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Global Sensitivity Analysis for Large Eddy Simulation Models

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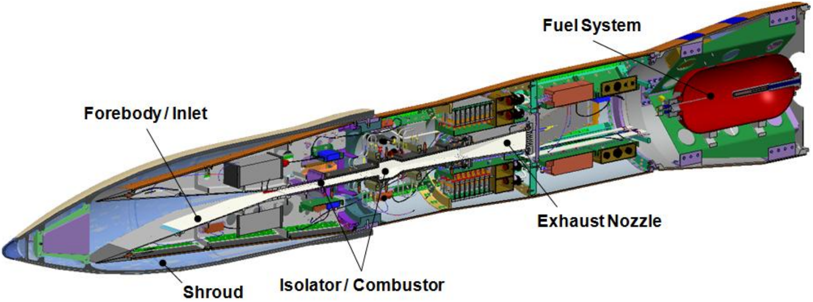
HIFiRE SCRAMJET

Development of SCRAMJET[2] engine involves

- flow simulations
- uncertainty quantification (UQ)
- design optimization

We focus on the HIFiRE[3] configuration:



[2] Supersonic Combustion RAMJET

[3] Hypersonic International Flight Research and Experimentation

Outline

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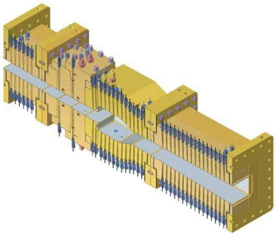
1. Flow Solver
2. Global Sensitivity Analysis
3. Results
4. Conclusions and Future Work

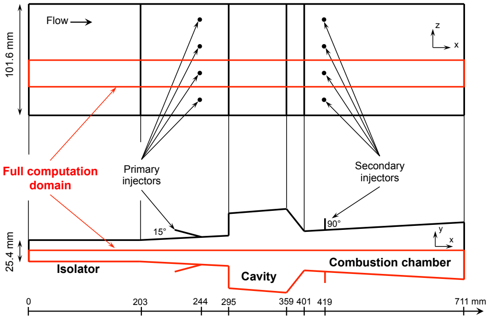
Computational domain of initial unit problem

Ultimate: simulation of full combustor domain, match experimental setup

Initial: primary injection section

- focus on interaction of fuel jet and supersonic air crossflow
- no combustion





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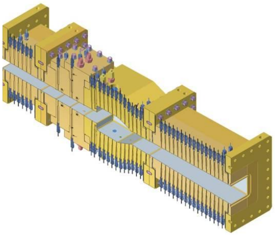
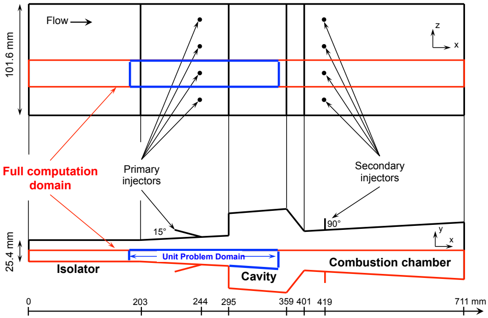




RAPTOR solver

RAPTOR: internal Sandia LES code by Oefelein *et al.* [Oefelein 06]

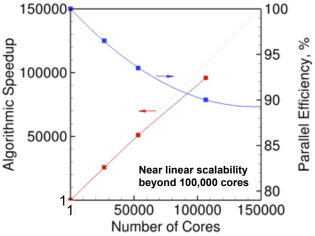
Theoretical:

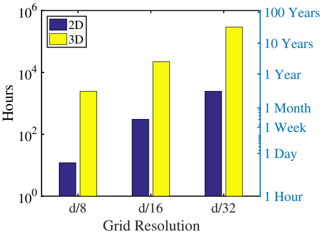
- Fully-coupled, compressible conservation equations
- Real-fluid equation of state
- Detailed thermodynamics, transport and chemistry
- Multiphase flow, liquid injection and sprays

Numerical:

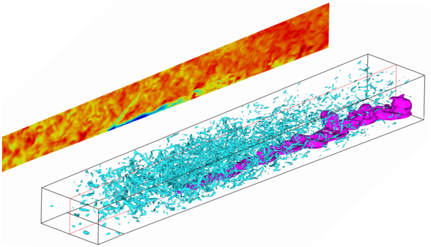
- Staggered finite-volume differencing
- Dual-time stepping with generalized preconditioning
- Complex geometry treatment

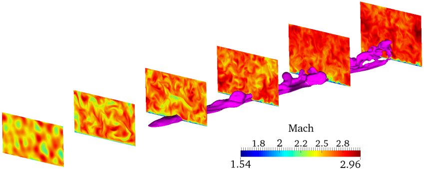
Highly-scalable but still **very expensive**





Sample solutions of unit problem





Fuel	purple iso-contour
Turbulence	blue iso-contour
Mach	cutting planes

High dimensional challenge for UQ

A **major challenge:** for uncertainty quantification

- Many uncertain parameters (high stochastic dimension)

Examples:

	Inflow boundary conditions	
Inlet	$p_0 = 1.48\text{MPa} \pm 5\%$	Stagnation pressure
(supersonic airflow)	$T_0 = 1550\text{K} \pm 5\%$	Stagnation temperature
	$M_0 = 2.51 \pm 10\%$	Mach number
	$\delta_a = (4.0 \pm 2.0)\text{mm}$	Boundary layer thickness
	$I_a = [0.0 - 0.05]$	Turbulence intensity: $I_a = u' / U_a$
	$Le_a = [0.0 - 8.0]\text{mm}$	Turbulence length scale
⋮	⋮	⋮
	Turbulence model parameters	
Static Smagorinsky	$C_R = [0.01 - 0.06]$	Modified Smagorinsky constant
	$Pr_t = [0.5 - 1.7]$	Turbulent Prandtl number
	$Sc_t = [0.5 - 1.7]$	Turbulent Schmidt number

UQ often involves some forms of "exploring" this parameter space (e.g., Monte Carlo, quadrature): *many* runs $\mathcal{O}(n^d)$ needed—**intractable!**

Outline

Find the important parameters

Possible approaches:

- Fast flow simulations (coarser grids, low-fidelity models/surrogates)
- Efficient "exploration" (adaptive sparse quadrature, QMC, MLMC)
- Dimension reduction (GSA, PCA, active subspace, manifolds)

Intuition: Not all parameters uncertainties are important

Question: Can we identify and retain only the important parameters?

Global sensitivity analysis (GSA) [Saltelli 04, Saltelli 08]

- For a given quantify of interest (QoI)
- Variance of QoI decomposed into contributions from each parameter
- Sobol sensitivity indices ranks parameters by their contribution magnitudes [Sobol 03]

Sobol sensitivity indices

Main effect $$S_i = \frac{\mathrm{Var}_{\lambda_i}\left(\mathbb{E}_{\lambda_{\sim i}}\left[f(\lambda)|\lambda_i\right]\right)}{\mathrm{Var}\left(f(\lambda)\right)}$$

Joint effect $$S_{ij} = \frac{\mathrm{Var}_{\lambda_{ij}}\left(\mathbb{E}_{\lambda_{\sim ij}}\left[f(\lambda)|\lambda_{ij}\right]\right)}{\mathrm{Var}\left(f(\lambda)\right)} - S_i - S_j$$

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

- Small S_{T_i}: low impact $\Rightarrow$ fix parameter, stochastic dim. eliminated
- Efficient Monte Carlo estimators [Sobol 90, Saltelli 02, Saltelli 10], but still prohibitive for LES model
- Plan: construct computationally-affordable surrogate model via polynomial chaos expansion (PCE)

Polynomial chaos expansions

Any random variable of finite variance can be expanded as follows

$$\lambda(\omega) = \sum_{|\beta|_1=0}^{\infty} \lambda_\beta \Psi_\beta(\xi_1, \xi_2, \ldots) \approx \sum_{\beta \in \mathcal{J}} \lambda_\beta \Psi_\beta(\xi_1, \xi_2, \ldots, \xi_{n_s})$$

$$\Psi_\beta(\xi_1, \xi_2, \ldots) = \prod_{j=1}^{\infty} \psi_{\beta_j}(\xi_j)$$

- $\lambda_\beta \in \mathbb{R}$
- ξ_j is a basis random variable that is easy to sample from
- Entries of β are the orders of ψ_{β_j}
- ψ_{β_j} is the β_jth order univariate orthogonal polynomial with respect to the PDF of ξ_j
- Series truncated to finite terms ($n_s \sim \#$ stochastic d.o.f.)

Polynomial chaos expansions: construction

For a QoI: $$f(\lambda) = \sum_{\beta \in \mathcal{J}} c_\beta \Psi_\beta(\xi_1, \xi_2, \ldots, \xi_{n_s})$$

Non-intrusive approach to compute expansion coefficients

- Projection (e.g., with sparse quadrature):

$$c_\beta = \frac{\mathbb{E}\left[f(\lambda)\Psi_\beta\right]}{\mathbb{E}[\Psi_\beta^2]} = \frac{\int_\Xi f\left(\lambda(\xi)\right)\Psi_\beta(\xi)p(\xi)\,d\xi}{\int_\Xi \Psi_\beta^2(\xi)p(\xi)\,d\xi}$$

- Regression $Gc = f$:

$$\begin{bmatrix} \Psi^{(1)}(\xi^{(1)}) & \cdots & \Psi^{(N)}(\xi^{(1)}) \\ \vdots & & \vdots \\ \Psi^{(1)}(\xi^{(M)}) & \cdots & \Psi^{(N)}(\xi^{(M)}) \end{bmatrix} \begin{bmatrix} c_{\beta^1} \\ \vdots \\ c_{\beta^N} \end{bmatrix} = \begin{bmatrix} f(\lambda(\xi^{(1)})) \\ \vdots \\ f(\lambda(\xi^{(M)})) \end{bmatrix}$$

Polynomial chaos expansions: extract Sobol indices

Can extract Sobol indices directly from the PCE coefficients:

$$S_i = \frac{1}{\mathrm{Var}\left(f(\lambda)\right)} \sum_{\beta \in \mathcal{J}_{S_i}} c_\beta^2 \, \mathbb{E}[\Psi_\beta^2], \qquad \mathcal{J}_{S_i} = \{\beta \in \mathcal{J} : \beta_i > 0, \beta_k = 0, k \neq i\}$$

$$S_{ij} = \frac{1}{\mathrm{Var}\left(f(\lambda)\right)} \sum_{\beta \in \mathcal{J}_{S_{ij}}} c_\beta^2 \, \mathbb{E}[\Psi_\beta^2], \qquad \mathcal{J}_{S_{ij}} = \left\{\beta \in \mathcal{J} : \beta_i > 0, \beta_j > 0, \beta_k = 0, k \neq i, k \neq j\right\}$$

$$S_{T_i} = \frac{1}{\mathrm{Var}\left(f(\lambda)\right)} \sum_{\beta \in \mathcal{J}_{S_{T_i}}} c_\beta^2 \, \mathbb{E}[\Psi_\beta^2], \qquad \mathcal{J}_{S_{T_i}} = \{\beta \in \mathcal{J} : \beta_i > 0\}$$

QoI variance: $$\mathrm{Var}\left(f(\lambda)\right) = \sum_{0 \neq \beta \in \mathcal{J}} c_\beta^2 \, \mathbb{E}[\Psi_\beta^2]$$

Compressed sensing

- Small number of LES evaluations available
- Large number of polynomial PCE basis
(p-3 20-d: total order 2925 terms, tensor-product 1.1×10^{12} terms)
- Extremely under-determined
- One approach: reduce the number of bases via sparsity
- Discover and retain only basis terms with high magnitude coefficients using **compressed sensing**

Compressed sensing

Different variants of the CS problem:

$$\min_c \| c \|_1 \quad \text{subject to} \quad Gc = f$$

$$\min_c \| c \|_1 \quad \text{subject to} \quad \| Gc - f \|_2^2 < \epsilon$$

$$\min_c \| Gc - f \|_2^2 \quad \text{subject to} \quad \| c \|_1 < t$$

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

Many algorithms available: e.g., LARS, OMP, FPC, ℓ_1-*magic*

Observation: with few data, solution often overfitted, not useful for interpolation

Current research: mitigate overfitting through Bregman inverse scale space (ISS) methods, and problem reformulations

Outline

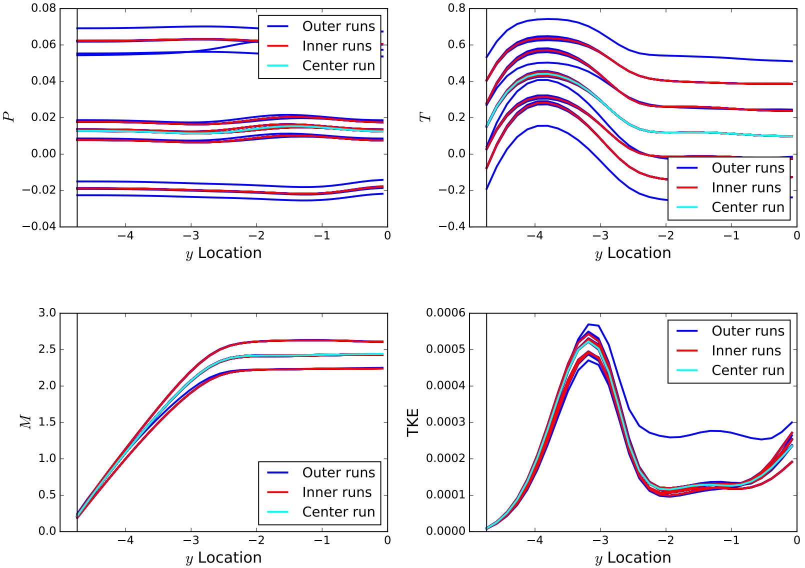
Initial study: 6 parameters

An initial 6 parameter study to exercise mechanics and verify our intuition

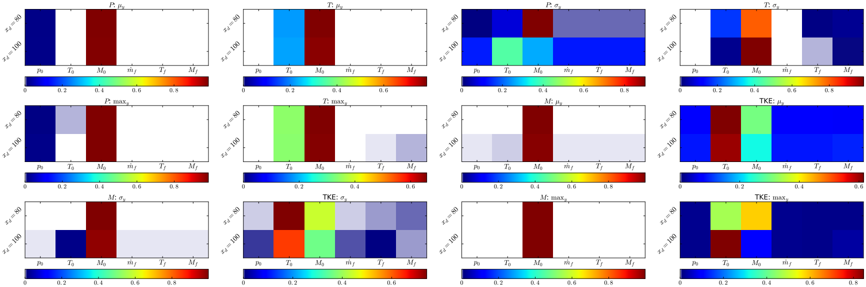
Type	Parameters and ranges	Description
	Inflow boundary conditions	
Inlet	$p_0 = 1.48\text{MPa} \pm 5\%$	Stagnation pressure
(supersonic airflow)	$T_0 = 1550\text{K} \pm 5\%$	Stagnation temperature
	$M_0 = 2.51 \pm 10\%$	Mach number
Fuel injection (1st row)	$\dot{m}_f = 7.37 \times 10^{-3}\text{kg/s} \pm 10\%$	Mass flux
JP-7 surrogate	$T_f = 300.0\text{K} \pm 5\%$	Static temperature
$(36\% CH_4 + 64\% C_2H_4)$	$M_f = 1 \pm 5\%$	Mach number

- 3D $d/8$-grid LES solves
- 73 runs at quadrature points
- 2nd order PCE

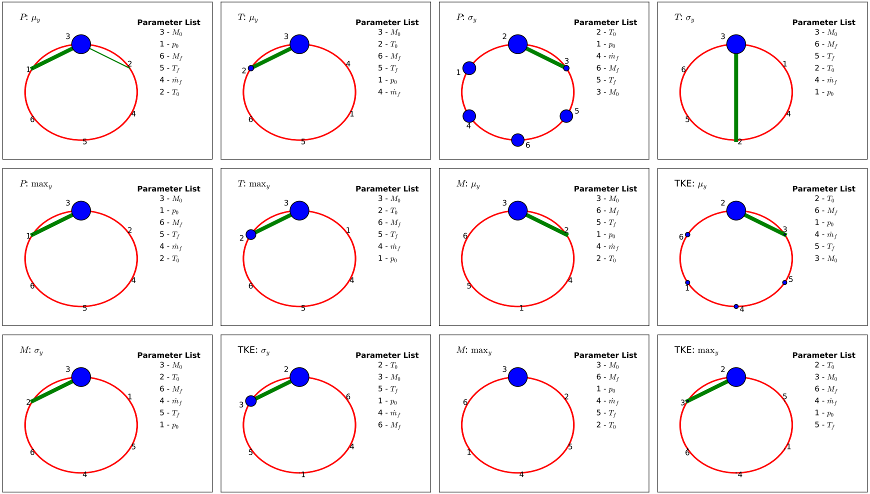
Solution profiles



Total sensitivity indices



Joint sensitivity indices



Outline

Conclusions

Conclusions:

- Demonstrated global sensitivity analysis framework
  - based on Sobol indices
  - applied to expensive LES simulations of SCRAMJET design
- Enabled tractable GSA computations with polynomial chaos expansions
- Verified highest sensitivity in initial non-combustion unit problem is to inlet Mach number

Future work:

- A 24-dimensional problem is in progress
- Employ compressed sensing
- Leverage different models/resolutions via multi-fidelity
- Full geometry with cavity
- Enabled combustion reactions (many more parameters!)

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