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Uncertainty Quantification in Large Scale Computational Models

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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

Challenges with Surrogate Construction

- Choice of surrogate function is informed by structure of $f(x)$
  - Structure of $f(x)$ not known *a priori*
  - Discontinuities, say at some x^*, require particular care
    - Local versus global surrogates
  - Nonlinearities, shape ...
    - *e.g.* polynomials have trouble with sigmoid response
    - Surrogate complexity can grow
- High dimensionality in x
  - Large number of uncertain parameters
  - Non-smooth random fields
- Large computational cost for $f(x)$
  - *e.g.* a global climate simulation
  - Can only afford a few samples

Role of Surrogates in Probabilistic UQ

Computational forward model, parameter vector λ

$$y = f(x, \lambda)$$

Forward UQ

- Given PDF $p(\lambda)$, estimate $p(y)$ or $M_q(y) = \mathbb{E}[y^q]$
- General *non-intrusive* methods rely on sampling λ
- Require many samples $(\lambda_k, f(x, \lambda_k))$, $k = 1, \dots, N$

Inverse UQ

- Given data $D := \{(x_i, y_i),\ i = 1, \dots, M\}$, estimate $p(\lambda|D)$
- Bayesian methods often use Markov Chain Monte Carlo (MCMC)
- Require many samples $(\lambda_k, f(x_i, \lambda_k))$, $k = 1, \dots, K$, $\forall i$

Require a cheap surrogate $S_\alpha(x, \lambda) \simeq f(x, \lambda),\ \alpha \in \mathbb{R}^L$

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
- Sparse-quadrature requires an unfeasible number of model evaluations for very high dimensional systems
- Monte Carlo requires similarly large number of samples when the number of important dimensions is very high
  - However, typically, physical model output quantities of interest are *smooth* $\Rightarrow$ Only a small number of inputs are important
- In this case, the way out is:
  - Use global sensitivity analysis (GSA) with Monte Carlo to identify important parameters
  - Use polynomial chaos expansions (PCE) with sparse quadrature on the reduced dimensional space for accurate forward UQ

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

S_{T_i} small $\Rightarrow$ low impact parameter $\Rightarrow$ fix value (eliminate dimension)

How to compute?

- Monte Carlo estimators (Saltelli:2002,2010) still prohibitive if used directly for large scale computational models

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

Estimation of GSA Sobol' Indices with PC regression

- When # samples is small, GSA indices can be computed with improved accuracy, relying on PC regression/smoothing
- Polynomial Chaos expansion (PCE): $u(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha}\in\mathfrak{I}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$
  - Germ: $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_d\}$, Multi-index $\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_d\}$,
  - Polynomials, orthogonal w.r.t. $p(\boldsymbol{\xi})$, $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{d} \psi_{\alpha_i}(\xi_i)$
- Use regression with MC samples to fit a PCE to the data

$$\underset{c_{\boldsymbol{\alpha}}}{\text{argmin}} \sum_{s=1}^{N} \left(f(\lambda(\boldsymbol{\xi}^{(s)}))) - \sum_{\boldsymbol{\alpha}\in\mathfrak{I}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(s)}) \right)^2$$

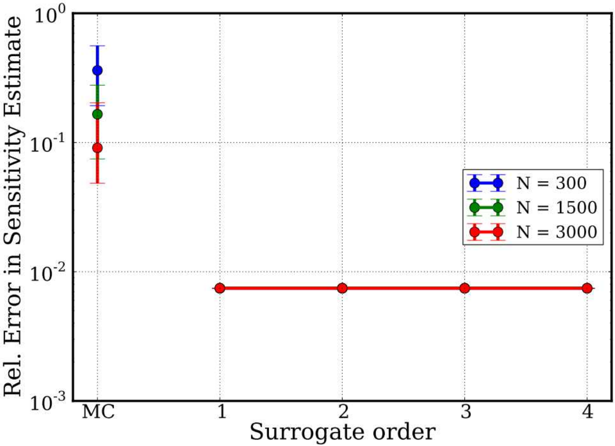
- Use PCE to evaluate Sobol indices

$$S_{T_i} = \frac{\sum_{\boldsymbol{\alpha}\in\mathfrak{I}|\alpha_i>0} c_{\boldsymbol{\alpha}}^2 \langle \Psi_{\boldsymbol{\alpha}}^2 \rangle}{\sum_{\boldsymbol{\alpha}\in\mathfrak{I}|\boldsymbol{\alpha}\neq\mathbf{0}} c_{\boldsymbol{\alpha}}^2 \langle \Psi_{\boldsymbol{\alpha}}^2 \rangle}$$

Sudret, 2008; Crestaux, 2009; Sargsyan, 2017; Ricciuto, 2018

Estimation of GSA Sobol' Indices with PC regression

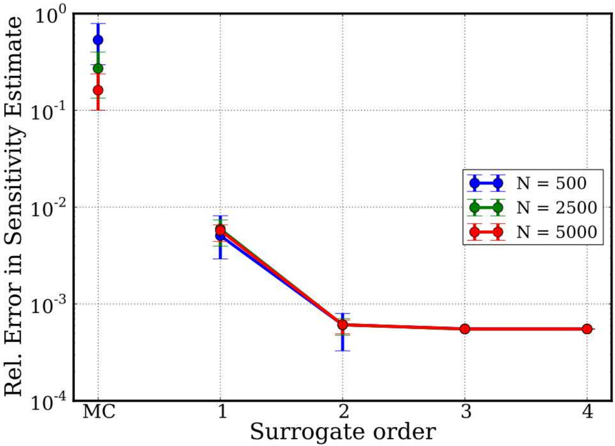
$d = 1$



Sargsyan, 2017

Estimation of GSA Sobol' Indices with PC regression

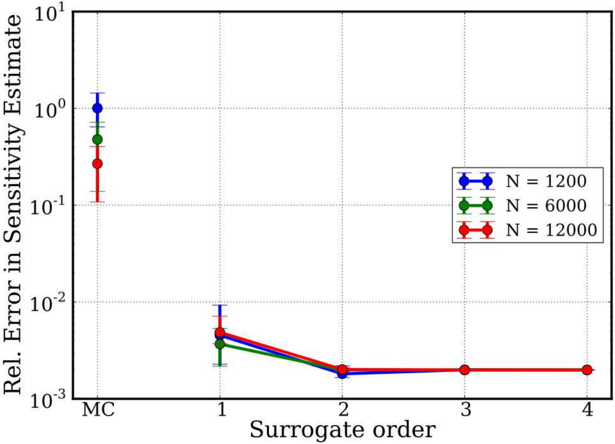
$d = 3$



Sargsyan, 2017

Estimation of GSA Sobol' Indices with PC regression

$d = 10$



Sargsyan, 2017

Sparse regression

Model: $$y = f(\boldsymbol{\xi}) \simeq \sum_{\boldsymbol{\alpha} \in \mathfrak{I}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

- With N samples $(\boldsymbol{\xi}^1, y^1), \ldots, (\boldsymbol{\xi}^N, y^N)$, estimate K terms $c_{\boldsymbol{\alpha}}$

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

With $N << K \Rightarrow$ under-determined, need regularization

- Use ℓ_1 norm regularization to discover sparsity
- Discover a sparse fitted PCE – many zero coefficients

Compressive Sensing; LASSO; basis pursuit; etc ...

$\min_{\boldsymbol{c}} \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2\}$	subject to $\|\boldsymbol{c}\|_1 \leq \epsilon$	LASSO
$\min_{\boldsymbol{c}} \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_1\}$		uLASSO
$\min_{\boldsymbol{c}} \{\|\boldsymbol{c}\|_1\}$	subject to $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{c}$	BP
$\min_{\boldsymbol{c}} \{\|\boldsymbol{c}\|_1\}$	subject to $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 \leq \epsilon$	BPDN

Unconstrained LASSO (uLASSO) – Practicalities

A broad range of methods exists for solving the optimization problem:

$$\boldsymbol{c}^* = \operatorname*{argmin}_{\boldsymbol{c}} \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_1 \right\}$$

l1_ls (Kim 2007), SpaRSA (Wright 2009), CGIST (Goldstein 2010), FPC_AS (Wen 2010), ADMM (Boyd 2010)

- Choice of $\lambda \geq 0$ controls the degree of overfitting vs underfitting
- This choice can be viewed as a model selection problem
    - Can base the choice on Bayesian model evidence maximization
- A cross-validation (CV) λ-choice strategy: minimize K-fold CV error

$$\lambda^* = \operatorname*{argmin}_{\lambda \geq 0} E_{\text{CV}}(\lambda)$$

- For expensive models, also target optimal data sample size
    - Increase sample size m adaptively
    - Stop sampling when the rate of decrease of λ-optimal CV error with increasing m drops below a given threshold Huan, SIAM JUQ 2018

Bayesian Regression

- Bayes formula

$$p(\boldsymbol{c}|D) \propto p(D|\boldsymbol{c})\pi(\boldsymbol{c})$$

- Bayesian regression: prior as a regularizer, *e.g.*
    - Log Likelihood $\Leftrightarrow$ $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2$
    - Log Prior $\Leftrightarrow$ $\|\boldsymbol{c}\|_p^p$
- Laplace sparsity priors $\pi(c_k|\alpha) = \frac{1}{2\alpha} e^{-|c_k|/\alpha}$
- uLASSO (Tibshirani 1996, Van den Berg 2008) ... formally:

$$\min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_1 \right\}$$

Solution $\sim$ the posterior mode of $\boldsymbol{c}$ in the Bayesian model

$$y \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{c}, I_N), \qquad c_k \sim \frac{1}{2\alpha} e^{-|c_k|/\alpha}$$

- Bayesian LASSO (Park & Casella 2008)

Bayesian Compressive Sensing (BCS)

- BCS (Ji 2008; Babacan 2010)— hierarchical priors:
  - Gaussian priors $\mathcal{N}(0, \sigma_k^2)$ on the c_k
  - Gamma priors on the σ_k^2

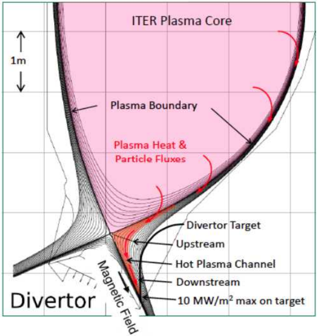
  $\Rightarrow$ Laplace sparsity priors on the c_k
- Evidence maximization establishes maximum likelihood estimates of the σ_k
  - many of which are found $\approx 0 \quad \Rightarrow \quad c_k \approx 0$
  - iteratively include terms that lead to the largest increase in the evidence
- Iterative BCS (iBCS) (Sargsyan 2012):
  - adaptive iterative order growth
  - BCS on order-p Legendre-Uniform PC
  - repeat with order-$p+1$ terms added to surviving p-th order terms

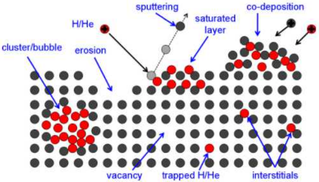
Demonstration in Cluster Dynamics Computations

- Material damage processes associated with plasma surface interactions in the ITER fusion reactor – He in W/Be
- Xe gas bubble transport in nuclear fuel rods in fission reactors
- "Xolotl" C++ cluster dynamics code for prediction of gas bubble evolution in solids
- Solves PDE (x, t) for concentration of clusters of different sizes
- 2D/3D - relies on PETSc solvers
- https://github.com/ORNL-Fusion/xolotl

Brian Wirth, Sophie Blondel – Oak Ridge National Lab

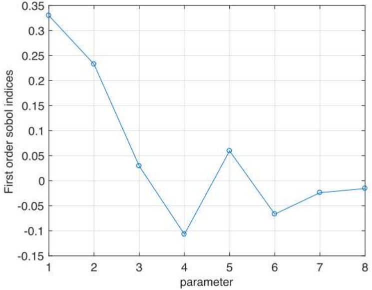
ITER Plasma Material Interface





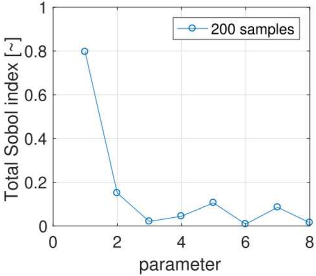
S. Blondel *et al.*, COSIRES, 2018

GSA in Xolotl

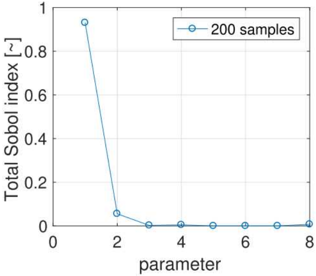


- 400 samples GSA MC study
- 8 parameters
- Noise/negativity in indices eliminated with sparse PC regression @ 200 samples

LSQ-PC: Total:



BCS-PC: Total:

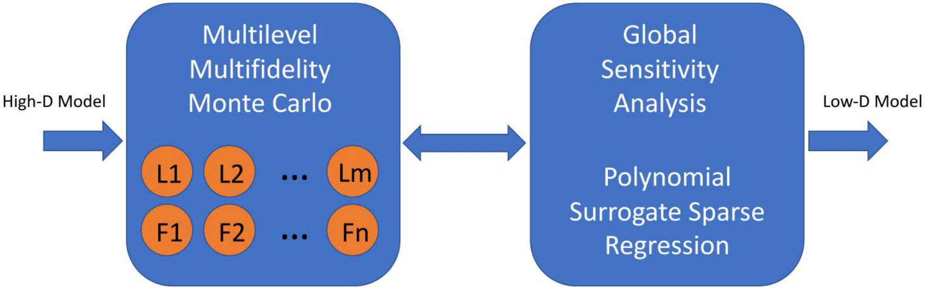


Multilevel Multifidelity (MLMF) Methods for UQ

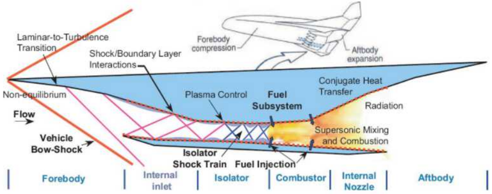
When the computational model is quite expensive, we still seek more reduction in the required number of expensive samples

- 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
- Choice of how many simulations to run at low and high fidelity/resolution is done adaptively

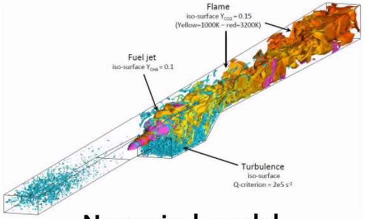
Forward UQ GSA Workflow



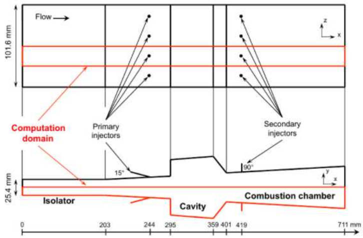
Supersonic Combusting **Ramjet** (scramjet)

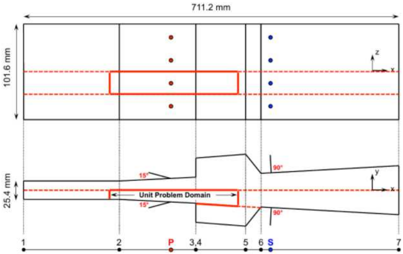


In flight



Numerical model

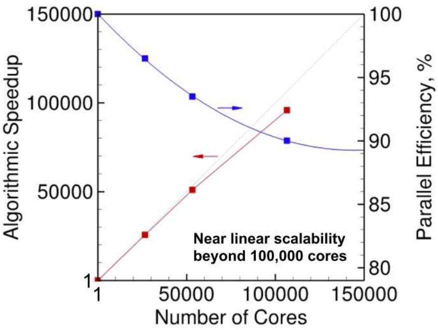




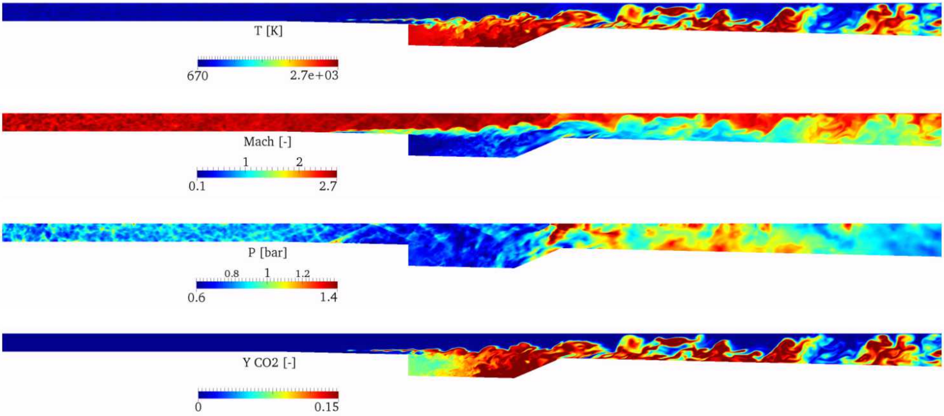
LES Performed using RAPTOR Code Framework

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

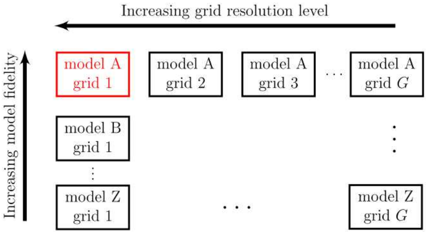
- **Theoretical framework … (Comprehensive physics)**
  - **Fully-coupled, compressible conservation equations**
  - **Real-fluid equation of state (high-pressure phenomena)**
  - **Detailed thermodynamics, transport and chemistry**
  - **Multiphase flow, spray**
  - **Dynamic SGS modeling (No Tuned 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)**



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



Multilevel and multifdelity forms



Telescopic sum:

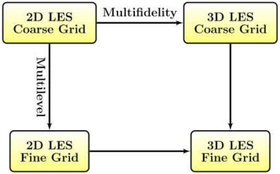
$$f_L(\lambda) = f_0(\lambda) + \sum_{\ell=1}^{L} f_{\Delta_\ell}(\lambda)$$

- 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 jet-in-crossflow problem (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.

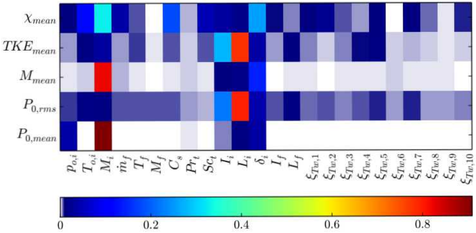
Optimize statistical accuracy given a limited number of high fidelity model evaluations by leveraging cheaper lower fidelity simulations.

Jet in crossflow problem: 24 parameters, 3^{rd}-order PCE

Parameter	Range	Description
	Inlet boundary conditions	
p_0	[1.406, 1.554] MPa	Stagnation pressure
T_0	[1472.5, 1627.5] K	Stagnation temperature
M_0	[2.259, 2.761]	Mach number
δ_a	[2, 6] mm	Boundary layer thickness
I_i	[0, 0.05]	Turbulence intensity magnitude
L_i	[0, 8] mm	Turbulence length scale
	Fuel inflow boundary conditions	
$\dot{m}_f$	[6.633, 8.107] $\times 10^{-3}$ kg/s	Mass flux
T_f	[285, 315] K	Static temperature
M_f	[0.95, 1.05]	Mach number
I_f	[0, 0.05]	Turbulence intensity magnitude
L_f	[0, 1] mm	Turbulence length scale
	Turbulence model parameters	
C_R	[0.01, 0.06]	Modified Smagorinsky constant
Pr_t	[0.5, 1.7]	Turbulent Prandtl number
Sc_t	[0.5, 1.7]	Turbulent Schmidt number
	Wall boundary conditions	
T_w	Expansion in 10 params of $\mathcal{N}(0,1)$	Wall temperature represented via Karhunen-Loève expansion

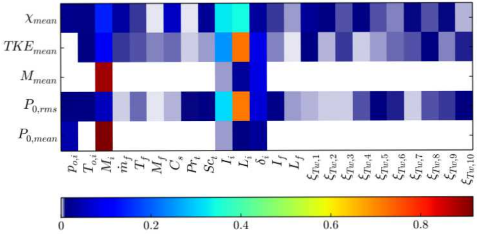
- QoIs computed at $x/d = 100$, averaged over (y, t)
- 2D runs: 1939 (coarse grid), 79 (fine grid)
- 3D runs: 46 (coarse grid), 11 (fine grid)

Unit problem: total sensitivity



Multilevel expansion of:

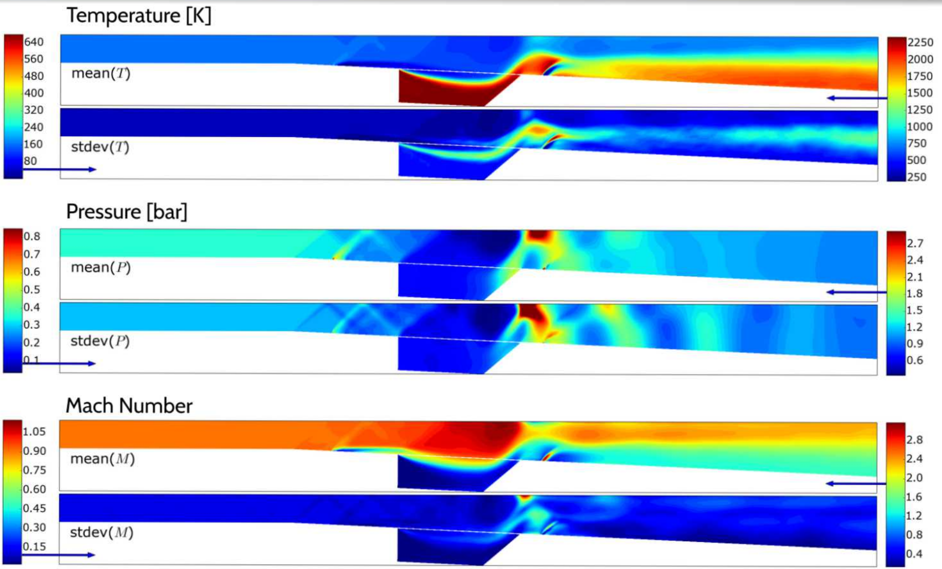
$$\widehat{f}_{2D,d/16} = \widehat{f}_{2D,d/8} + \widehat{f}_{\Delta_{2D,d/16-2D,d/8}}$$



Multifidelity expansion of:

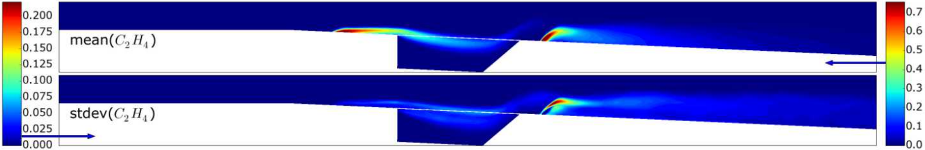
$$\widehat{f}_{3D,d/8} = \widehat{f}_{2D,d/8} + \widehat{f}_{\Delta_{3D,d/8-2D,d/8}}$$

MC-Predicted Uncertainty in Mean Flow Quantities – 3D

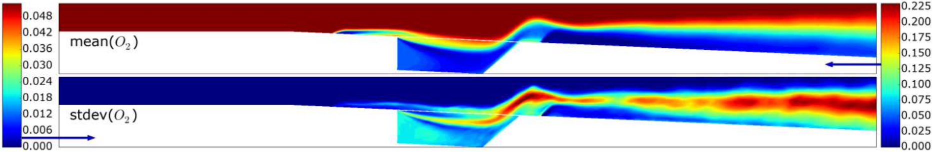


MC-Predicted Uncertainty in Mean Flow Quantities – 3D

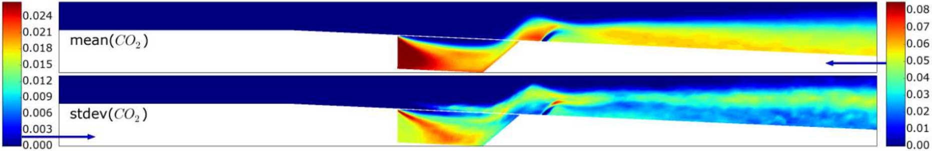
Ethane



Oxygen



Carbon Dioxide



Discussion and Closure

- Necessary workflow for UQ in large-scale computational models
  - Global sensitivity analysis to cut dimensionality, assisted by
    - Polynomial Chaos regression
    - ℓ_1-norm regularization / compressive sensing
    - Multilevel Monte Carlo & Multifidelity
  - Adaptive sparse quadrature forward UQ on reduced dimensional space
  - Resulting PC surrogate can be used in Bayesian inference on model parameters and optimization under uncertainty
- Other avenues to re-cast the problem in low-D:
  - Basis adaptation & active subspace methods
  - Manifold discovery, e.g. via Isomap or diffusion maps
  - Low rank tensor methods, etc
- Caution: Noisy computational QoIs due to finite averaging windows