When the number of feasible samples for GSA is highly limited due to computational costs:

- Reliable MC-estimation of sensitivity indices requires regularization
- Presuming smoothness, use MC samples to fit a PCE, which is subsequently used to estimate the sensitivity indices
- Employ ℓ_1-norm constrained regression to discover a sparse PCE
  - compressive sensing
- Employ Multilevel Monte Carlo (MLMC), as well as Multilevel Multifidelity (MLMF) methods
  - Optimal combination of coarse/fine mesh and low/high fidelity models to minimize computational costs for a given accuracy

Similarly for forward PC UQ:

- Employ generalized adaptive non-isotropic sparse quadrature with MLMF methods on reduced dimensional input space

Learning from Limited Sparse Noisy Data

- We often need to use data to estimate quantities of interest
- Experimental data can be inherently noisy
  - Randomness in physical system
  - Instrument noise
- It can also be sparse – data gaps
  - e.g. data (x_i, y_i) on small subsets of some domain $\mathcal{D}$
- Even when the data is from computations, it can be "noisy"
  - Statistics computed from simulation outputs can be noisy due to limited averaging time windows
  - Discrepancies between computational simulation outputs and some fit-model of interest can be treated as noise
- Generally, learning from small number of data points, especially when sparse and noisy, can be a major challenge
  - Little information available from data

Learning from data with limited information

- Generally we address "Learning" in the context of estimation of statistics, and fitting
- Consider data $(x_1^{(i)}, \cdots, x_n^{(i)}, y^{(i)})$, $i = 1, \cdots, N$
  - $x \in \mathbb{R}^n$ are independent variables
  - $y \in \mathbb{R}$ is the dependent variable
- We might be interested in statistics $s = (s_1, \cdots, s_n)$
  - with, e.g., $s_i = V[E(y|x_i)]$
- Or fitting function $y = f(x; c)$, to estimate $c = (c_0, \cdots, c_P)$
  - with, e.g. $f(x; c) = \sum_{k=0}^{P} c_k \Psi_k(x)$
  - with either least-squares fitting, or Bayes
- In all cases, the accuracy of the estimate of c or s depends on the "quality" of the data
  - data noise, coverage, range, quantity

Estimation of GSA Sobol' Indices with PC regularization

- When the number of samples is small, the GSA sensitivity indices can be computed with improved accuracy, relying on regularization
- Use regression with MC samples to fit a Legendre-Uniform PCE to the data

$$u(\boldsymbol{\xi}) = \sum c_k \Psi_k(\boldsymbol{\xi})$$

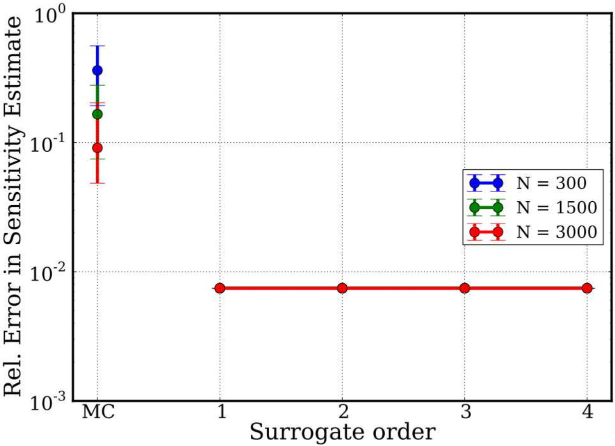
- Use PCE to evaluate Sobol Indices directly

Sargsyan, 2017

- Example results illustrate significant improvement over the direct estimation from samples

Estimation of GSA Sobol' Indices with PC regularization

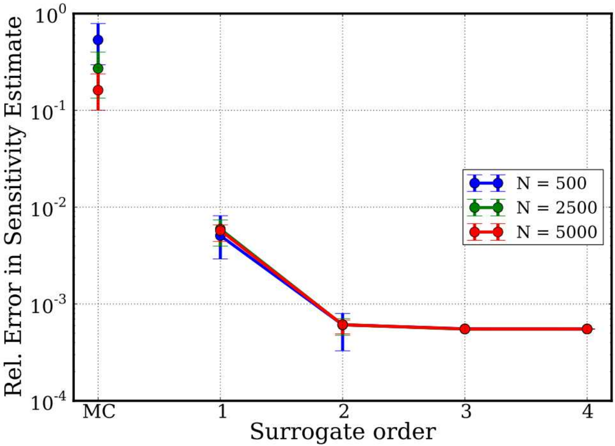
$d = 1$



Sargsyan, 2017

Estimation of GSA Sobol' Indices with PC regularization

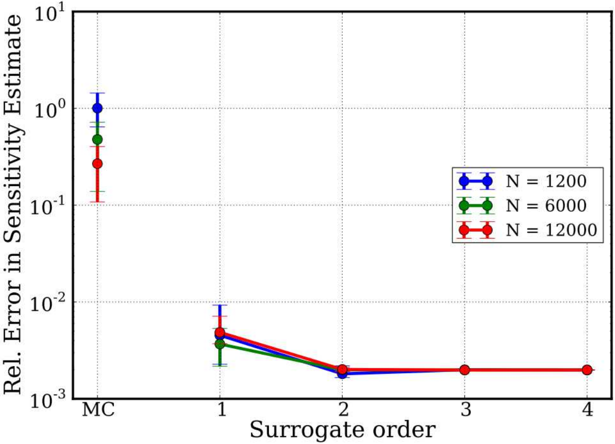
$d = 3$



Sargsyan, 2017

Estimation of GSA Sobol' Indices with PC regularization

$d = 10$



Sargsyan, 2017

Need for regularization in fitting/inversion

- Sometimes the fitting problem is ill-posed ... non-uniqueness
  - Multiple values of c give the same $f(x;c)$ over a range of x
- More often the problem is ill-conditioned
  - The amount of information in the data is small relative to the number of parameters we are interested in learning
    - For example $N << P + 1$
- Ill-conditioning can manifest itself in sensitivity to
  - Initial guess choice in least-squares fitting
  - Prior choice in Bayesian fitting
  - Specific choice of data set
- Ill-conditioning can lead to poor convergence in the iterative solution or to poor mixing in MCMC
- Regularization is often useful to deal with these challenges

Regularization in Learning from Data

- Regularization involves adding some information into the problem
- Of course, the choice of the form of $f(x;c)$, or the value of P, also provide explicit regularization
- Regularization allows enforcement of desired traits in the solution
  - Smoothness, positivity, ...
  - Introduces bias, destroys consistency
- Example: Tikhonov-type regularization:

$$c = \operatorname*{argmin}_{c'} \left(\|f(x,c) - y\|_2^2 + \alpha L(c') \right)$$

- How to choose regularization form, L, α ? – Somewhat arbitrary
- $L(t) := \|t\|_2^2 \Rightarrow$ favor solutions with small ℓ_2 norm
- $L(t) := \| \max_x \nabla_x f(x,t)\|_2^2 \Rightarrow$ favor smooth functions
- $L(t) := \|t\|_0 \Rightarrow$ favor solutions with small # of non-zero elements
  - sparse solutions

Regularization in Learning from Data

- Employing the ℓ_0 constraint is a problem because the resulting constrained optimization is not convex
- It turns out that it's possible to use the ℓ_1-norm, with good sparsity selection
    - This problem is indeed convex
- Hence the use of the ℓ_1 norm in sparse regression
    - Compressive Sensing, LASSO
    - Bayesian compressive sengin, Bayesian LASSO

Sparse regression

Model:

$$y = f(x) \simeq \sum_{k=0}^{K-1} c_k \Psi_k(x)$$

with $x \in \mathbb{R}^n$, Ψ_k max order p, and $K = (p+n)!/p!/n!$

- N samples $(x_1, y_1), \ldots, (x_N, y_N)$
- Estimate K terms $c_0, \ldots, c_{K-1}$, s.t.

$$\text{min } ||\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}||_2^2$$

where $\boldsymbol{y} \in \mathbb{R}^N$, $\boldsymbol{c} \in \mathbb{R}^K$, $\boldsymbol{A}_{ik} = \Psi_k(x_i)$, $\boldsymbol{A} \in \mathbb{R}^{N \times K}$

With $N << K \Rightarrow$ under-determined

- Need some form of regularization

Regularization – Compressive Sensing (CS)

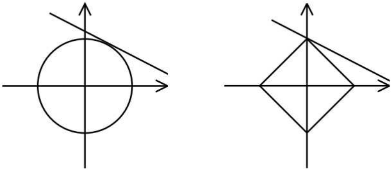
- ℓ_2-norm – Tikhonov regularization; Ridge regression:

$$\min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_2^2\}$$

- ℓ_1-norm – Compressive Sensing; LASSO; basis pursuit

$$\begin{aligned} \min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_1\} & \\ \min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2\} & \quad \text{subject to } \|\boldsymbol{c}\|_1 \leq \epsilon \\ \min \{\|\boldsymbol{c}\|_1\} & \quad \text{subject to } \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 \leq \epsilon \end{aligned}$$

$\Rightarrow$ discovery of sparse signals



Multilevel Multifidelity (MLMF) Methods – 1

We evolved MC estimation of the Sobol' sensitivity indices in two steps

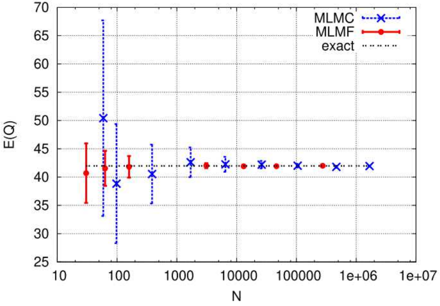
- We introduced the fitting of a PCE as a primary step, before using the PCE to estimate the sensitivity indices
  - This helps, but more is needed
- We introduced the regularization of the PCE fitting by introducing a norm of the solution vector into the objective function, or constraint
  - ℓ_2 and ℓ_1 norm
- ℓ_1-norm constrained regression facilitates the discovery of a *sparse* PCE that has good fit to the data
  - This helps, providing fitted sparse PCEs given available data

Multilevel Multifidelity (MLMF) Methods – 2

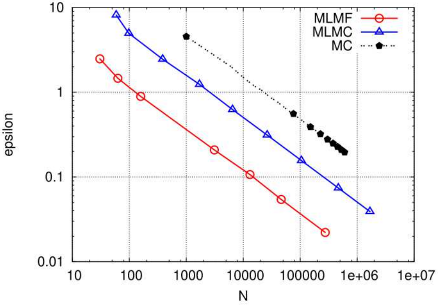
In particular, when the computational model is quite expensive, we still seek more reduction in the required number of samples

- Multilevel Multifidelity (MLMF) methods allow further savings by combining information judiciously from low/high-resolution and how/high-fidelity models
- Use many low resolution/fidelity model computations and a minimal necessary number of high resolution/fidelity model computations to achieve target accuracy with MC

Heat equation–MLMF vs. MLMC vs. plain MC

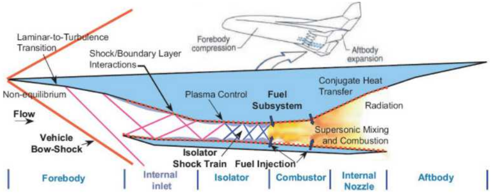


Expected Value

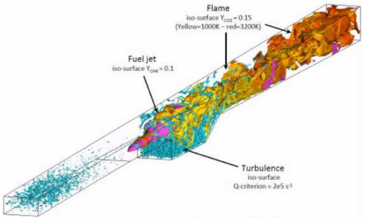


Accuracy ε

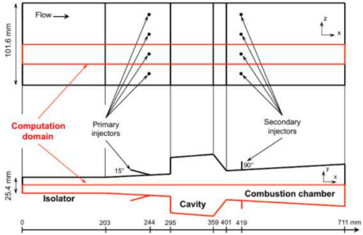
Supersonic Combusting Ramjet (scramjet)

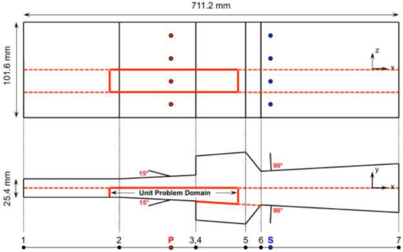


In flight



Numerical model





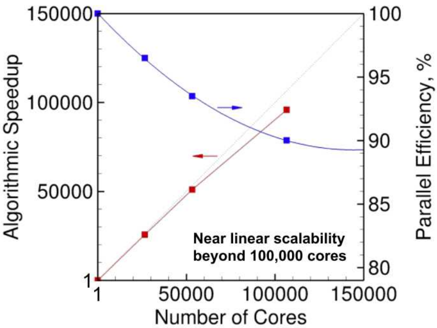
Scramjet–24 uncertain parameters

Parameter	Symbol	Range
Inflow boundary conditions		
Inlet		
Stagnation pressure	$p_{0,i}$	1.48 MPa $\pm 5\%$
Stagnation temperature	$T_{0,i}$	1550 K $\pm 5\%$
Mach number	M_i	$2.51 \pm 10\%$
Turbulence intensity	$I_i = u'_i/U_i$	$[0.0 - 0.05]$
Turbulence intensity ratio	$I_r = v'_i/u'_i$	1.0
Turbulence length scale	L_i	$[0.0 - 8.0]$mm
Boundary layer thickness	δ_i	$[2.0 - 6.0]$mm
Fuel injection $(36\%CH_4, 64\%C_2H_4)$		
Mass flux	$\dot{m}_f$	7.37×10^{-3} kg/s $\pm 10\%$
Static Temperature	T_f	300.0 K $\pm 5\%$
Mach Number	M_f	$1.0 \pm 5\%$
Turbulence intensity	$I_f = u'_f/U_f$	$[0.025 - 0.075]$
Turbulence length scale	L_f	$[0.02 - 1.0]$ mm
Wall boundary conditions		
Wall Temperature	T_w	Profile from KLE Expansion (10 params)
Turbulence model parameters		
Static Smagorinsky		
Modified Smagorinsky constant	C_R	$[0.01 - 0.016]$
Turbulent Prandtl number	Pr_t	$[0.5 - 1.7]$
Turbulent Schmidt number	Sc_t	$[0.5 - 1.7]$

LES Performed using RAPTOR Code Framework

Joe Oefelein – Sandia National Labs. – currently at Georgia Tech

- **Theoretical framework … (Comprehensive physics)**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (No Tuned Constants)
- **Numerical framework … (High-quality numerics)**
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Detailed treatment of geometry, wall phenomena, transient BC's
- **Massively-parallel … (Highly-scalable)**
  - Demonstrated performance on full hierarchy of HPC platforms (e.g., scaling on ORNL CRAY XK7 TITAN architecture shown below)
  - Selected for early science campaign on next generation SUMMIT platform (ORNL Center for Accelerated Application Readiness, 2015 – 2018)



Global sensitivity analysis: Sobol indices

Global sensitivity analysis (GSA) (Saltelli:2004,2008)

- For a given quantify of interest (QoI) ...
- QoI variance decomposed into contributions from each parameter
- Sobol indices rank parameters by their contributions (Sobol:2003)

Total effect $$S_{T_i} = \frac{\mathbb{E}_{\lambda_{\sim i}}[\text{Var}_{\lambda_i}(f(\lambda)|\lambda_i)]}{\text{Var}(f(\lambda))}$$

S_{T_i} small $\Rightarrow$ low impact parameter $\Rightarrow$ fix value (i.e. dim. eliminated)

How to compute?

- Monte Carlo estimators (Saltelli:2002,2010) still prohibitive for LES
- **Our approach:** construct affordable surrogate models via polynomial chaos expansion (PCE)

Polynomial chaos expansions

A QoI (output) random variable can be expanded as follows:

$$f(\lambda(\xi)) = \sum_{\beta \in \mathcal{J}} c_\beta \Psi_\beta(\xi)$$

- c_β: PCE coefficients
- ξ: reference random vector (e.g., uniform, Gaussian)
- Ψ_β: multivariate orthonormal polynomial (e.g., Legendre, Hermite)
- β: multi-index, reflects order of polynomial basis

Orthonormality property
$\Rightarrow$ extract Sobol indices analytically from coefficients (no Monte Carlo!):

$$S_{T_i} = \frac{1}{\text{Var}(f(\lambda))} \sum_{\beta \in \mathcal{J}:\beta_i>0} c_\beta^2 \qquad \text{where} \qquad \text{Var}(f(\lambda)) = \sum_{0 \neq \beta \in \mathcal{J}} c_\beta^2$$

Sparse polynomial chaos expansions

Non-intrusive regression to compute expansion coefficients $Gc = f$:

$$\underbrace{\begin{bmatrix} \Psi_{\beta^1}(\xi^{(1)}) & \cdots & \Psi_{\beta^N}(\xi^{(1)}) \\ \vdots & & \vdots \\ \Psi_{\beta^1}(\xi^{(M)}) & \cdots & \Psi_{\beta^N}(\xi^{(M)}) \end{bmatrix}}_{G} \underbrace{\begin{bmatrix} c_{\beta^1} \\ \vdots \\ c_{\beta^N} \end{bmatrix}}_{c} = \underbrace{\begin{bmatrix} f(\lambda(\xi^{(1)})) \\ \vdots \\ f(\lambda(\xi^{(M)})) \end{bmatrix}}_{f},$$

Challenges:

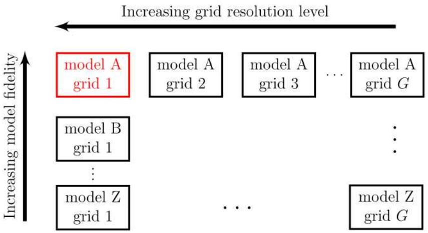
- Very few LES flow solves (data) available
- Large number of polynomial PCE basis (e.g. total-order degree 3 in 24 dimensions: 2925 terms)
- Extremely under-determined system ($N \gg M$)

Our approach: use compressed sensing to find sparse solution

$$\min_c \frac{1}{2}\| c \|_1 + \tau \| Gc - f \|_2^2$$

discover and retain only basis terms with high magnitude coefficients

Multilevel and multifdelity forms



Telescopic sum:

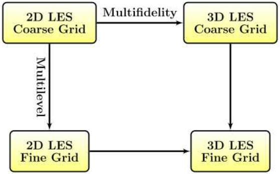
$$f_L(\lambda) = f_0(\lambda) + \sum_{\ell=1}^{L} f_{\Delta_\ell}(\lambda)$$

- ℓ indicates different grid levels or fidelity of models
- Δ_ℓ indicates difference between models ℓ and $\ell - 1$

Function approximation:

$$f_L(\lambda) \approx \hat{f}_L(\lambda) = \hat{f}_0(\lambda) + \sum_{\ell=1}^{L} \hat{f}_{\Delta_\ell}(\lambda)$$

High-D – ML/MF UQ Results



Two model forms and two mesh discretization levels

- Model form: 2D (LF) and 3D (HF) LES
- Meshes: $d/8$ and $d/16$

The P1 problem is considered (24 inputs).
Five QoIs extracted over a plane at $x/d = 100$.

- $\mathbb{E}_{y,t}$ stagnation pressure ($P_{0,mean}$)
- $\mathbb{E}_{y}$ RMS$_t$ stagnation pressure ($P_{0,rms}$)
- $\mathbb{E}_{y,t}$ Mach number (M_{mean})
- $\mathbb{E}_{y,t}$ turbulent kinetic energy (TKE$_{mean}$)
- $\mathbb{E}_{y,t}$ scalar dissipation rate (χ_{mean})

	2D	3D
$d/8$	1	204
$d/16$	25.5	1844

Relative computational cost for the model forms and discretization levels.

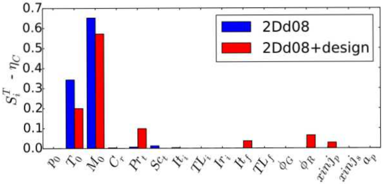
Optimize statistical accuracy given a limited number of high fidelity model evaluations by leveraging cheaper lower fidelity simulations.

GSA: uncertain + design parameter space (16d); 2D flow

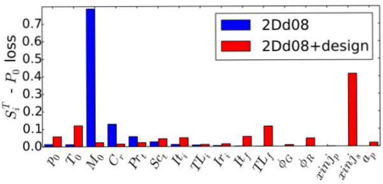
Setup

- Design parameters:
  - global equivalence ratio (ϕ_G)
  - ratio of equivalence ratios primary/secondary (ϕ_R)
  - location of primary and secondary injectors ($xinj_P$, $xinj_S$)
  - angle of primary injector (a_P).
- 220 simulations

Combustion Efficiency

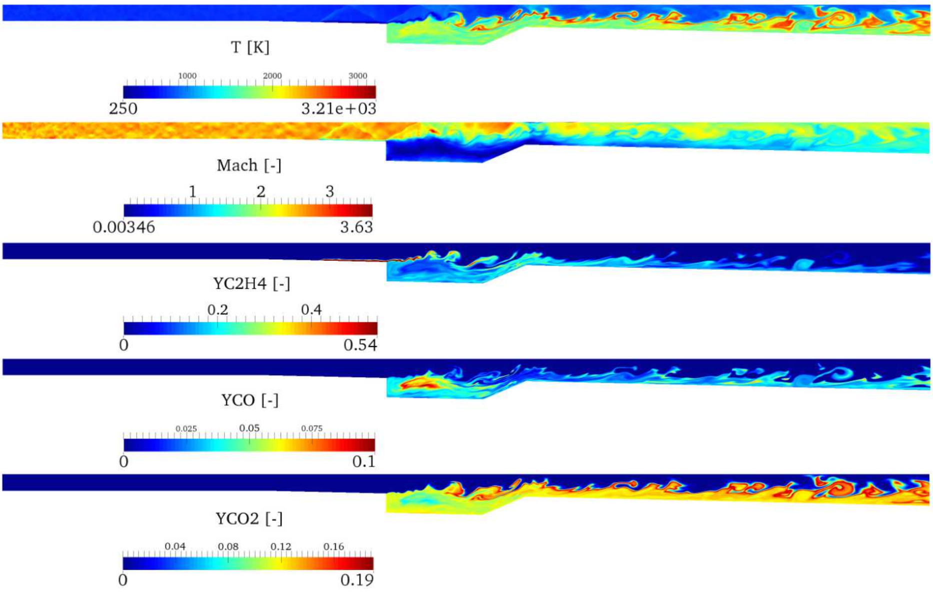


Stagnation Pressure Loss

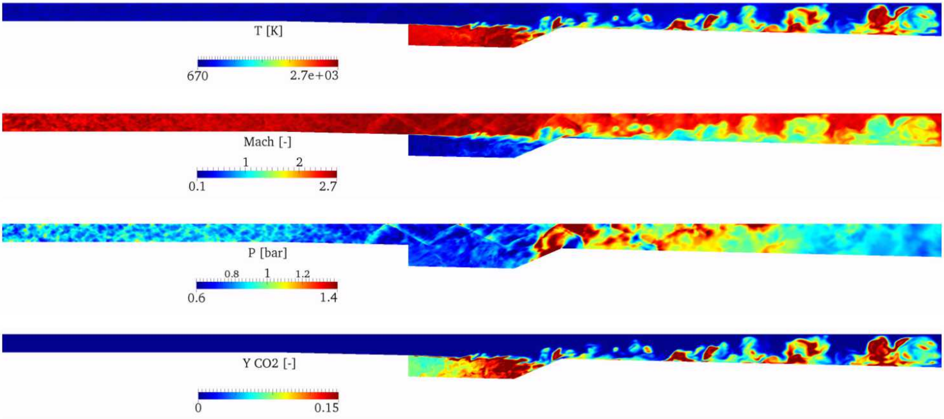


- Inlet Mach number (M_o) and stagnation temperature (T_o) remain dominant
- Location of the second injector important for ΔP_{stag}

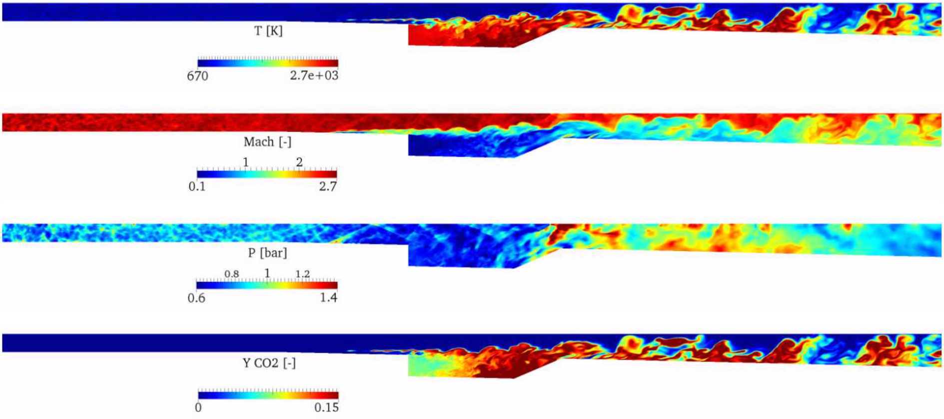
Instantaneous Flow Structure – 2D d32



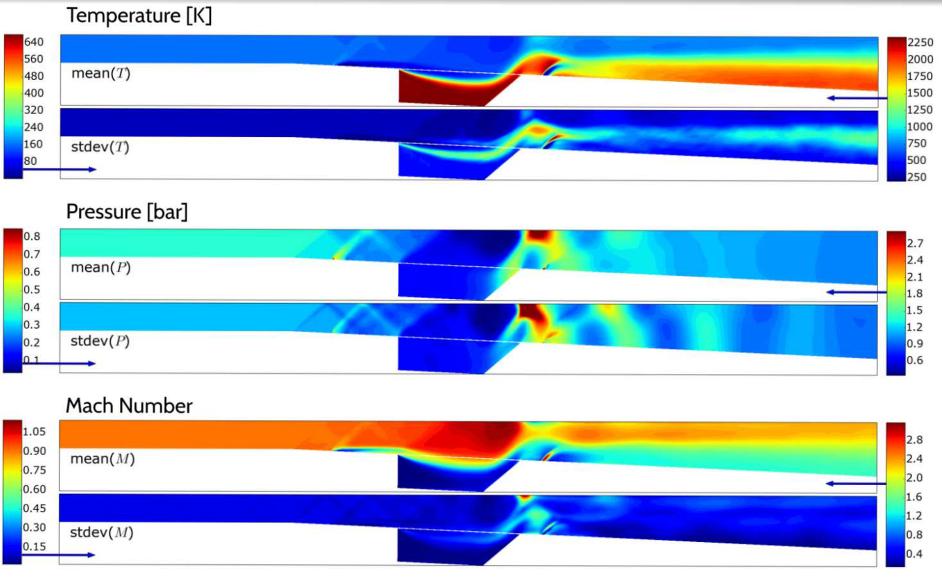
Instantaneous Flow Structure – z-0-cut – 3D d16



Instantaneous Flow Structure – z-inj-cut – 3D d16

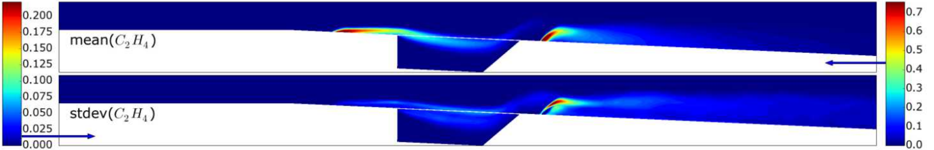


MC-Predicted Uncertainty in Mean Flow Quantities – 3D

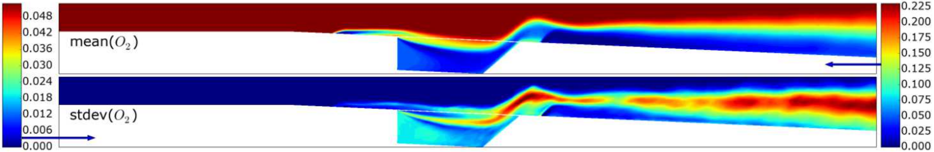


MC-Predicted Uncertainty in Mean Flow Quantities – 3D

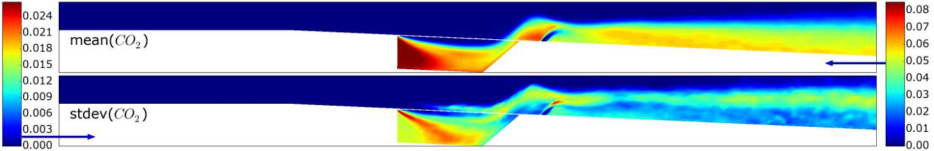
Ethane



Oxygen



Carbon Dioxide



Optimization Under Uncertainty – strategies

- Design parameters ϕ
- Uncertain parameters λ
- OUU statement ... example

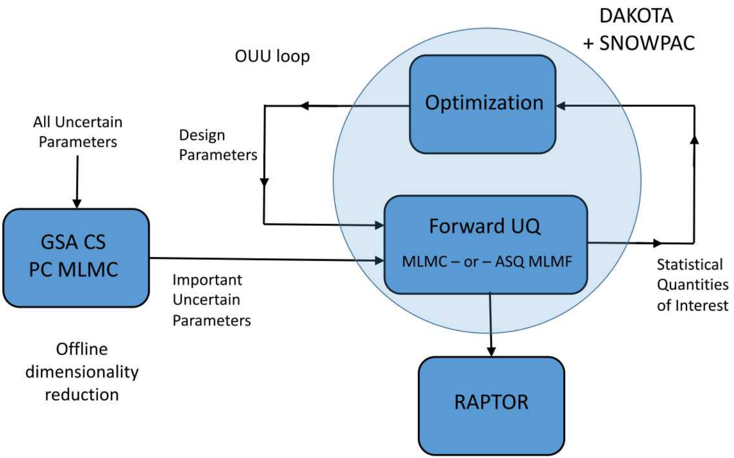
$$
\begin{aligned}
\phi^* &= \underset{\phi}{\operatorname{argmin}} \, \mathbb{E}_\lambda[f(\phi, \lambda)] \\
s.t. \quad & \mathbb{E}_\lambda[g(\phi, \lambda)] + 3\mathbb{V}^{\frac{1}{2}}[g(\phi, \lambda)] < \alpha \\
& \mathbb{E}_\lambda[h(\phi, \lambda)] - 3\mathbb{V}^{\frac{1}{2}}[h(\phi, \lambda)] > \beta
\end{aligned}
$$

  Many other statements, probabilistic, risk analysis, are possible
- Each step in the optimization strategy requires solving the forward UQ problem for the given ϕ
- Inherits and magnifies all the difficulties of forward UQ in high-dimensional complex models

Elements of OUU in large scale models

- We rely on two software libraries under development
  - DAKOTA – https://dakota.sandia.gov
  - SNOWPAC – https://bitbucket.org/fmaugust/nowpac.git
- Offline GSA/PC-smoothing/CS/MLMF and dimensionality reduction for uncertain parameters
- Reliance on surrogates and simplified models where possible
- Noise in objective function due to finite time-window averaging for flow statistics of interest
- Code/model failures are often encountered when exploring parameter spaces
- When noise is high and/or have failures, use MC/MLMC for forward UQ – build a Gaussian process over ϕ with MLMC – SNOWPAC
- If noise is small enough, and no failed samples, can use forward-UQ with PCE adaptive sparse quadrature (ASQ) and MLMF – DAKOTA
- DAKOTA handles overall optimization strategy

Optimization under uncertainty workflow



Closure

- Relevance of UQ in computational science
- Challenges
  - High dimensionality
  - Model complexity
  - Optimization under uncertainty
- Discussed
  - GSA, PC smoothing, CS, MLMC, MLMF
  - OUU, finite averaging noise, code failures
- Ongoing application for UQ & OUU in Scramjet design
- A highly multidisciplinary enterprise – applied math, probability, statistics, information theory, computations, data, physical modeling