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Uncertainty Quantification in Large Scale Computational Models

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

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 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

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

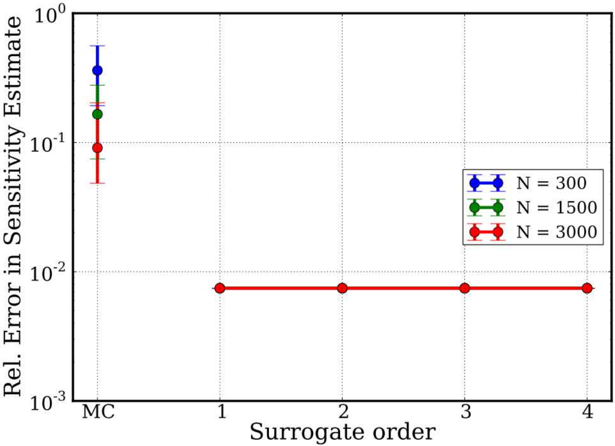
- Use PCE to evaluate Sobol Indices directly

Sargsyan, 2017

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

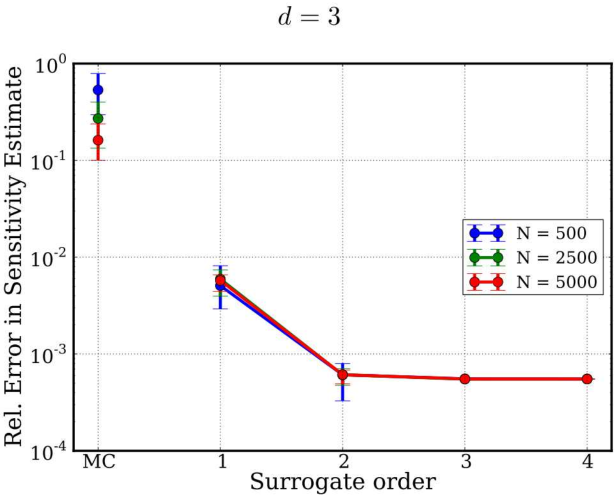
Estimation of GSA Sobol' Indices with PC regularization

$d = 1$



Sargsyan, 2017

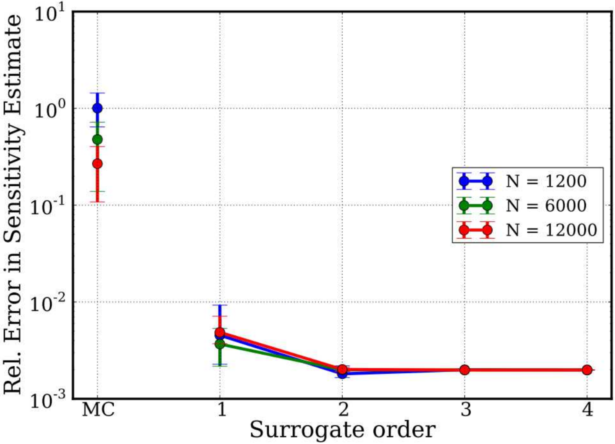
Estimation of GSA Sobol' Indices with PC regularization



Sargsyan, 2017

Estimation of GSA Sobol' Indices with PC regularization

$d = 10$



Sargsyan, 2017

Sparse regression

Model:

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

- With N samples $(\boldsymbol{\xi}^1, y^1), \ldots, (\boldsymbol{\xi}^N, y^N)$, estimate K terms $c_0, \ldots, c_{K-1}$

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

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

- Use ℓ_1 norm regularization to discover sparsity
- Compressive Sensing; LASSO; basis pursuit

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

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

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

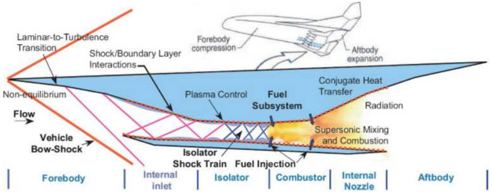
- Discover a sparse fitted PCE – many zero coefficients

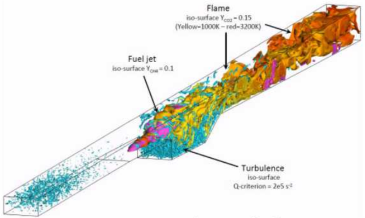
Multilevel Multifidelity (MLMF) Methods for UQ

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

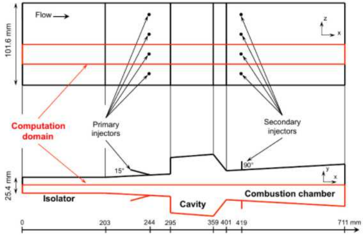
Supersonic Combusting Ramjet (scramjet)

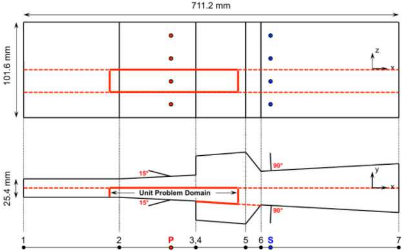




In flight

Numerical model

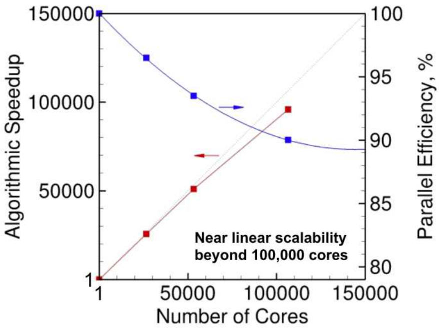




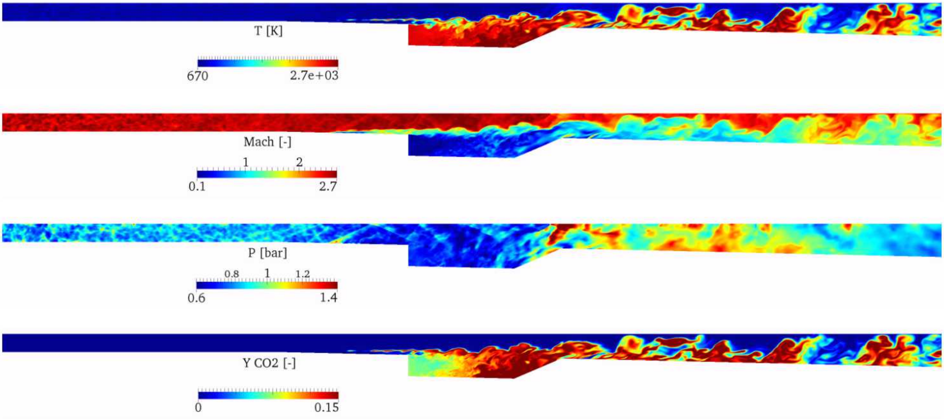
LES Performed using RAPTOR Code Framework

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

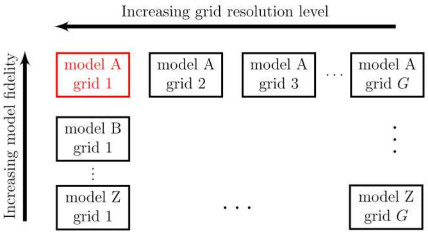
- **Theoretical framework … (Comprehensive physics)**
  - **Fully-coupled, compressible conservation equations**
  - **Real-fluid equation of state (high-pressure phenomena)**
  - **Detailed thermodynamics, transport and chemistry**
  - **Multiphase flow, spray**
  - **Dynamic SGS modeling (No Tuned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



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



Multilevel and multifdelity forms



Telescopic sum:

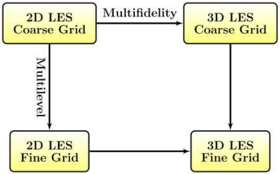
$$f_L(\lambda) = f_0(\lambda) + \sum_{\ell=1}^{L} f_{\Delta_\ell}(\lambda)$$

- 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 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.

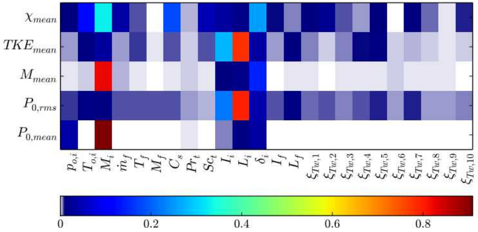
Optimize statistical accuracy given a limited number of high fidelity model evaluations by leveraging cheaper lower fidelity simulations.

Jet in crossflow unit problem: 24 parameters

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

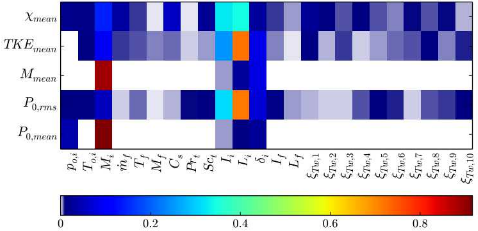
- QoIs: P_{stag}, $P_{stag,rms}$, M, TKE, χ
  - fixed at $x/d = 100$, averaged across y/d and t
- 3rd-order PCEs
- 2D runs: 1939 (coarse grid), 79 (fine grid)
- 3D runs: 46 (coarse grid), 11 (fine grid)

Unit problem: total sensitivity



Multilevel expansion of:

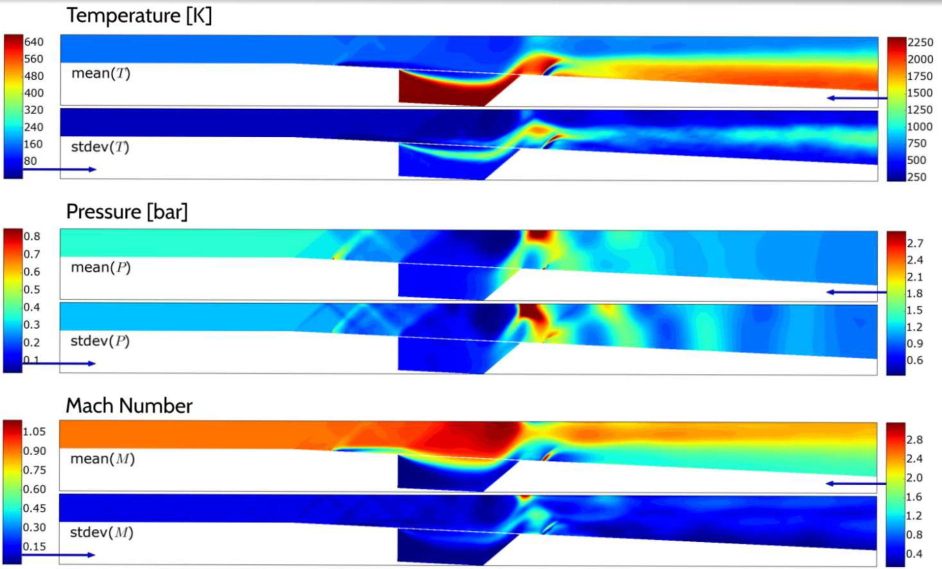
$$\hat{f}_{2D,d/16} = \hat{f}_{2D,d/8} + \hat{f}_{\Delta_{2D,d/16-2D,d/8}}$$



Multifidelity expansion of:

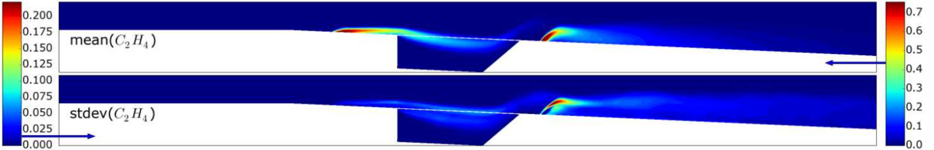
$$\hat{f}_{3D,d/8} = \hat{f}_{2D,d/8} + \hat{f}_{\Delta_{3D,d/8-2D,d/8}}$$

MC-Predicted Uncertainty in Mean Flow Quantities – 3D

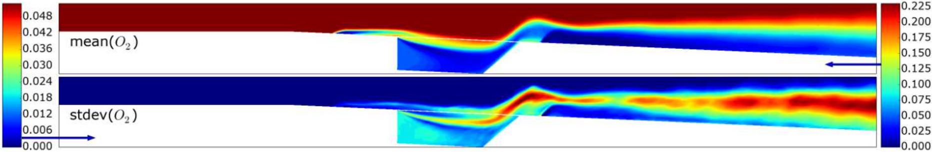


MC-Predicted Uncertainty in Mean Flow Quantities – 3D

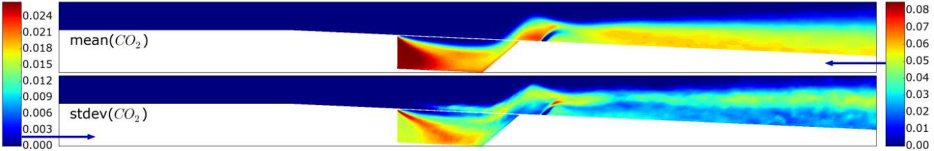
Ethane



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
- Caution: Noisy computational QoIs due to finite averaging windows
- Other surrogate options beside PC include local interpolants, Padé, RBFs, GPs, neural networks, etc