Verification and Validation in Simulations of Complex Engineered Systems

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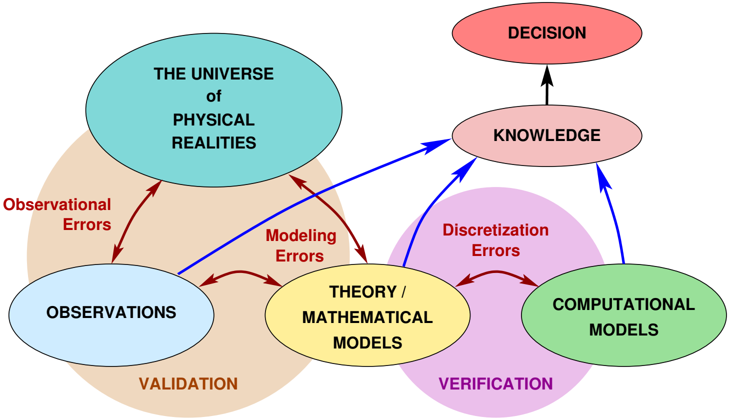
Imperfect Paths to Knowledge and Predictive Simulation



Predictive Simulation: the treatment of model and data uncertainties and their propagation through a computational model to produce predictions of **quantities of interest with quantified uncertainty**.

Quantities of Interest

Simulations have a purpose: to inform a decision-making process

- Quantities are predicted to inform the decision
- These are the Quantities of Interest (QoI's)
- Models are not (evaluated as) scientific theories

Acceptance of a model is conditional on:

- its purpose
- the QoI's to be predicted
- the required accuracy

What are Predictions?

Prediction

Purpose of predictive simulation is to predict QoI's for which measurements are **not** available (otherwise predictions not needed)

Measurements may be unavailable because:

- instruments unavailable
- scenarios of interest inaccessible
- system not yet built
- ethical or legal restrictions
- it's the future

How can we have confidence in the predictions?

Problem Statement

“A theory is something nobody believes, except the person who made it.
An experiment is something everybody believes, except the person who made it.”
[Attributed to Albert Einstein]

What are the **necessary conditions** that entitle us to make predictions and what are the **sufficient conditions** to trust those predictions?

We are concerned with developing a methodology capable to provide a **credible** and **defensible** level of confidence regarding the predictive capability of a model.

Best Estimate + Uncertainty + Confidence Level

Model Pedigree

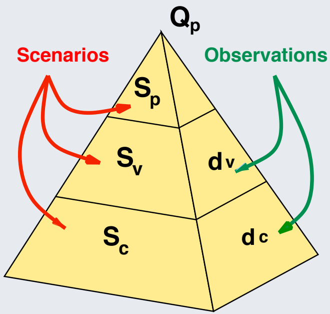
- **(M1) Pure Physics.** Models are accepted as established laws of nature by the scientific community in their domain of applicability (Eq. Newtonian and Quantum mechanics).
- **(M2) Models with Localized Model Error.** Examples are models derived from fundamental laws such as conservation of mass, but solved together with phenomenological constitutive relations which are uncertain (Eq. RANS). **This is the common case**
- **(M3) Pure Empirical.** Models in this category are data driven-models, thus their domain of applicability is solely defined by the input data (Eq. data reduction models).

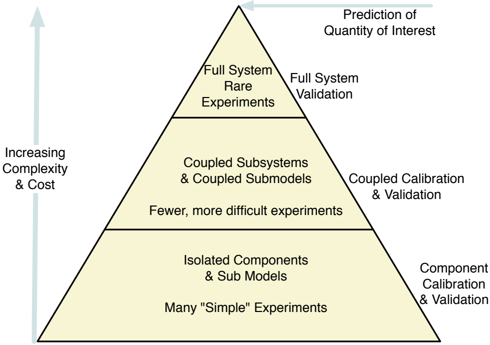
Model Error: concerned with **source**, structure

Extrapolation to new scenarios is only justified for models of type **M1** and **M2**. This is what makes **prediction** possible.

Validation for Complex Systems

Observables and Scenario Parameters





Validation is hierarchical

Processes for Confidence Building

Calibration - tuning to match observations

- Calibration within the domain of applicability
- Optimal Experimental Design
- Infer the structure of model error

Validation - challenge wrt Observable

- Comparison of observations with model predictions
- No data then No validation
- Not invalidated = Conditionally valid
- Model error still consistent with validation data

Predictive Assessment - challenge wrt QoI

- Mostly via Sensitivity Analysis
- Effect of model error on model predictive capability
- More conclusive via Accreditation Experiments

Uncertainty

Need to Treat Uncertainty in Calibration and Validation

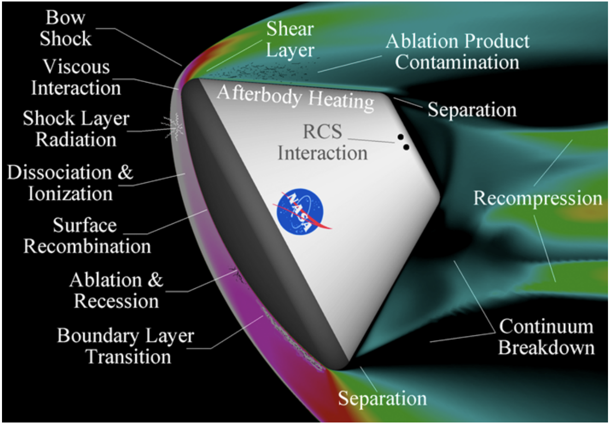
- Mathematical representation of uncertainty (Bayesian probability)
- Uncertainty models (e.g. data, model inadequacy)
- Probabilistic calibration & validation processes (Bayesian inference)

Uncertainty considerations can inform modeling

- How does the data inform the models?
- What new/better data are needed?
- What are the nature & consequences of model inadequacies?

Atmospheric Reentry

- RV problems present physical modeling challenges at multiple scales
- Models involve numerous uncertain parameters
- Models are not always reliable (e.g. turbulence)



Predictive Simulation Target (QoI's)

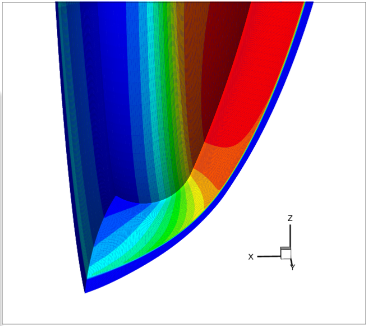
We will simulate

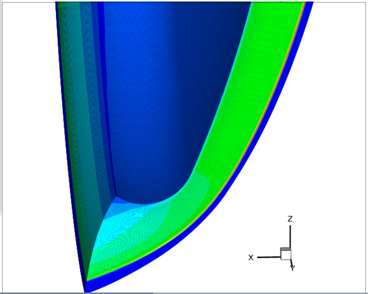
- Earth reentry vehicle with ablative TPS
- ISS and Lunar return trajectories
- The thermal environment
  - Radiative
  - Convective
  - Chemical
- The (peak) heat loads on the vehicle (QoI)
- The (peak) consumption of ablative TPS (QoI)
- During the peak heating regime

Forward Uncertainty Propagation

Calibrated Input Parameter PDF $\rightarrow$ Output QoI Statistics

Uncertain Parameters





Submodel Uncertainties

- Hypersonic Flow
  - Chemical reaction rates
  - Diffusive flux model coefficients
  - Turbulent mixing augmentation
- Radiation
  - Absorptivity/Model Error
- Ablation
  - Virgin, char densities
  - Reaction rate, equilibrium constants

~ 300 independent parameters

Challenges

Uncertainty Quantification

- High individual forward solve cost
- High parameter count

Verification

- Code complexity
- Lacking analytical solutions to complex physics
- Sole interest: Quantity of Interest functionals

Validation

- Validation processes are cyclical
  - Modeling informs research informs modeling
  - FSS results inform model development, data collection

Code verification

To create a suite of representative test problems that are simple and whose solutions are (partially) known.

Methodology:

- Problems for which special features of the solution are known
- Problems with manufactured solutions
- Problems with known rates of convergence
- Benchmark problems

Example: Method of Manufactured Solutions

- Assume form of solution (guess)
- Non-trivial to solve by hand - use symbolic manipulation software packages (Maple)
- This method can be extended to complex systems of equations (Navier-Stokes w/ chemistry)

Manufactured Analytical Solutions Abstraction Library

Features

- Provides standardized interface for all MMS across the center
- C++, C, Fortran90 bindings
- Supports gnu, Intel, portland group compilers
- Meet or exceed all PECOS software standards
- Released under LGPL 2.1: red.ices.utexas.edu/projects/software
- Performance is not principle consideration

Equations	Dimensions	Coordinate System
Euler (+ chemistry)	1,2,3	Axisymmetric, Cartesian
Navier-Stokes (+ ablation)	1,2,3	Axisymmetric, Cartesian
Heat	1,2,3	Cartesian
Sod Shock Tube	1	Cartesian
RANS: SA (+ wall)	1	Cartesian

Solution Verification

Estimate numerical errors

- Consider $u = u^h$ to be a numerical approximation to u
- Estimate error in the QoI $\mathcal{E} = Q(u) - Q(u^h) \approx \mathcal{R}(u^h; p)$
- Is error in QoI within acceptable tolerance?

Goal-Oriented Adaptive Refinement

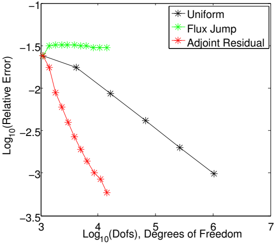
Goal: Construct a sequence of numerical representations to systematically reduce the error in the QoI

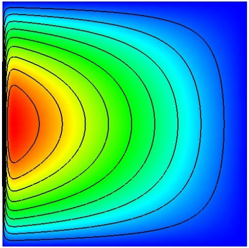
- The adjoint solution p indicates where the QoI is sensitive to numerical errors
- Use to drive adaptive refinement to reduce errors in the QoI

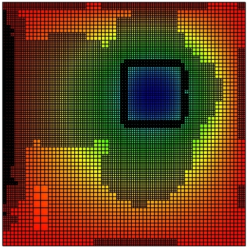
Example: Goal-Oriented Refinement

Adaptive Discretization

- Estimate error on each cell
  - Patch recovery on forward solution
- Estimate each cell error contribution to QoI
  - Patch recovery on adjoint solution
- Refine highest contribution cells first



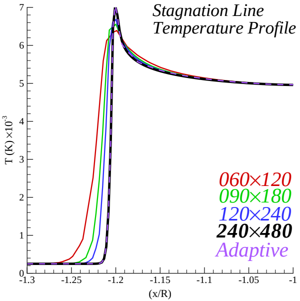


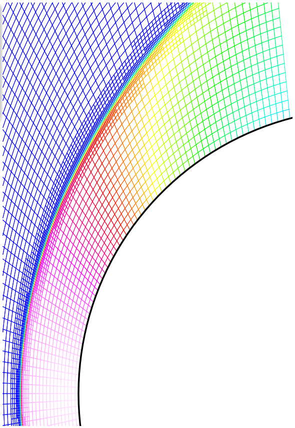


Example: FIN-S and Adaptivity

Solution verification in libMesh

- Uniform, adaptive mesh refinement
- Adjoint-based error estimation





Example: 4.75 km/sec inviscid 5-species air flow around a cylinder
Fine grid: 116K nodes AMR grid: 13K nodes

Calibration and Validation

Process of Predictive Simulation

- Identify QoI's: reflects the purpose of the simulations
- Calibration: models and error models are informed by observations
- Validation: models and error models are challenged by observations
- Predictive Assessment: assess ability of models to predict QoI's

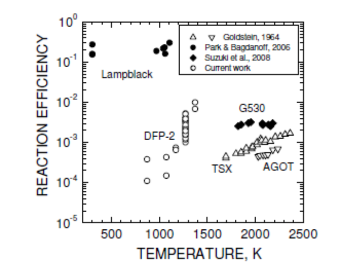
Expectations of data

- Properly calibrated data reduction model (calibration should be interpolative, not predictive!)
- **Validated data reduction model for scenarios of interest**
- Uncertainty information on output quantities

Example: Surface/Wall Catalysis

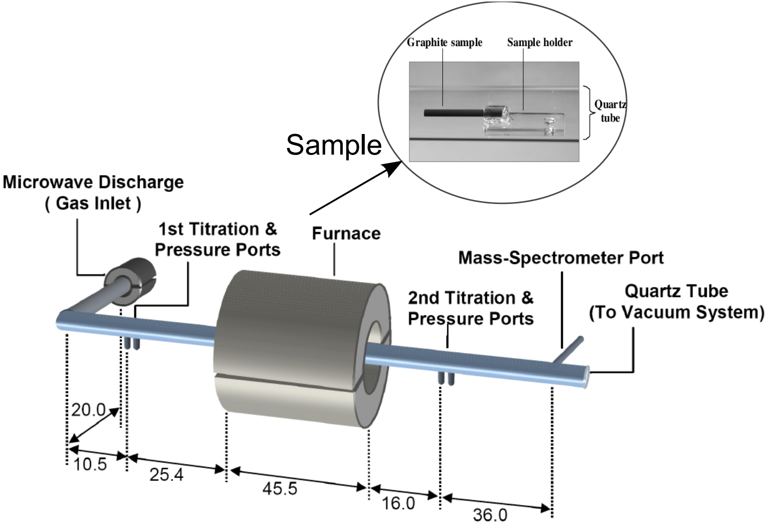
Motivation

- Surface/wall catalysis plays a critical role in surface heat flux on a re-entry vehicle
- Reported estimates of surface reaction efficiency vary by few orders of magnitude[1] (often supercatalytic wall is assumed[2])



[1] Zhang et. al. AIAA-2009-4251
[2] Wright et. al. AIAA-2004-2455

Experimental Setup[1]



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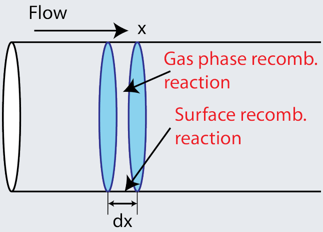
Plug Flow Reactor Model (1D) – PFRM



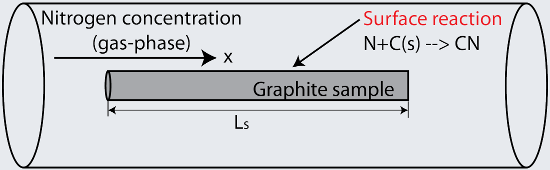
$$d(vC_N)/dx = -\bar{\gamma}_N \bar{v}_N^{th} C_N / d_{eff} - 2k_{NN} C_N^2 C_{N_2}$$

Two recombination mechanisms:

- Recombination at tube surface: $\bar{\gamma}_N = \gamma_N T^{n_N}$
- Recombination in gas-phase: $k_{NN} = A_{NN} e^{(-E^a_{NN}/(RT))}$

where, C_j is concentration of species j with no radial gradients, v is bulk flow velocity, and d_{eff} is effective diameter

Carbon Mass Loss



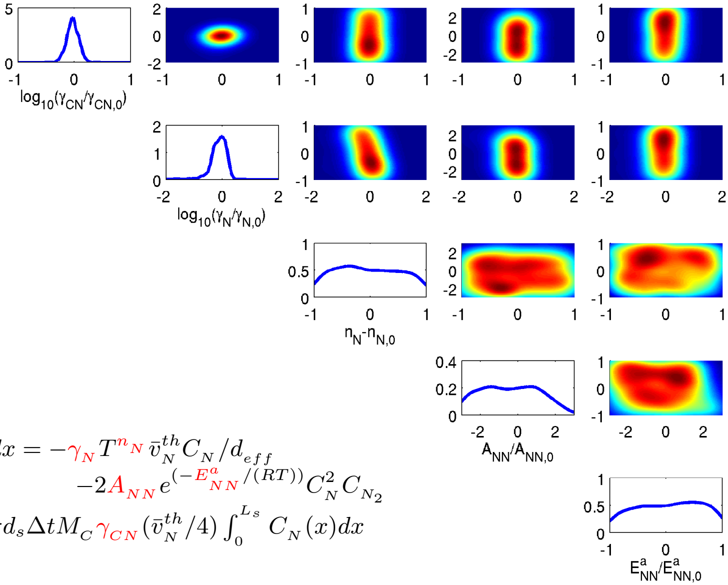
$$\Delta m_C = \pi d_s \Delta t M_C \int_{L_s} R_s(x)dx$$

Gas-surface mechanism:

- Reaction flux: $R_s(x) = \gamma_{CN} \bar{v}_N^{th} C_N(x)/4$

where, gas-surface interaction is based on a simplified flux model in which we assume $C_{N,w_s}(x) = C_N(x)$ and $k_{eq}(T)$ to be large

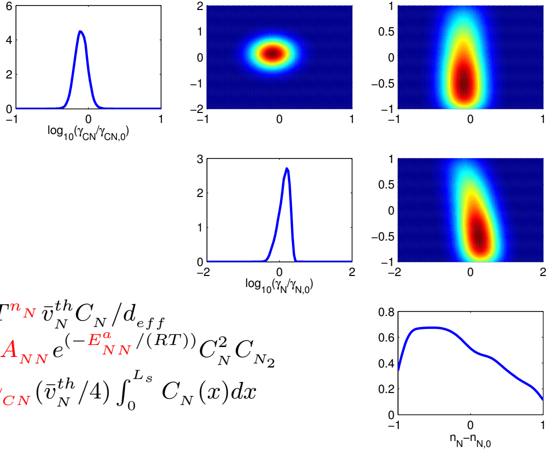
Synthetic Data : Joint PDFs of Parameters



$$d(vC_N)/dx = -\gamma_N T^{n_N} \bar{v}_N^{th} C_N / d_{eff}$$
$$-2A_{NN} e^{(-E^a_{NN}/(RT))} C_N^2 C_{N_2}$$
$$\Delta m_C = \pi d_s \Delta t M_C \gamma_{CN} (\bar{v}_N^{th}/4) \int_0^{L_s} C_N(x) dx$$

Observed Data (35 runs) : Joint PDFs of Parameters

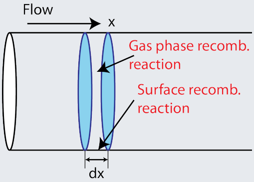
- A model ignoring inadequacy ($d_{\Delta m} = \epsilon \, y_{\Delta m}$) has null plausibility
- Up to 1 million samples in the last level

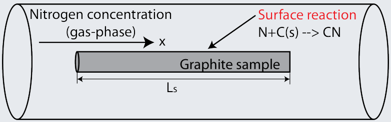


$$d(vC_N)/dx = -\gamma_N T^{n_N} \bar{v}_N^{th} C_N / d_{eff} - 2A_{NN} e^{(-E^a_{NN}/(RT))} C_N^2 C_{N_2}$$

$$\Delta m_C = \pi d_s \Delta t M_C \gamma_{CN} (\bar{v}_N^{th}/4) \int_0^{L_s} C_N(x) dx$$

A Look Back at Modeling Assumptions





Assumptions:

- *no radial gradients in species concentration:* $C_N(x)$
- *bulk flow velocity:* $v(x)$
- *effective diameter:* d_{eff}
- *concentration at sample surface is same as bulk:* $C_{N,w_s}(x)$

GRINS: General Reacting Incompressible Navier-Stokes

Plan

- Develop GRINS code on top of libMesh to perform modeling and analysis of laminar, non-isothermal, low Mach number, reacting flows
- Support general problem cases: axisymmetric, two-dimensional or fully three-dimensional
- Use GRINS code for joint calibration of model parameters as well as for optimal design of experiments (jointly with J. Marschall; for both nitridation and oxidation)

Example: Spalart-Allmaras (SA) Model Calibration

Why start with SA?

- Widely used in aerospace applications
- Relatively easy to implement and robust
- Roy and Blottner [2001, 2003] find reasonable performance for hypersonic boundary layers

SA implemented in FIN-S for FSS and implementation verified via MASA

Mach number

Kinematic eddy viscosity

Calibration Data

Experiment

Data in supersonic TBL experimental literature found insufficient

- Requirements for calibration data very difficult to satisfy
  - Fully characterized BCs
  - Systematic and quantitative uncertainty analysis
- Often data only available in outer layer
  - Leads to pathological behavior in calibrated parameters (e.g., $\kappa < 0.3$)
- Novel PIV technique under development (Sharma and Clemens) intended to enable resolved velocity measurements down to $y^+ \approx 22$

Direct Numerical Simulation

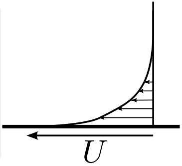
Currently pursuing DNS as primary calibration data source

- Obtain data arbitrarily close to wall
- Simulation complicated by streamwise inhomogeneity
- Develop “slow growth” approach to avoid this complication

Temporal Slow Growth Formulation

Motivating flow: Rayleigh Problem

- At $t = 0$, impulsively start infinite plate with velocity U
- Homogeneous in streamwise direction but not stationary



Slow temporal development

- Define two time variables: $t_f = t$, $t_s = \epsilon t$ where $\epsilon \ll 1$
- Assume mean and RMS depend only on slow time variable
- Navier-Stokes equations become

$$\frac{\partial U}{\partial t_f} + \epsilon \frac{\partial U}{\partial t_s} + N(U) = 0$$

- Idea: Simulate at single point in slow time
- Procedure: Use similarity assumption to develop model for slow time development

DNS Mean Flow Results

Case scenarios very loosely based on CEV BL conditions for ISS return

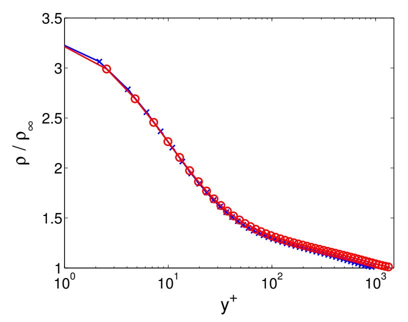
Case 1

- $M_\infty \approx 0.925$, $T_w/T_\infty \approx 0.285$,
- $Re_{\delta^*} \approx 262$, $Re_\tau \approx 916$

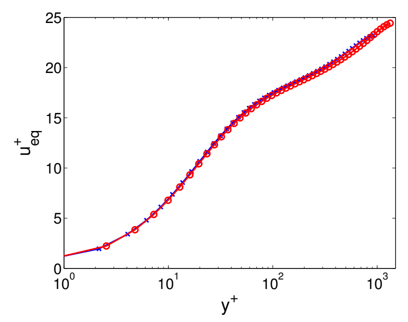
Case 2

- $M_\infty \approx 1.17$, $T_w/T_\infty \approx 0.285$,
- $Re_{\delta^*} \approx 501$, $Re_\tau \approx 1330$

Density



Van Driest Velocity



Uncertainty Models

Model Uncertainty

$$\rho_{\text{true}} = (1+\epsilon_\rho)\rho_{\text{rans}}; \quad \rho u_{\text{true}} = (1+\epsilon_{\rho u})\rho u_{\text{rans}}$$

Two zero-mean Gaussian stochastic models for ϵ_ρ and $\epsilon_{\rho u}$

- Independent at observation points: $\epsilon_\rho \sim N(0, \sigma_\rho^2 \delta(y-y'))$
- Correlated with two-length structure: $\epsilon_\rho \sim N(0, k(y,y'))$ where

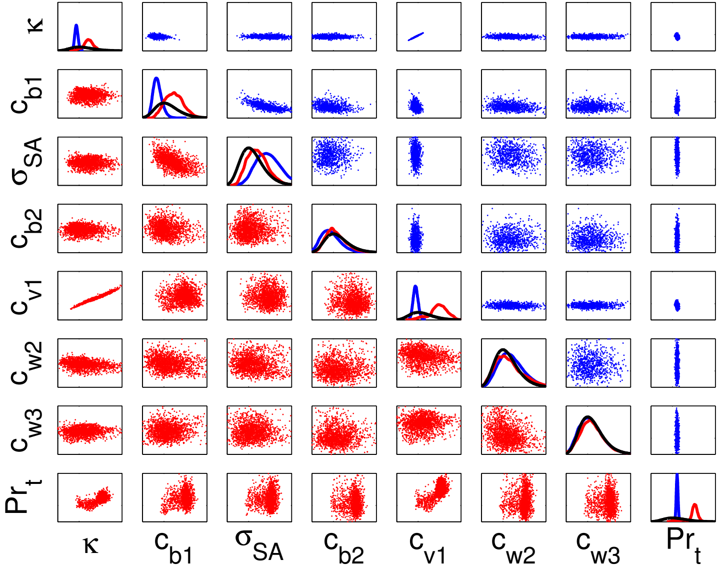
$$k(y,y') = \sigma_\rho^2 \left(\frac{2\ell(y)\ell(y')}{\ell^2(y)+\ell^2(y')} \right)^{1/2} \exp\left[\frac{-(y-y')^2}{\ell^2(y)+\ell^2(y')} \right]$$

Data Uncertainty

- Now: Assume Gaussian with σ of 0.1% of reported value
- Soon: Estimate uncertainty in DNS sample statistics

Model uncertainty + Data uncertainty $\Rightarrow$ Likelihood function

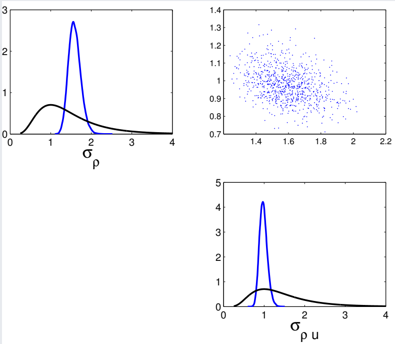
Physical Parameter PDFs



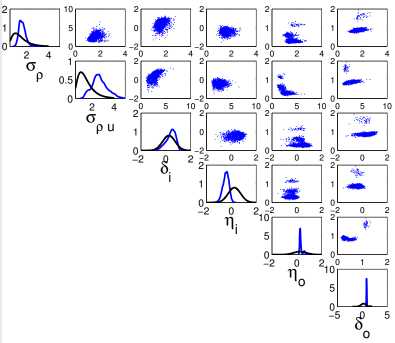
Blue = Independent model uncertainty; Red = Correlated model uncertainty

Uncertainty Parameter PDFs

Independent



Correlated



Correlated model sees more uncertainty, particularly in ρu

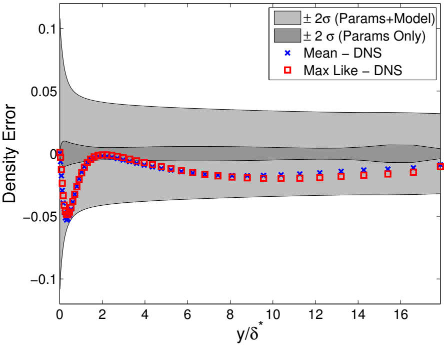
Model Comparison Results

	SAB+IND	SAB+COR	SAC+IND	SAC+COR
$\log p(D\|M_j)$	558.6	982.5	557.6	982.0
$P(M_j\|D,\mathcal{M})$	≈ 0	0.61	≈ 0	0.39

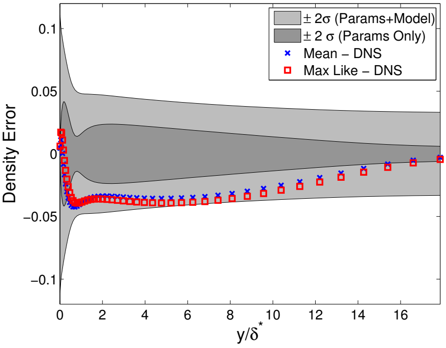
SAB = Spalart-Allmaras; SAC = SA with Catris-Aupoix correction
IND = Independent model uncertainty; COR = Correlated model uncertainty

- Catris-Aupoix correction makes virtually no difference
- Independent uncertainty model highly implausible relative to correlated
  - Parameter uncertainty + white noise does not explain the data
- Correlated uncertainty model best of this set

Density Calibration Data Comparison



Independent

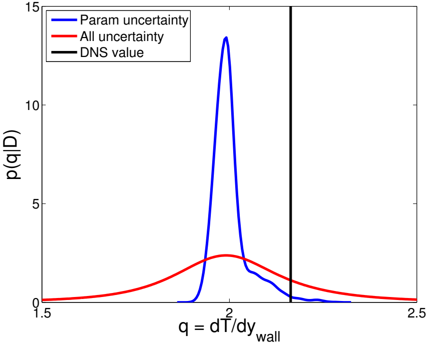


Correlated

- Parameter uncertainty **does not capture** data
- Must propagate model uncertainty

QoI Results

- QoI $= \frac{\partial T}{\partial y}\Big|_{wall}$ at $M_\infty = 0.925$
- Only correlated uncertainty model
  - Represents data better
  - Cannot propagate model uncertainty to this QoI for independent model



- DNS value in tail of PDF given by parameter uncertainty only
- Model uncertainty critical again
- Model uncertainty possibly overestimated here... multiplicative uncertainty model for density breaking down near the wall?

Recall: Full System Simulation

We will simulate

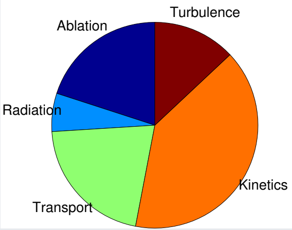
- Earth reentry vehicle with ablative TPS
- ISS and Lunar return trajectories
- The thermal environment
  - Radiative
  - Convective
  - Chemical
- The heat loads on the vehicle
- The consumption of ablative TPS
- During the peak heating regime

Forward Uncertainty Propagation

Calibrated Input Parameter PDF $\rightarrow$ Output QoI Statistics

Sensitivity Analysis from Calibrated Component Physics

Physics: Calibrated Sensitivity Results

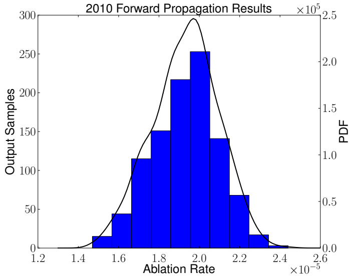


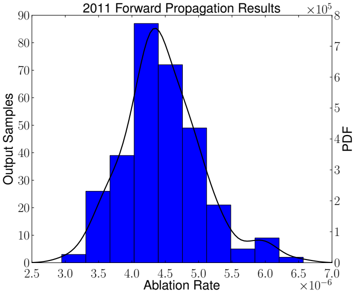
- Kinetics parameter uncertainty largest
  - Need data on carbon reactions
- Confirmed nitridation insensitivity
- Turbulence model parameter uncertainty less important than model uncertainty

Algorithms

- Monte Carlo sampling is expensive
- Push development of adjoint-enhanced sensitivity methods

Calibrated Forward Propagation Results





UQ Output

- Much lower mean ablation mass loss than with uncalibrated submodels
  - 2010 peak: $\approx 1.97 \times 10^{-5}$
  - 2011 peak: $\approx 4.37 \times 10^{-6}$
- Primary driver: $100\times$ lower nitridation coefficient than initial prior
- New nitridation sensitivity: negligible

Discussion

What is **necessary** to entitle making predictions

- Reliable physics models, possibly with embedded less reliable models, used in domain of applicability
- Less reliable embedded models & modeling assumptions identified:
  - augmented with model inadequacy models & formulated to use in prediction
  - uncertainty estimates for model parameters (due to calibration)
  - calibrated with data from scenarios relevant to the prediction
- Models with all uncertainty models consistent with all available data

What is sufficient for **confidence** in predictions

- Errors to which the QoI's are sensitive have been modeled
- All model assumptions and empirical sub-models (including uncertainty models) challenged in scenarios relevant to prediction

Lessons Learned

- MMS quickly become intractable for multiphysics problems
  - MASA software infrastructure helps
  - Divide and conquer strategies
- Data reduction modeling (DRM) is critical but very difficult
  - Build close relationships with experimentalists
  - Work with them to improve DRM
- Model inadequacy models needed, but not well developed
  - Construct to respect what is known about the models – this is a further physical modeling challenge
- Inadequacy models lead to stochastic models (e.g. stochastic PDE's)
  - Need new Bayesian inference algorithms to avoid nested sampling
- Model comparison, model evidence and information theory are critical "validation" tools

Thank you!

Questions?