Uncertainty Quantification in LES Computations of Turbulent Multiphase Combustion in a Scramjet Engine

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– ScramjetUQ –

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Quarterly DARPA Review

Motivation

- Uncertainty quantification (UQ) in computational predictions of physical systems is useful for
  - Hypothesis testing, model comparison, and validation
  - Decision support
  - Estimation of model error
  - Optimal experimental design
  - Optimization under uncertainty (OUU)

- Challenges for UQ in systems of practical interest arise from:
  - High dimensionality
  - Model complexity and computational cost
  - Optimization under uncertainty

- Scramjet application
  - Challenging computational problem
  - Relevant engineered system of practical interest
  - Limited data available from ground and flight testing – high uncertainty
  - Challenging design under uncertainty problem

Project Goals

- Advance the state of the art in UQ methods and software, targeting challenges with
  - High dimensionality
  - Model complexity and computational cost
  - Optimization under uncertainty
- Demonstrate these capabilities, with effective handling of these challenges, in Large Eddy Simulation (LES) of a laboratory scale Scramjet combustor
  - NASA Langley Hypersonic International Flight Research and Experimentation (HIFiRE) configuration
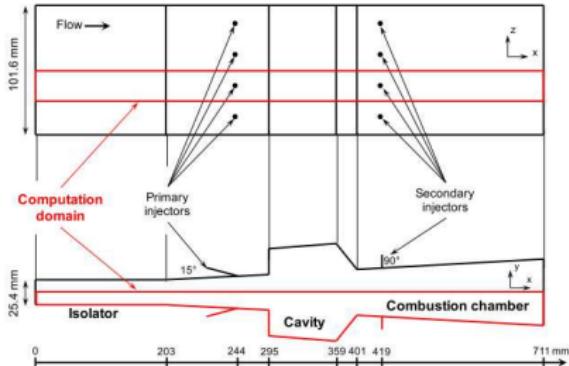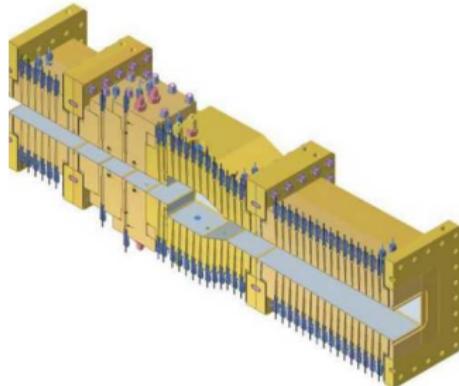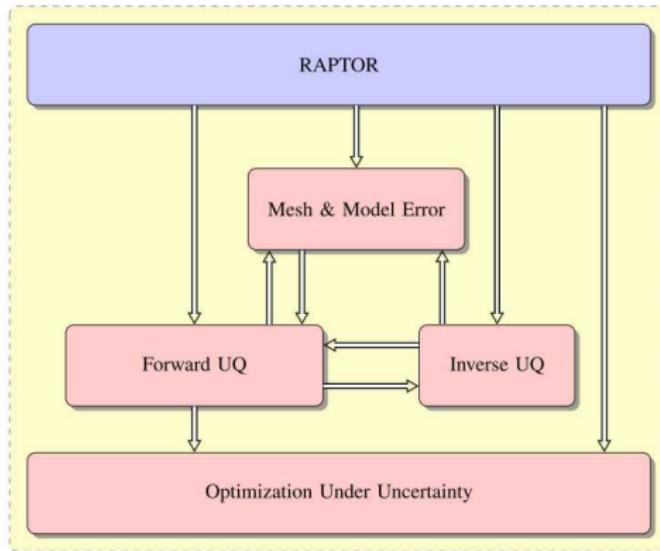
Approach

- Employ RAPTOR LES code for Scramjet flow computations
  - 3D hypersonic multiphase turbulent combustion
  - Adapt as needed for UQ purposes
  - Evolve from simpler jet-in-crossflow problem to full Scramjet flow
- High Dimensionality – identify important uncertain parameters
  - Global sensitivity analysis, PC regularization, compressive sensing
  - Adaptive selection of computational sparse quadrature samples
  - Adaptive basis and low-dimensional manifold samplin
  - Multi-level Multi-fidelity (MLMF) methods
- Model complexity
  - Employ statistical embedded model-error constructions
  - Account for uncertainty due to discretization error given coarse meshes
  - MLMF methods minimize #requisite fine-mesh high-fidelity runs
- Optimization under uncertainty
  - DAKOTA library for MLMF & UQ/statistics evaluation
  - SNOWPAC library for stochastic optimization
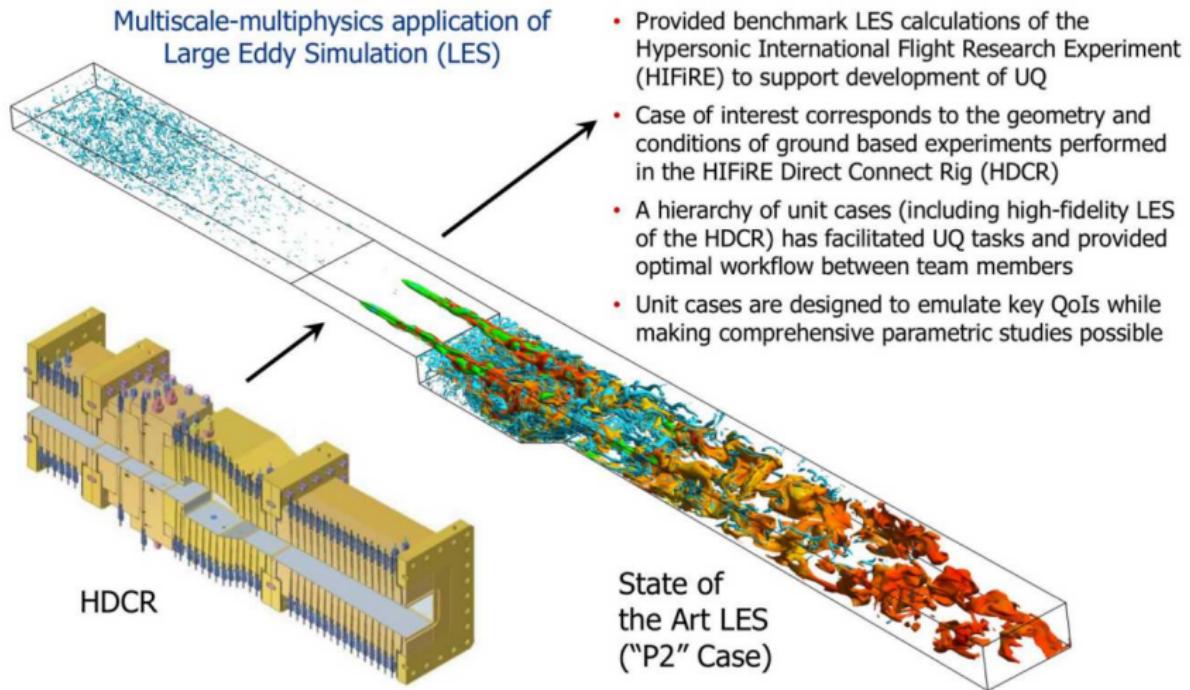 - Develop software workflows coupling DAKOTA, SNOWPAC, & RAPTOR

Integrated Project Structure

- The application code, RAPTOR, is central to all activities
- Inverse UQ estimates uncertain inputs, and model and mesh error
- Mesh and model error sources of uncertainty feeding to forward UQ.
- Forward UQ provides estimation of uncertainty in model outputs
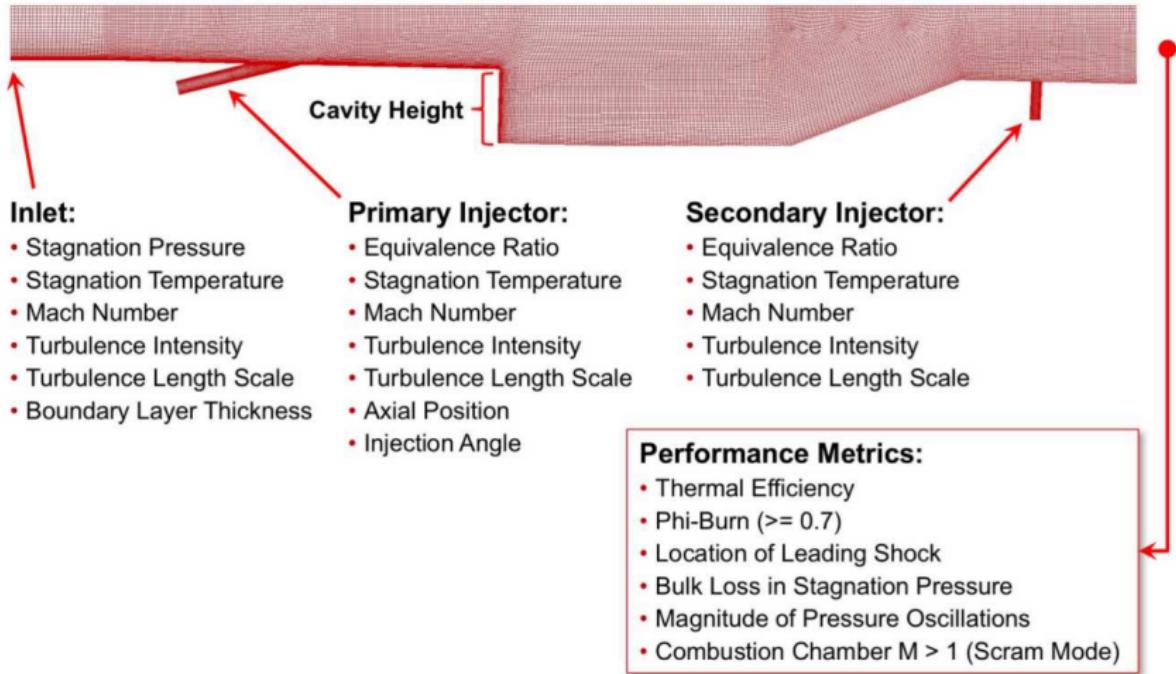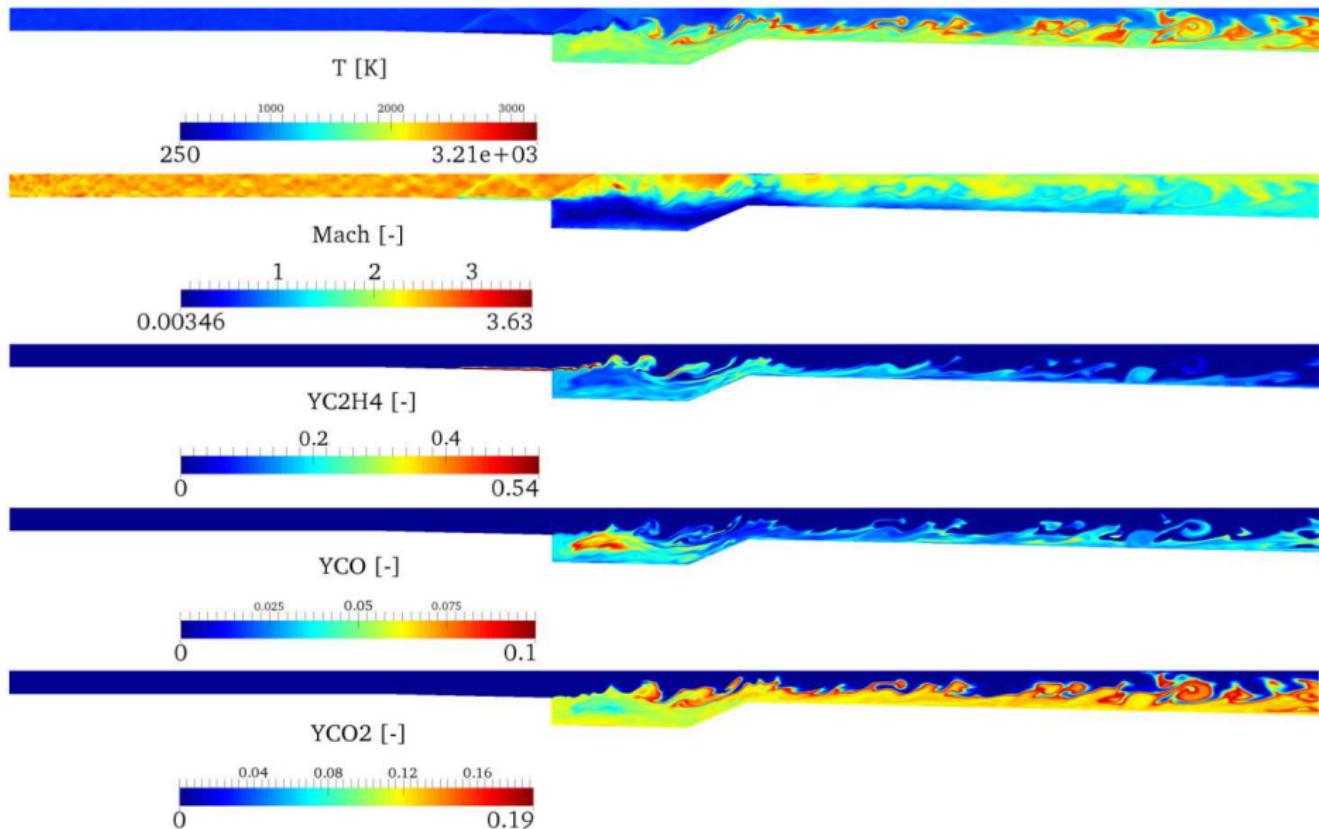- Optimization under uncertainty couples all the above

Multiscale-multiphysics application of Large Eddy Simulation (LES)

- Provided benchmark LES calculations of the Hypersonic International Flight Research Experiment (HIFiRE) to support development of UQ

- Case of interest corresponds to the geometry and conditions of ground based experiments performed in the HIFiRE Direct Connect Rig (HDCR)

- A hierarchy of unit cases (including high-fidelity LES of the HDCR) has facilitated UQ tasks and provided optimal workflow between team members

- Unit cases are designed to emulate key QoIs while making comprehensive parametric studies possible

HDCR

State of the Art LES ("P2" Case)

Cavity Height

Inlet:
- Stagnation Pressure
- Stagnation Temperature
- Mach Number
- Turbulence Intensity
- Turbulence Length Scale
- Boundary Layer Thickness

Primary Injector:
- Equivalence Ratio
- Stagnation Temperature
- Mach Number
- Turbulence Intensity
- Turbulence Length Scale
- Axial Position
- Injection Angle

Secondary Injector:
- Equivalence Ratio
- Stagnation Temperature
- Mach Number
- Turbulence Intensity
- Turbulence Length Scale

Performance Metrics:
- Thermal Efficiency
- Phi-Burn (>= 0.7)
- Location of Leading Shock
- Bulk Loss in Stagnation Pressure
- Magnitude of Pressure Oscillations
- Combustion Chamber M > 1 (Scram Mode)

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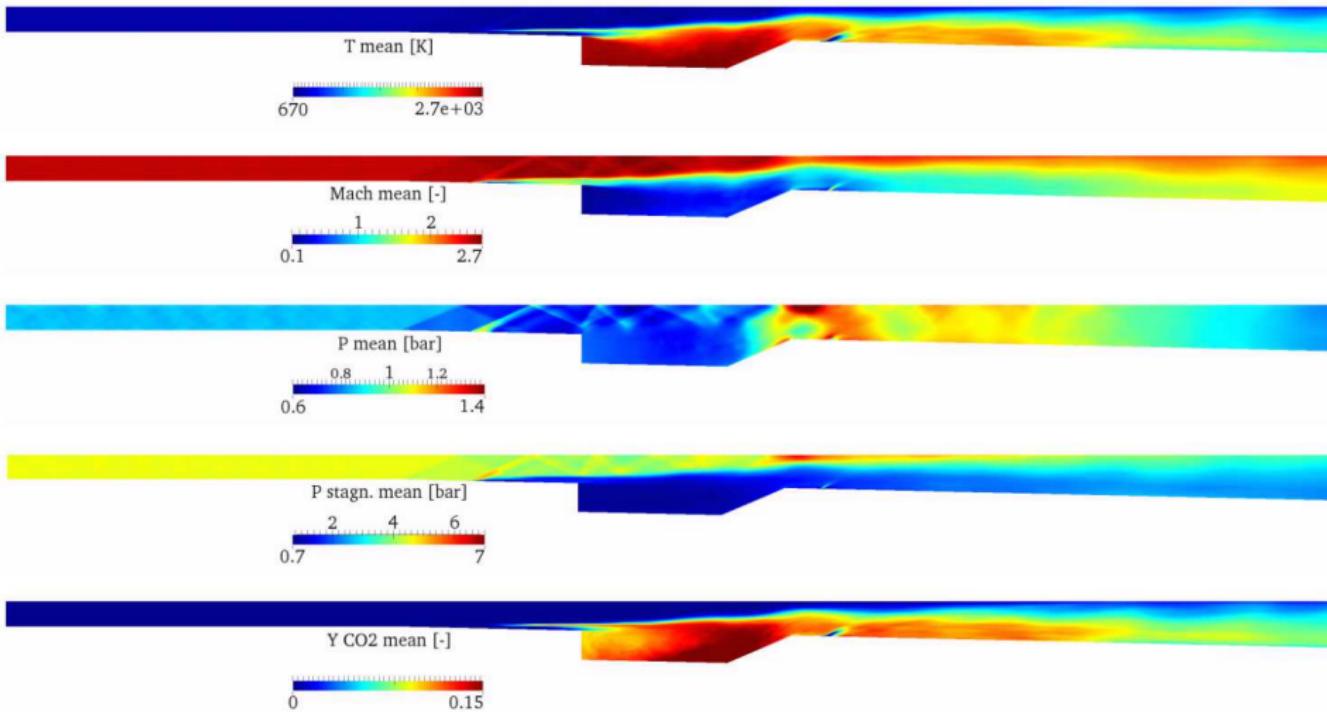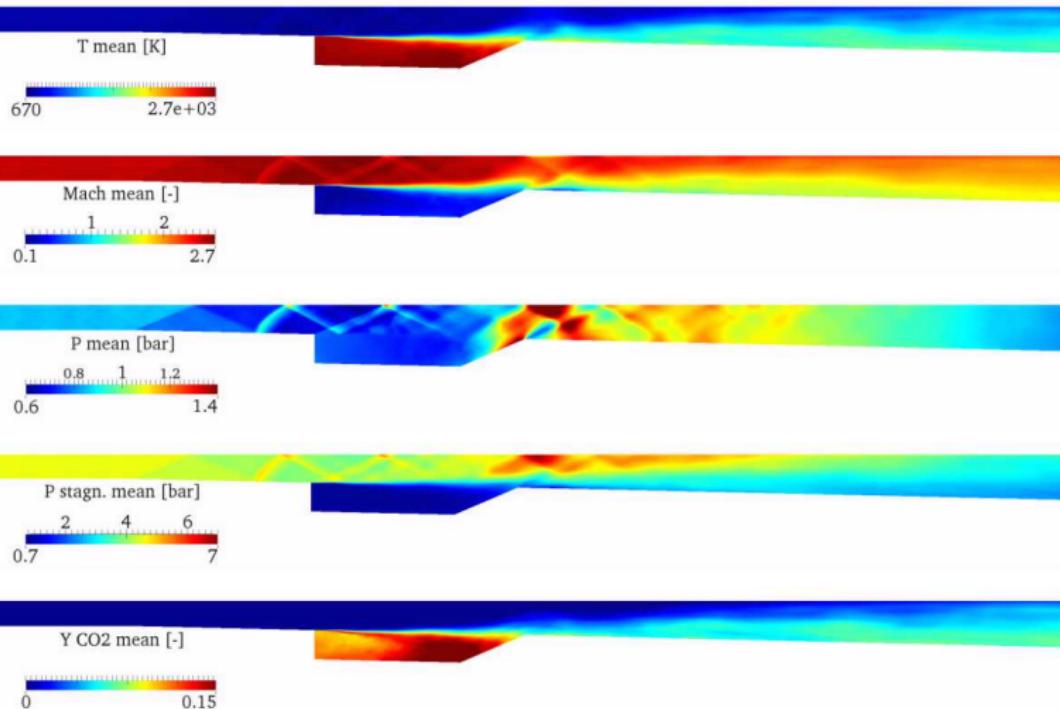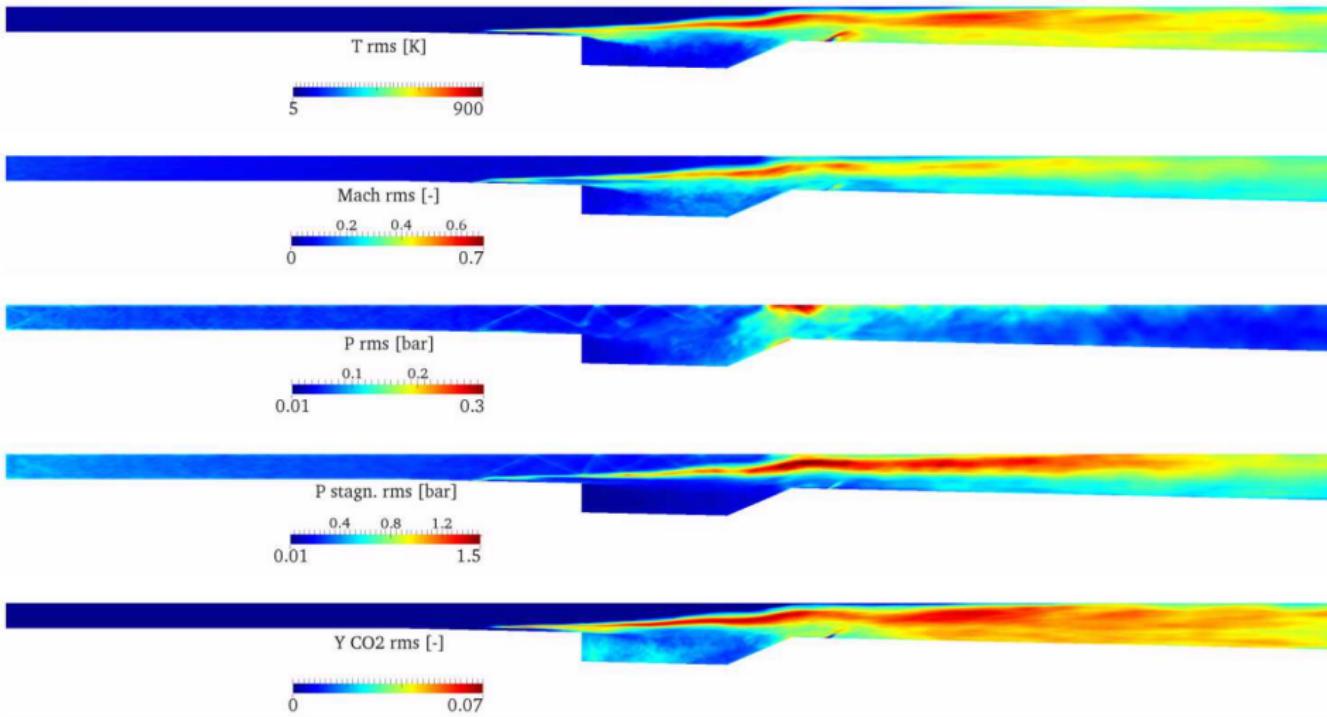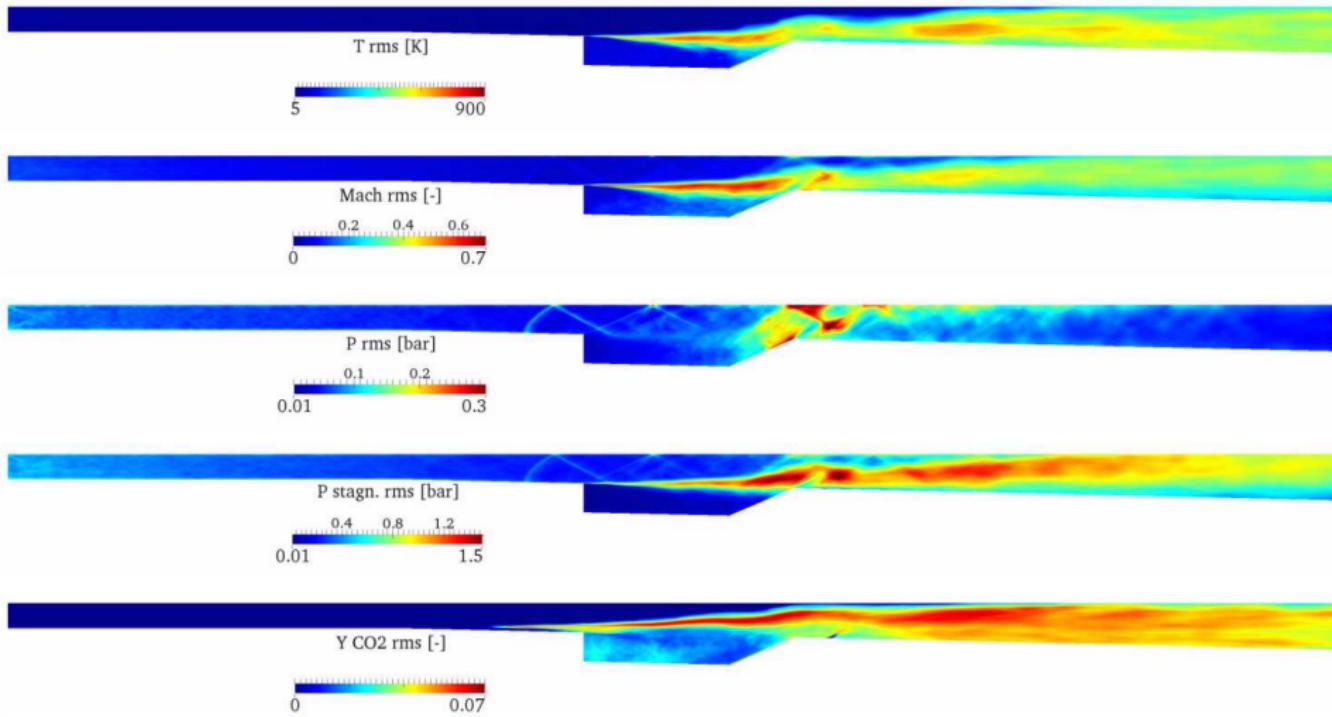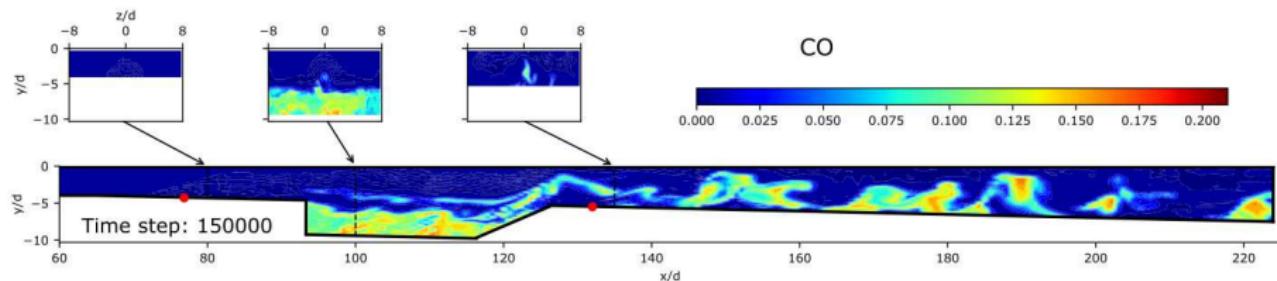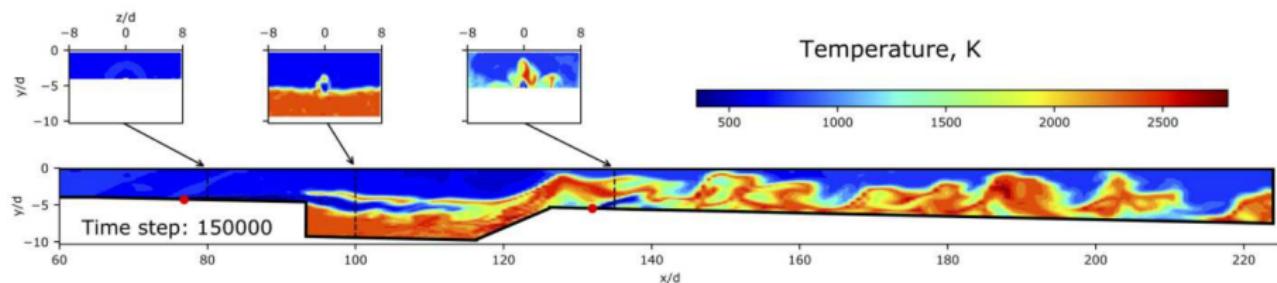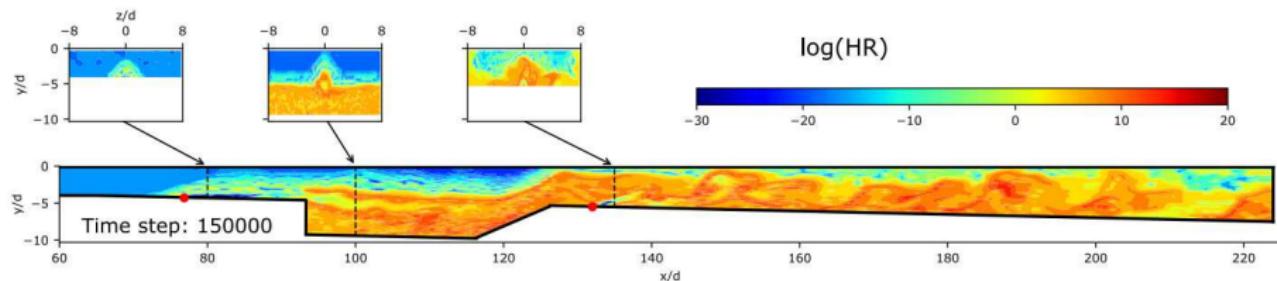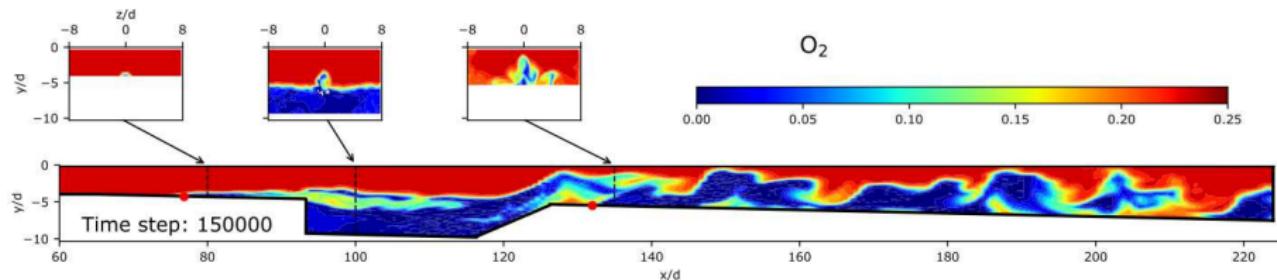
Computational Considerations

- 3D d08 : $\Delta x \sim 0.4$ mm, $\Delta t \sim 47$ ns
- $Re_{\mathrm{air}} \sim$ 380,000 and $M_{\mathrm{air}} \sim$ 2.5
- Meshes and CPU cost:

Grid Spacing	Total Cells in 2D Grids		Total Cells in 3D Grids	
$d_p/8$	64,500	(20 CPU-Hrs/FTT)	4,128,000	(10,240 CPU-Hrs/FTT)
$d_p/16$	258,000	(160 CPU-Hrs/FTT)	33,024,000	(163,840 CPU-Hrs/FTT)
$d_p/32$	1,032,000	(1,280 CPU-Hrs/FTT)	264,192,000	(2,621,440 CPU-Hrs/FTT)
$d_p/64$	4,128,000	(10,240 CPU-Hrs/FTT)	2,113,536,000	(41,943,040 CPU-Hrs/FTT)

CPU hours given for 1 flow-through-time (FTT) in P2 geometry.

- Global chemistry model:

$$CH_4 + \tfrac{3}{2}\,O_2 \quad \rightarrow CO + 2\,H_2O$$
$$C_2H_4 + 2\,O_2 \quad \rightarrow 2\,CO + 2\,H_2O$$
$$2\,CO + O_2 = CO_2$$
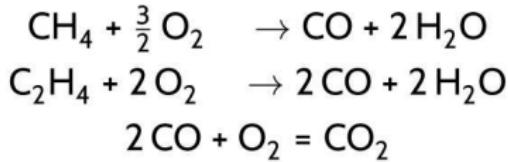
Our UQ vision – High Dimensionality and Forward UQ

- Intrinsic dimensionality for smooth observables from physical systems is generally *low*
- Employ a suite of methods and robust software for discovering underlying low-dimensional sparse representation
  - Global sensitivity analysis
  - Polynomial Chaos (PC) surrogates
  - Compressive sensing – ℓ_1-norm regression
  - Greedy basis growth
  - Multilevel Multifidelity (MLMF) strategy for computational samples
- Forward UQ; adaptive sparse quadrature; reduced parameter space
- Develop new methods for basis adaptation
  - Discover optimal basis rotation for low-order representations
- Develop new methods for discovery of low-dimensional manifolds
  - Data analysis; discover manifold structure in computational results

Our UQ vision – Model Error

- Designate complex model as "truth"
- Designate simple model of interest as "model"
- Represent the discrepancy between model predictions and truth as a statistical model, embedded in the governing equations
  - Embed in model components where approximations have been made
- Estimate parameters of model error representation using Bayesian inference, given truth data
- Goal is to ensure that predictions with the calibrated model exhibit a degree of uncertainty that is representative of the discrepancy from the truth
- Analysis of model-error embedding in different submodels allows diagnostic exploration after the component where model misspecification is most responsible for discrepancy in predictions

Our UQ vision – Mesh Error

- Large-scale models of physical systems are often run at coarse-mesh resolution due to computational feasibility constraints
  - Results are a function of the mesh
  - Mesh error is not "small"
  - Models are calibrated for a given mesh – e.g. climate models
- Mesh discretization error needs to be estimated and incorporated as part of the uncertainty in predictions
- We are developing and evaluating two approaches for estimation of mesh error
  - Random field modeling
  - Variational multiscale method

Our UQ vision – Bayesian Inference

- Uncertain model parameters need to be estimated using a combination of
  - Expert knowledge
  - Experimental HIFiRE data
- Rely on Bayesian inference, addressing:
  - High-dimensionality
  - Computational cost
- Use Markov chain Monte Carlo (MCMC)
- Employ polynomial chaos model surrogates, built from GSA/ForwardUQ, instead of RAPTOR, in the Likelihood function
- Advance the state of the art in Likelihood Informed Subspace (LIS) methods to non-intrusively identify relevant, hopefully low-dimensional, parameter subspaces where data is informative

Our UQ vision – Model Complexity

- Make use of computations over a range of
  - mesh resolution
  - model fidelity

  to provide information on uncertain predictive QoIs
- Rely on multi-level multi-fidelity (MLMF) UQ methods
- Incorporate MLMF strategies wherever possible
  - Global sensitivity analysis
  - Sparse quadrature and forward UQ/surrogate construction
  - Optimization under uncertainty (OUU)
- Explore connections between MLMF, model error, and mesh error methods

Our UQ vision – Optimization Under Uncertainty (OUU)

- Optimization under uncertainty is required for ensuring that optimal designs are robust to uncertainty/variability in parameters and/or operating conditions
- Uncertainty raises the need for risk-aware optimization targets
- Uncertainty increases the difficulty of the optimization problem
  - Increases dimensionality: design + uncertain params
  - Integration over uncertain parameters for each design point
- Statistical QoIs from large-scale models are typically *noisy*
  - Spatiotemporal averaging with finite sample size
- Employ surrogates, constructed from model runs, as needed
- Rely on MLMF and Trust Region Model Mgmt (TRMM) methods
- Couple DAKOTA with SNOWPAC stochastic optimization library