Experiences & Expectations

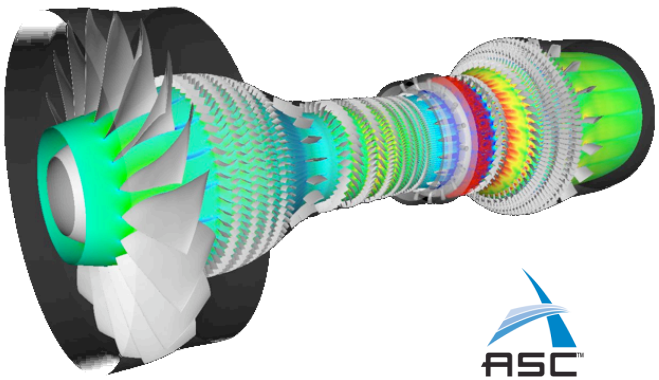
Stanford ASC Center

Gianluca Iaccarino
Center for Turbulence Research
Mechanical Engineering Dept.
Stanford University

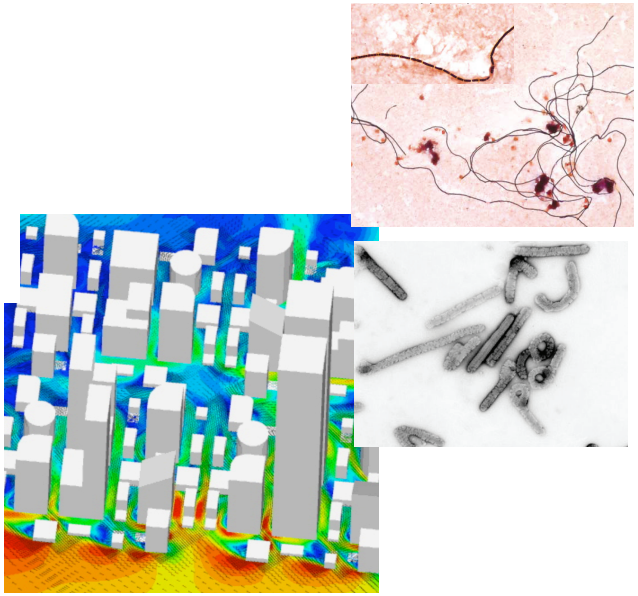
Sandia Workshop on MMVV - 14-16 August 2007

Physical Problems

Large scale thermal/fluid systems dominated by turbulence transport (strongly non-linear PDEs) and multiscale phenomena (combustion, multiphase interfaces, shocks, etc.)



Flow and heat transfer in a jet engine



Dispersion of complex biological agents

Heat transfer on ablating thermal protection systems

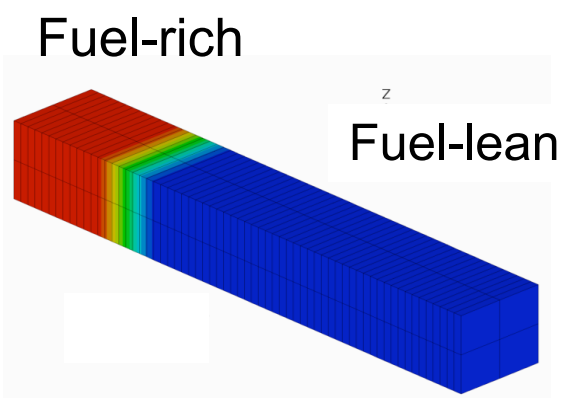
Verification

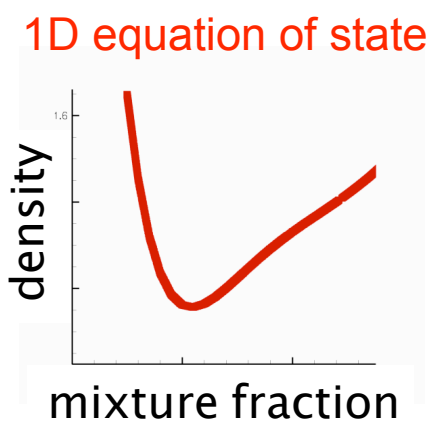
Formulate (physics-based) manufactured solutions that include multiple physical processes in realistic conditions

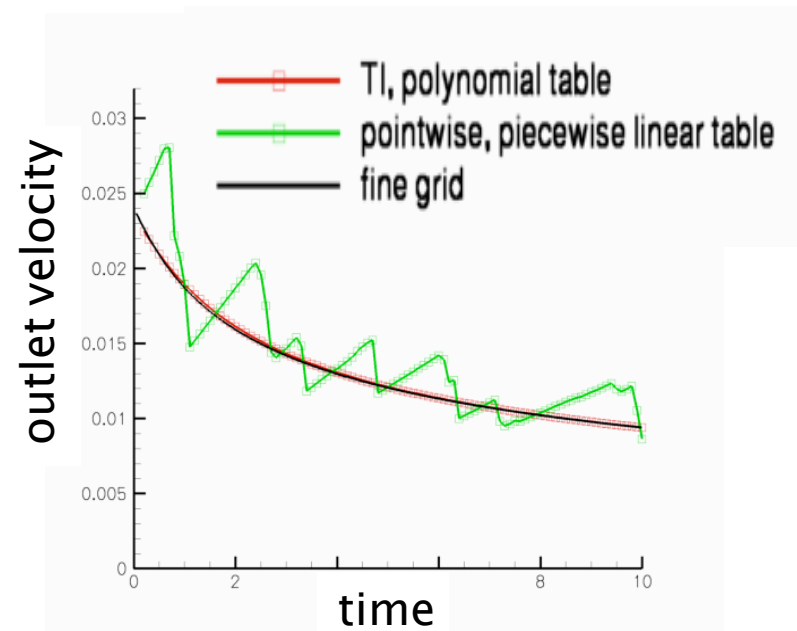
Objective I: algorithmic correctness - order of accuracy

Objective II: algorithm appropriateness - robustness and physical "fidelity" (parameter sensitivity)

Example: L. Shunn (Sandia summer intern) with P. Knupp - work on compressible, rective flows with complex, non-linear (tabulated) equation of state.



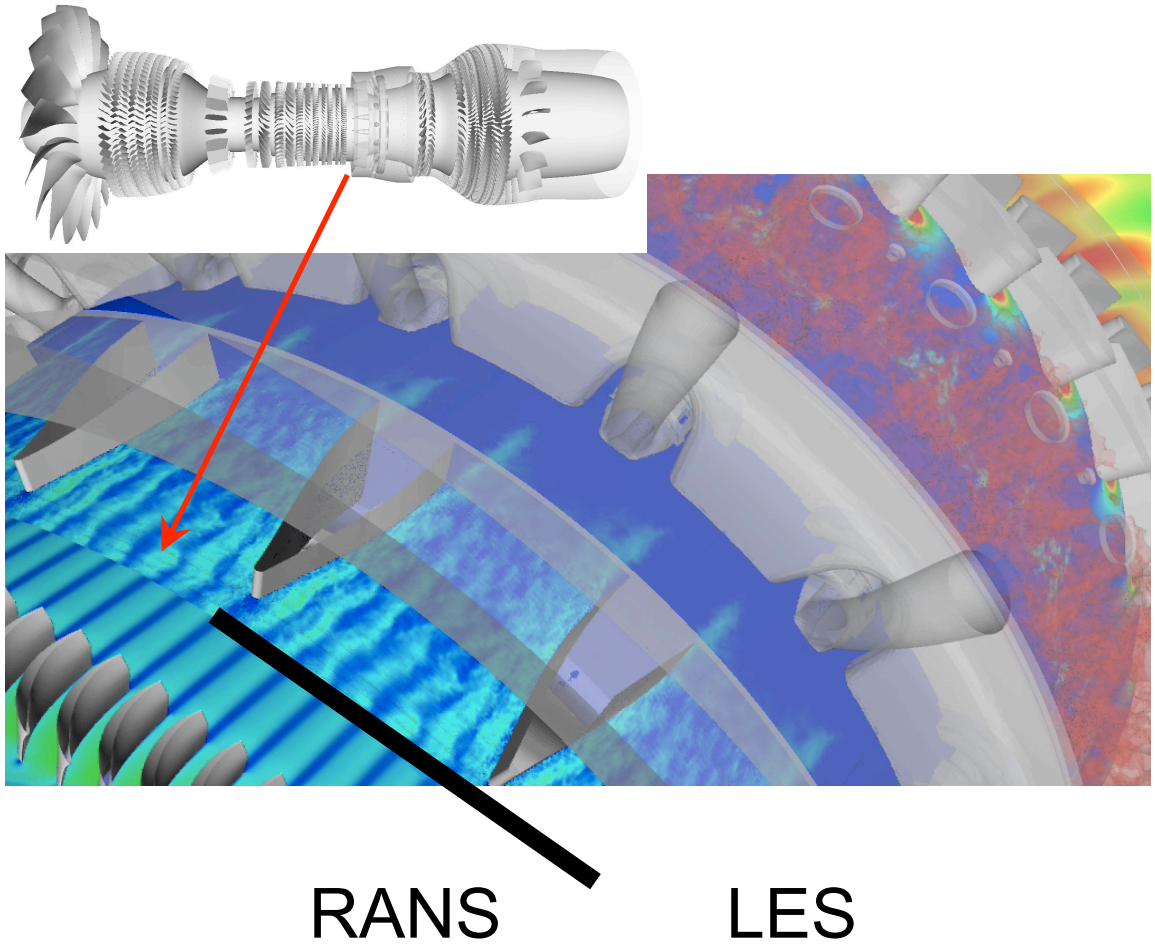




Validation

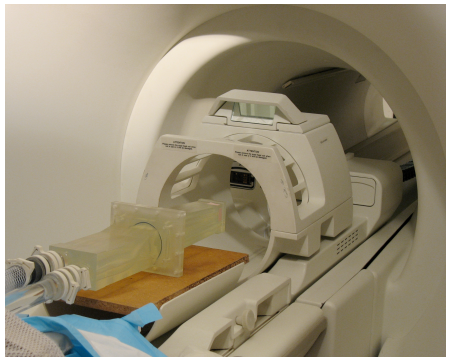
Perform accreditation tests for physical models based in close interactions with experimentalists

Example: interface between two subsystems characterized by different turbulence modeling approaches

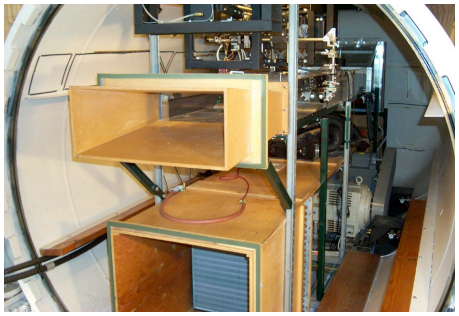


Validation

Multiple Experimental Facilities/Diagnostics

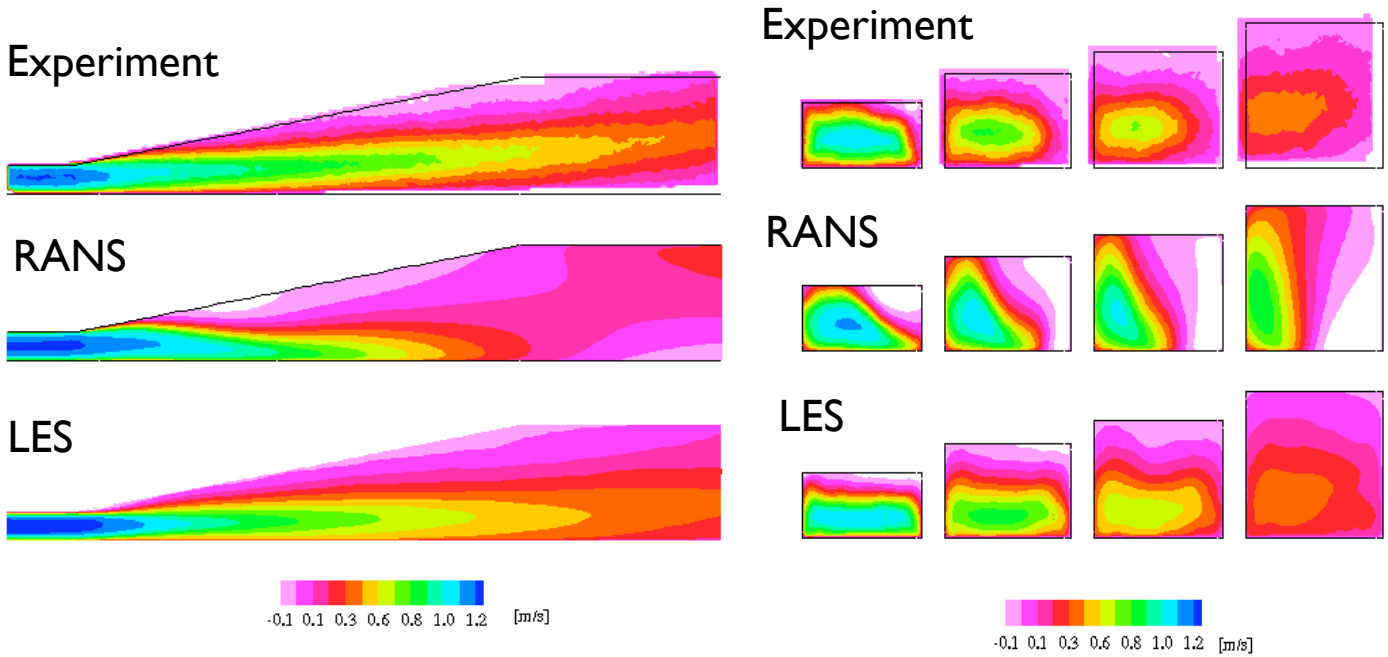


Magnetic Resonance Velocimetry



Particle Image Velocimetry

Large Experimental Datasets & Multiple Physical Models



Streamwise Velocity

Uncertainty Quantification

Rather new activities, not originally part of the ASC program.

For our problems

Uncertainty Quantification

Rather new activities, not originally part of the ASC program.

For our problems

- Very expensive deterministic solution evaluations
  - Naive MC is unfeasible
- Very complex and extensive application codes
  - Intrusive methods are not attractive
- Potentially large uncertainty in the parameters
  - Sensitivity Derivative (Perturbation Method) can be inaccurate
- Very large number of uncertain parameters
  - PC is too expensive

Uncertainty Quantification

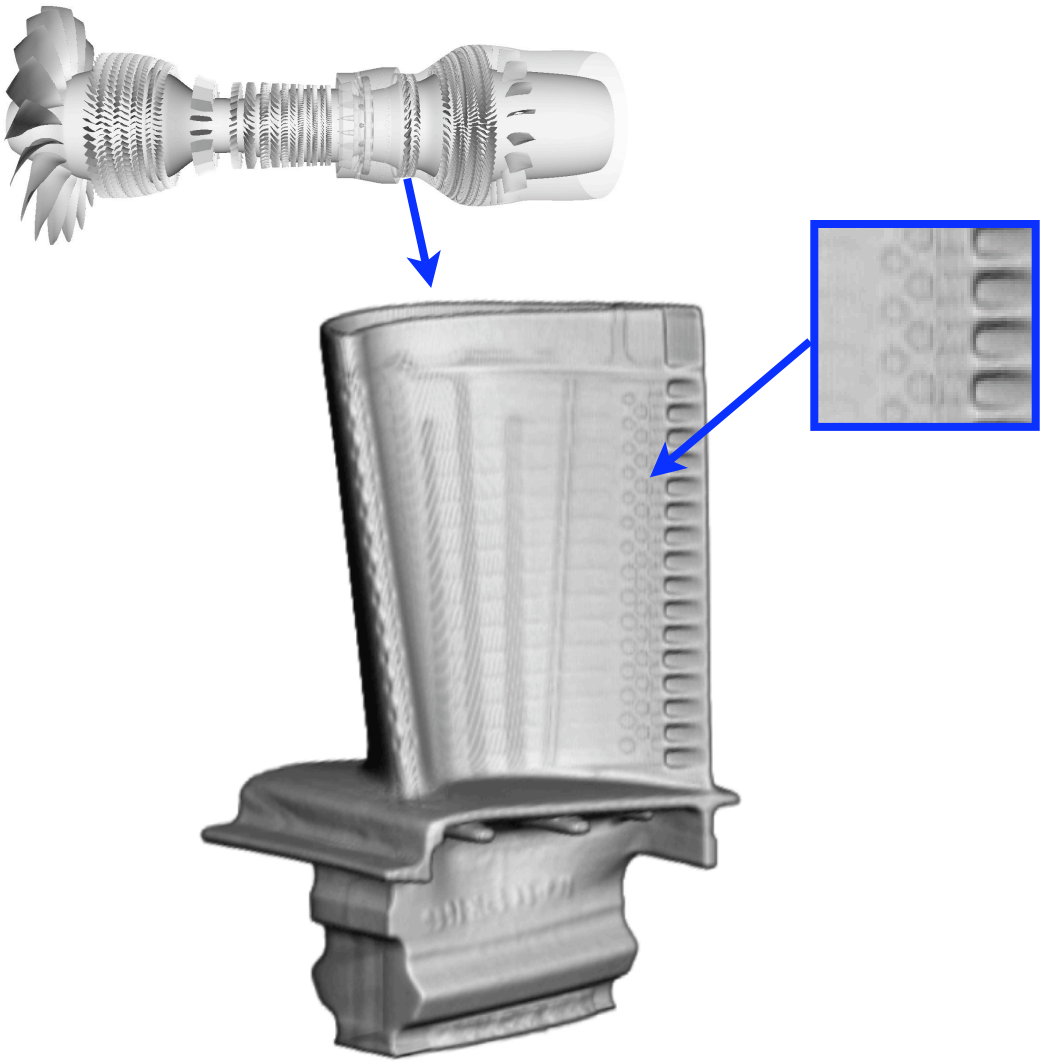
Current focus is on non-intrusive approaches

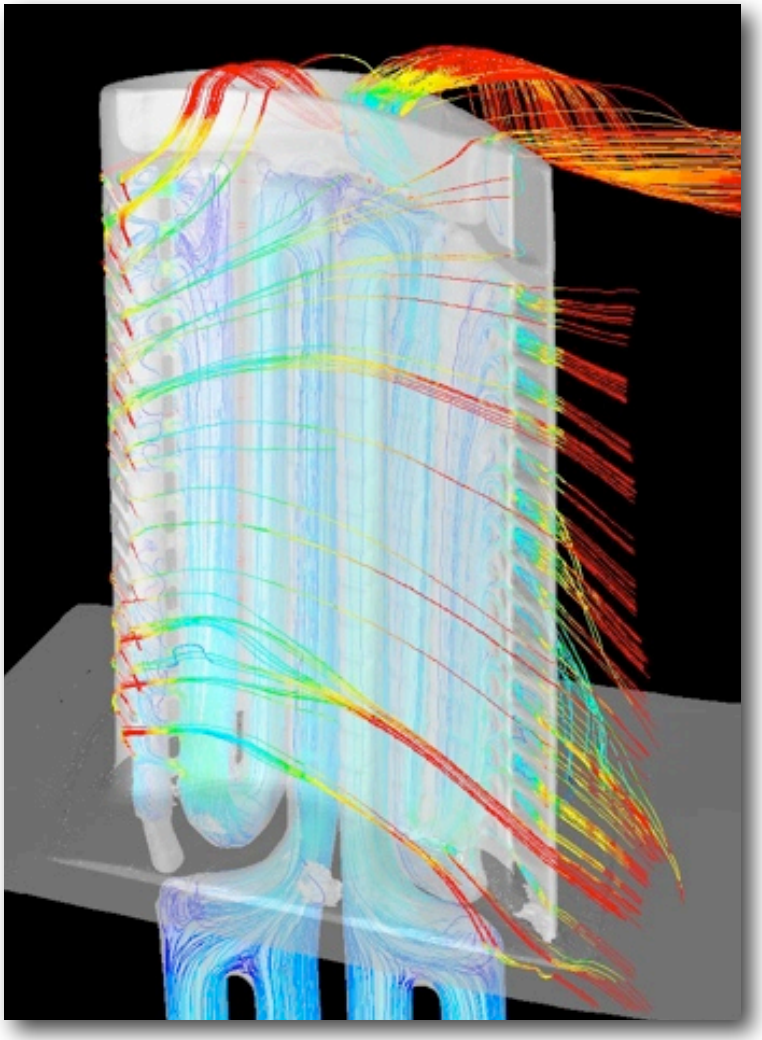
- Effect of quadrature rules in high order stochastic colocation (P. Constantine - Sandia summer intern)
- Pade-Legendre colocation for strongly non-linear problems with discontinuities in probability space (T. Chantrasmi)
- Combined Adjoint/Polynomial Chaos method for turbulent flow simulations (Q. Wang)

Stochastic Colocation

Mean and variance are "just" integrals: we can use quadrature rules to compute them accurately. Evaluate choices of 1D integration rule and multi-dimensional extensions

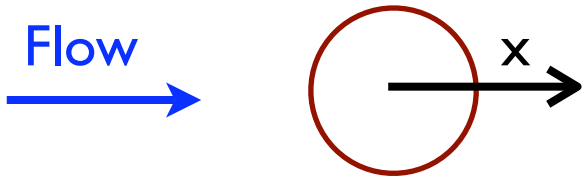
Turbine blade cooling passages



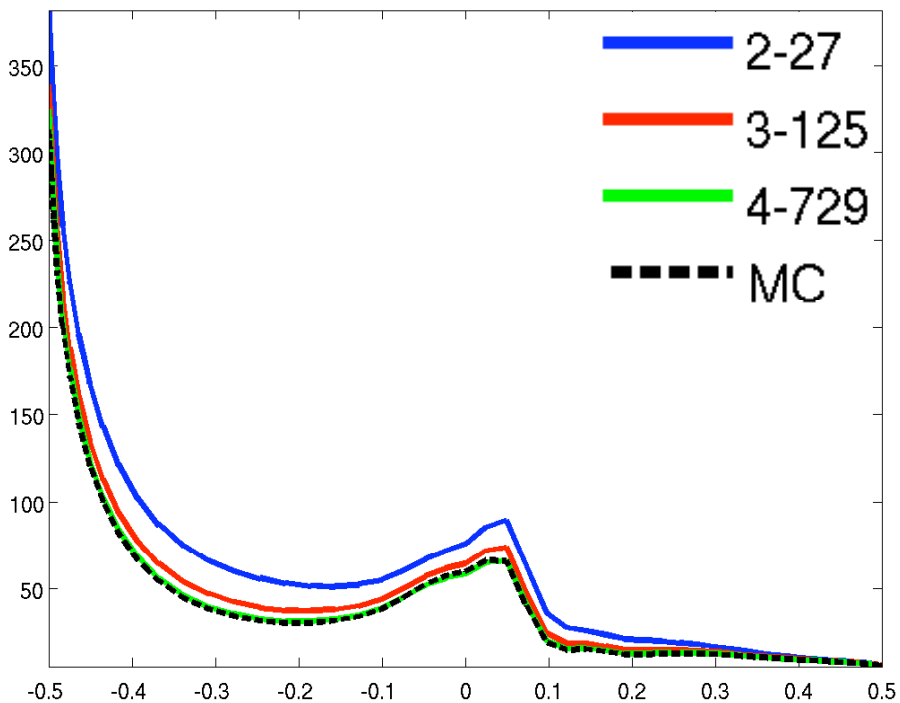


Stochastic Colocation

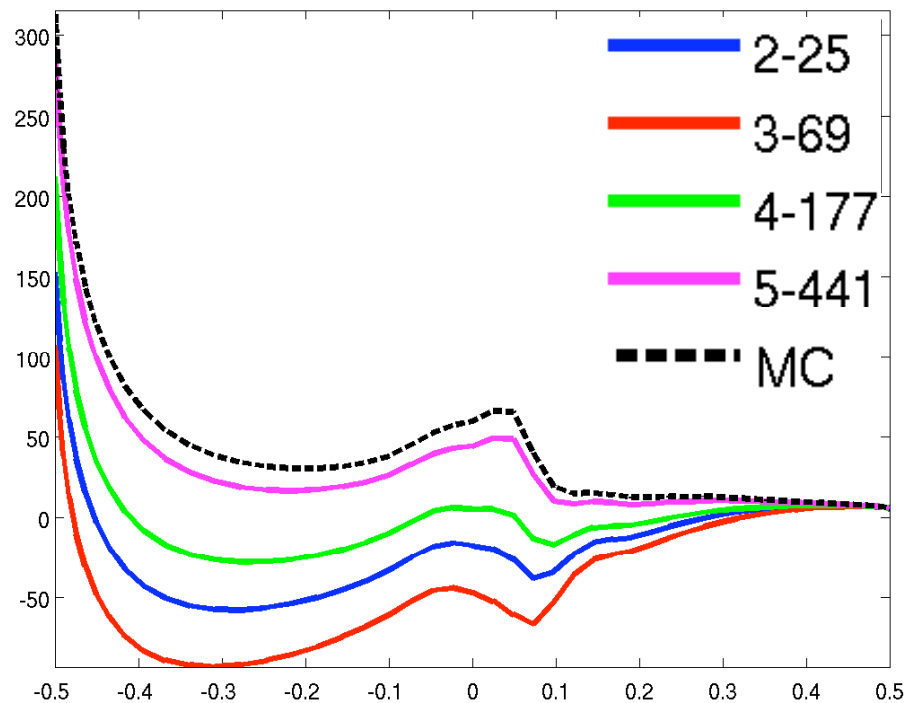
Example: Turbulent flow around an array of heated cylinders with uncertain inlet velocity and wall heat flux



Wall Temperature Variance



Gauss + Tensor Product Grid



Clenshaw-Curtis + Smolyak Grid

Discontinuities in Probability Space

develop a method to handle functions with *discontinuities in the probability space as well as physical domain* but smooth away from the discontinuities. Discontinuity in probability space not uncommon for non-linear systems: change of system behavior, transitions, flow separation, etc.

- Does *not* require a-priori knowledge of the discontinuities
- Works with multiple spatial and stochastic dimensions
- Wants a non-intrusive method
- Global polynomial/Spectral representation of Non-smooth functions is not straightforward (Gibbs phenomena)

Possible remedies

Enrichment techniques

Local (zonal) representations

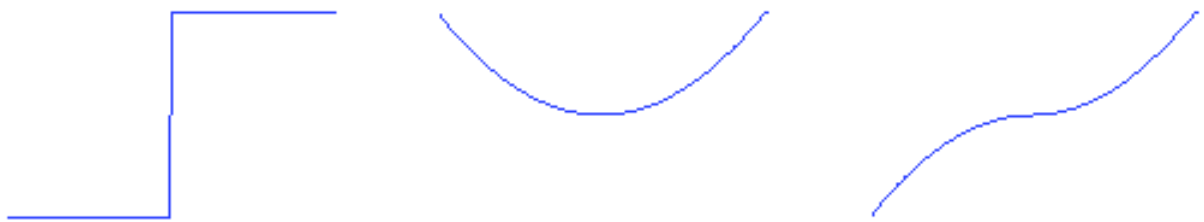
Pade-Legendre approximates

Pade-Legendre Polynomial Chaos Approach

$$R(u) = \frac{P}{Q} \quad \text{where} \quad P, Q \text{ polynomials of degrees } M, L$$

$$\langle P - Qu, \varphi \rangle = 0 \quad \text{where } \varphi \text{ polynomial of deg} < N$$

$$\forall x \in [-1,1]: \quad Q(x) > 0$$

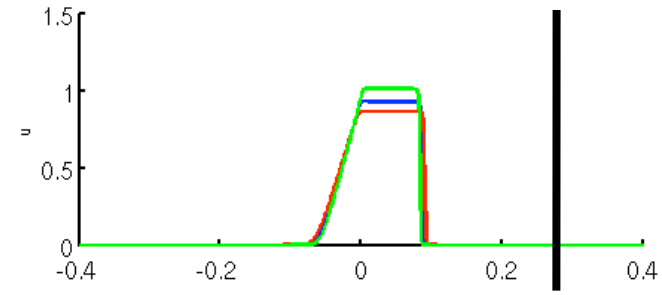


u **Q** **uQ ~ P**

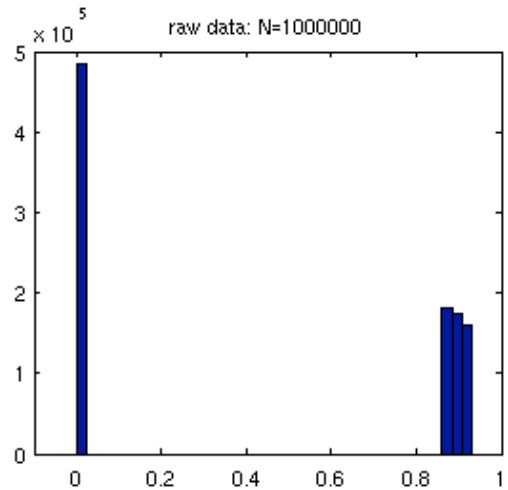
Which is much smoother than u

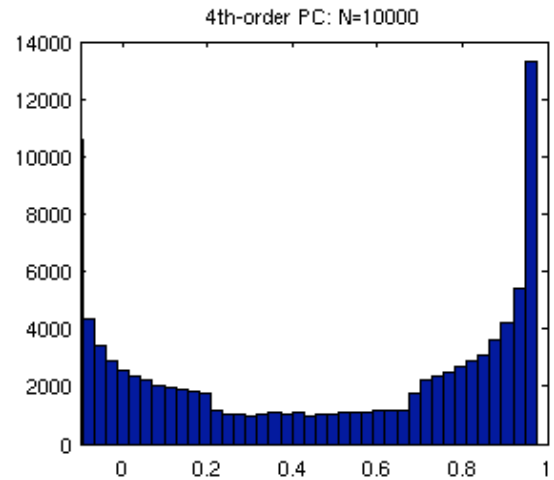
Example

Shock tube problem with uncertain equation of state



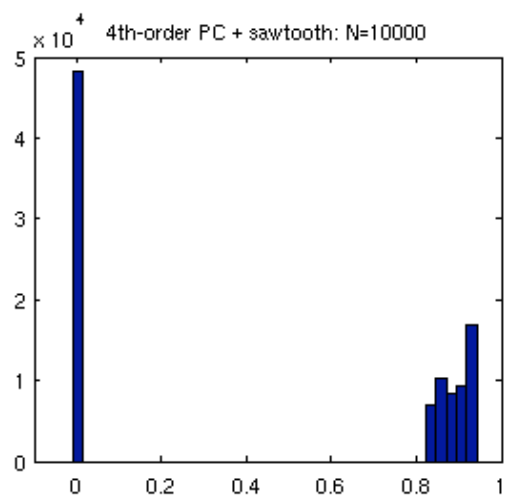
MC

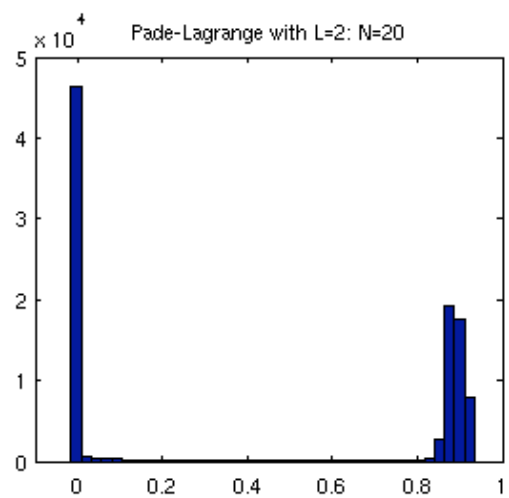




PC (4)

PC (4) + Sawtooth





PL (2)

What are the expectations?

Beyond the simplistic view: "*add error bars to the computational results*"

Objective assessment of the predictive capabilities of the computational models: validation metrics and confidence bounds (Oberkampf & Barone, 2006), uncertainty propagation, data assimilation (Ghanem & Doostan, 2006)

Identify areas of model inadequacy in the physical models and develop "modeling-error" estimates.

- Should validation be limited to comparing the quantity of interest?
- What about modeling error cancelation?
- Does the model works for the right reasons?

Perspectives

Our research focus has been traditionally on pursuing improving the physical models - typically increasing the fidelity by adding more and more "scales"

UQ of an existing model is not considered as rewarding as the development of a brand-new physical model (cultural problem) and the research agenda of many funding agency (NASA, AirForce, DARPA) has a limited focus on UQ

Need to show the advantages of doing UQ beyond the decision making

Opportunity: develop model improvements using ideas originated from UQ methodologies. One simple idea is to substitute "deterministic-type" hypothesis with probabilistic statements or theoretical bounds (interval analysis)

Education

Need to bring together computational mathematics, engineering, physics and statistics educational curriculum

Stanford's Institute for Computational Mathematical Engineering (http://icme.stanford.edu) has been designed around this idea. Two ICME PhD candidate are now directly involved in UQ activities within Stanford's Alliance Center

Verification and Validation awareness starts early in the CFD classes but there is much more than is required.

We do not formally offer an UQ-methodology class but we are organizing one in collaboration with Applied Math Dept. (hopefully starting next year)

Acknowledgments

DOE support (and guidance) within the ASC Alliance program

PhD Students	PostDocs
Paul Constantine	Alireza Doostan
Qiqi Wang	Debraj Ghosh
Tonkid Chantrasmi	Frank Ham
Lee Shunn	

...more

Combined Adjoint Polynomial Chaos Analysis

Combined Adjoint/PC Analysis

Observation

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

Goal: reduce the number of uncertain parameters

- Evaluate the ones that contribute the most to the output uncertainty

Step 1: Sensitivity analysis: use Adjoints

Step 2: Perform PC on

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

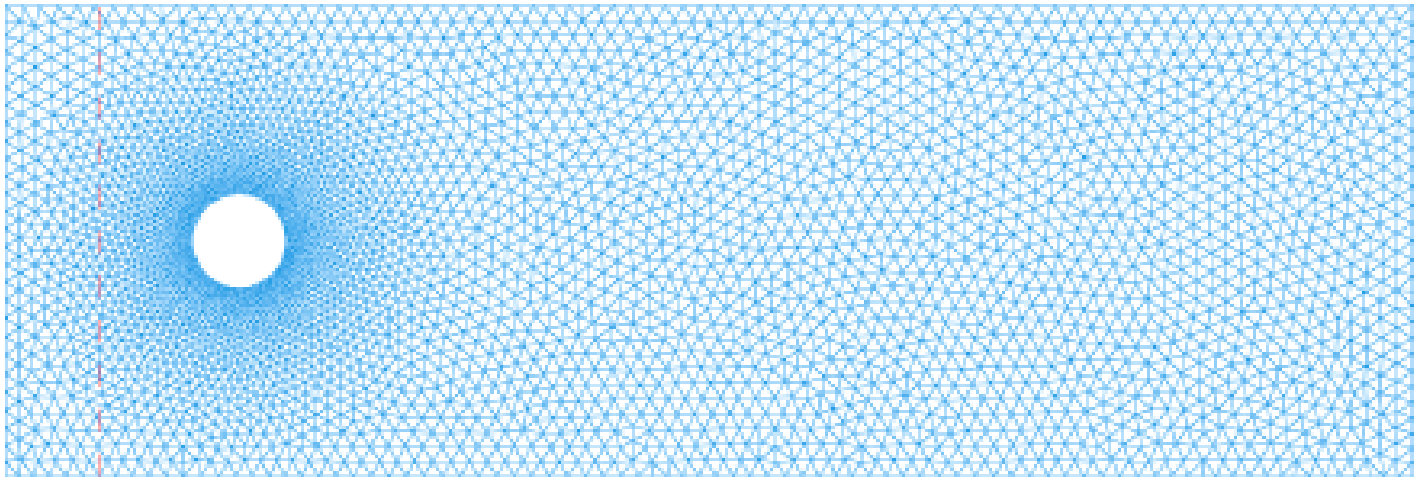
Step 3: Combine the results

Application

Vortex shedding around cylinder (Re=100)

Uncertain inflow conditions (non uniform inflow) - modeled using 10 parameters - KL expansion

Objective: evaluate the uncertainty in the time-averaged pressure drag coefficient



Combined Adjoint/PC Analysis

- Uncertainty of objective function based on adjoint analysis:

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

where $F^{(0)} = F(\xi_1^{(0)}, \cdots, \xi_m^{(0)})$.

- Uncertainty of objective function based on PC analysis:

$$F = F^{(pc)}(\xi_1, \cdots, \xi_k)$$

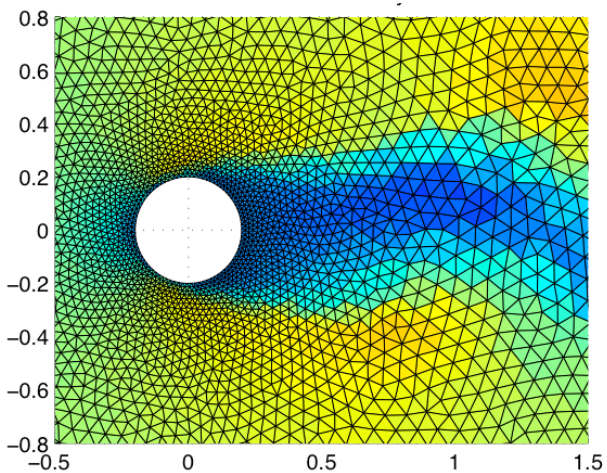
where $\xi_1, \cdots, \xi_k$ are the important parameters determined by adjoint analysis.

- Combined result:

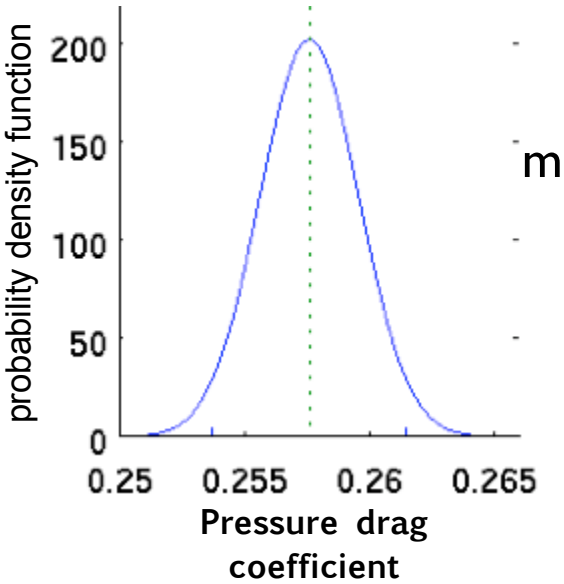
$$F = F^{(pc)}(\xi_1, \cdots, \xi_k) + \frac{\partial F}{\partial \xi_{k+1}}(\xi_{k+1} - \xi_{k+1}^{(0)}) + \cdots + \frac{\partial F}{\partial \xi_m}(\xi_m - \xi_m^{(0)})$$

Combined Adjoint/PC Analysis

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



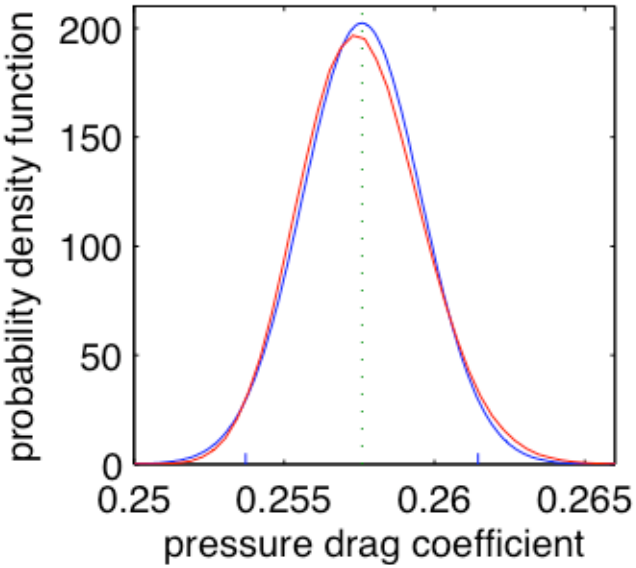
Adjoint Solution



Downselect to three most important parameters

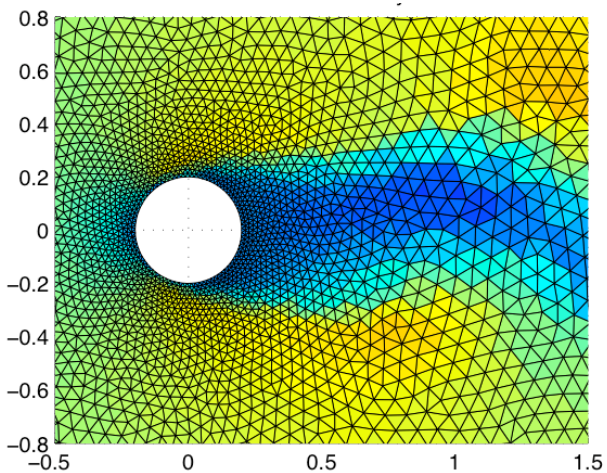
"Small" Uncertainty

Polynomial Chaos

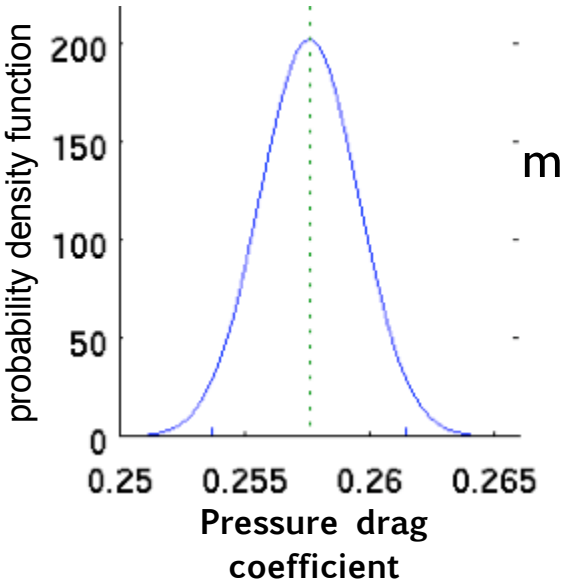


Combined Adjoint/PC Analysis

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



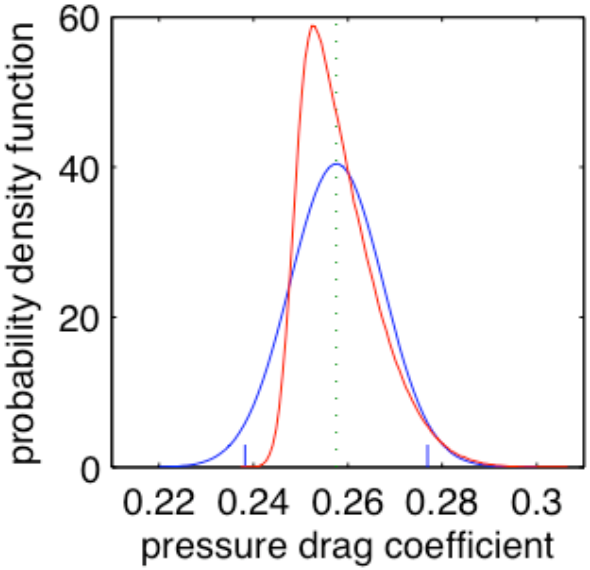
Adjoint Solution



Downselect to three most important parameters

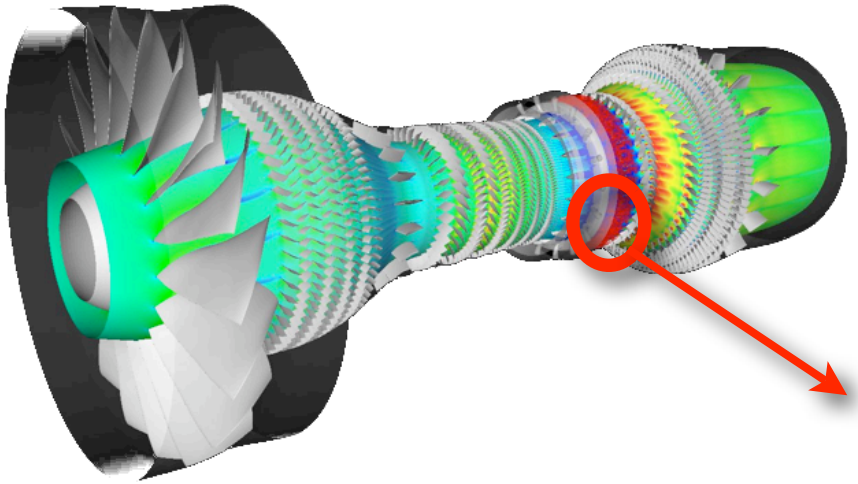
"Large" Uncertainty

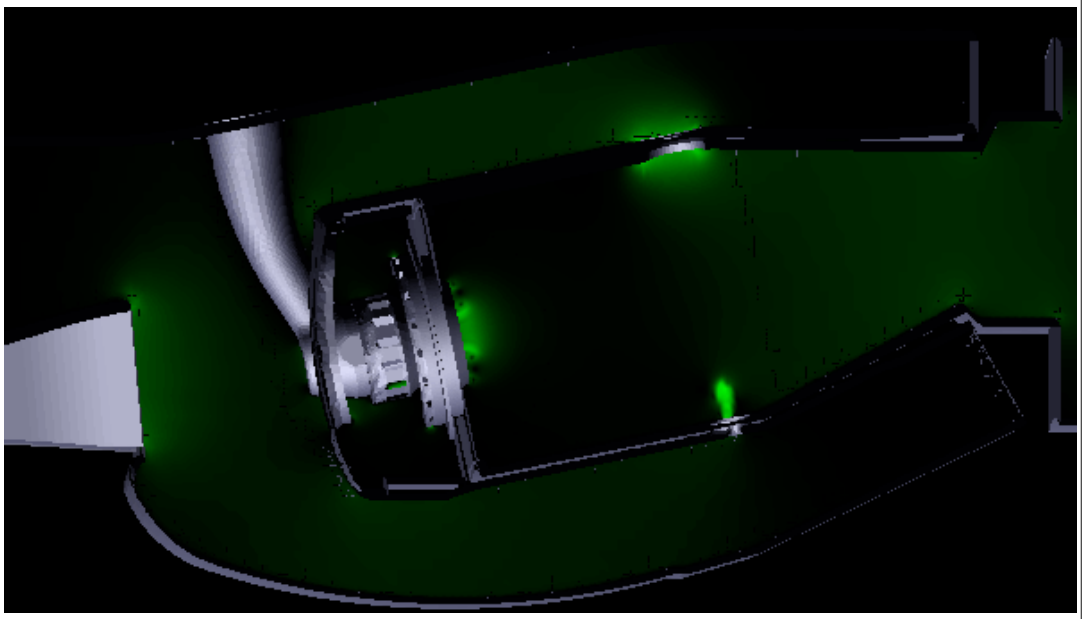
Polynomial Chaos



On-going Work

- Completion of MC sampling to verify the accuracy of the combined Adjoint/PC expansion
- Extensions to three-dimensional turbulent flows
- Development of efficient methods to solve the adjoint system for unsteady problems



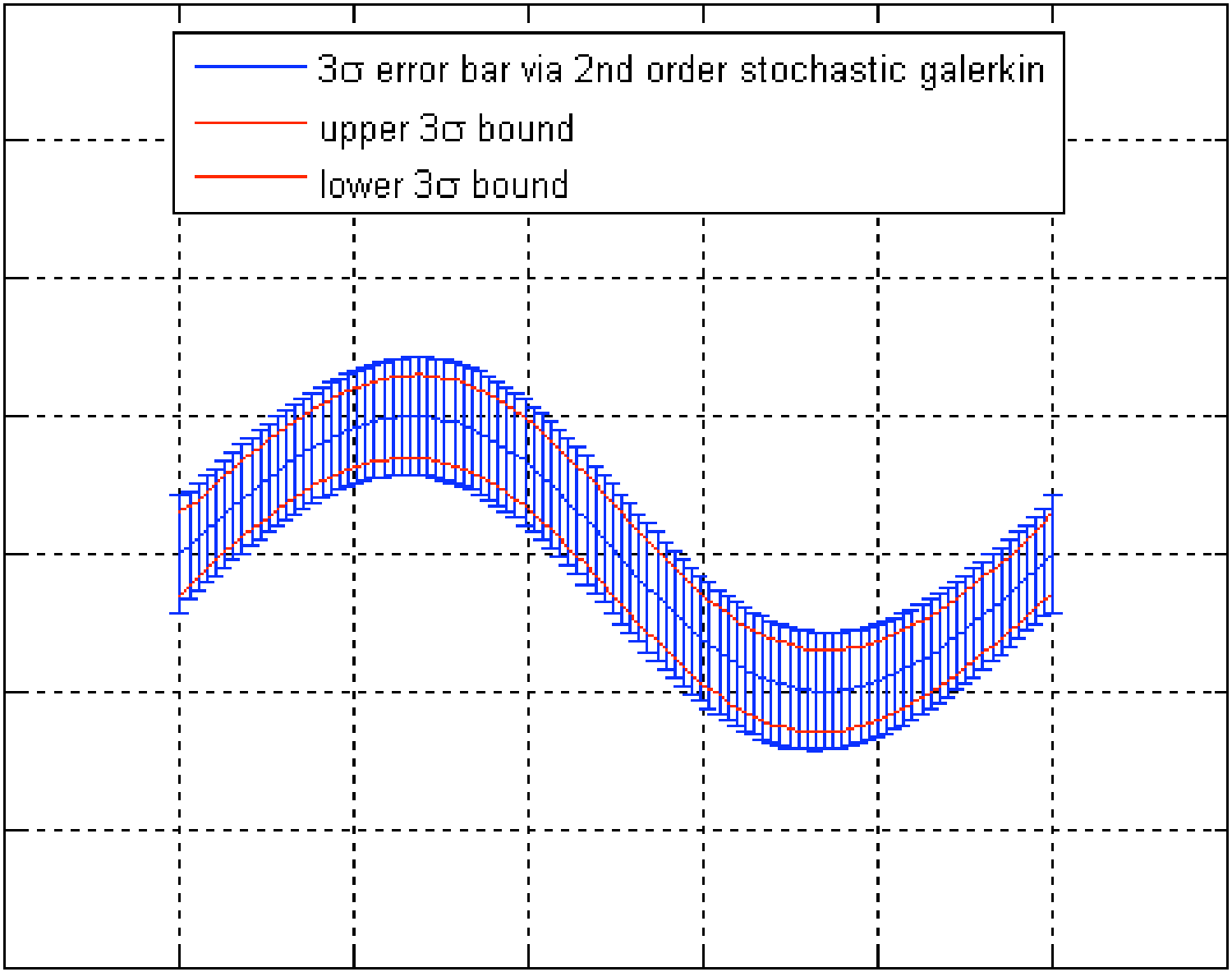


Turbulent Reactive Flow in the Combustion Chamber

Uncertainty Propagation for Strongly Non Linear Problems

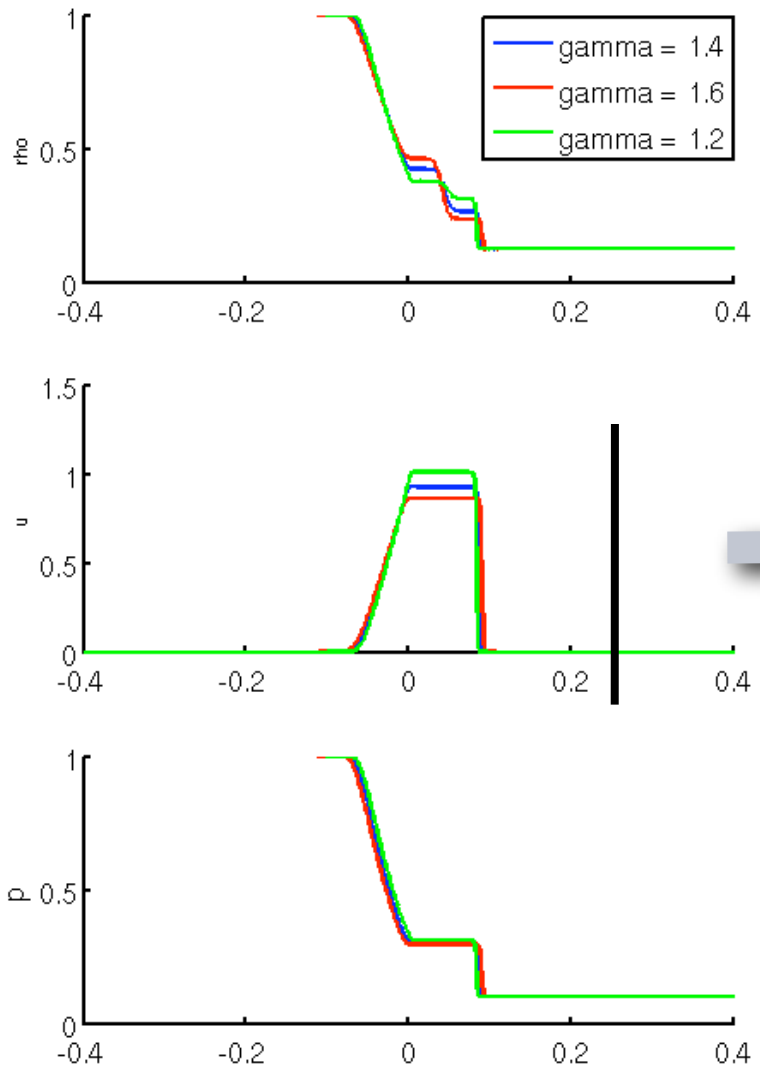
Discontinuity in Physical Space

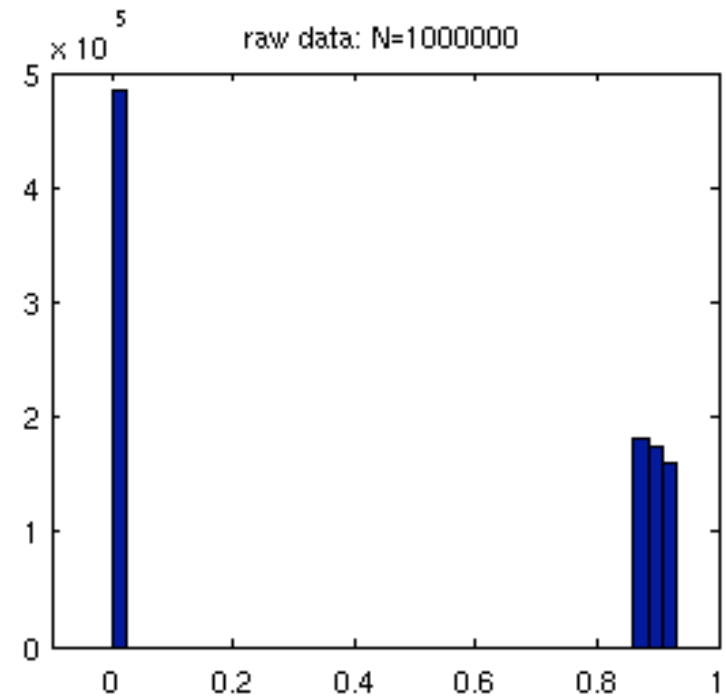
Burgers Eq. with "Noisy" initial data



Discontinuity in Probability Space

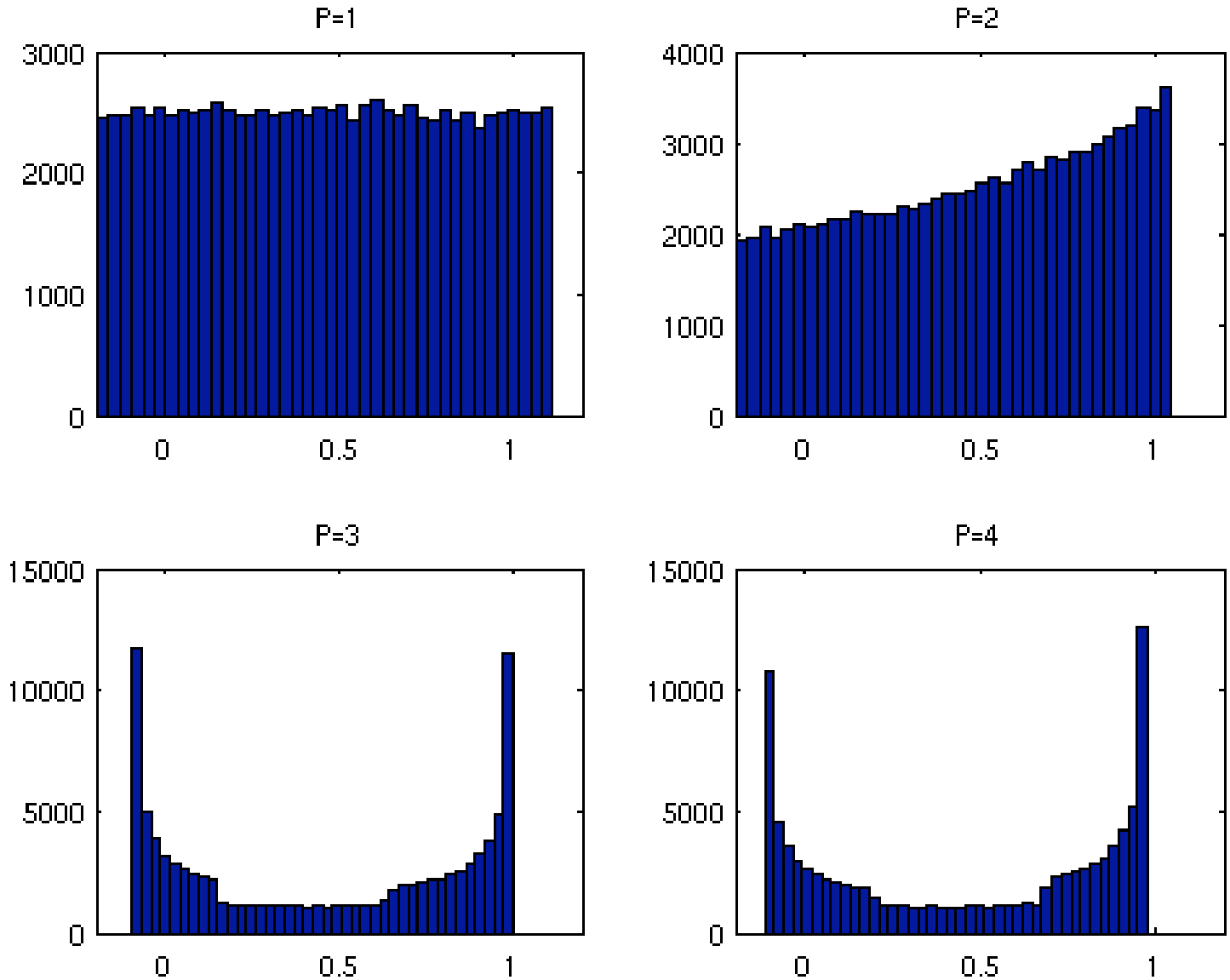
Shock-Tube Problem with uncertain gas properties





Discontinuity in Probability Space

"Classical" Polynomial Chaos Approach



Discontinuity in Probability Space

"Classical" Polynomial Chaos Approach

- Global polynomial/Spectral representation of Non-smooth functions is not straightforward (Gibbs phenomena)
- Discontinuity in probability space not uncommon for non-linear systems: change of system behavior

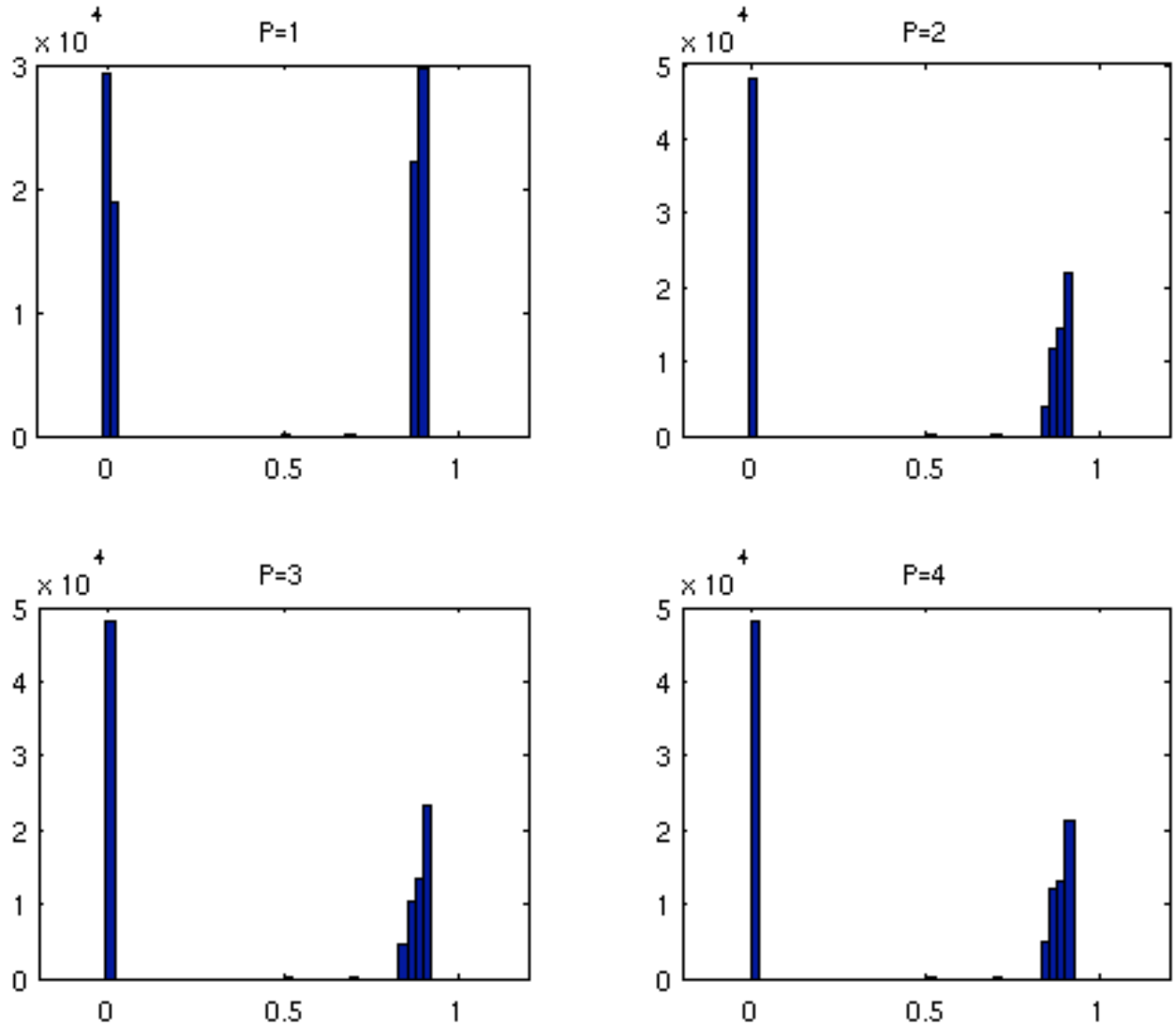
Possible remedies

Enrichment techniques
Local (zonal) representations
Pade-Legendre approximates

"Enriched" Polynomial Chaos Approach

$$\mathbf{u}(x,t,\omega) = \sum_{i=0}^{P} u_i(x,t)\Phi_i(\xi) + u_{P+1}\Psi(\xi)$$

Saw-tooth

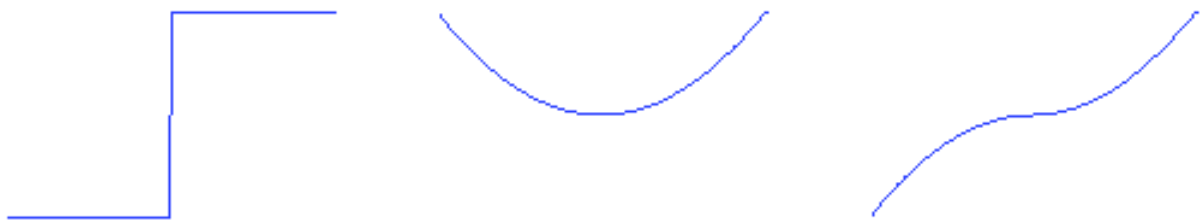


Pade-Legendre Polynomial Chaos Approach

$$R(u) = \frac{P}{Q} \quad \text{where} \quad P, Q \text{ polynomials of degrees } M, L$$

$$\langle P - Qu, \varphi \rangle = 0 \quad \text{where } \varphi \text{ polynomial of deg} < N$$

$$\forall x \in [-1,1]: \quad Q(x) > 0$$

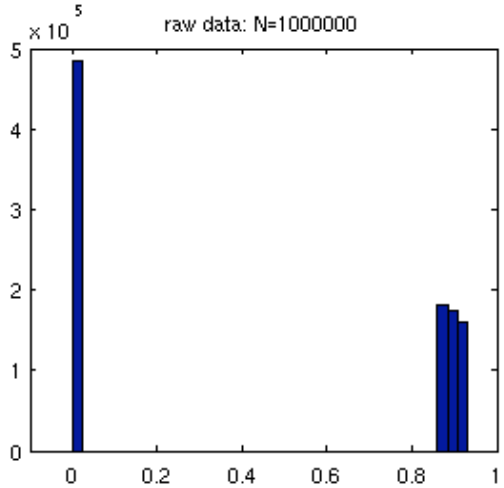


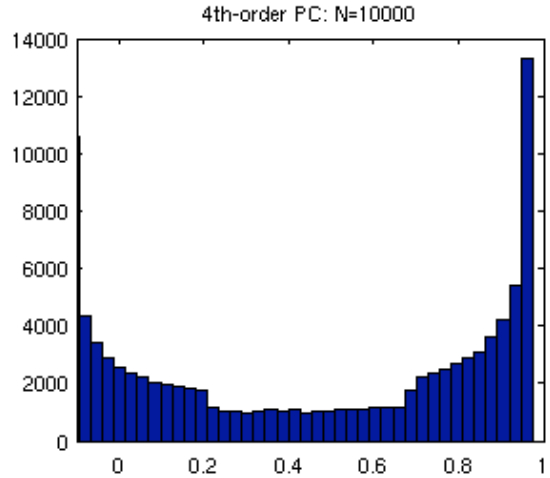
u **Q** **uQ ~ P**

Which is much smoother than u

Discontinuity in Probability Space

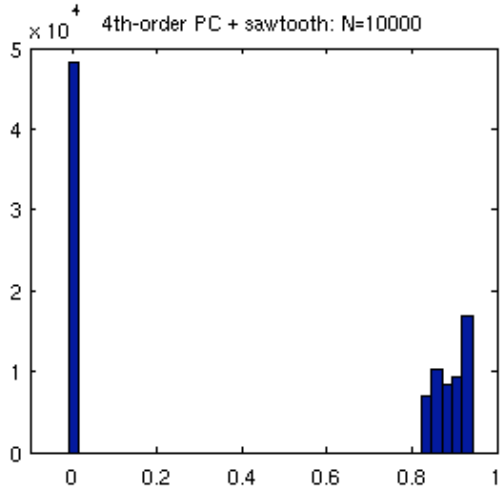
MC

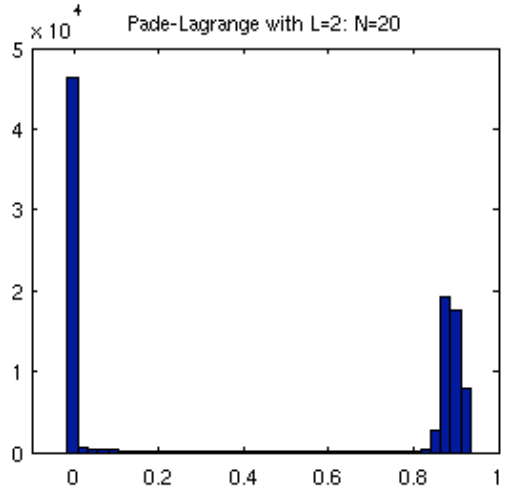




PC (4)

PC (4) + Sawtooth

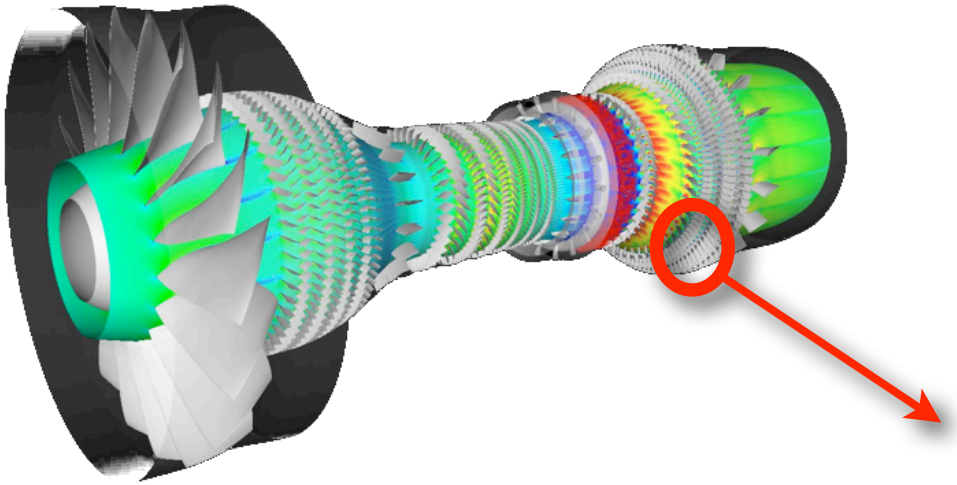




PL (2)

On-going Work

- Extension of the PL-expansions in multiple stochastic and physical dimensions
- Robust choice of the denominator polynomial order



Turbine Blades Heat Transfer