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Computational Mathematics

Date: 4 March 2013

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2013 AFOSR SPRING REVIEW



NAME: **Fariba Fahroo**

BRIEF DESCRIPTION OF PORTFOLIO:

Discover Mathematical Algorithms and Develop Computational Techniques that Provide More **Accurate, Reliable, and Efficient** Algorithms for Modeling and Simulation and Design of Complex Systems for the U.S. Air Force with radical cost and turn-time improvements.

LIST SUB-AREAS IN PORTFOLIO:

➔ **Multi-Scale Modeling** (*materials, plasma, structures, fluids, combustion*)

➔ **Multi-Physics Modeling** (*fluid-structure interactions, particle-fluid models*)

➔ **Uncertainty Quantification**

➔ **Multidisciplinary Optimization and Control** (*Design Under Uncertainty*)

New Emphasis on Scalable Algorithms in All These Sub-Areas



Comp Math Transformational Opportunities for the AF



Goal: Simulation, Analysis and Design of complex systems with radical cost and turn-time improvements

Needs for Computational Math: Support for Accurate, Reliable, and Efficient novel, mathematically sound, and verified algorithms for complex AF applications such as in plasma, structures, combustion, fluids, and so on.

AF Examples: 1) Simulations of High Power Microwaves (Dr. Luginsland)

– Need for 3D, high-fidelity, parallel modeling of high energy density fields and particles in complex geometry --- AFOSR comp math support

2) “Digital Twin” (Dr. Stargel): Real Time, High-Fidelity Operational Decisions for Individual Aircraft Enabled by Tail Number Health Awareness : Need for Material Scale modeling, Deterministic Multiscale Modeling, Uncertainty quantification – Key research areas in comp math supported for several years.

3) Turbulence Combustion (Dr. Li): Need for new numerical and mathematical approaches for multiscale, multiphysics modeling – Key research area in comp math

4) Aerospace Materials for Extreme Environments (Dr. Sayir): Need for theoretical and computational tools that aid in the discovery of new materials and Mathematics to quantify the microstructure --- A new research thrust



Transformational Opportunities for Computational Math



Predictive High-Fidelity Simulations for AF Applications

- More computing power based on emerging heterogeneous computing architecture BUT *computing power isn't everything*
- **Challenges** : Issues with system **Power**, Slower growth in **Memory** bandwidth, Cost of **data movement**, Slower growth in clock rate and move to **Concurrency** of higher number of nodes and threads, Slower growth in **I/O bandwidth**, **Resiliency and Reliability** of the computing systems

We Need Fundamental Paradigm Shifts in Algorithms, Software, Architecture Design

- **2 Basic Research Initiatives in 2012 → Ultra-scale Algorithms(with Dr. Luginsland), and Co-Design (with Drs. Luginsland, Smith, Stargel)**
- For Co-Design, the emphasis was on integration of research threads into a coherent agenda for **specialized**, high-performance computing architectures for Air Force and DoD applications.
- For Ultra-Scale Algorithms the focus was on mathematical aspects of scalable solvers with emphasis on **parallelism across scales (spatial and temporal)**, high-order discretization, and multi-level domain decomposition techniques.



Portfolio's Focus Areas and Outline of Research Highlights



- **High-Order Methods of Accuracy**(the sole funding agency to support these methods across various application areas such CFD, Structures, Plasma, Combustion) :
 - An interplay of Efficiency ,Accuracy and Robustness---- Serious need for mathematical development of these methods for capturing complex multiscale physics in an accurate AND efficient way
 - **Highlight of a CFD effort**
 - **Highlight of a Combustion effort**
- **Multiscale Methods: Materials** – need for more mathematical and computational techniques for bridging the scales
- **Uncertainty Quantification:** Need for more mathematics in modeling and analysis of stochastic phenomena
 - **Design Under Uncertainty -- a 2012 BRI topic**
 - **Bayesian Framework for UQ** → **a MURI 2012 in Material Science**
 - **Scalable Algorithms for Inverse Problems**

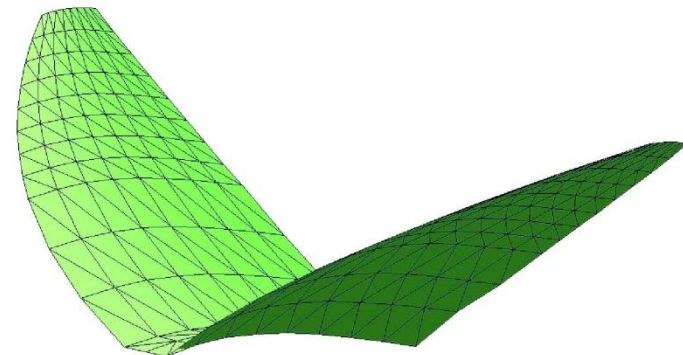


A High-Order IMEX Scheme for FSI

Persson (UC Berkeley)



- Many important problems require predictions of **fluid-structure interaction (FSI)**:
 - Oscillatory interactions in engineering systems (e.g. aircraft, turbines, and bridges) can lead to failure
 - The blood flow in arteries and artificial heart valves is highly dependent on structural interactions
- Two main numerical approaches for the coupling:
 - Fully coupled (monolithic): Solve the fluid/structure equations simultaneously. Accurate, but requires specialized codes and solvers are often slow.
 - Weakly coupled (partitioned): Use standard solvers for fluid/structure and apply a separate coupling scheme, often together with sub-iterations. Efficient and simple, but issues with accuracy and stability.
- **Approach:** Use Implicit-Explicit (IMEX) schemes to obtain high-order accuracy without coupled solvers or iterations
- Using high-order spatial DG and FEM schemes for the fluid and the structure, up to 5th order of temporal accuracy with the IMEX scheme is obtained

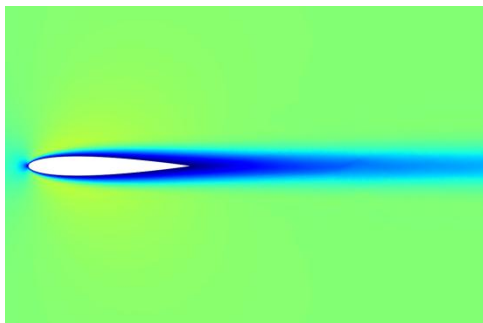
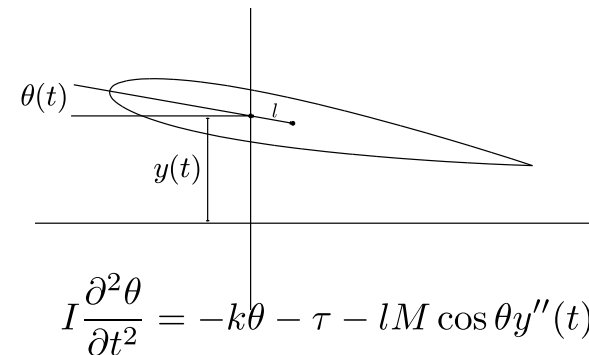




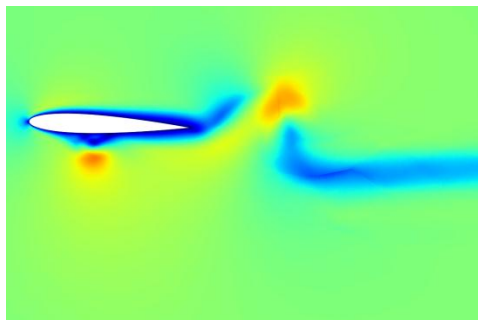
Benchmark Airfoil System



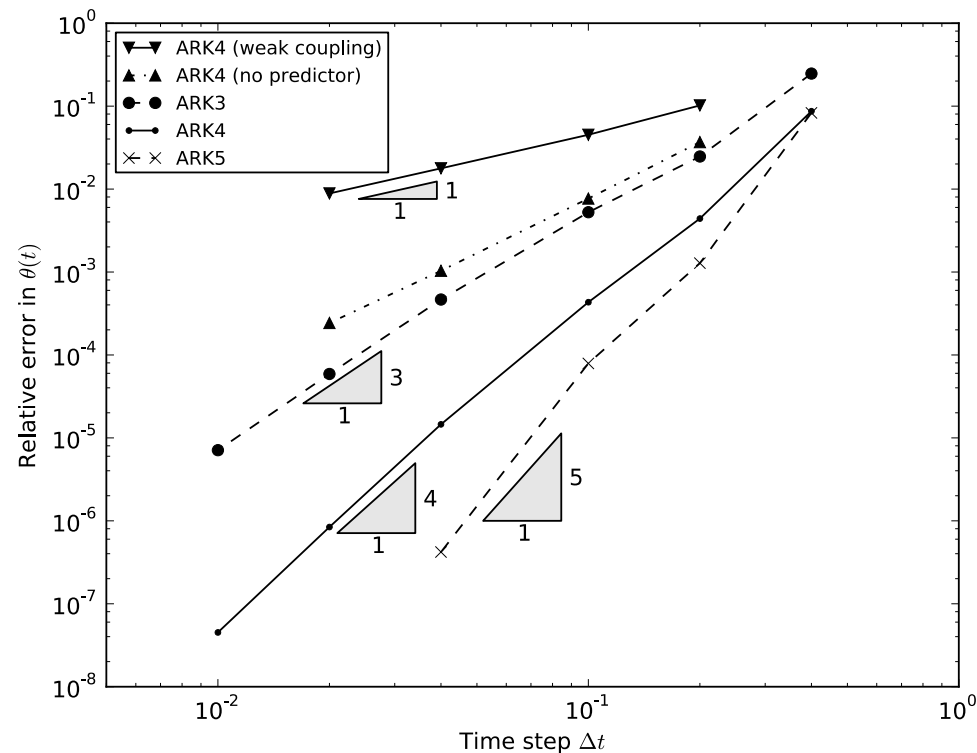
- High-order DG for Navier-Stokes, ALE for moving domain
- Rigid pitching/heaving NACA 0012 airfoil, torsional spring
- Up to 5th order of convergence in time
- Without the predictor, at most 2nd order of convergence



$t = 0.0$



$t = 1.2$

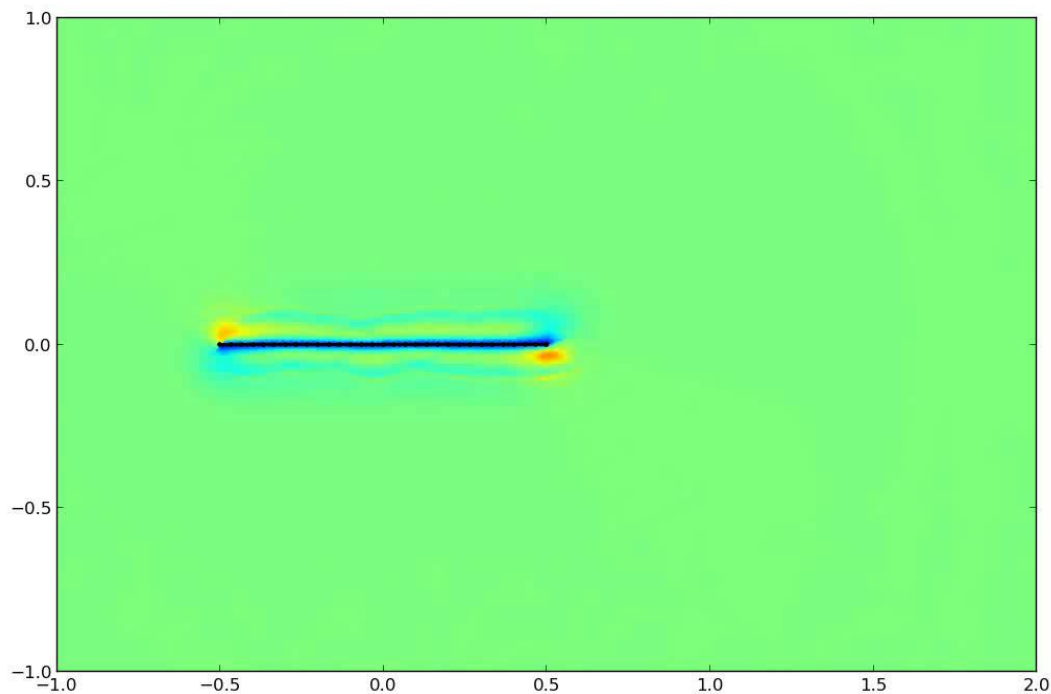




Fluid/Membrane Interaction



- Hyper-elastic neo-Hookean membrane with viscous, fluid-like, dissipation
- Membrane ends are held fixed but allowed to rotate
- Fluid has 20 degree angle of attack and Reynolds number 2,000
- Implicit schemes easily handle complex behavior with large time-steps





Flame Roll Up in a Vortex: Overview

Mitchell D. Smooke --- Yale University



- Optimal numerical methods for chemically reacting flows will ultimately have to be both **locally adaptive** and **high order**
- **Diffusion Flame-Vortex Interaction**
 - Canonical configuration facilitating a first-principles understanding of aspects of turbulent combustion (e.g., flame stretch, local extinction, soot production)



Hsu, et al., *Phys. Fluids A* (1993)

- **Simplified Flame-Vortex Models**

- Convection-diffusion-reaction equations with imposed flow field
- One-step or multi-step finite-rate Arrhenius chemistry
- Variable mechanical timescale related to a vortex Reynolds number
- Benefits of simplified models:
 - Faster development of tailored numerical methods for complex problems
 - Imposing the flow facilitates joint theoretical and computational work

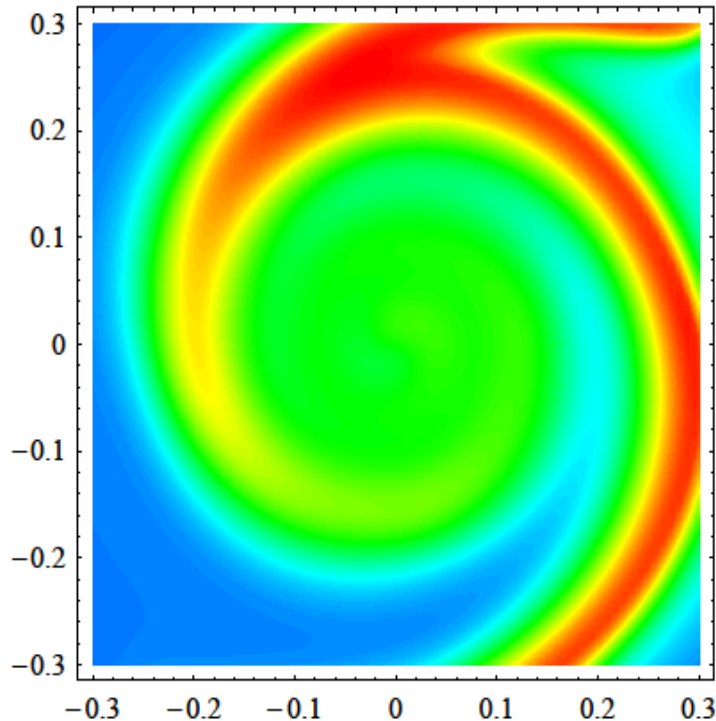


Flame Roll Up in a Vortex – $Re = 600$

Conventional method under grid refinement



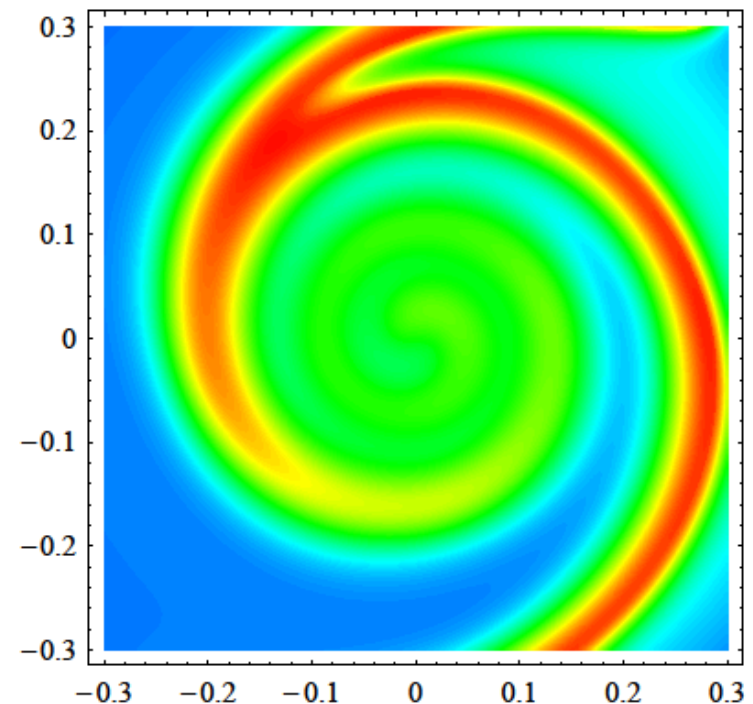
LO, base grid, $t=3.00d-4$



Spatial discretization

- Grid: quasi-uniform, $\Delta x \approx 0.008$
- Order: 1st (upwind scheme)
- CPU factor: 1

LO, refined grid, $t=3.00d-4$



Spatial discretization

- Grid: quasi-uniform, $\Delta x \approx 0.004$
- Order: 1st (upwind scheme)
- CPU factor: 15.3

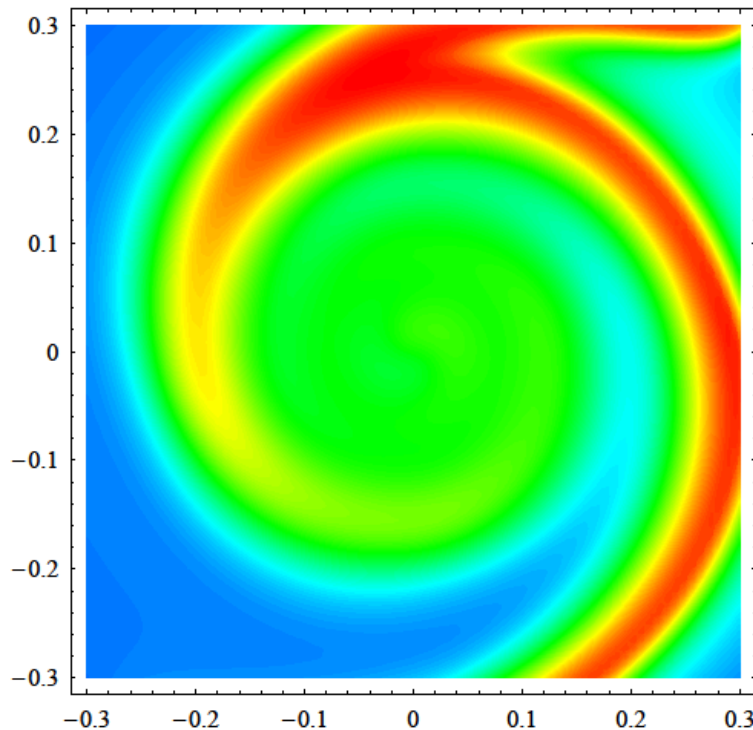


Flame Roll Up in a Vortex – $Re = 600$

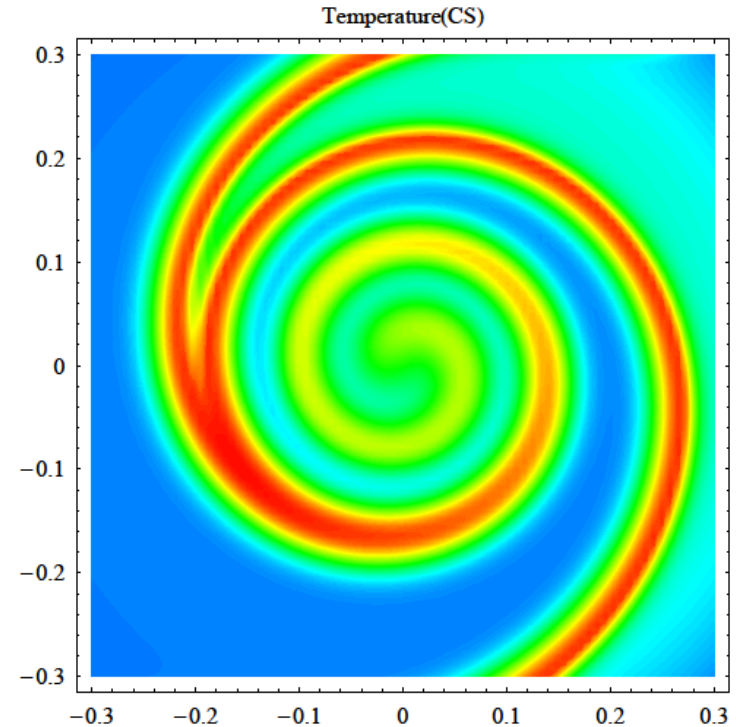
Conventional vs. implicit-compact method



LO, $t=3.00d-4$
Temperature(LO)



CS, $t=3.00d-4$
Temperature(CS)



Spatial discretization

- Grid: quasi-uniform, $\Delta x \approx 0.008$
- Order: 1st (upwind scheme)
- CPU factor: 1

Spatial discretization

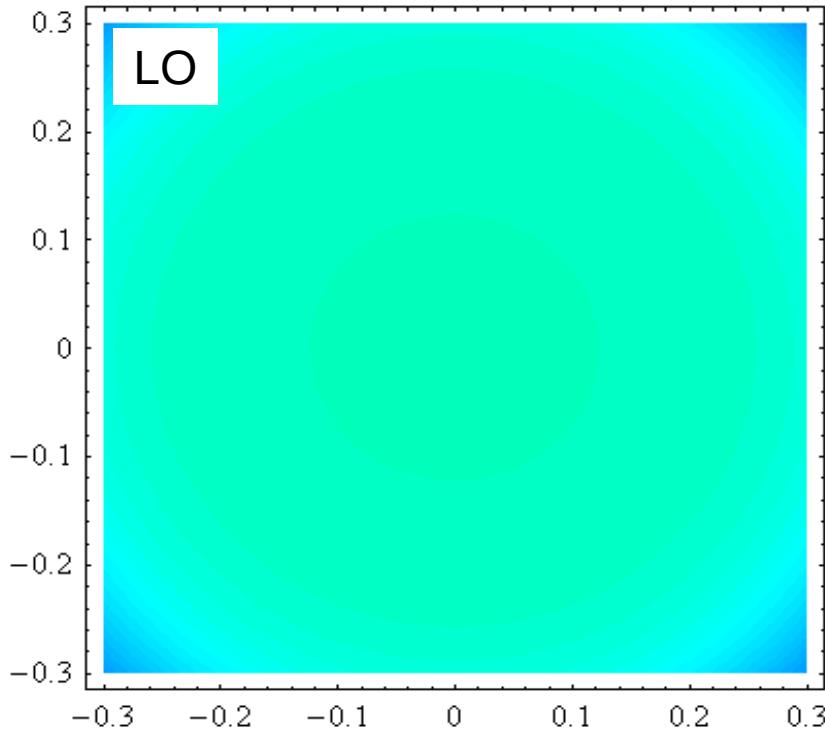
- Grid: quasi-uniform, $\Delta x \approx 0.008$
- Order: 4th – 6th (compact scheme)
- CPU factor: 1.2



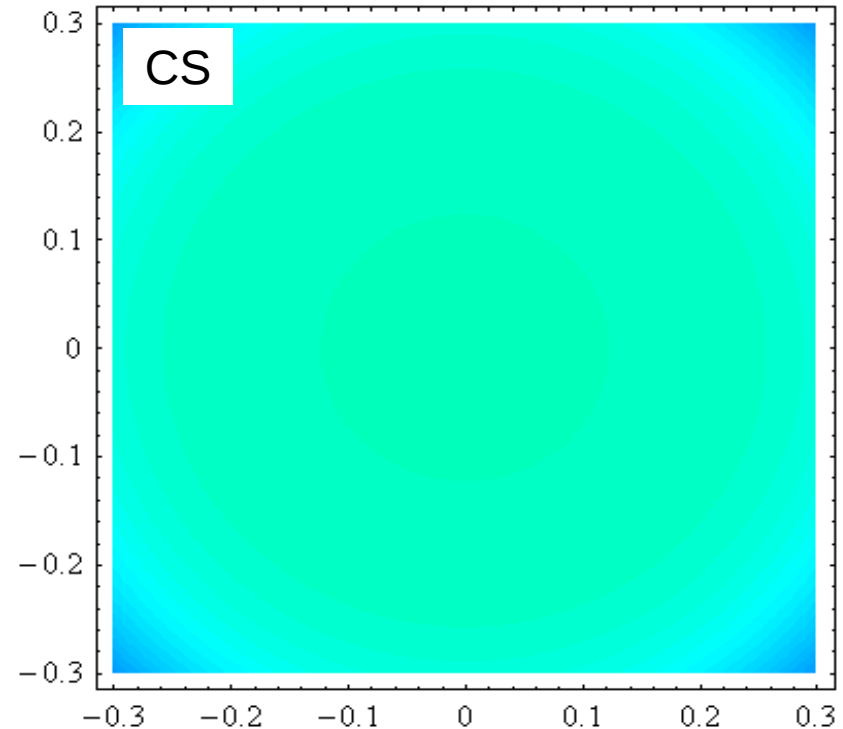
Flame Roll Up in a Vortex – $Re = 600$



$t=0.00d-4$



$t=0.00d-4$



Spatial discretization

- Grid: quasi-uniform, $\Delta x \approx 0.008$
- Order: 1st (upwind scheme)
- CPU factor: 1

Spatial discretization

- Grid: quasi-uniform, $\Delta x \approx 0.008$
- Order: 4th – 6th (compact scheme)
- CPU factor: 1.2



Multiscale Modeling and Computation for Materials



- **New research thrust** – New core projects, a MURI 2012 in Managing Data Complexity in Predictive Material Science, and a COE on Integrated Computational Material Science and Engineering (**ICMSE**), 2013 MURI on Peridynamics
- *“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations that are much too complicated to be soluble.”* P. A.M. Dirac, Proc. Royal Soc. 123 (1929), 714-733
- Dirac’s quote true today, and relevant. Most new technologies of interest to the Air Force can be analyzed by equations known (in 1929) to be accurate and predictive, but we are unable to do it: **The discipline that is needed most: Computational Mathematics**
- **Approach:**
 - 1) By evaluating all competing multiscale methods on the basis of rigorous error analysis and systematic numerical testing
 - 2) New multiscale approaches for design of new materials – Objective Structures

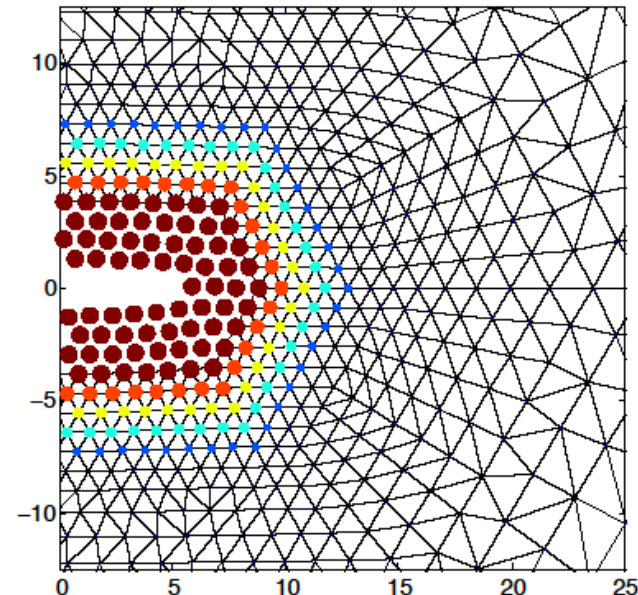
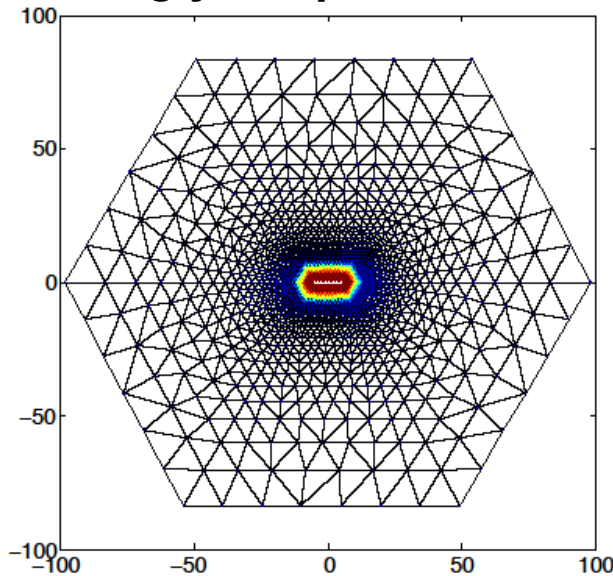


Multi-scale Materials Computing



Mitch Luskin (Univ of Minnesota)

- Multiscale computational methods for materials need to be validated by benchmark numerical experiments designed and evaluated on the basis of theoretical error analysis.
- **Theory-based benchmarking for material failure**
- Crystal defects such as grain boundaries, cracks, and dislocations play a central role in determining material behavior for Air Force applications. The key difficulty in simulation is that crystal defects affect elastic fields far beyond their immediate atomistic neighborhood and give rise to strongly coupled **multi-scale** systems.

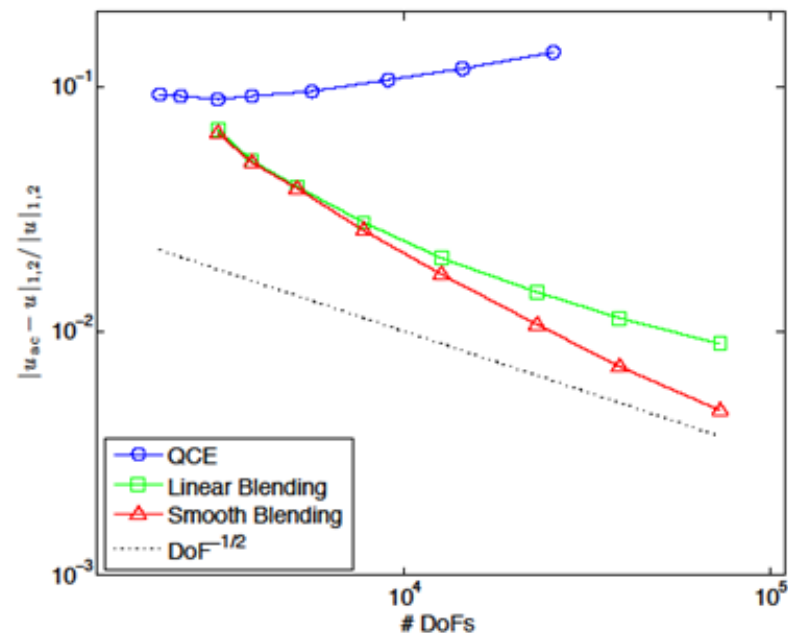
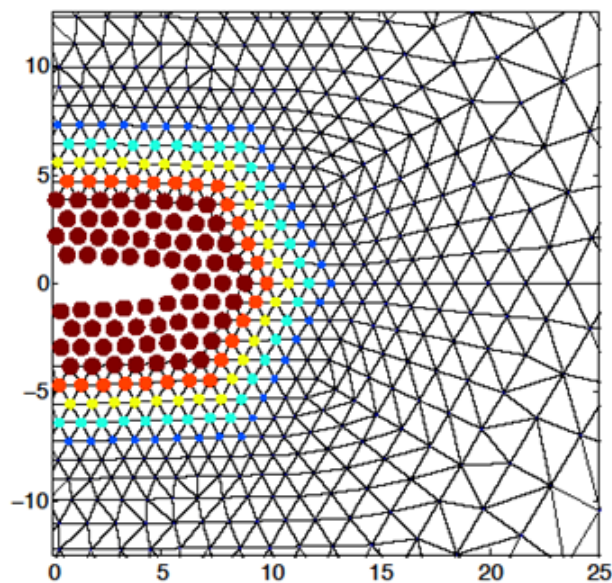




Computational Complexity of Defects



- Identify the **quantity of interest** (material failure, strength, toughness, etc.) and utilize multiscale error analysis to determine the **complexity** (number of degrees of freedom) to compute the quantity of interest to the required tolerance.
- The Blended Quasicontinuum Energy is the first atomistic-to-continuum energy for many-body interactions and multi-lattices with a controllable error. Numerical results for a microcrack are exactly predicted by theoretical complexity estimates.





Multiscale Methods for Materials,

Kaushik Dayal (CMU) & Richard D. James (UMN)



- Approach: use the underlying **invariance*** of quantum mechanics as the main principle for simplification

* Frame-indifference and permutation invariance

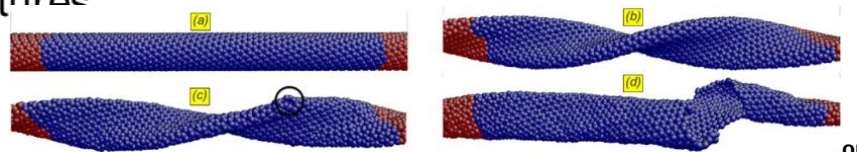
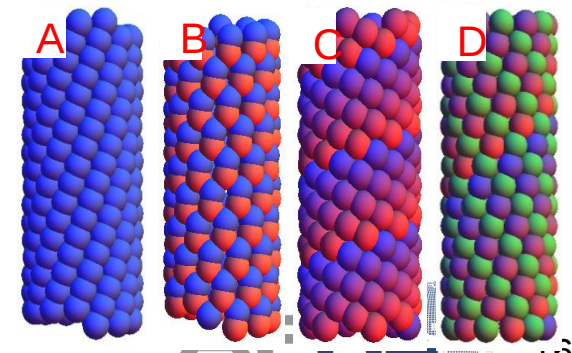
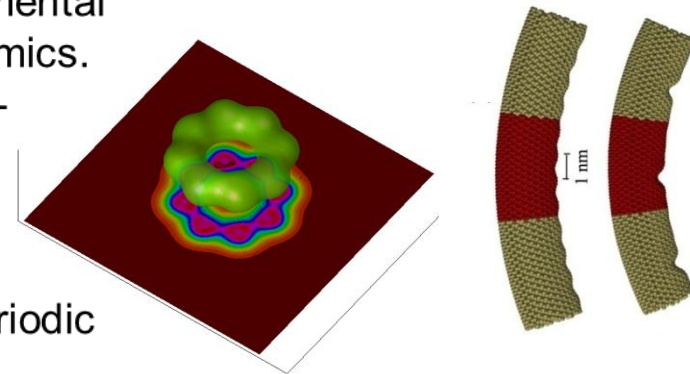
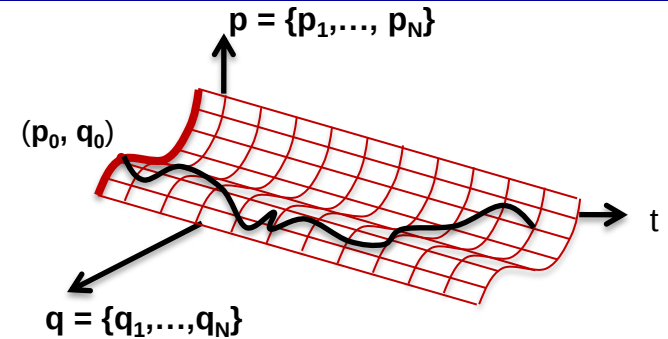
- Some current implementations of this idea

- **Objective molecular dynamics.** Based on a fundamental invariant manifold of the equations of molecular dynamics.

TO: a method for simulation of macroscopic, far-from-equilibrium fluid flows of **any fluid** using only a few “simulated atoms”. **TO:** a method for simulation of **nonequilibrium properties of nanostructures**

- **Objective DFT:** An advanced DFT method for nonperiodic nanostructures. **TO:** predict collective properties (**ferromagnetism, ferroelectricity, flexoelectricity**, etc.) of nanostructures from first principles

- **Objective self-assembly:** **TO:** predictive **design** of functional macromolecules to enable tailored self-assembly of nanostructures

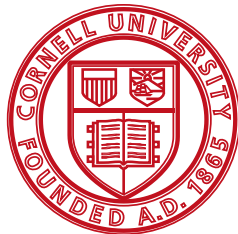




Uncertainty Quantification Efforts – MURI '09 and Core Projects



- **Uncertainty Quantification (UQ):** The process of quantifying uncertainties associated with model calculations of true, physical Quantities of interest (QOIs) with the goal of accounting for all sources of uncertainties and quantifying the contributions of specific resources to the overall uncertainty. *From “Assessing the Reliability of Complex Models” – NRC report in 2012*
- **MURI Effort:** To develop rigorous **theory, algorithms and software** for UQ management in a **computationally scalable way**. – **A unique effort in terms of its breadth of topics and approaches, and its impact on the field.**
- 5 Research Thrusts:
 - Mathematical Analysis and Multiscale Formulation of SPDEs
 - Numerical Solution of SPDEs
 - Reduced-Order Modeling
 - **Design & Control Under Uncertainty***
 - **Multiscale Property Estimation****





Research Highlights



- **Mathematical Theory:** Quantization-renormalization of SPDEs; New evolution equations for joint-pdf of SPDEs; Nonlinear Malliavin calculus
- **Reduced Basis Methods (RBM):** Integral equations and multi-scattering problems; Robust design, parameter estimation, and model uncertainty
- **Adaptive ANOVA:** Convergence theory; Parameter compression and RBM; Fluid flows, porous media, multi-scattering
- **Bayesian Framework:** Coarse-graining; Active learning + SPDEs; Adaptive SMC, dependent random variables, Model uncertainty in inverse problems
- **Design Under Uncertainty: Multi-Fidelity approaches**
- **Numerical SPDEs:** Data-driven stochastic multiscale method, Multiscale multilevel MC, **Probabilistic graphical models**, Long-time integrators of SPDEs
- **Software:** MEPCM library; Reduced basis method libraries - RBOOMIT, RBAppMIT; **Akselos, Inc**; Random poly-crystals - RPCrystal



Design Under Uncertainty

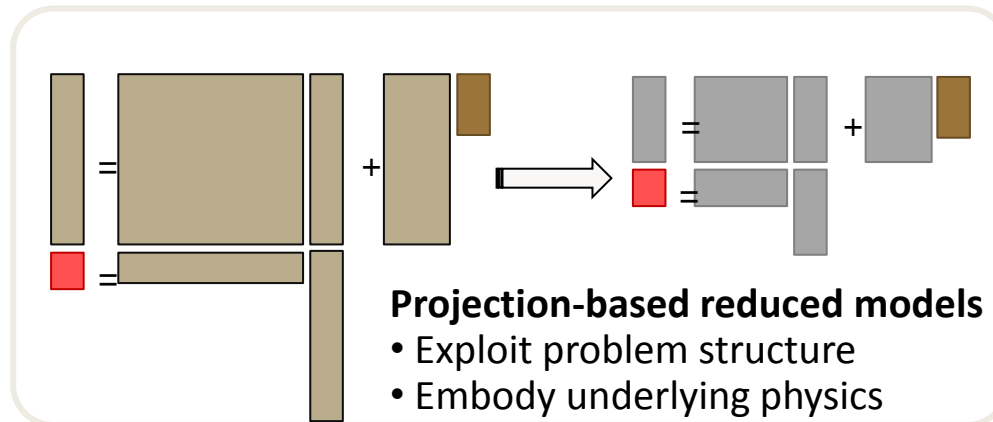
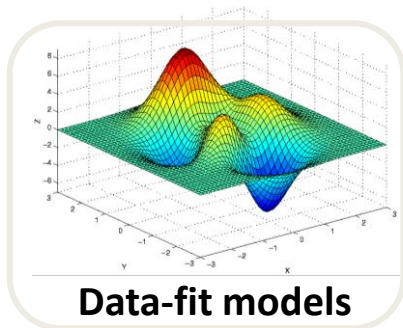
P Huynh, C Lieberman, L Ng, K Willcox (PI)



Multifidelity approaches: How should we best use all available models *and data* in concert to achieve:

Better decision-making (optimization, control, design, policy)

Better understanding of modeling limitations



Research objectives: Develop and apply new multifidelity methods for design under uncertainty

Multifidelity model construction (certified reduced basis models)

Quantification of uncertainty and model fidelity (how good is a model for a given purpose)

Multifidelity model management (which model to use when, convergence guarantees, model adaptation, model-data fusion)

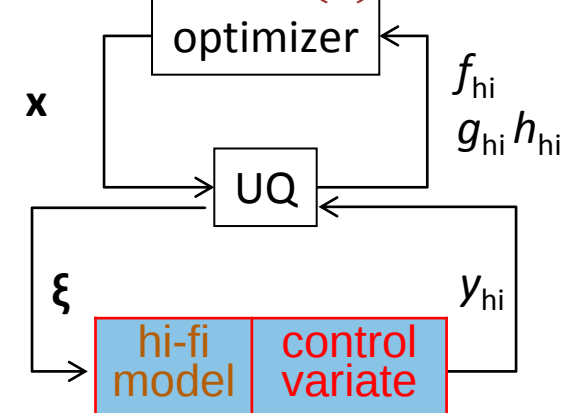
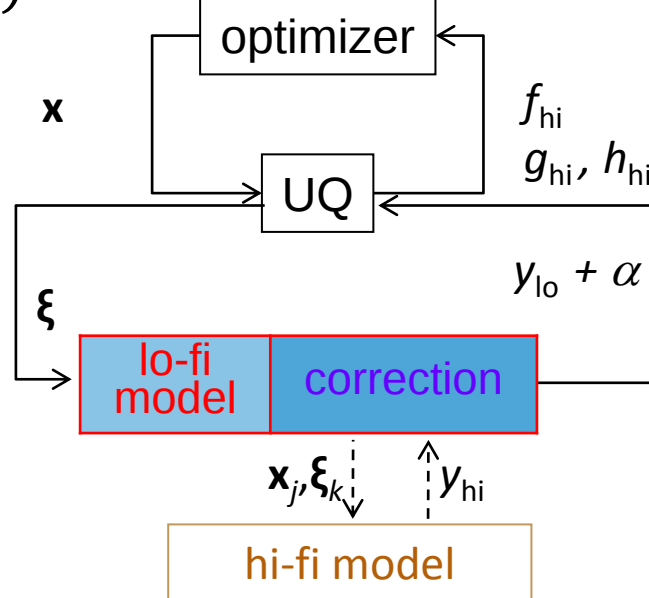
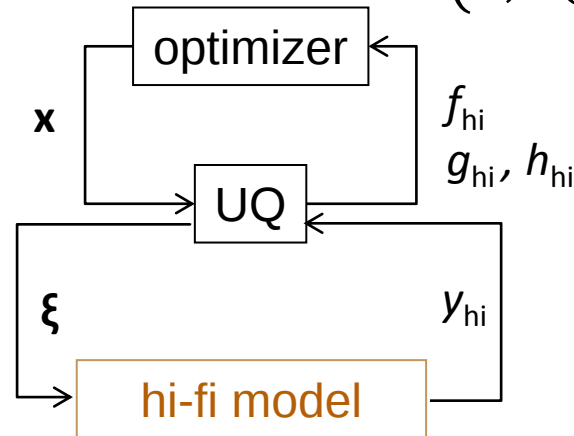


Multifidelity Optimization under Uncertainty



$$\begin{aligned} \min_x & f(x, s(x)) \\ \text{s.t. } & g(x, s(x)) \leq 0 \\ & h(x, s(x)) = 0 \end{aligned}$$

Design variables x
Uncertain parameters ξ
Model outputs $y(x, \xi)$
Statistics of model $s(x)$



Traditional OUU methods

- Require thousands of high-fidelity model evaluations at each optimization iteration

Adaptive corrections: Exploit model local accuracy

- Computed using occasional recourse to high-fidelity model

Control variates: Exploit correlation between high- and low-fidelity models

- Reduce high-fidelity samples needed at optimization iterations

Surrogates constructed to have desirable properties (e.g., for convergence)



Multifidelity methods lead to large computational savings, making optimization under uncertainty tractable



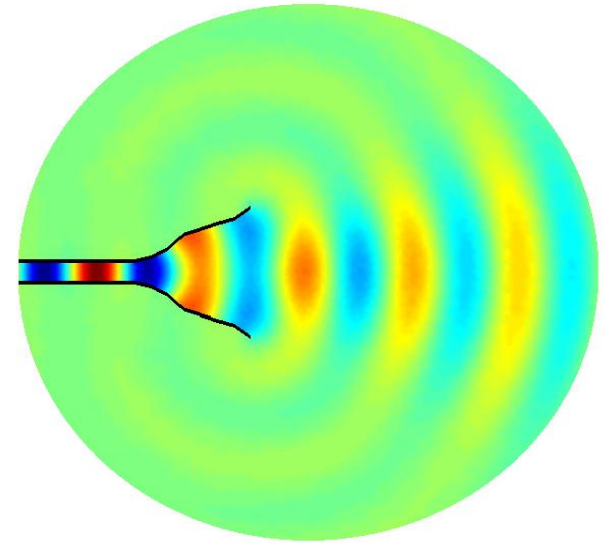
Design under uncertainty of an acoustic horn.

Decision variables: horn geometry, b

Uncertainty: wavenumber, wall impedances

Output of interest: reflection coefficient, s_r

$$\min_b \mathbb{E}[s_r] + \sqrt{\text{Var}[s_r]}$$



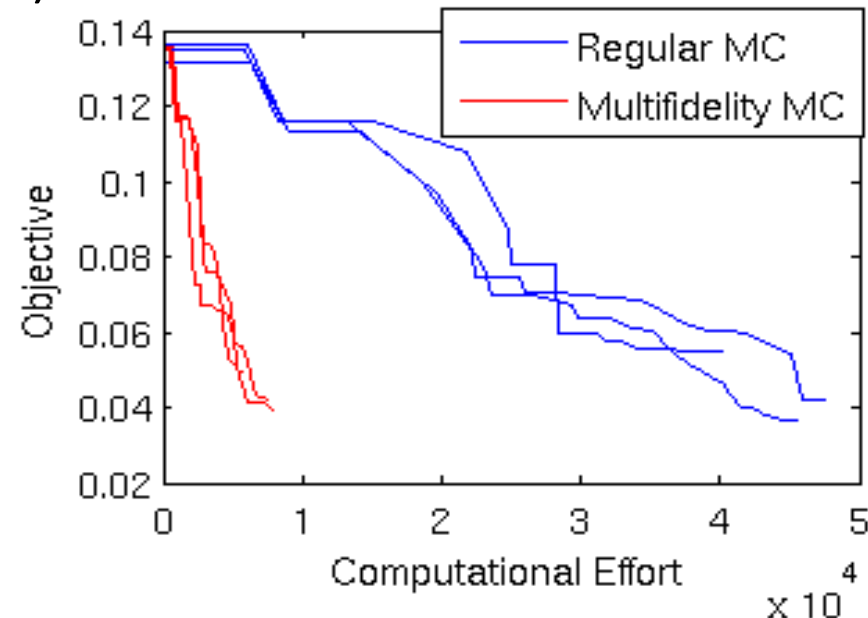
Multifidelity models:

Finite element model (35,895 states)

Reduced basis model (30 states)

Multifidelity approach:

Control variates



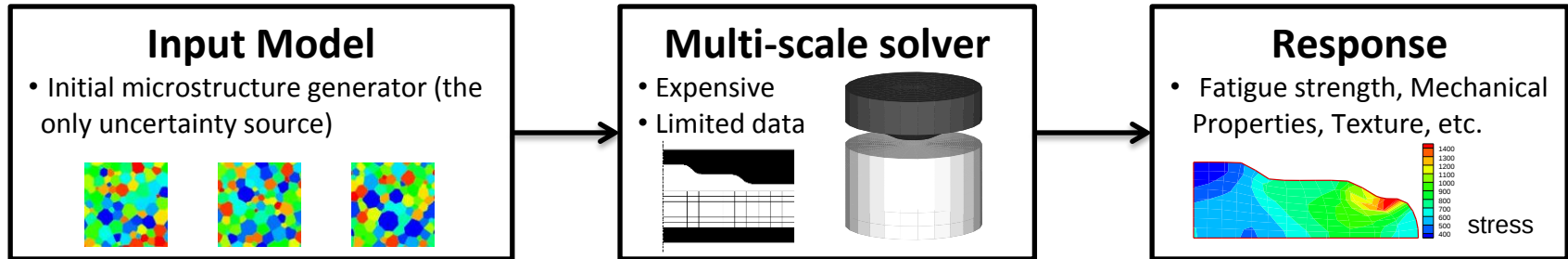
	Equivalent number of hi-fi evaluations
Regular Monte Carlo	44,343
Multifidelity Monte Carlo	6,979 (-84%)



Uncertainty propagation using probabilistic graphical models



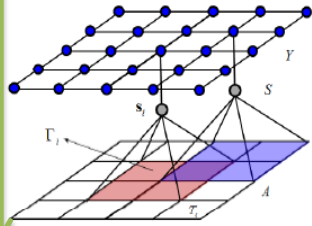
Application: Multiscale aircraft engine disk forging problem



Probabilistic Graphical model framework

Structure design

- Decompose the joint distribution on a graph using localized potentials

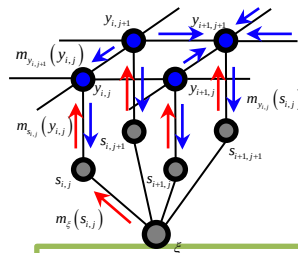


Model Reduction

- Localized model reduction scheme

Inference

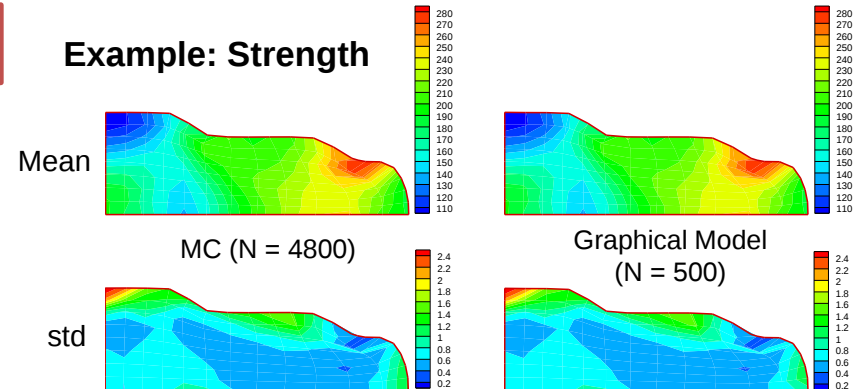
- Infer the marginal distribution of the response (calculate the statistics)



Graph Learning

- Learning all the unknown parameters in the graph (EM)

Example: Strength



Surrogate model

New Observation of the input

Localized Input Model Reduction

Inference

- Infer the conditional distribution



Ultra-Scalable Algorithms for Large-Scale Uncertainty Quantification in Inverse Wave Propagation



G. Biros, T. Bui-Thanh, L. Demkowicz, O. Ghattas, J. T. Oden, G. Stadler (UT-Austin)

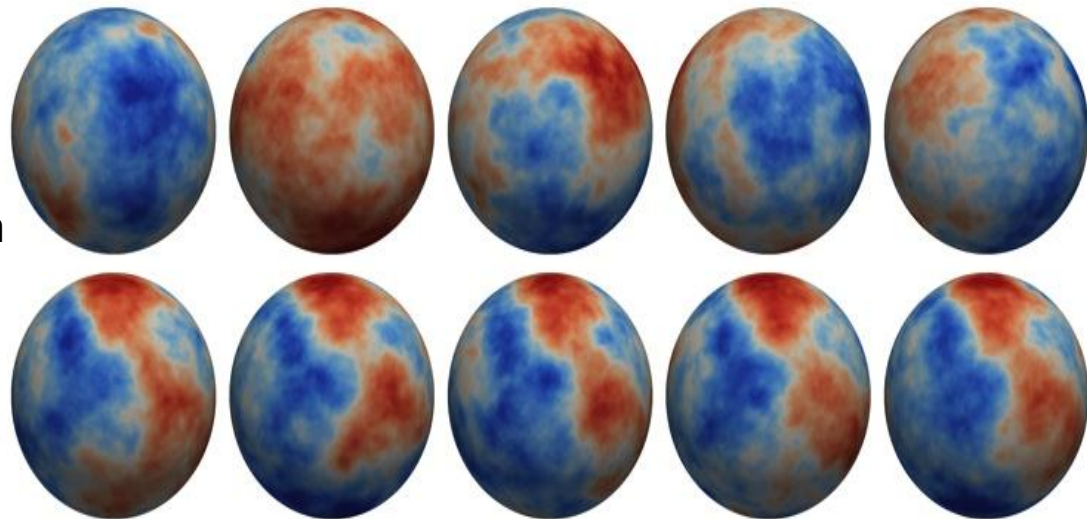
- **Problem:** Address **inverse problem** (aka calibration or parameter estimation) in the framework of **Bayesian inference**: given a model with uncertain parameters and noisy observations of model outputs, estimate the model parameters and quantify uncertainties in the estimate
- Current state-of-the-art Markov chain Monte Carlo (MCMC) methods **are prohibitive**
- The issue with current MCMC methods : their **inability to exploit problem structure**
- The overarching goal is to overcome the “curse of dimensionality” by **exploiting the structure of the posterior probability density function (pdf)**
 - Insight: **Hessian operator** of the parameter-to-observable map defines local correlation structure of posterior pdf, and can be used **to accelerate MCMC sampling**
 - Construct **adjoint-based low-rank approximation of Hessian** to make tractable
 - Develop theory at **infinite dimensional level**, ensure mesh-independence of finite dimensional discretization
 - Develop **parallel implementations** that scale to the limits of modern supercomputers



Transformational Opportunities



- Tailor theory to structure of **inverse wave propagation** problems
 - Estimate heterogeneous material properties from scattered waves
- Preliminary results demonstrate **1000X speedups** on small problems relative to conventional MCMC methods; permit solution of large problems that were **previously intractable**
- **Million-parameter example** from acoustic wave propagation: infer global heterogeneous wave speed from surface observations of seismic waveforms
 - 1.07 million uncertain parameters
 - 630M states, 2400 time steps
 - Observations only in N Hemisphere
 - 100K cores on Jaguar Cray XK6
 - 2000X effective dimension reduction
 - Top row: samples from the prior
 - Bottom row: samples from posterior
 - Differences between rows indicate knowledge gained from data





Summary



- Continued support of **high-order methods** in multiscale and multiphysics modeling, support in **time-integration** methods
- Continued emphasis on **UQ** and **V&V**
 - New approaches for reducing the curse of dimensionality (**PDF methods**), Optimal Statistical Estimators, Sampling methods, **Design under Uncertainty**
- Algorithms for multi-core platforms: GPU computing
- Emphasis on **scalability** of algorithms for ultra-parallel large scale computing
- Understanding the impact of **geometric discretization** on the fidelity of the analysis and computation