Uncertainty Quantific SAND2016-2802C Computations of Turbulent Multiphase Combustion in a Scramjet Engine

— ScramjetUQ —

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Quarterly Review
Stanford University, Palo Alto, CA

Outline

Current ScramjetUQ Project Team

Team includes Sandia (Livermore + Albuquerque), Duke, MIT, and USC.

Institution	Expertise	**Participants**
Sandia	UQ + Comb	**Habib Najm**, Bert Debusschere, Cosmin Safta, Khachik Sargsyan *Xun Huan*
	LES + SprayComb	Joe Oefelein, Guilhem Lacaze *Zachary Vane*
	UQ + Optim	Mike Eldred *(+pd tbd)*
Duke	UQ + Comb	**Omar Knio**, *Ihab Sraj*
	LES	Guglielmo Scovazzi, *Oriol Colomés*, *(+tbd)*
MIT	UQ + Optim	**Youssef Marzouk**, *Olivier Zahm*, *Florian Augustin*
USC	UQ + Optim	**Roger Ghanem**, *(+pd tbd)*

Project Goals

For UQ in coupled multiphysics problems, address challenges of:

- High dimensionality
  - Forward UQ
  - Mesh discretization error
  - Inverse UQ
- Model complexity
  - Model error
  - Multifidelity UQ
- Design optimization
  - Optimization under uncertainty

Demonstrate capabilities on unit problems leading to:

- Problem P1: Turbulent jet in cross flow – Phase I
- Problem P2: Scramjet problem – Phase II

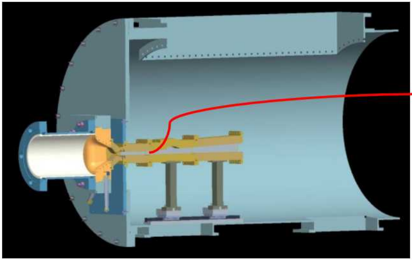
Project Outline

- Three-year project plan with specified tasks and milestones
- Year-1:
    - LES code development for P1 & P2 including unit problems
    - UQ methods development and tests on P1 unit problems
    - Demo on a simplified P1 unit problem
- Year-2:
    - Testing and demonstration on full P1
    - UQ developments and tests on P2 unit problems
- Year-3:
    - UQ developments and tests on unions of P2 unit problems
        - increasing complexity
    - Demonstration on full P2

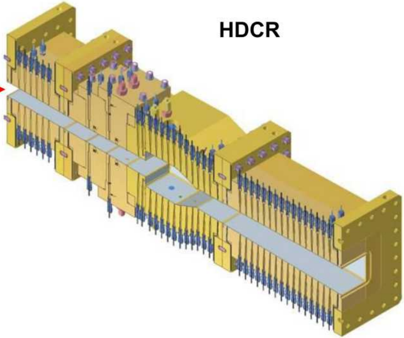
HIFiRE Experiments

- HIFiRE experiments provide data for extrapolating results of ground tests to flight hardware and validation of numerical simulation tools
  - Cavity-based hydrocarbon-fueled dual-mode scramjet combustor
  - Emulates complex transition from subsonic to supersonic combustion
  - Characterized by nonlinear coupling between multiscale physics
  - Turbulence and shock interactions intricately coupled to combustion, heat transfer, and thermodynamics
- Involve both flight and ground based experiments via HIFiRE Direct Connect Rig (HDCR) ... this project is focused on HDCR
  - Test facility has generated a large body of publications and recognized as a key experiment for hypersonic science
  - Available data includes static pressure and temperature distributions along wall and wall heat flux
  - Additional quantities of interest can be extracted from LES

Geometry

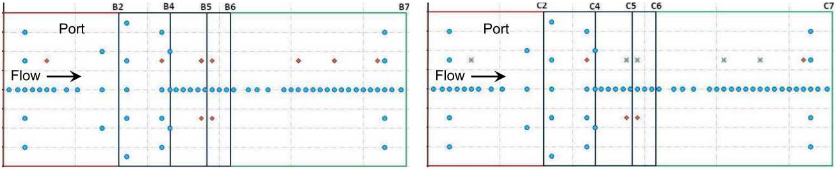


Arc-Heated SCRAMJET Test Facility (AHSTF) … NASA LaRC



Flow path constructed with 50.8 mm (2 inch) thick copper walls thermally protected with zirconium dioxide coating (144 static pressure ports, 19 flow path surface thermocouples, 4 heat flux gauges)

Available Data (Provided by Hass et al., NASA LaRC)

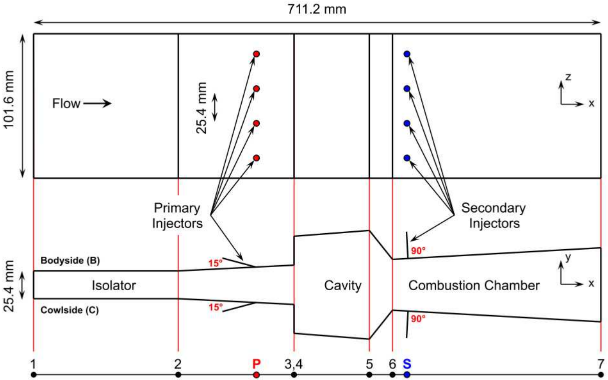


Bodyside Instrumentation Layout

Cowlside Instrumentation Layout

- **144 static pressure ports (blue circles)**
- **19 flow path surface thermocouples (red diamonds)**
- **4 heat flux gauges (X boxes)**
- **Also “port” and “starboard” sidewall thermocouples**
- **Both fueled and “tare” (no fuel) measurements available**

HDCR Flow Path



	x [mm], (x/d_p)	y [mm], (y/d_p)
B1	0.000 (0.000)	12.7 (4.000)
B2	203 (63.94)	12.7 (4.000)
BP	244 (76.85)	13.6 (4.283)
B3	295 (92.91)	14.8 (4.661)
B4	294 (92.60)	31.9 (10.05)
B5	359 (113.1)	33.4 (10.52)
B6	401 (126.3)	17.2 (5.417)
BS	419 (132.0)	17.6 (5.543)
B7	711 (223.9)	24.2 (7.622)
C1	0.000 (0.000)	−12.7 (−4.000)
C2	203 (63.94)	−12.7 (−4.000)
CP	244 (76.85)	−13.6 (−4.283)
C3	295 (92.91)	−14.8 (−4.661)
C4	294 (92.60)	−31.9 (−10.05)
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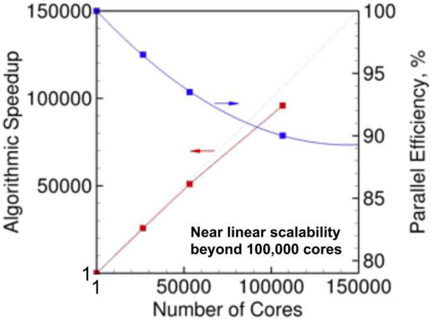
CS	419 (132.0)	−17.6 (−5.543)
C7	711 (223.9)	−24.2 (−7.622)

$d_p = 3.175$ mm, $d_s = 2.3876$ mm.

LES Performed using RAPTOR Code Framework

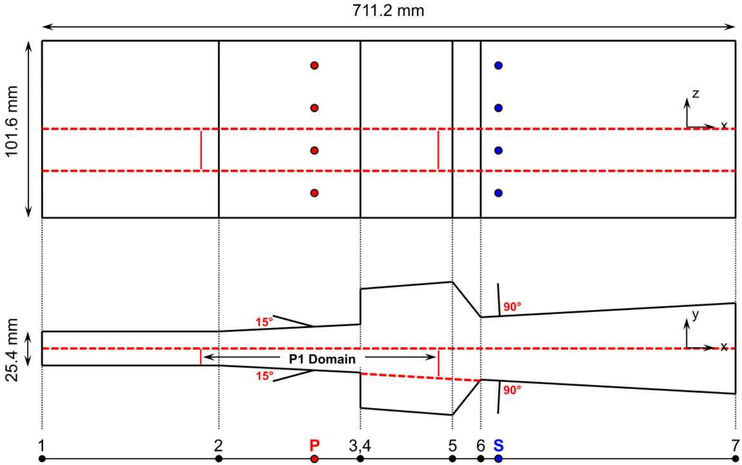
- **Theoretical framework … (Comprehensive physics)**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray (Lagrangian-Eulerian)
  - Dynamic SGS modeling (No Tuned 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 hierarchy of HPC platforms (e.g., scaling on ORNL TITAN)
  - Selected for early science campaign on next generation SUMMIT platform (ORNL Center for Accelerated Application Readiness, 2015 – 2018)



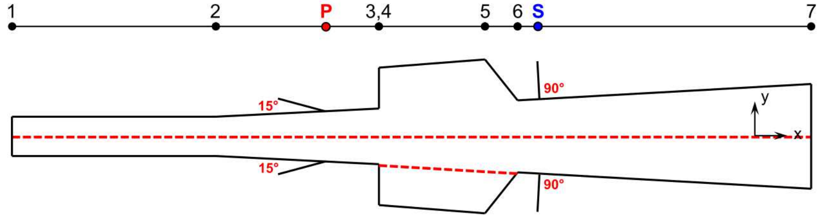
LES unit problems

- LES of P1, P2 cases performed over hierarchy of grid resolutions to establish benchmarks (e.g., 3D # d/64, d/32, d/16, d/8)
- Benchmarks post-processed and analyzed in detail to establish and characterize QoIs (including comparisons with available data)
- Expensive calculations, data generation, and/or analysis requiring significant HPC resources performed by LES group
- Affordable UQ relevant unit cases designed and justified from established set of high-fidelity benchmarks
- Temporal convergence analysis: 10 flow-through-times (of the air stream) required to get converged RMS.
- Unit cases are designed to emulate key QoIs while at the same time facilitating detailed parametric studies

Progressive Simplifications (1/8th domain, 3D periodic, 2D, etc.)



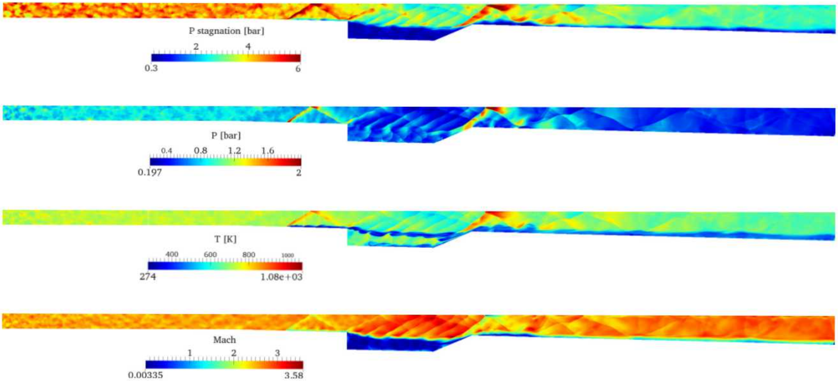
Grids For 1/8th Domain Periodic and 2D Cases



Grid Spacing	nx	ny	nz	Total (2D)	Total (3D)
$d_p/8$	1,800	32	64	57,600	3,686,400
$d_p/16$	3,600	64	128	230,400	29,491,200
$d_p/32$	7,200	128	256	921,600	235,929,600
$d_p/64$	14,400	256	512	3,686,400	1,887,436,800

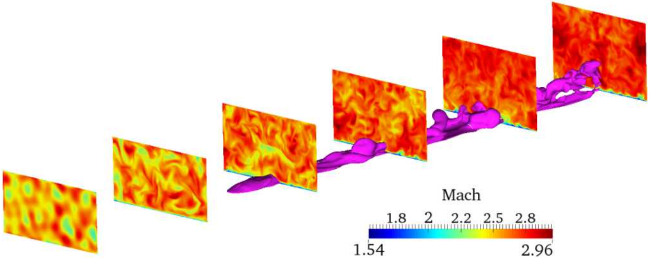
Does not include cavity.

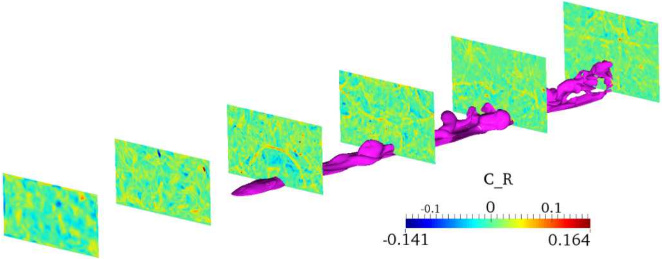
Both Baseline P1 (d/32, 3D) and Initial P2 (d/32, 2D) Cases Running



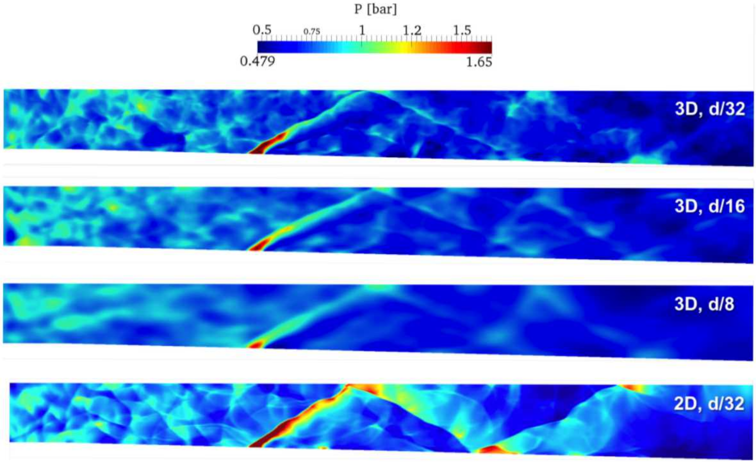
P2, d/32, 2D

P1 Domain is Cut at x/d = 60, 110 with Cavity Removed

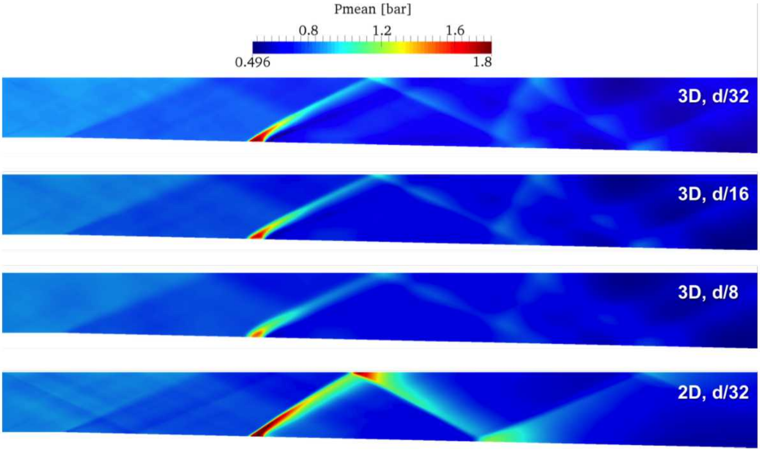




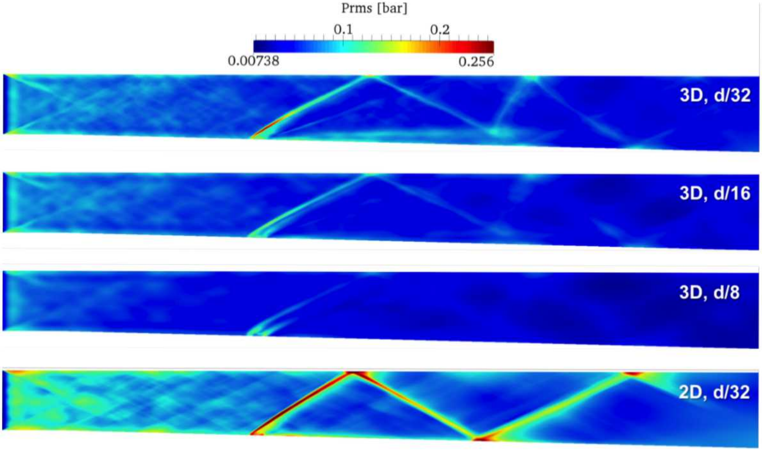
Instantaneous Pressure



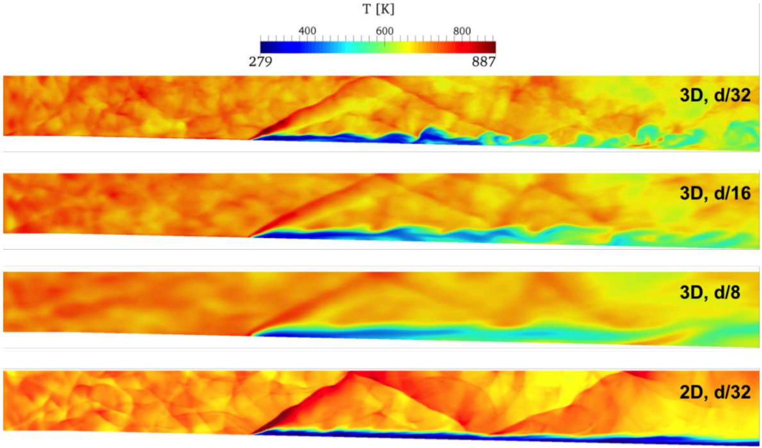
Mean Pressure



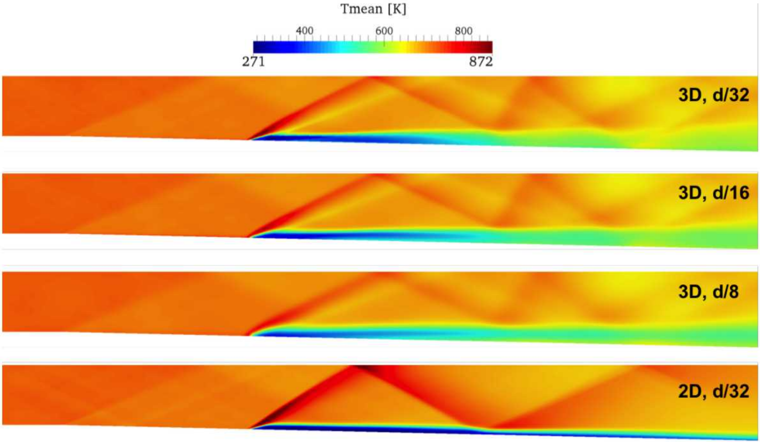
RMS Pressure



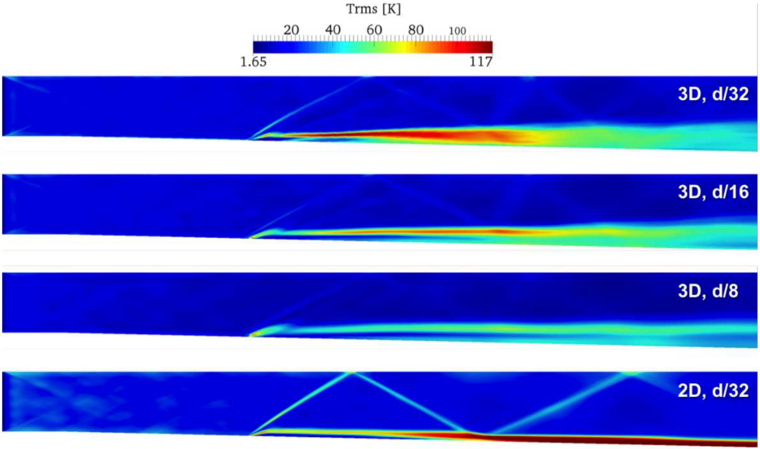
Instantaneous Temperature



Mean Temperature



RMS Temperature



Summary Completed LES Tasks

- Benchmark calculations performed to-date have served to define affordable unit cases that emulate key physics
- Insights have demonstrated tradeoffs related to resolution and geometry (P1 geometry defined and running)
- Will continue to add complexities and work toward full reacting P2 while progressively staging P1 unit cases
- Sparse quadrature simulations of P1 unit cases aimed at forward UQ baseline, dimensionality reduction, and model error in progress
- Managing the balance between computational cost and the progression of UQ tasks/needs is key to success

High Dimensionality – Parameter Space

- The number of (lumped) uncertain parameters is:
  30-50 for P1 and **60-90** for P2.
  - The number depends on which physical models are activated
    - e.g. non-reacting vs reacting, wall models, etc
- The number of modes in the representation of random fields further increases the dimensionality
  - We will employ Karhunen-Loève expansions for representation of random fields to tackle dimensionalities $\mathcal{O}(10^5 - 10^7)$ for
    - wall boundary conditions
    - model error representation
    - mesh discretization error representation
- The requisite number of runs for forward UQ renders the straightforward application of isotropic sparse quadrature techniques prohibitive for 3D LES.

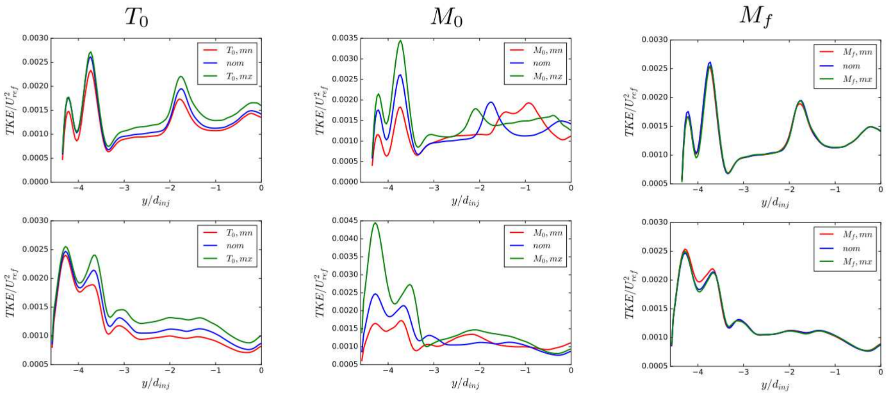
Parameter Space - Baseline UQ study for P1

Limited dimensionality study to determine the effects of select input parameters on several QoIs relevant to the Scramjet configuration.

- Employing isotropic sparse quadrature (Gauss-Kronrod-Patterson) to estimate polynomial chaos expansions (PCEs) for the selected QoIs
- Progressively increasing the number of parameters
    1. 2D, non-reacting, 1 row of fuel injectors, *6 uncertain parameters*: About **70 LES runs/70K CPU hours** for 2nd order PCE.
    2. Same setup as above, with *10 parameters*. The additional parameters pertain to the turbulence intensity and lengthscale. Computational budget: **200 runs/200K CPU hours**
    3. Same as above, adding sub-sgrid scale model parameters to the list of uncertain parameters, for a total of *14 parameters*. Computational budget: **400 runs/400K CPU hours**
    4. 3D, non-reacting, 1 row of fuel injectors. Setup TBD

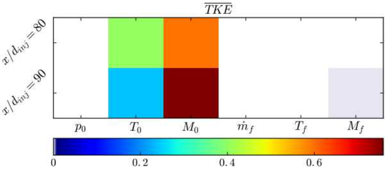
Baseline UQ study for P1 - Preliminary Results

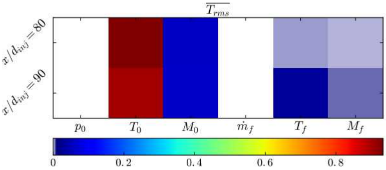
- Baseline UQ study in progress; some runs are completed
  - Illustration of influence of individual parameters: T_0, M_0, M_f below
- QoI: turbulent kinetic energy (TKE) crosswise profiles, shown below
  - at $x/d_{inj} = 80$ (top row) and $x/d_{inj} = 90$ (bottom row)



Baseline UQ study for P1 - Preliminary Results

- First order PCEs are constructed for several QoIs using a preliminary set of LES simulations
- Total order Sobol indices indicate that uncertainties in oxidizer inlet Mach number M_0, and stagnation temperature T_0, control most of the variance in the selected QoIs.
  - $\overline{TKE}$ and $\overline{T_{\text{rms}}}$
- Since the flow is non-reacting, uncertainties in fuel inflow parameters have a negligible impact on the selected QoIs.





Techniques for Dimensionality Reduction

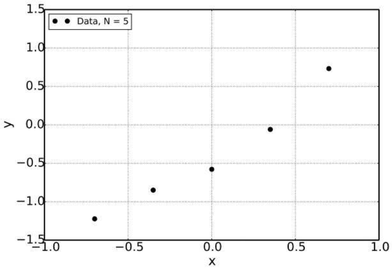
- Karhunen-Loève expansions for random fields
  - Spatio-temporal boundary conditions
  - Mesh-based quantities (subgrid params, model & mesh errors)
- Compressed Sensing (CS) to discover and fit sparse surrogates
  - Explore and compare OMP, LARS, and BCS algorithms
  - Explore algorithm enhancements that reduce overfitting
    - e.g. Inverse Scale Space mehods
- Leverage experience of collaborators
  - Basis Adaptation – with R. Ghanem, USC
  - Low-rank tensor representations – with P. Rai, SNL

Model error – Main target

Model error = deviation from 'truth', or from a higher-fidelity model

- Represent and estimate the error associated with
  - Mathematical formulation, theoretical framework
  - Assumptions, parameterizations
  - Geometric simplifications (*e.g.* 3D-vs-2D)
  - Numerical discretization – connection to Mesh Discretization Error Task
- ...will be useful for
  - Model validation, comparison and improvement
  - Reliable computational predictions: *i.e.* require
    low-fidelity model uncertain prediction to be consistent with
    high-fidelity simulations – connection to Multifidelity UQ Task
- Inverse modeling context
  - Given experimental or higher-fidelity model data,
    estimate the model error – connection to Inverse UQ Task

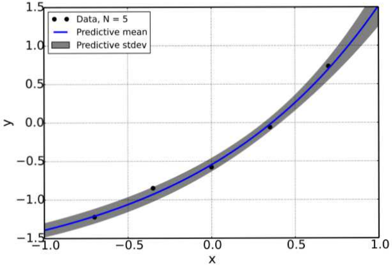
Model error – Motivation



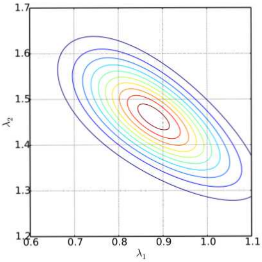
Model-data fit

- Given noisy data – Gaussian noise
- $y = g_{\text{true}}(x) + \epsilon$

Model error – Motivation



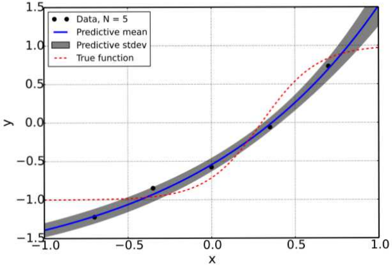
Model-data fit



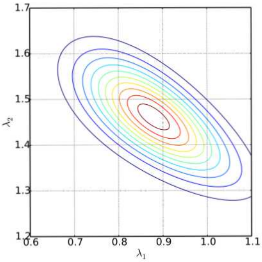
Posterior on parameters

- Employ Bayesian inference to fit an exponential model – $y_{\mathrm{m}} = f(x, \lambda)$
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\mathrm{d}}$
- Plotted:
  - Posterior density on the parameters
  - Preditive mean and standard deviation

Model error – Motivation



Model-data fit



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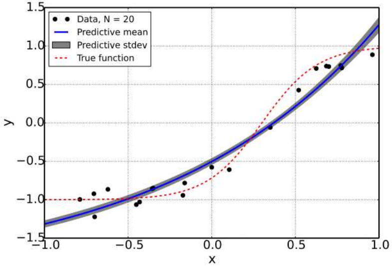
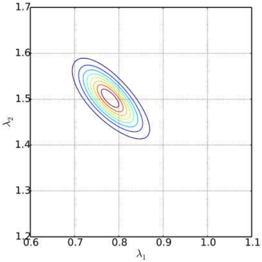
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\rm d}$
- True model $g(x)$ – dashed-red – differs from fit model $f(x, \lambda)$
- Actual discrepancy includes both data and model errors

Model error – Motivation



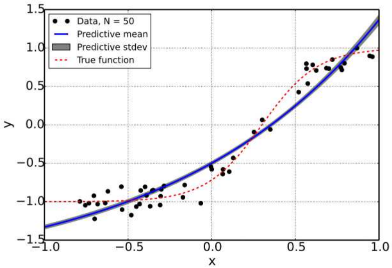
Model-data fit



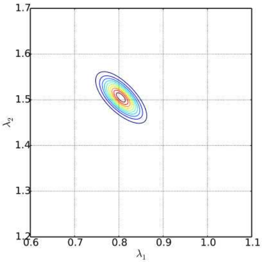
Posterior on parameters

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model

Model error – Motivation



Model-data fit



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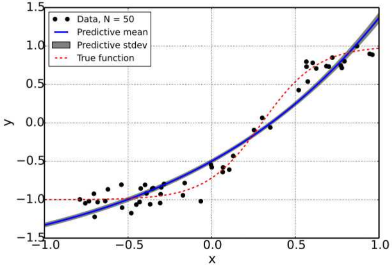
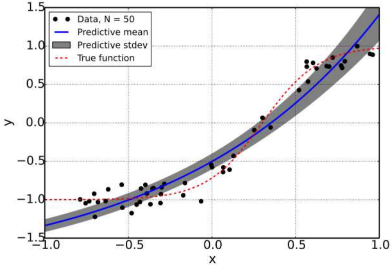
Model error – Motivation



Model-data fit



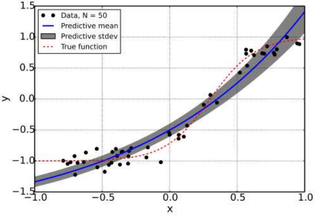
What we want

- If the model has structural uncertainty, more data leads to biased and overconfident results
- We want to quantify model-vs-truth discrepancy in a rigorous and systematic way
    - Cannot ignore model error

Model Error – Challenges with current methods

Total error budget

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{Truth } g(x_i)} + \epsilon_i$$



- Ignoring model error $\delta(x)$ leads to incorrect predictive errors
- Conventional statistical modeling (Kennedy and O'Hagan, 2001)
  - makes it difficult to disambiguate model/data errors
  - may violate physical constraints
  - not meaningful for prediction of other QoIs
- Issue is highlighted in model-to-model calibration ($\epsilon_i = 0$)
  - no a priori knowledge of the statistical structure of the discrepancy

Model Error – Key idea: probabilistic embedding

Cast input parameters λ as a random variable Λ

$$y_i = f(x_i;\lambda) + \delta(x_i) + \epsilon_i \longrightarrow y_i = f(x_i;\Lambda) + \epsilon_i$$

- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
  - turbulent model constants
- Allows placement of model error term in locations where key modeling assumptions and approximations are made
  - as a correction or high-order term
  - as a possible alternate phenomenology
- Naturally preserves model structure and physical constraints
- Disambiguates model/data errors

Model Error – Bayesian density estimation

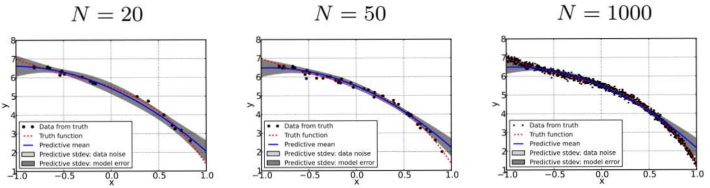
$$y_i = f(x_i; \Lambda) + \epsilon_i$$

- Parametrize embedded random variable Λ:
  - PDF form $\pi_\Lambda(\cdot; \alpha)$
  - Polynomial Chaos (PC): $\Lambda = \sum_k \alpha_k \Psi_k(\xi)$
  - Multivariate Normal (MVN): $\begin{cases} \Lambda_1 = \alpha_{10} + \alpha_{11}\xi_1 \\ \Lambda_2 = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ \quad \vdots \\ \Lambda_d = \alpha_{d0} + \alpha_{d1}\xi_1 + \alpha_{d2}\xi_2 + \cdots + \alpha_{dd}\xi_d \end{cases}$
- Inverse modeling context
  - Parameter estimation of $\lambda \Rightarrow$ PDF estimation of $\Lambda \Rightarrow$ parameter estimation of α
  - Bayesian formulation

$$\underbrace{p(\alpha|y)}_{\text{Posterior}} \propto \underbrace{L_y(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$

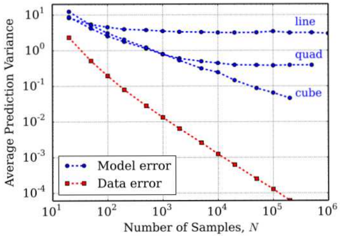
More data leads to ‘leftover’ model error

Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. ‘truth’ $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.



Summary of features:

- Well-defined model-to-model calibration
- Model-driven discrepancy correlations
- Respects physical constraints
- Disambiguates model and data errors
- Calibrated predictions of multiple QoIs



Model Error – LES subgrid static/dynamic modeling

- Problem Focus: P1 Jet in Crossflow problem – $3D$, $d/8$ grid resolution
- LES subgrid parameters (C_R, Pr_t, Sc_t)
- LES model fidelity
  - Dynamic: subgrid parameters variable in space/time
  - Static : subgrid parameters constant in space/time
- Target: Calibrate a static model against a dynamic model
  - accounting for model error
- Setup:
  - Consider dynamic model as the truth model $g(x)$
  - Fit parameters of static model $f(x, \lambda)$ w.r.t. data from dynamic model simulations
    - $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1})$
- In principle:
  - Proceed by embedding PCE for λ in static model governing equations

Model Error – Embed it in turbulent closure constants

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\overline{\tau} - \mathbf{T}) = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] - \overline{\rho}\left(\widetilde{\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}}} - \tilde{\tilde{\mathbf{u}}}\otimes\tilde{\tilde{\mathbf{u}}}\right) - \frac{1}{3}\overline{\rho} q_{\text{sfs}}^2\,\mathbf{I}$$

- Energy Flux:

$$\vec{\mathcal{Q}}_e = (\overline{\mathbf{q}}_e - \mathbf{Q}) = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr}\right)\frac{1}{Re}\nabla\tilde{h} + \sum_{i=1}^{N}\tilde{h}_i\vec{\mathcal{S}}_i - \overline{\rho}\left(\widetilde{\tilde{h}\tilde{\mathbf{u}}} - \tilde{\tilde{h}}\tilde{\tilde{\mathbf{u}}}\right)$$

- Mass Flux:

$$\vec{\mathcal{S}}_i = (\overline{\mathbf{q}}_i - \mathbf{S}_i) = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i}\right)\frac{1}{Re}\nabla\tilde{Y}_i - \overline{\rho}\left(\widetilde{\tilde{Y}_i\tilde{\mathbf{u}}} - \tilde{\tilde{Y}}_i\tilde{\tilde{\mathbf{u}}}\right)$$

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$$\begin{cases} C_R = \alpha_{10} + \alpha_{11}\xi_1 \\ Pr_t^{-1} = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ Sc_t^{-1} = \alpha_{30} + \alpha_{31}\xi_1 + \alpha_{32}\xi_2 + \alpha_{33}\xi_3 \end{cases}$$

Model Error – Embed it in turbulent closure constants

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Computational cost of LES – Use of Surrogates

Major challenge:

- Static model $f(x;\lambda)$ is still expensive
  - a single run for a fixed λ is ~ 3 hours on 480 proc
- Default strategy:
  - Embed model error a few parameters at a time, $\lambda \to \Lambda$
  - Define PCE $\Lambda = \sum_k \alpha_k \Psi_k(\xi)$ and push forward through $f(x;\Lambda)$
  - Infer PC coefficients α

  is infeasible with direct use of static model in the likelihood

Resolution:

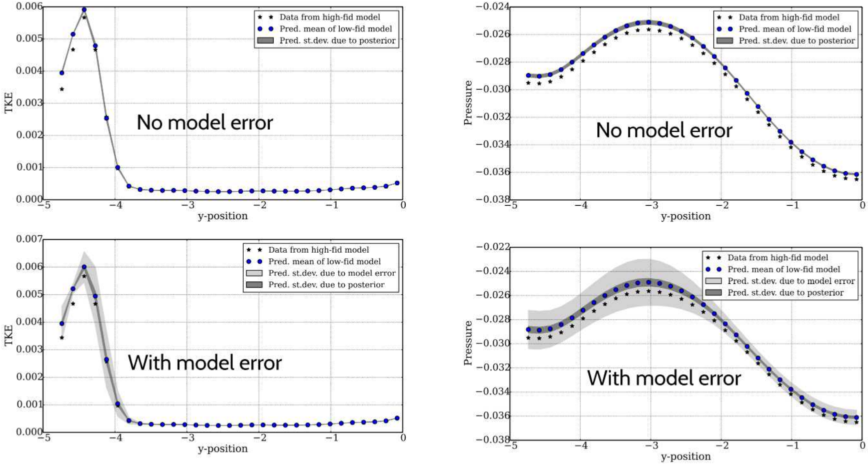
- Pre-build a 3-parameter surrogate $f_s(x;\lambda) \approx f(x;\lambda)$
  - Ranges selected from baseline computations: $C_R \in [0.005, 0.08]$, $Pr_t^{-1}, Sc_t^{-1} \in [0.25, 2.0]$
  - A total of $64 = 4^3$ runs **in progress**
- Employ $f_s(x,\Lambda)$ in the inference for α

Preliminary results – embed model err in C_R

Calibrate with TKE data, predict both TKE and Pressure

Pushed forward posterior

TKE | Pressure



Mesh Discretization Error (MDE) – Framework

Goal: Probabilistic quantification of *mesh discretization errors* (MDE) ...as manifested at the *production run resolution*

- Clear distinction with "sub-grid physics": we are *not* after modeling of subgrid scales
- At the same time, methodology should (i) apply to and (ii) link with model error representations

Approach:

- Random-field representation of MDE (dynamical forcing)
- Consider and contrast finite-difference/variational methods in uniform and variable resolution settings
- Downselect and extend to extreme-scale multiphysics simulations

Mesh Discretization Error – Approaches

Random Field (RF) approach:

- Apply a "downscaling" approach to estimate local discretization errors
- Use error estimates to infer a low-dimensional representation of stochastic source term
- Apply a sampling strategy to quantify the impact on QoIs

Variational Multiscale (VMS) Formalism:

- Provides explicit error estimator based on the convolution of a simple kernel with the residual of the mesh scale (coarse scales) equations
- Naturally links with model-error estimation, namely by incorporating model parametrization into residual
- Error estimates are represented using low-dimensional RF:
  - leads to stochastic forcing of coarse-mesh dynamics

Mesh Discretization Error – Key Steps

Consider canonical problem:

$$\frac{\partial u}{\partial t} - \alpha \Delta u = F(u)$$

where F is a non-linear (transport and/or reaction) source term
Given estimates $\epsilon(x,t)$ for MDE error on the production grid:

- *View:* $\dot{\epsilon}$ as an *approximate* source ("nudging") term in the equation
- *Challenge:* $\dot{\epsilon}$ is inherently a high-dimensional object, at least as many dofs as the solution!
- *Treat* $\dot{\epsilon}$ data as a realization of a random-field $s(x,t,\omega)$ to be inferred
- *Use a semi-intrusive strategy* to propagate uncertainty into the solution, i.e. consider a finite size ensemble of trajectories:

$$\frac{\partial u}{\partial t} - \alpha \Delta u = F(u, \Sigma) + s(x, t, \omega_i)$$

$i = 1, \ldots, N$ where N is the ensemble size

Mesh Discretization Error – Illustration

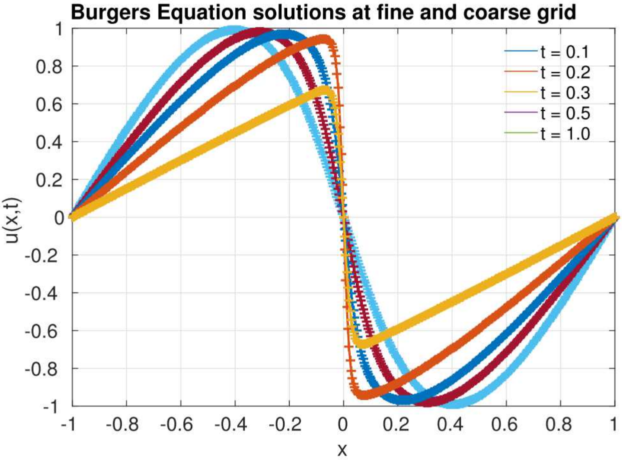
Consider Burger's equation in 1D:

$$\frac{\partial u}{\partial t} - \nu \Delta u = F(u), \qquad F(u) \equiv -u\frac{\partial u}{\partial x}$$

- on the interval $[-1, 1]$ with homogeneous Dirichlet boundary conditions
- initial condition $u(x, 0) = -\sin(\pi x)$
- Set $\nu = 0.01$ and $h = 0.008$
- Second-order time integration with $\Delta t = 10^{-4}$

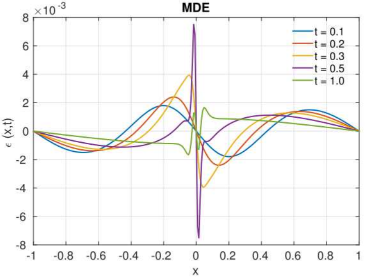
Mesh Discretization Error – Illustration

Behavior of solution

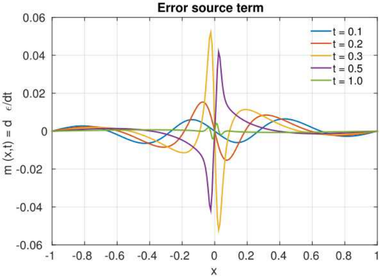


Mesh Discretization Error – Illustration

Solution error and forcing term



Solution error, estimated by downscaling the equations

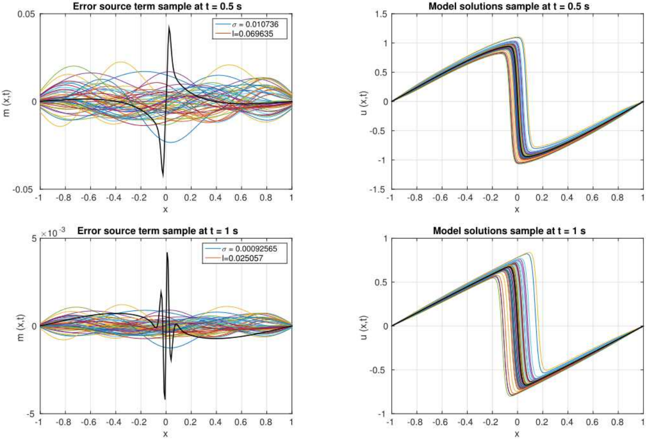


Solution estimates shown on the left are differentiated in time, to generate data for the source field

Mesh Discretization Error – Illustration

Error samples and solution ensemble:

- Matérn 3/2 covariance
- KL representation of random source term



Mesh Discretization Error – Illustration

Elliptic problem:

$$\boldsymbol{\nabla} \cdot (\kappa(\boldsymbol{x}) u(\boldsymbol{x})) = -f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \Omega = [0,1],$$

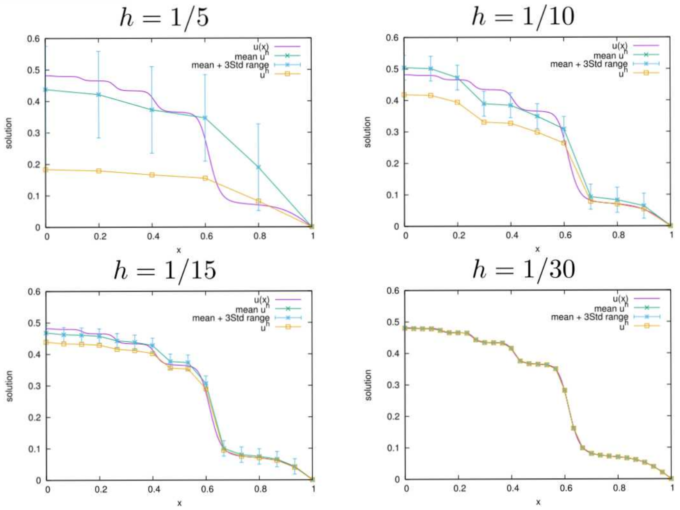
- $\log \kappa(x) = 2 \sin(10\pi(1-x)^2)$, $f(x) = 1 + 5 \exp(-(x-0.5)^2/.005)$
- Dirichlet and / or Neuman type bc
- P1 finite element solution

Gaussian Process correction:

$$F(\boldsymbol{x},\omega) = f(\boldsymbol{x}) + \delta F(\boldsymbol{x},\omega), \quad \delta F \sim \mathcal{G}(\delta f, \Sigma_f^2).$$

- δF squared-exponential Matérn covariance structure
- correlation length, variance, and hyper-parameter inferred from error estimates

Mesh Discretization Error – Illustration



- Corrected solution endowed with uncertainty reflecting its error
- Corrected solution approximates exact solution with decreasing h
  - Both mean error and uncertainty go to zero

Mesh Discretization Error – Next Steps

- Refine random source field modeling:
  - Contrast performance of Bayesian PCA and LIS approaches
  - Explore more elaborate source field models, particularly to enable enforcement of solution constraints
- Apply VMS methodology to:
  - develop local error estimates
  - extend framework to combined mesh and model error UQ
- Extend framework to canonical problems involving parametrized subgrid representations

Optimization – Challenges and Approach

Challenges:

- OUU further amplifies UQ expense
- Complex design process must effectively manage:
  - multiple simulation fidelities and UQ resolutions
  - uncertainty due to model error
  - dimensionality of both random and design domains

Approach:

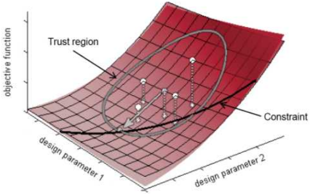
- Develop and deploy provably-convergent derivative-free optim. (DFO) framework that manages multiple levels of approximation
  - Efficient DFO algorithms provide solver foundation
  - Meta-algorithms manage model hierarchy
- ***Theory:*** Establish rigorous (local) convergence
  - Extend deterministic theory to include stochastics
- ***Scale:*** Extend DFO to higher dimensions
  - Leverage sparse surrogates (ℓ_1-regularization)
- ***Multifidelity:*** Manage multiple fidelities and UQ resolutions

Optimization – Efficient DFO with NOWPAC/SNOWPAC

No adjoints at simulation level → OUU approaches must be derivative-free or use derivatives inferred from surrogates.

Nonlinear Optimization with Path-Augmented Constraints (NOWPAC)

- TR approach for nonlinear constrained DFO
- Non-intrusive optimization framework
- New way of handling constraints using an inner boundary path
- Provable convergence to a first order local optimal design



NOWPAC framework

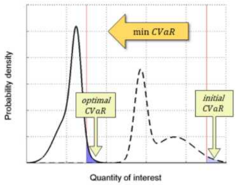
- Build fully linear surrogate models of objective and constraints
- Find improved designs by minimizing surrogate models

Optimization – Efficient DFO with NOWPAC/SNOWPAC

Optimization under uncertainty requires the quantification of risk

- Expectation optimization and variance minimization
- Risk minimization using CVaR
- Chance constraints

Example: minimize CVaR



Sample approximations of risk / deviation measures are noisy

- Only a small number of PDE simulations available
- Estimate statistical error using confidence intervals

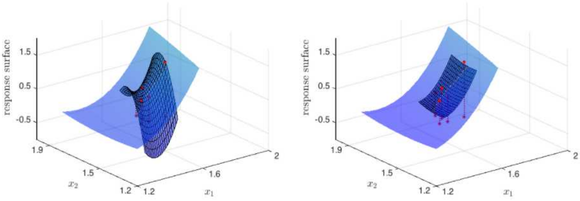
Stochastic NOWPAC

- Generalized framework to handle noise in objective and constraint evaluations

Optimization – Efficient DFO with NOWPAC/SNOWPAC

SNOWPAC framework

- Build regularized surrogate models
- Adapt trust region management to noise estimates
- Introduce Gaussian process surrogate models
    - Reduce noise in sample approximations of QoIs
    - Make efficient use of PDE simulations by exploiting information from neighboring runs



minimum-Frobenius norm models vs. regularized surrogate models

Optimization – Efficient DFO with NOWPAC/SNOWPAC

SNOWPAC framework

- Build regularized surrogate models
- Adapt trust region management to noise estimates
- Introduce Gaussian process surrogate models
  - Reduce noise in sample approximations of QoIs
  - Make efficient use of PDE simulations by exploiting information from neighboring runs

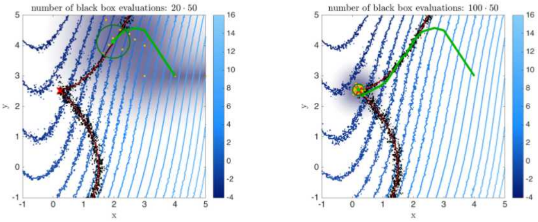
- $\mathcal{S}_{err}$: structural error in surrogate approximations
- $\mathcal{I}_{err}$: statistical estimate of the sampling noise
- Ensure $\mathcal{S}_{err} \approx \mathcal{I}_{err}$
  - Need a lower bound on trust region size dependent on $\mathcal{I}_{err}$

Optimization – Efficient DFO with NOWPAC/SNOWPAC

SNOWPAC framework

- Build regularized surrogate models
- Adapt trust region management to noise estimates
- Introduce Gaussian process surrogate models
  - Reduce noise in sample approximations of QoIs
  - Make efficient use of PDE simulations by exploiting information from *neighboring* runs

- Blend Gaussian process mean with sample estimates of QoIs



Optimization – Efficient DFO with NOWPAC/SNOWPAC

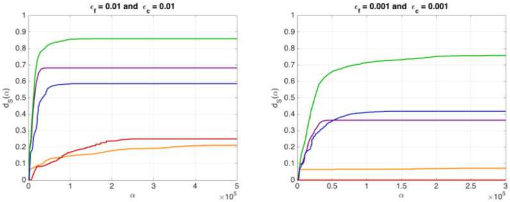
SNOWPAC benchmark performance

- Use data profile to compare performance based on 2400 optimization runs

$$d_S(\alpha) = \frac{1}{2400}\left|\left\{p \;:\; \frac{t_{p,S}}{n_p+1} \le \alpha\right\}\right|,$$

  - n_p: dimension of the design space of benchmark problem p
  - $t_{p,S}$: min number of simulations solver S needs to solve problem p
- An optimization problem is deemed "solved" if the error is below ε_f and the constraint violation is less than ε_c

Performance comparison between (S)NOWPAC (green), COBYLA (purple), NOMAD (blue), SPSA (orange) and KWSA (red).



Optimization – Meta-Algorithms for Model Management

New Dakota infrastructure available for multiple model forms, each with multiple discretization levels.

- enable algorithms that exploit special discretization structure

Nonlinear Optim. by Mesh Adaptive Direct search (NOMAD):

- Provable convergence based on pattern search theory
- Generalizing Dakota capability for multifidelity search plug-in
  - 0^{th}-order multifidelity trust-region (TR) approach provides heuristic *search* accelerator, with fallback to rigorous *poll*

First-order TR model management w/ combined stoch expansions:

TRMM with gradient-based minimizers, enabled by combined design/uncertain stochastic expansions: $R(\boldsymbol{\xi}, \boldsymbol{d}) \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}, \boldsymbol{d})$

- Expectations over ξ can be differentiated over d
- UQ is *derivative-free*; Opt is *derivative-inferred*.
- Accuracy of inferred moment derivatives managed by design TR size

Optimization – Meta-Algorithms for Model Management

Multigrid optimization (MG/Opt) exploiting discretization hierarchies:

- Specialization of TRMM exploits special structure
  - Apply multigrid V cycle to hierarchy of optim. problems
  - Line search ensures fine-grid impr. from coarse-grid step
- prototype MG/Opt now available to test DFO sub-problem optimizers (NOWPAC)

Efficient global optimization (EGO) with multifidelity GPs:

- Optimize expected impr. fn. (EIF) from GP mean & pred. variance
- Extend for hierarchical prediction variance from multifidelity
  - Simple: LF + discrepancy GP (single prediction variance)
  - Advanced: multi-GP with adaptive level refinement

Candidate approaches to be down-selected based on performance on model problems and emerging Scramjet OUU problem characteristics.

Optimization – Progress and Plans

Progress:

- DFO solvers: NOWPAC $\rightarrow$ SNOWPAC
- Model management meta-algorithms
  - Exploiting infrastructure for model forms / discretizations
  - Generalizing NOMAD for multifidelity search plug-in
  - Deploying MG/Opt prototype with DFO solvers
- OUU & model hierarchy problem definitions

Plans:

- *OUU development*
  - SNOWPAC development
  - MG/Opt with DFO, including NOWPAC
- *OUU deployment for P1*
  - Robust design with initial prototype of P1
  - Evolve towards full P1 complexity
- *OUU deployment for P2 (Phase 2)*
  - Demonstrate OUU for unions of P2 unit problems
  - Device performance optimization for HIFiRE

Closure

- The project is underway with progress on all tasks
- Demonstrated 3D liquid-jet in crossflow problem P1 at supercritical conditions $\Rightarrow$ Milestone
  - Preliminary P2 runs in progress
- Initial UQ baseline and GSA study with P1-2D
- Initial demonstration of model error estimation and propagation with P1-3D
- Initial demonstration of mesh error estimation and propagation in model problems
- Progress on tools for derivative-free stochastic optimization under uncertainty