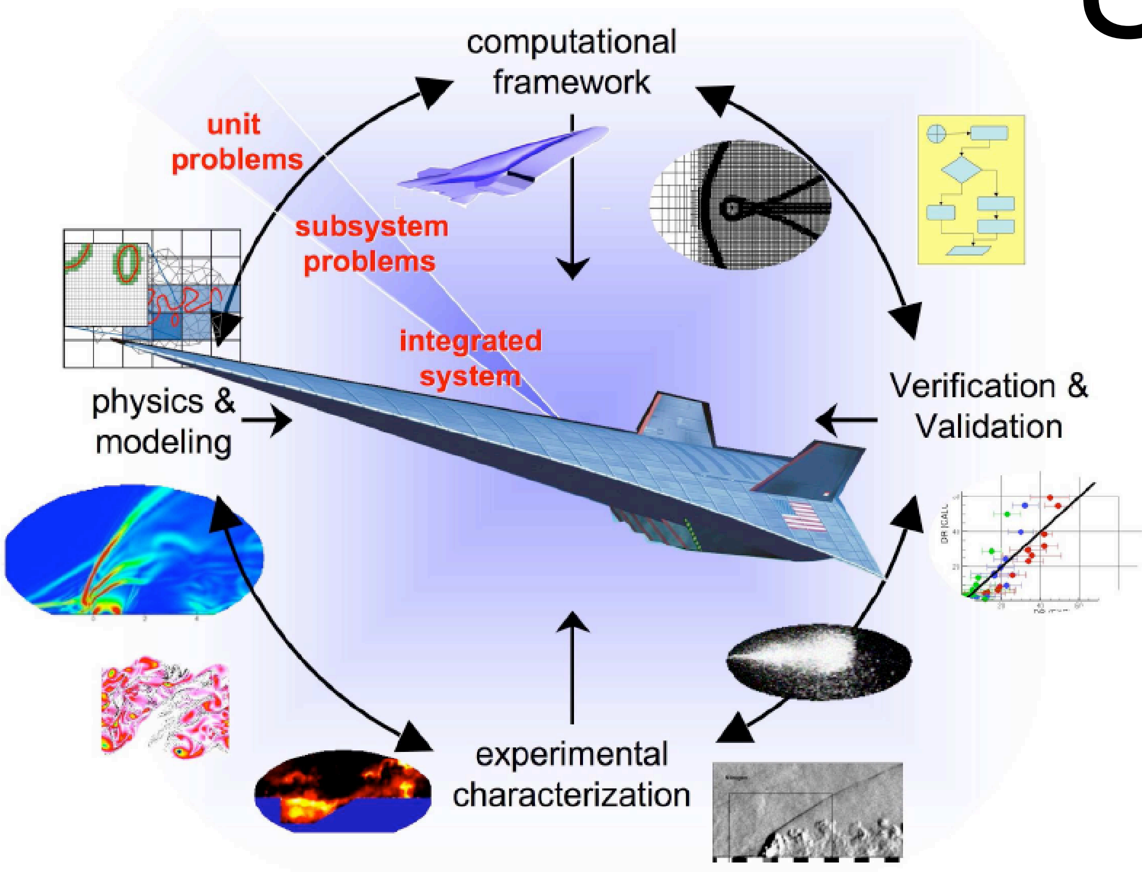
Stanford's UQ Plan



PSAAP KickOff Meeting - July 8-9, 2005

UQ Challenges - a roadmap

Challenges are common to all large-scale engineering applications

Very expensive solution evaluations

Very complex and extensive application codes

Very large number of uncertain parameters

Non-smooth system response (discrete events)

UQ Challenges - a roadmap

Challenges are common to all large-scale engineering applications

Very expensive solution evaluations

- Naive MC is infeasible] Use ROMs and LAPS

Very complex and extensive application codes

- Intrusive methods are not attractive] Non-intrusive colocation, hybrid methods

Very large number of uncertain parameters

- Curse of dimensionality] Parameter downselect using adjoints] Approximations in high-dimensions (ALS)

Non-smooth system response (discrete events)

- Difficult to interpolate] Use Pade-type global approximation

Subsystem/Unit Level UQ

Use a suite of UQ methodologies for uncertainty propagation

- Tailor/Optimize them to the specific component to be analyzed
- Example: isolator/inlet shock dynamics under uncertainty
  - Discontinuous system response
  - PDFs of shock location known to be very challenging to compute
  - We developed a Pade/Legendre-based stochastic colocation approach
  - Considerably more accurate that conventional methods for large uncertainty
  - Plan to collaborate with experimentalists to assess prediction quality

Clear distinction between aleatory and epstemic uncertainty

- Use data assimilation techniques to describe distributions driven *only* by data
- Represent both within the same context, e. g. using PCE

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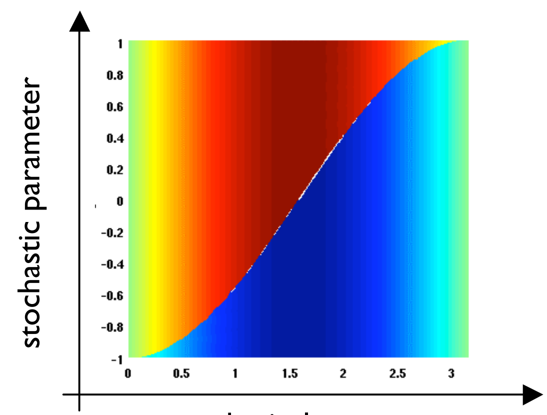
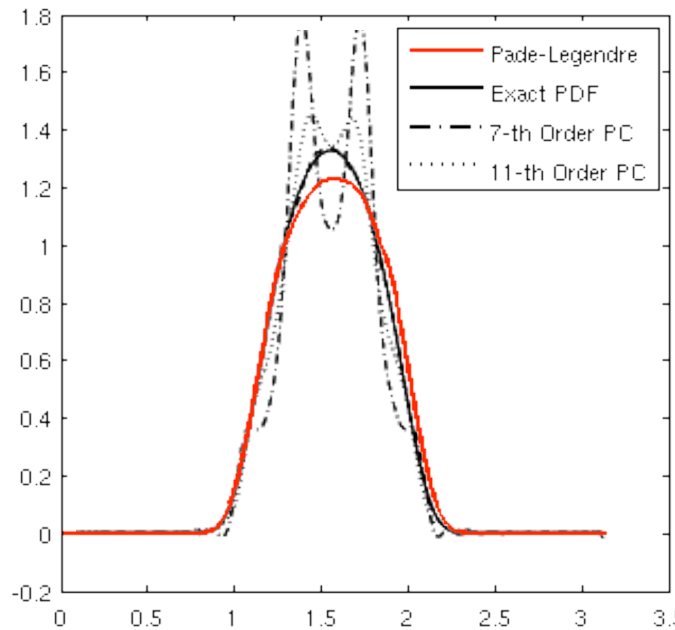
1. Ghanem, R., & Doostan, A. "On the construction and analysis of stochastic models: characterization and propagation of the errors associated with limited data. J. Comp. Phys. Vol. 217, 2006.
2. Chantrasmi, T., Doostan, A., Iaccarino, G. "Analysis of stochastic systems in the presence of discontinuities", 9th USCCM, 2007.

PDF of Shock Location

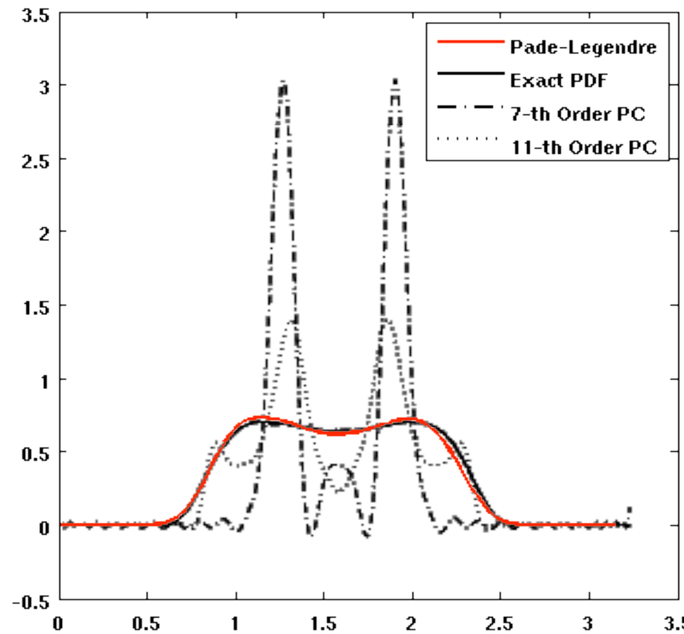
Simplified problem: Burgers equations with random forcing - exact solution with discontinuity in both physical and stochastic dimension

Present Pade-Legendre is a non-intrusive method.





"small" uncertainty



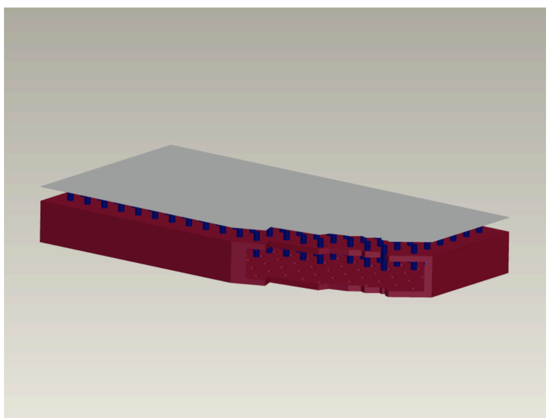
"large" uncertainty

1. Chen, Q. Y., Gottlieb, D., Hesthaven, J. S. "Uncertainty Analysis for Steady-State Inviscid Burgers Equation". JCP Vol. 204, 2005.
2. Chantrasmi, T., Doostan, A., Iaccarino, G. "Analysis of stochastic systems in the presence of discontinuities", 9th USCCM, 2007

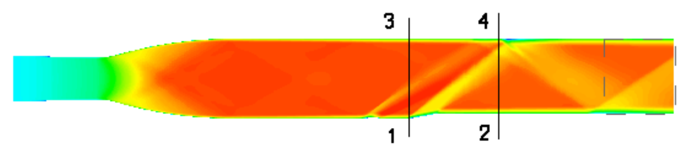
Experimental support for UQ

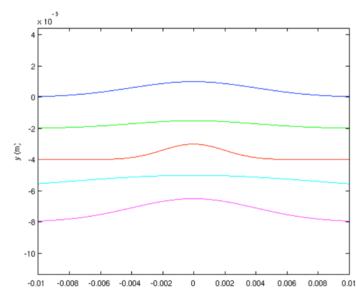
Tight coupling between experiments and computations - from the experiment design phase…

Prof. Eaton's Shock/Boundary layer interaction test will include features to accurately control the inflow turbulence and boundary geometry (Physical Monte Carlo)



Individually adjustable pins for surface geometry perturbation





Geometry perturbations
Are designed using CFD

Objective is to validate single-realization as well as distributions

System Level UQ

The plan is to develop two independent UQ approaches

ROM-based UQ

- Simulate full system with reduced complexity in each component
- Reduced models of component coupling
- Calibration via higher-fidelity subsystem models
- Simple and inexpensive to compute
- Comprehensive exploration of the input parameter space possible
- Identification of system-level failure modes, QMU

LAPS-based UQ (Likelihood Averaging in Probability Space)

- Formulated on the basis of expansion of the solution in mean and fluctuations
- Requires closure models calibrated in unit/subsystem test
- Built on top of the high-fidelity computational model
- Only used selectively in parameter space
- Provide insights in the physics behind failure modes

Combined ROM and LAPS

Total analysis error = physical space errors + probability space errors

ROM-based UQ : small probability-space errors

- Accurate identification of the cliffs in probability space
- Provide information for improving the closure models in LAPS

LAPS-based UQ : small physical-space errors

- Improve the accuracy of the physics reduction in ROMs

ROM-based UQ

LAPS-based UQ

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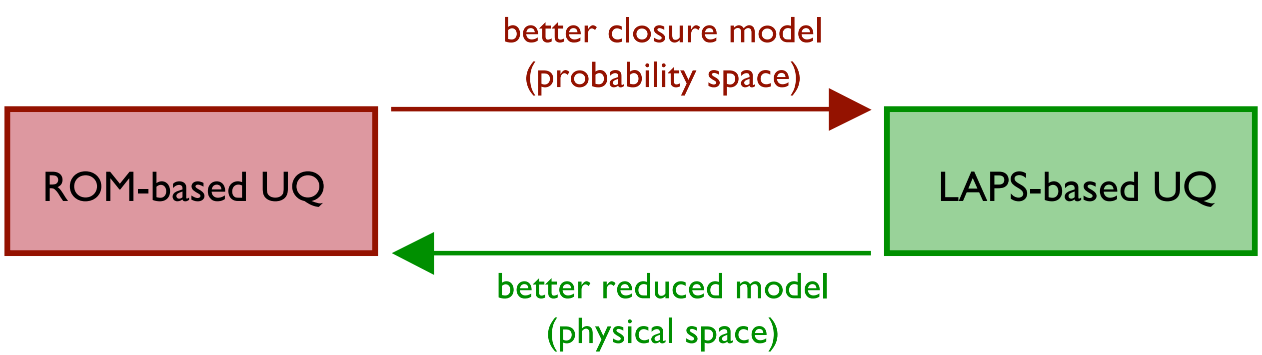
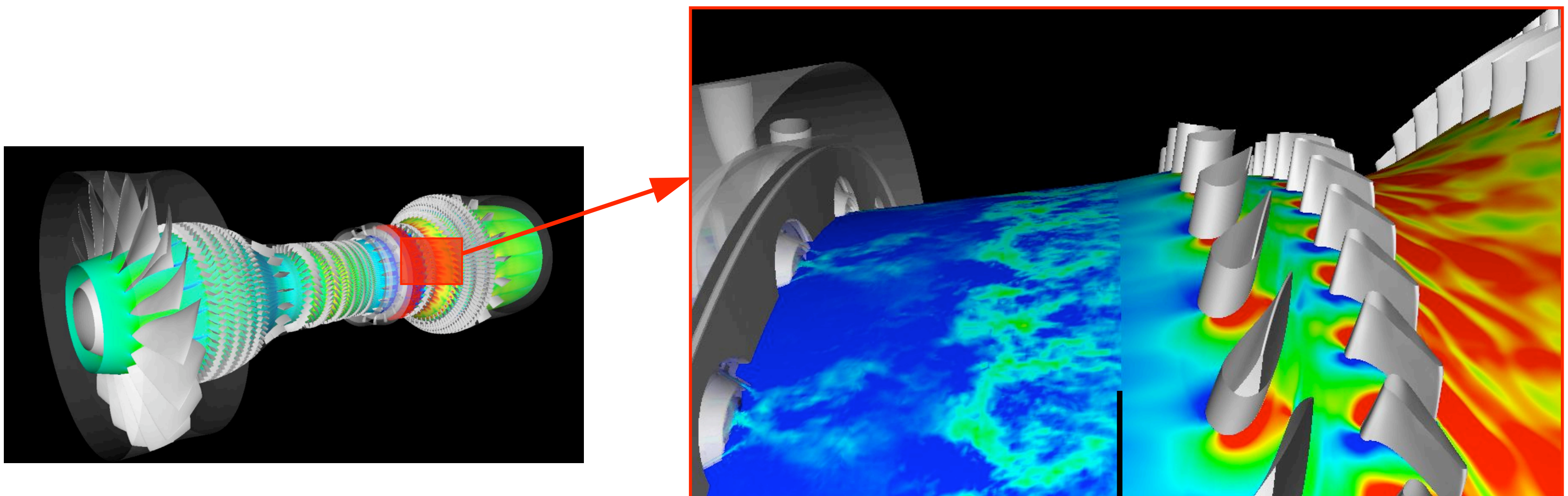


Successive use of ROMs and LAPS is a path towards “converged” high-fidelity predictions

Hybrid UQ in Multiphysics Problems

- Complex simulations place conflicting demands on numerical methods
- Hybrid methods attempt to address this conflict:
  - Apply the “best” method to each aspect of the problem, and
  - Communicate between methods such that the overall simulation is stable, accurate, convergent
- Within the ASC program at Stanford we have developed a stable framework to couple tools

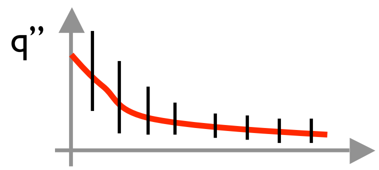


“Broad-spectrum” representation (LES)

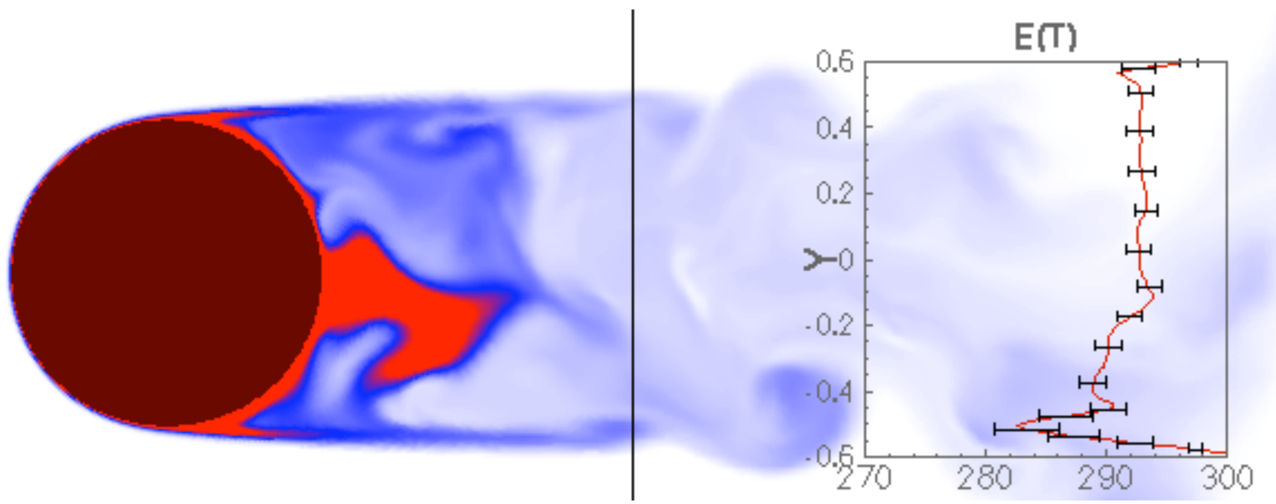
Reduced statistical representation (RANS)

Hybrid UQ in Multiphysics Problems

- Can we take the same approach for UQ?
  - Objective: build a UQ coupling framework.
  - Use best method for subsystems - MC or PCE could be doable and effective at small scale
  - Derive formal coupling procedures to combine different stochastic representations at interfaces
  - Initial results for loosely coupled problems are encouraging.



LES of turbulent flow and heat transfer around a bluff body subject to uncertain heat loading



1. Constantine P. et al, "A Hybrid Uncertainty Propagation Scheme for Convective Heat Transfer Problems", AIAA 2008-1723.

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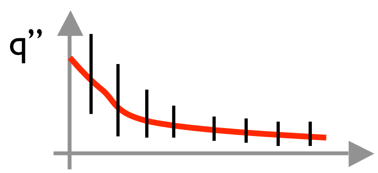

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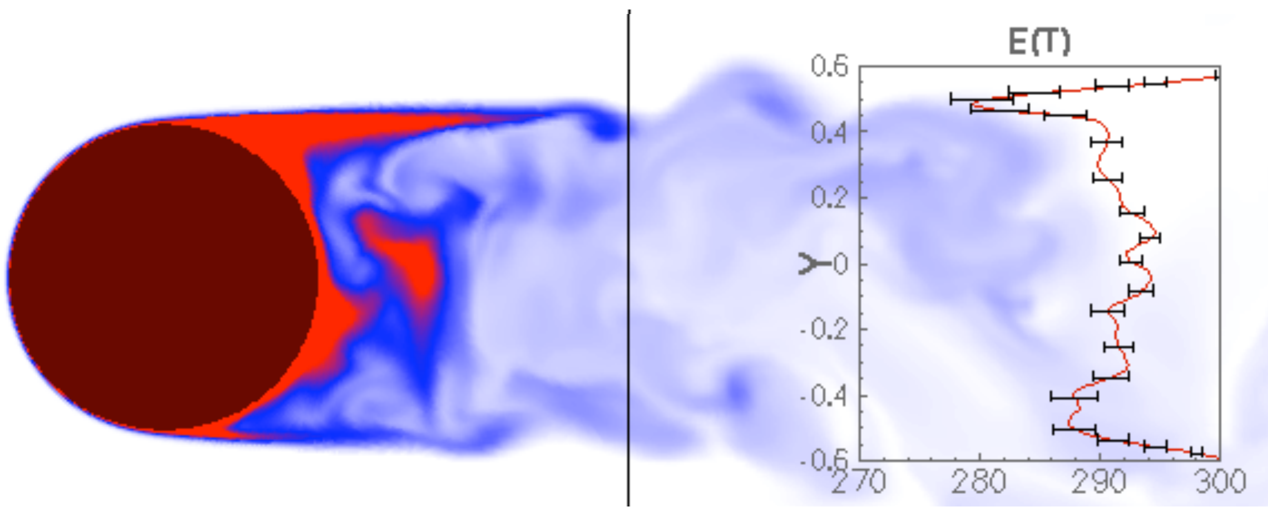

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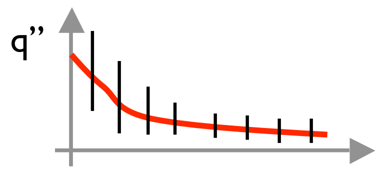

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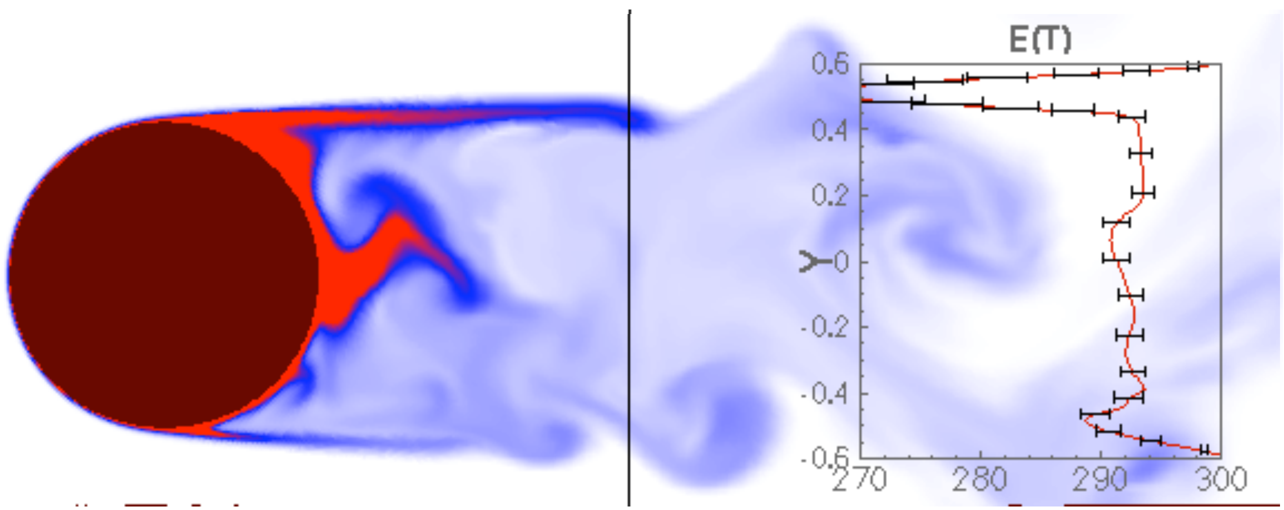

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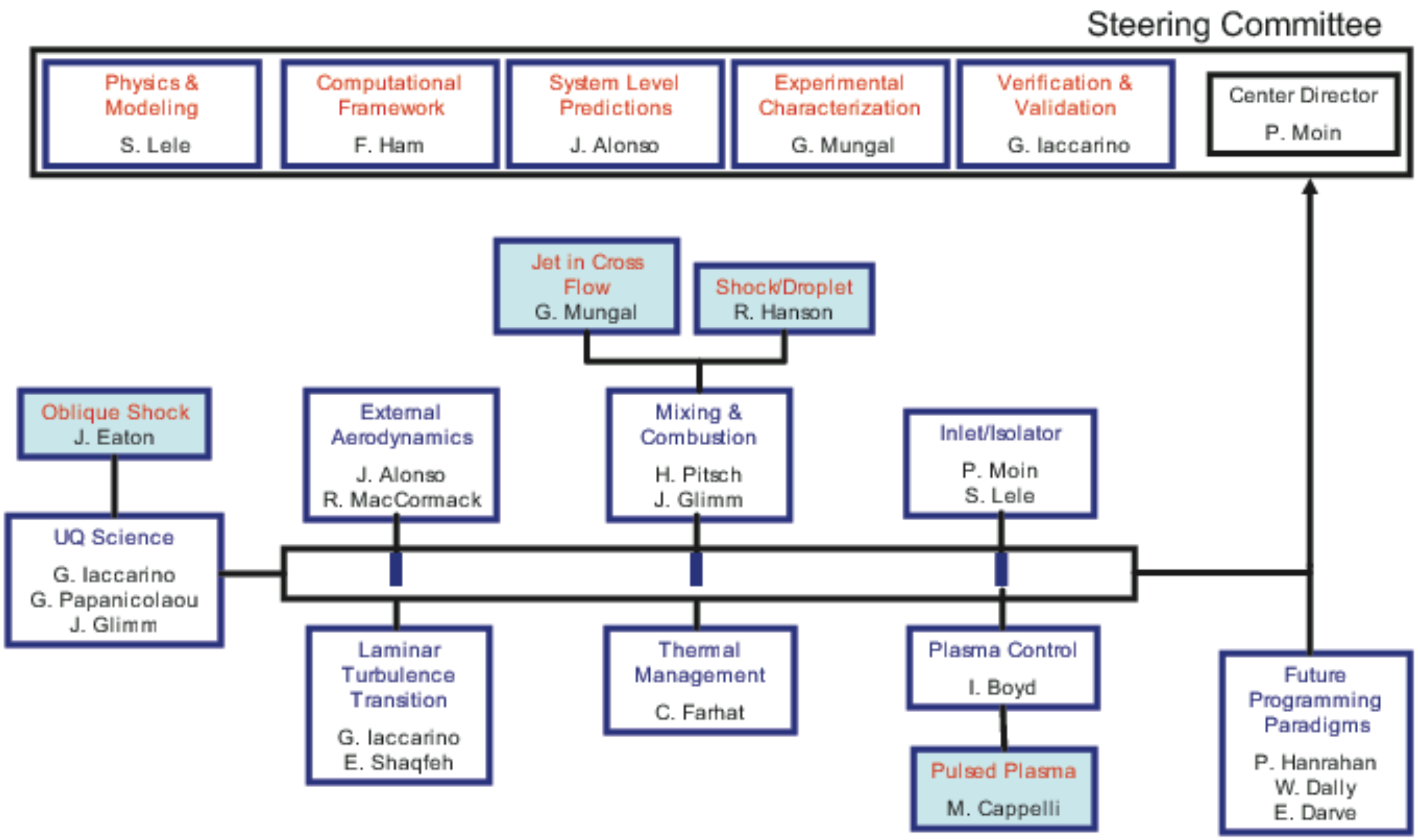
V&V/UQ Role in the Center



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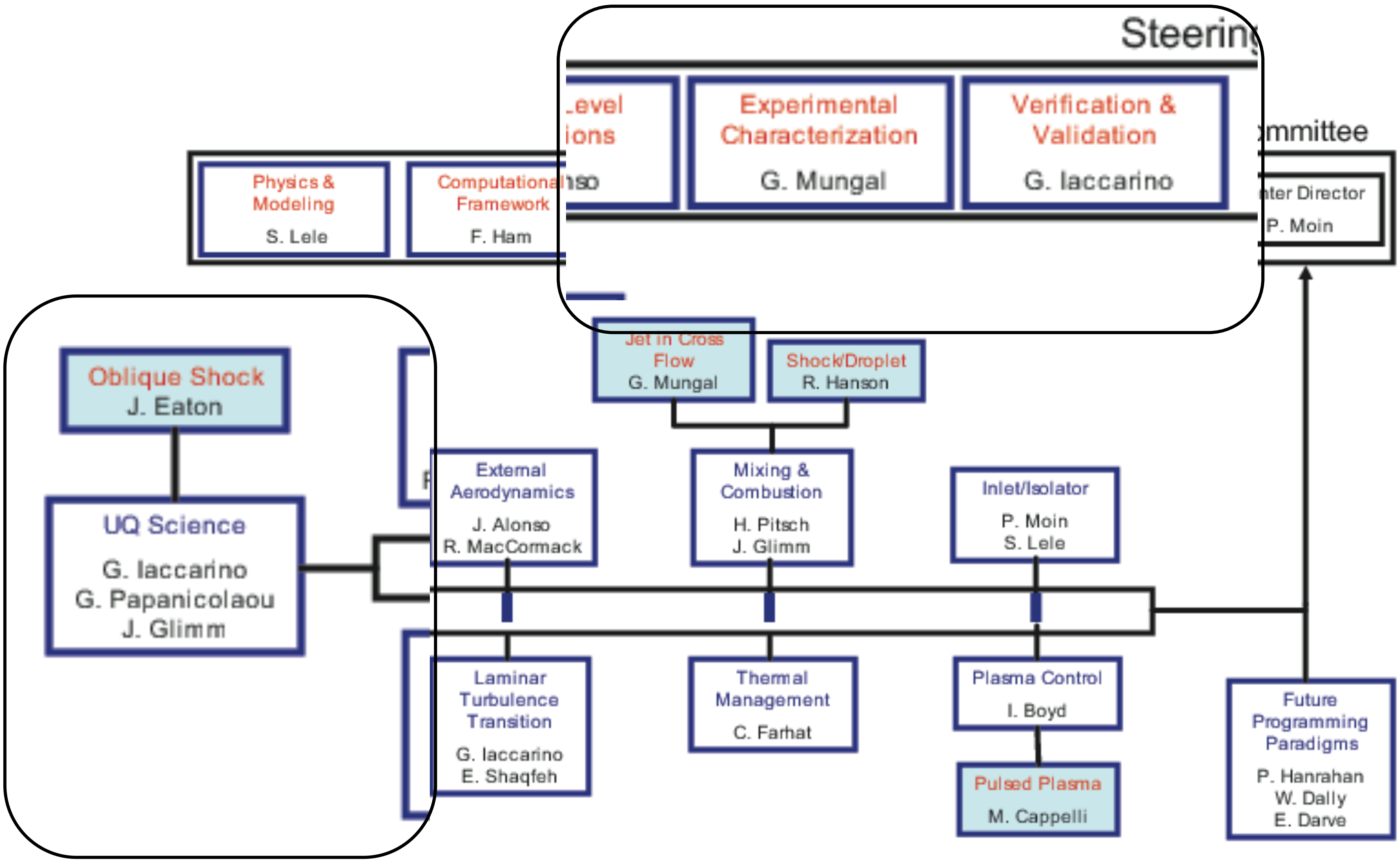
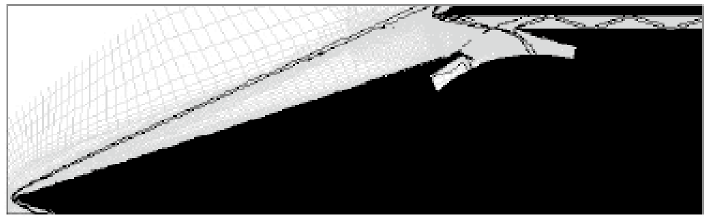


Uncertainty Analysis in Complex, Multi-Physics Applications

Stanford PSAAP Center

July 25-26 2008
Stanford University
Stanford CA



HyShot Hypersonic Vehicle Simulations

R. Ghanem, USC
O. Knio, J. Hopkins
R. Tempone, Florida State
B. Rozowsky, Brown
D. Estep, Colorado State
G. Papanicolaou, Stanford

J. Glimm, SUNY Stony Brook
O. Ghattas, UT Austin
H. Owhadi, Caltech
M. Eldred, SNL
C. Tong, LLNL
T. Wallstrom, LANL
M. Wright, NASA

16 Lectures (40 minutes) on research directions and ideas in UQ

Extra Slides

Uncertainty Sources

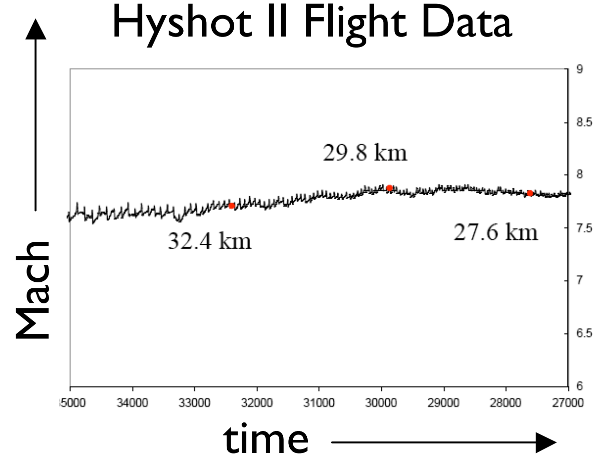
- Imprecise characterization of the environment
  - speed of sound
  - angle of attack
  - temperature fluctuations

  …
- *Static* characterization of the vehicle components
  - structure and material imperfections/inhomogeneity
  - fuel mixture imperfections
  - surface rougheness and out-of-spec geometry

  …
- Thermal-fluid processes during operation
  - fuel injection rate
  - fuel temperature
  - combustion process
  - thermodynamic non-equilibrium effects

  …

Hyshot II Flight Data



1. Boyce, R. R., et al.. "The HyShot Scramjet Flight Experiment", AIAA2003-7029

Combined Adjoint/PC Analysis

Observation

	Polynomial chaos	Adjoint method
Accuracy	Spectral	First order
Computational Cost	Exponential	Constant

Address curse of dimensionality by identifying the parameters that contribute the most to the output uncertainty

Step 1: Sensitivity analysis: use Adjoints

$$F = F^{(0)} + \frac{\partial F}{\partial \xi_1}(\xi_1 - \xi_1^{(0)}) + \cdots + \frac{\partial F}{\partial \xi_m}(\xi_m - \xi_m^{(0)})$$

Step 2: Perform non-intrusive PC on

- Parameters that have considerable sensitivity
- Parameters that have large uncertainty

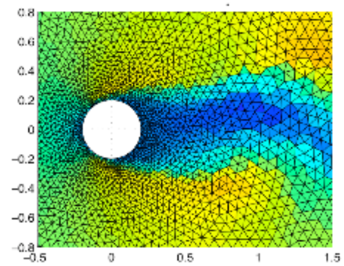
$$(\xi_1^{(0)}, \cdots, \xi_m^{(0)}) \xrightarrow{\text{downselect } (k << m)} (\xi_1, \cdots, \xi_k)$$

Step 3: Combine the results

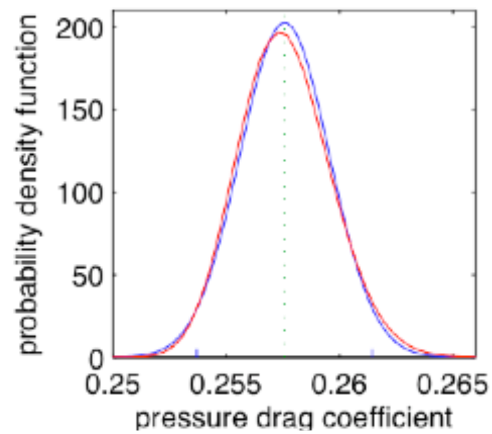
$$F = F^{(pc)}(\xi_1, \cdots, \xi_k) + \frac{\partial F}{\partial \xi_{k+1}}(\xi_{k+1} - \xi_{k+1}^{(0)}) + \cdots + \frac{\partial F}{\partial \xi_m}(\xi_m - \xi_m^{(0)})$$

Combined Adjoint/PC Analysis

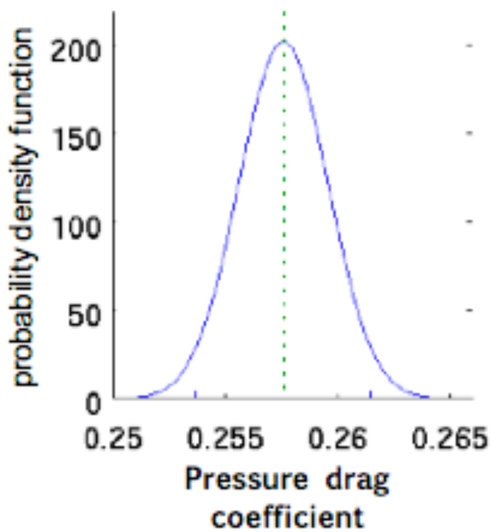
Uncertainty in the drag of a cylinder in response to variability in the inlet conditions (10 parameters)



Polynomial Chaos Solution

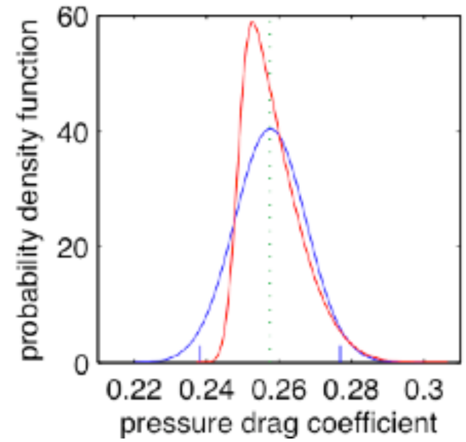


Adjoint Solution



"Small" Uncertainty

"Large" Uncertainty



Downselect to three most important parameters

Alternating Least Square

Separated Representation of Functions:

$$u(y_1, \cdots, y_d) \approx u_1(y_1) \cdots u_d(y_d)$$

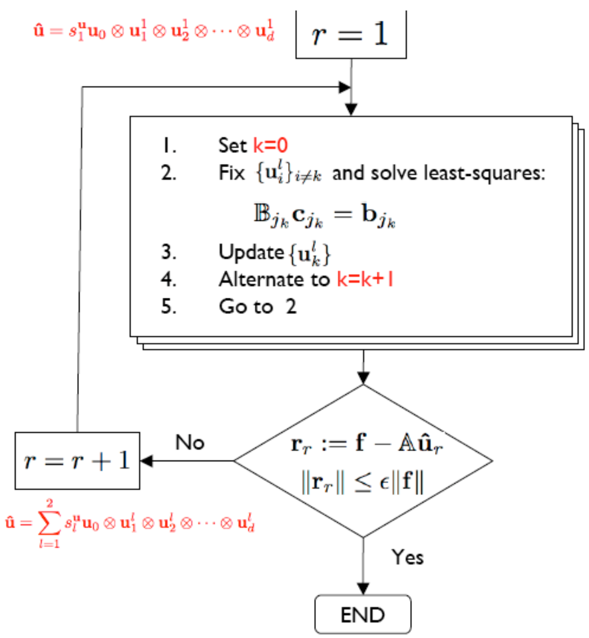
Rank *1* approximation

$$u(y_1, \cdots, y_d) = \sum_{l=1}^{r} s_l u_1^l(y_1) \cdots u_d^l(y_d) + \mathcal{O}(\epsilon)$$

Rank *r* approximation

$$= \sum_{l=1}^{r} s_l \mathbf{u}_1^l \otimes \mathbf{u}_2^l \otimes \cdots \otimes \mathbf{u}_d^l + \mathcal{O}(\epsilon)$$

Rank *r* approximation on the tensor-product grid



1. For each rank solve a least-square problem to find the best approximation
2. Alternate among directions - searching on one direction while freezing the solution on the others
3. Once exhausted the directions check that the residual is decreasing - and then repeat from k=0
4. If the current residual is still high and the residual reduction is small, then the rank must be increased

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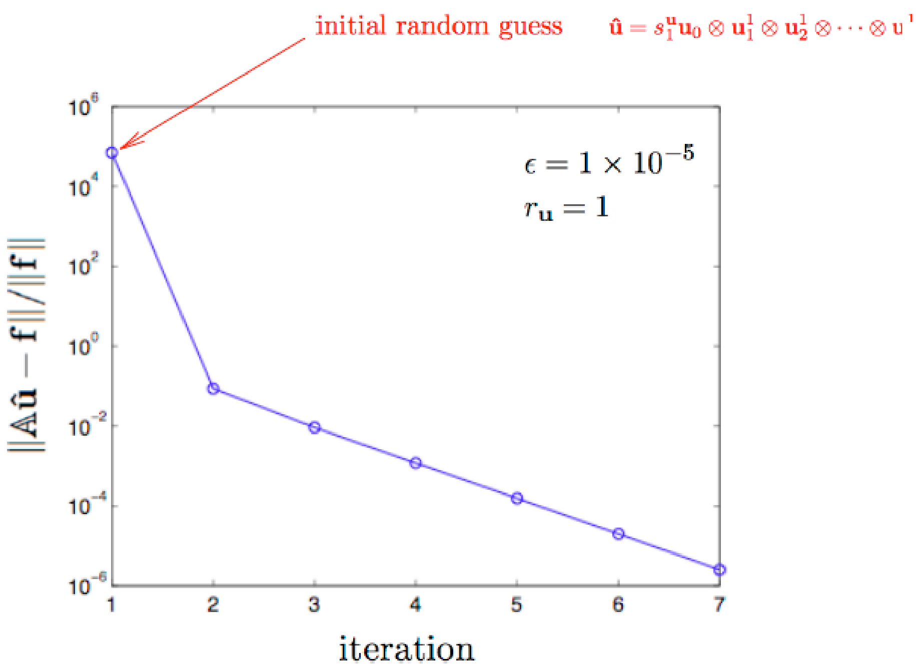
G. Beylkin & M. J. Mohlenkamp, "Separated Rank Representation", PNAS, 2002

Alternating Least Square

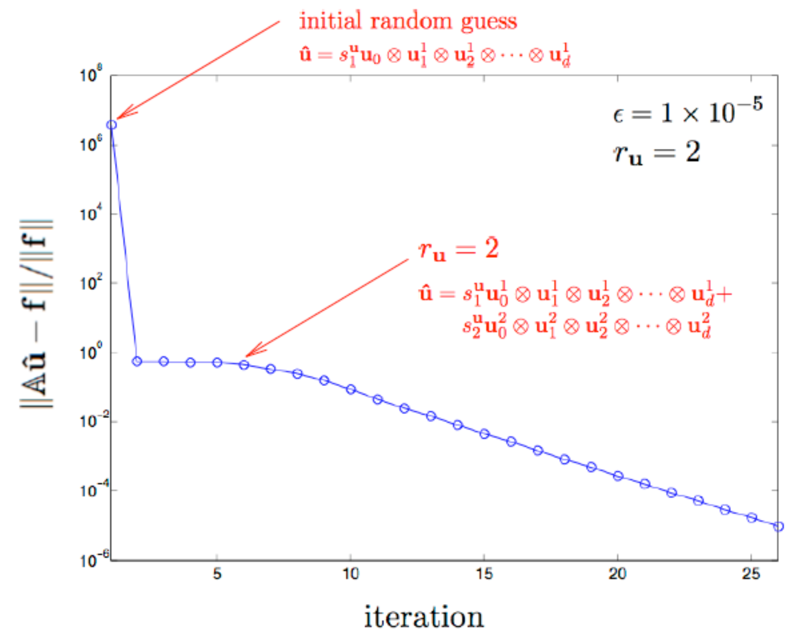
Example: Elliptic problem with uncertain diffusion coefficient (random process - KL with 10 coefficients) - Use MMS with different rank

Rank 1 MMS



$$u_m(x,\omega) = \sin(\pi x) y_1^2(\omega) y_2^2(\omega)$$

Rank 2 MMS



$$u_m(x,\omega) = \sin(\pi x) y_1^2(\omega) y_2^2(\omega) + 0.1 \sin(10\pi x) y_4^2(\omega) y_5^2(\omega)$$

A. Doostan & G. Iaccarino, "A Least Square Approximation of High Dimensional Uncertain Systems", WCCM 2008

ROM-based UQ

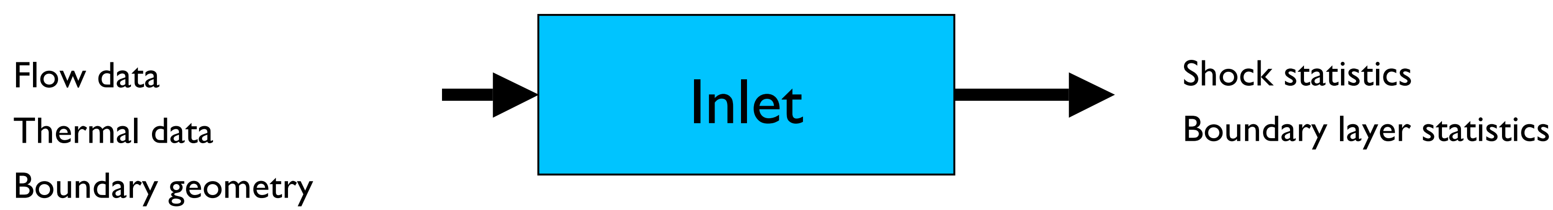
Stochastic Markovian model for system-level UQ

- Nodes on a directed graph represent reduced models of the subsystems

  e.g. grid coarsening, RANS, simplified physical assumptions, engineering models
- Links represent reduced models of subsystem coupling with uncertainty

  e.g. shock location statistics, low order statistics of thermal state, statistics of boundary layers, etc.
- Response function of each node calibrated by high-fidelity unit models

  Adjoint and Polynomial Chaos analysis used to select low order representation of output variability.



Reduced order model

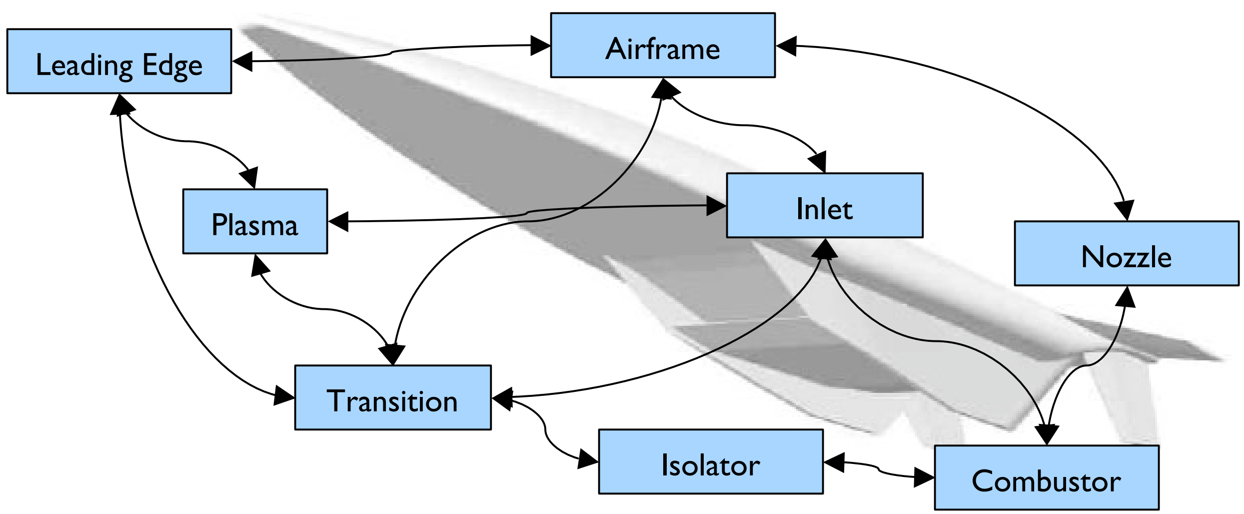
ROM-based UQ

Additional noise terms used to model uncertainty introduced by model reduction and to probe for abnormal behavior or "cliffs"

Propagate uncertainty through the entire graph via Monte Carlo

- Initial states chosen according to statistics determined experimentally and by high-fidelity subsystem models.

Identify transition from normal operation and margins of uncertainty



LAPS-based UQ

LAPS (Likelihood Averaging in Probability Space) is an approximated approach to evaluate mean and low-order statistics

Similar in spirit to Reynolds-averaging in turbulence physics

- Fundamentally requires a closure.
- It does not rely on Taylor series expansions around the mean (like in moments methods)
- Retains the non-linearity of the original problem
- Built upon the high-fidelity physics simulation tools

Closure terms in the LAPS formulation need to be evaluated and calibrated on the basis of MC sensitivity analysis and MC/PCE propagation techniques.

We plan to use Stanford's long-history in the field to identify feasible and accurate closures.

LAPS-based UQ

Example: Burgers equations with uncertain initial conditions

Decompose and define

$$u = \bar{u} + u'.$$

$$\bar{u} \equiv \langle u \rangle = \int_{\omega \in \Omega} u dP(\omega)$$

$$\hat{u} \equiv \mathrm{var}(u) = \frac{1}{2} \int_{\omega \in \Omega} (u - \bar{u})^2 dP(\omega).$$

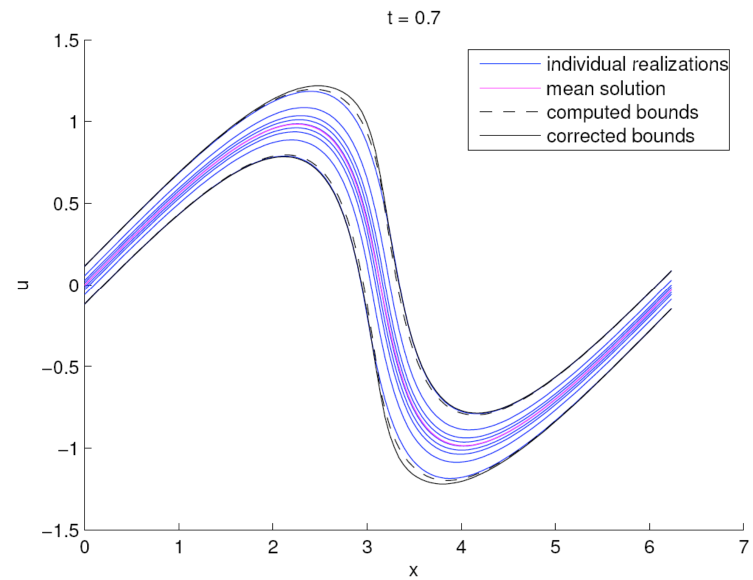
Plug in the governing eqns.

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} = - \int_{\omega \in \Omega} u' \frac{\partial u'}{\partial x} dP(\omega)$$

$$\frac{\partial \hat{u}}{\partial t} + \bar{u} \frac{\partial \hat{u}}{\partial x} + 2\hat{u} \frac{\partial \bar{u}}{\partial x} = - \int_{\omega \in \Omega} u' u' \frac{\partial u'}{\partial x} dP(\omega)$$

Closure problem!

LAPS predicted uncertainty bounds



1. Chatrasmi T. et al, "UQ Analysis for Linear and Non-Linear Problems ", CTR Annual Research Brief 2005.