# Poster Blitz Session 2

Posters number 48 to 97

Regency Ballroom A

# Fast and Robust Computation of Stochastic Transcendentals

Kevin Long and Kaleb McKale (Texas Tech University)

## Transcendental functions of polynomial chaos expansions (PCE)

- Problem: compute PCE representation of $f(x(\xi))$, where $x(\xi)$ is a PCE
- Existing methods: line integration, sparse quadrature
- New method: modified arithmetic-geometric mean iteration applied to PCE
- Requires only arithmetic and square root operations
- Converges in a few iterations

## Borchardt-Gauss iteration with Carlson acceleration

$$a_{n+1} = \frac{1}{2}(a_n + g_n)$$

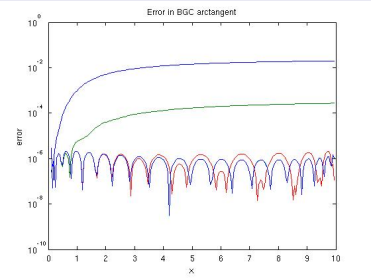
$$g_{n+1} = \sqrt{a_{n+1} g_n}$$

$$B(a_0, g_0) = \lim_{n \to \infty} a_n$$

- Any inverse transcendental (*e.g.* log, arctan) can be computed via BG iteration
- For example: $\log(x) = (x-1)/B(\frac{x+1}{2}, x)$
- BG iteration with Carlson acceleration: very fast convergence (contraction by $\sim 10^{-3}$ per iteration)

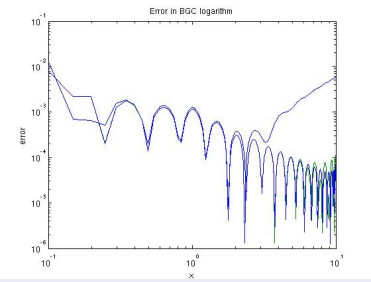
## BGC Computation of PCE Arctangent

- Convergence in 4 BGC iterations




## BGC Computation of PCE Logarithm

- Convergence in 3 BGC iterations

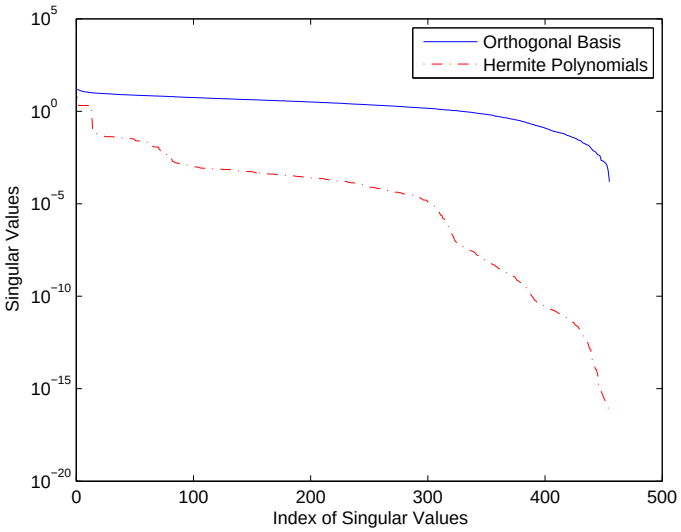


# Poster #49 — Fred J. Hickernell, IIT
# Efficient Construction of Surrogates for Computer Experiments with Gradient Information

- Realistic nuclear reactor simulations take a lot of time.
- Need a cheap approximation for $f : \mathbb{R}^d \to \mathbb{R}$ from computer experiment data.
- Adjoint methods provide $\nabla f(\boldsymbol{x}_i)$ ($d$ more data) in addition to $f(\boldsymbol{x}_i)$ for $\approx 100\%$ more cost.
- Use a polynomial basis for regression that is orthogonal with respect to

$$\langle f, g \rangle_{\mathcal{G}} = \langle f, g \rangle_{\mathcal{L}_2} + \sum_{\ell=1}^{d} \frac{1}{\lambda_\ell} \left\langle \frac{\partial f}{\partial x_\ell}, \frac{\partial g}{\partial x_\ell} \right\rangle_{\mathcal{L}_2}$$

  to reduce the condition number of the information matrix.

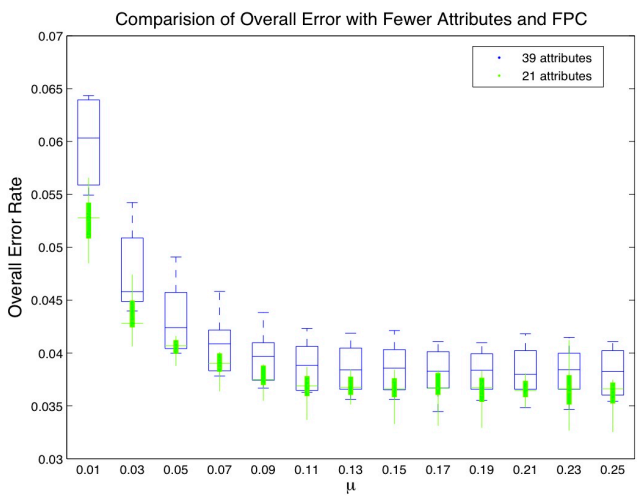



- Choose sample points that are evenly spread (low discrepancy) to control the condition number of the information matrix regardless of model.

# #50 – Orianna DeMasi

# Dimension Reduction Using the Rule Ensemble Machine Learning Method

Orianna DeMasi, Juan Meza, David Bailey




Application on supernova data culls 39 attributes to 21 while decreasing the overall error rate

- Model is a linear sum of rules

$$r_k(\mathbf{x}_i) = \prod_j I(x_{ij} \in p_{kj})$$

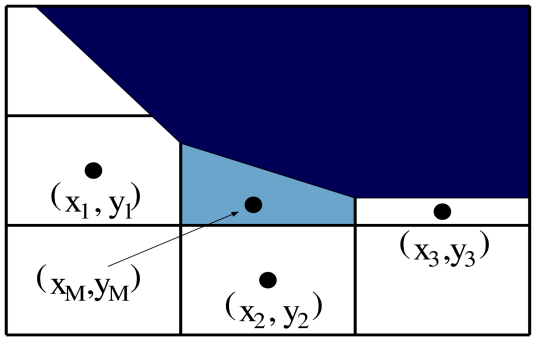
- Consider how to construct rules and weights
- The weight indicates a rule's importance
- Importance of rules used to prune attributes

Poster 51: *Sandra May* and Marsha Berger
Courant Institute, NYU

# Slope Limiters for Finite Volume Schemes on Non-coordinate-aligned Meshes

## Goal:

Construct **gradient** on **cutcell** respecting monotonicity conditions




## Approach:

**Limit** gradient estimate ($D_x$,$D_y$) by scalars $(\phi_x, \phi_y)$ which solve a **Linear Program**

e.g.

$$\max \ \phi_x |D_x| + \phi_y |D_y|$$
$$s.t.$$
$$0 \le \phi_x, \phi_y \le 1,$$
$$\text{for } j = 1, \text{neighbors } (\text{assume } u_M \le u_j):$$
$$u_M + \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix} \cdot \begin{bmatrix} D_x (x_j - x_M) \\ D_y (y_j - y_M) \end{bmatrix} \le u_j.$$

## Result:

+ Ensures monotonicity
+ Adaptable for specific needs

## Family of LP limiters

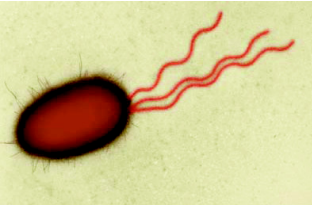
+ Good for Cartesian embedded boundary grids
+ Limits x- and y-slope independently (not scalar)

# Coarse-graining computation of collective swimming in biosuspensions. L. Berlyand, Penn State

PSU Students: B.Haines, S.Ryan, DOE Collaborators: I.Aranson, D.Karpeev (ANL)

Phys. Rev. E **80**, 041922 (2009); Comm. Pure Appl. Anal., (2012), Phys. Rev E **83**, 050904(R) (2011), ARMA (2010)

**Objective:** Develop computational models that reveal mechanisms behind collective swimming. Explain striking experimental results.
**Challenge:** Computationally prohibitive fine scales.



- **Dilute** suspensions - no interactions. Obtained additional term in Einstein's formula for effective viscosity – due to self-propulsion; homogenization, multi-scale analysis.
- **Semidilute**: Add mean field interactions and develop a computational model. Include soft collisions and dipolar interactions - accounts for full range of exp. concentration.
- **Current Work: Beyond mean field**. Capture critical concentration for onset of collective motion, correlations, fluctuations.
- **PDEs with many non-separated scales** Irregular coefficients: classical FEM and homogenization do not work. Designed shape functions that capture scales. Extend to moving fine-grained boundaries, evolving shape functions to track swimming bacteria.

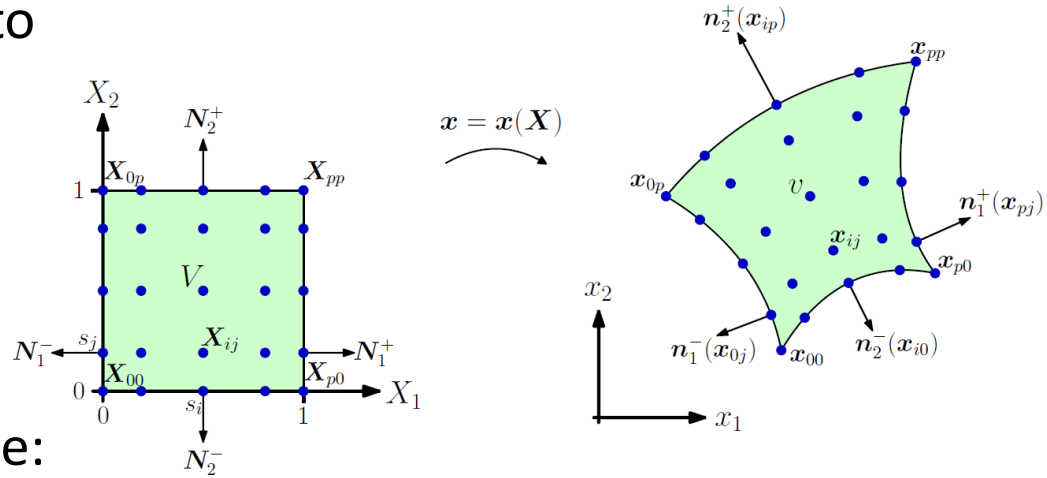
Poster 53: Per-Olof Persson, UC Berkeley, LBNL

# Sparse Line-Based Discontinuous Galerkin Discretizations and Efficient Time-Integration

Map system of conservation laws to a reference element:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0}$$

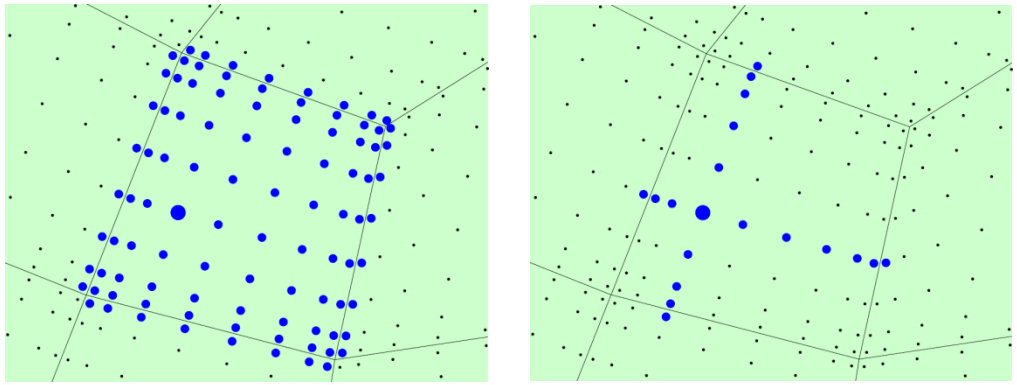
$$J\frac{\partial \boldsymbol{u}}{\partial t} + \nabla_X \cdot \widetilde{\boldsymbol{F}}(\boldsymbol{u}) = \boldsymbol{0}$$

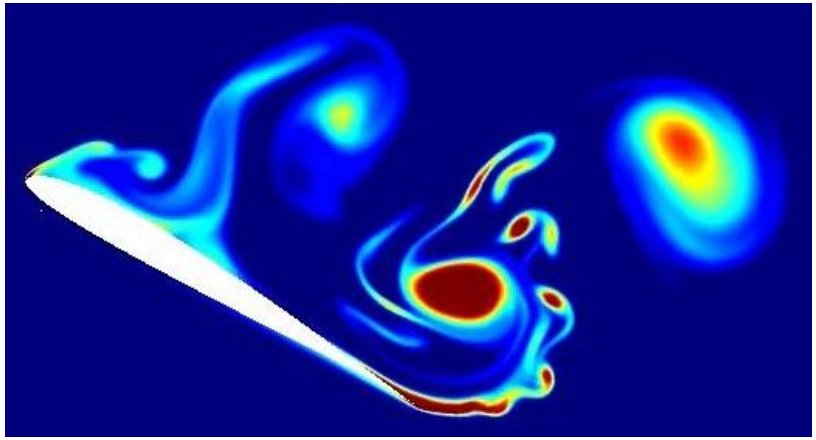



Apply 1-D Discontinuous Galerkin schemes along each coordinate line:

$$J_{ijk}\frac{d\boldsymbol{u}_{ijk}}{dt} + \sum_{n=1}^{3} \boldsymbol{r}_{ijk}^{(n)} = \boldsymbol{0}$$

- Magnitudes sparser Jacobians
- Simple scheme: Only 1-D integrals
- LDG-type second order terms





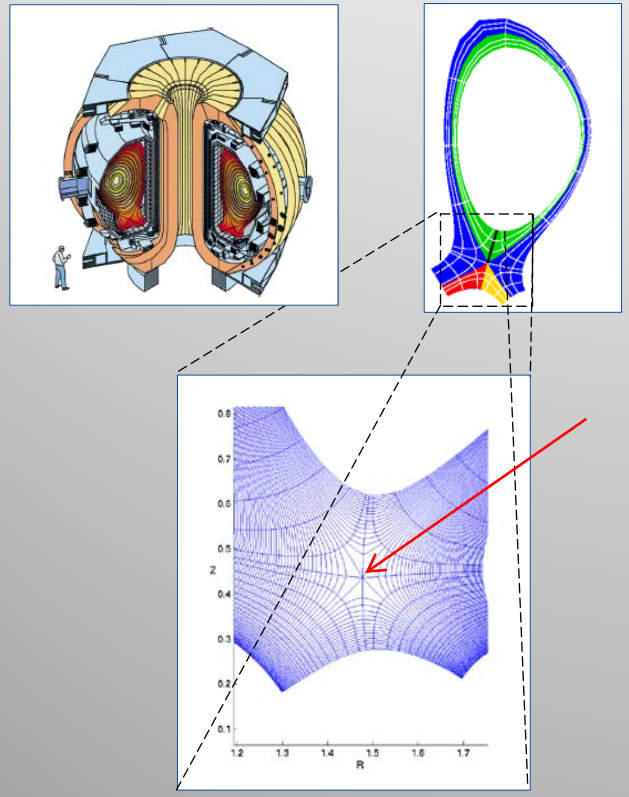
# connectivities / node (3-D hexahedrals)

| Polynomial order $p$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Line-DG connectivities | 10 | 13 | 16 | 19 | 22 | 25 | 28 | 31 | 34 | 37 |
| Nodal-DG connectivities | 32 | 81 | 160 | 275 | 432 | 637 | 896 | 1215 | 1600 | 2057 |

# Poster 54: Milo Dorr
# High-Order, Mapped-Multiblock, Finite-Volume Discretization of Gyrokinetic Systems Near the X Point of a Diverted Tokamak Geometry

Collaborators: John Compton, Jeffrey Hittinger (LLNL), Phil Colella, Peter McCorquodale (LBNL)

Field-aligned coordinates help accommodate strong anisotropy in solving PDEs on edge plasma domains defined by magnetic flux surfaces:




X point:

- Poloidal field component vanishes (no need to stay field aligned)
- Field line projections become progressively kinked, leading to large derivatives in coordinate mappings

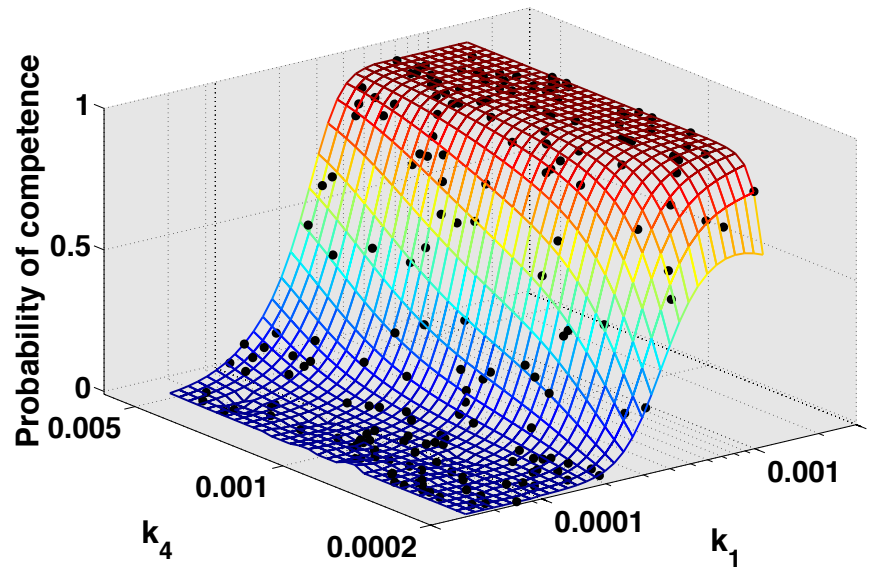
This poster describes how we address this issue in the development of *fourth-order, mapped-multiblock, finite-volume discretizations* of advection operators in this *unique geometry*.

55. Bert Debusschere

# Bayesian Quantification of Uncertainty in Systems with Intrinsic Noise

Khachik Sargsyan, Cosmin Safta, Bert Debusschere, Habib Najm
Sandia National Laboratories, Livermore, CA
{ksargsy, csafta, bjdebus, hnnajm}@sandia.gov

- Goal:
  - Uncertainty quantification in high-dimensional stochastic systems
- Challenges:
  - Large number of parameters, i.e. the curse of dimensionality
  - Intrinsic noise makes sparse quadrature methods infeasible
  - Nonlinear output observables
- Approach:
  - Polynomial Chaos (PC) representation
  - Bayesian inference of PC modes
  - Nearest-neighbor based mixture PC
  - Outcome: *uncertain* response surface



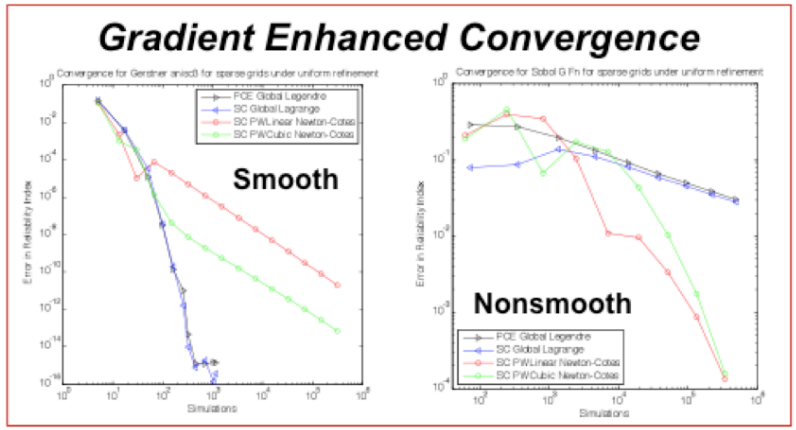

**Mixture PC response surface of competence probability in Bacillus subtilis with respect to two influential rate constants.**

Sargsyan *et al.*, J. Comp. Theor. Nanosci., 6(10), 2009
Sargsyan *et al.*, SIAM J. Sci. Comp., 31(6), 2010
Sargsyan *et al.*, in preparation for Biophys. J, 2011

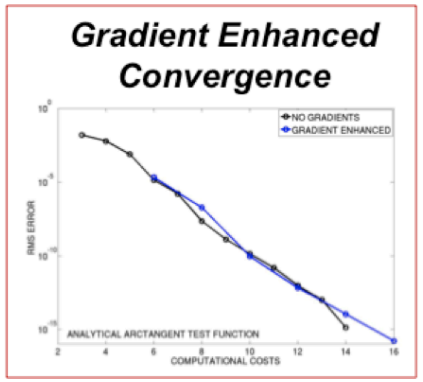
# Large-Scale Uncertainty and Error Analysis for Time-dependent Fluid/Structure Interactions in Wind Turbine Applications

## Uncertainty Quantification Methodology

**The use of gradient evaluations as a enhancement to classic stochastic collocation techniques is one of the main drivers of the algorithmic development**




**As a more flexible alternative to hypercube-based discretization of the parameter space we are considering the Simplex Stochastic Collocation method**




## Research Team


Juan J. Alonso, Gianluca Iaccarino, Karthik Duraisamy, Jeroen Witteveen, Giovanni Petrone, Gart Tang

Michael Eldred, Matthew Barone Stefan Domino

Dongbin Xiu

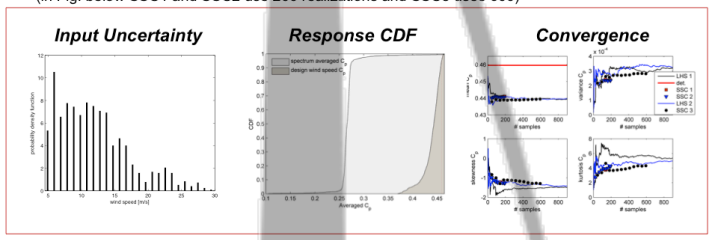
Purdue University

Sandia National Laboratories


## Uncertainty Quantification for Wind Turbine

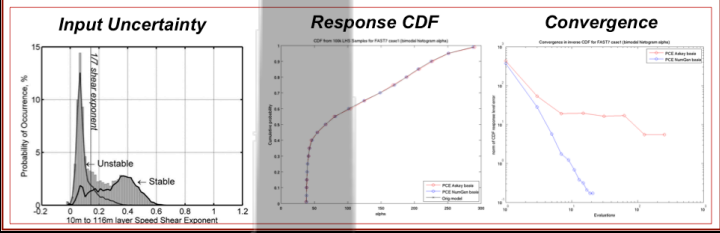
**Evaluation of energy extraction and noise under uncertainty in wind condition (speed) and surface perturbations (dust, bugs)**

- **Input Uncertainty**: Speed velocity as a discrete histogram distribution and geometry perturbations as "assumed" continuous distributions (3 input variables).
- **Output Metric**: Energy extraction (aerodynamic loading) and noise
- **UQ Methods**: LHS and SSC (adaptive with 24/48 realizations added at each iteration)
- **Response function evaluations**: 1k LHS samples for moments evaluation; up to 600 for SSC/PCE (in Fig. below SSC1 and SSC2 use 200 realizations and SSC3 uses 600)




**Evaluation of fatigue under uncertainty in wind condition (shear)**

- **Input Uncertainty**: Speed shear exponent as continuous histogram distribution.
- **Output Metric**: Blade root out-of-plane bending moment amplitude during steady limit cycle.
- **UQ Methods**: LHS and PCE with Askey/Gauss-Patterson or numerically generated/Gauss using p-refinement (isotropic/anisotropic/generalized essentially equivalent for 1-D).
- **Response function evaluations**: 100k LHS samples for PDF/CDF eval (truth or approx); up to 255 for Askey PCE (level w=7); up to 21 for NumGen PCE (level w=10).



# Positivity-preserving high order well-balanced method for the shallow water equations

## ASCR- Applied Mathematics Highlight

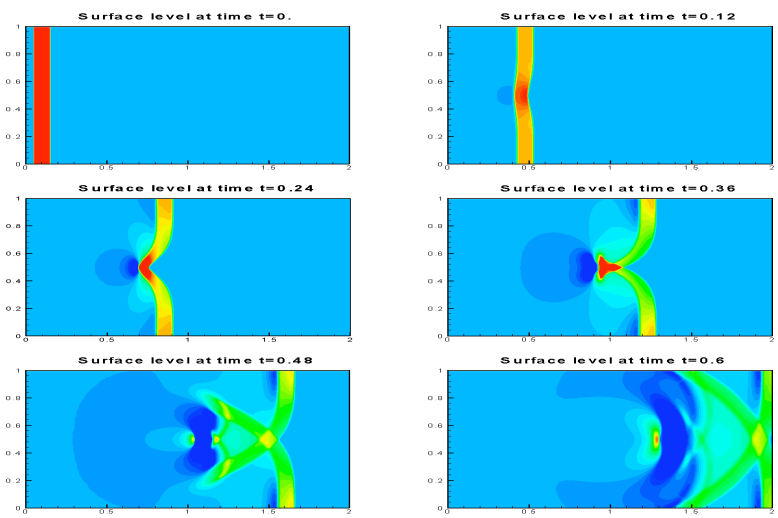
### *Objectives*

- Develop accurate and efficient numerical methods for the shallow water equations, which can
  - take care of the dry area automatically;
  - capture the steady state exactly.

### *Impact*

- Enable stable and efficient simulations to the shallow-water equations and their applications in dam break problem and tsunamis wave prediction
- Similar technique can be extended to the MHD model in plasma, gas dynamics model in astrophysics and other hyperbolic system with source terms

Time history of a small perturbation to the equilibrium state




### *Accomplishments*

- Provide positivity-preserving limiters for the shallow-water equations
- Y. Xing, X. Zhang and C.-W. Shu, *Positivity-preserving high order well-balanced discontinuous Galerkin methods for the shallow water equations,* **Advances in Water Resources,** v33 (2010), pp.1476-1493
- Y. Xing, C.-W. Shu and S. Noelle, *On the advantage of well-balanced schemes for moving-water equilibrium of the shallow water equations,* **Journal of Scientific Computing,** v48 (2011), pp.339-349
- Y. Xing and C.-W. Shu, *High-order finite volume WENO schemes for the shallow water equations with dry states*, **Advances in Water Resources**, v34 (2011), pp.1026-1038

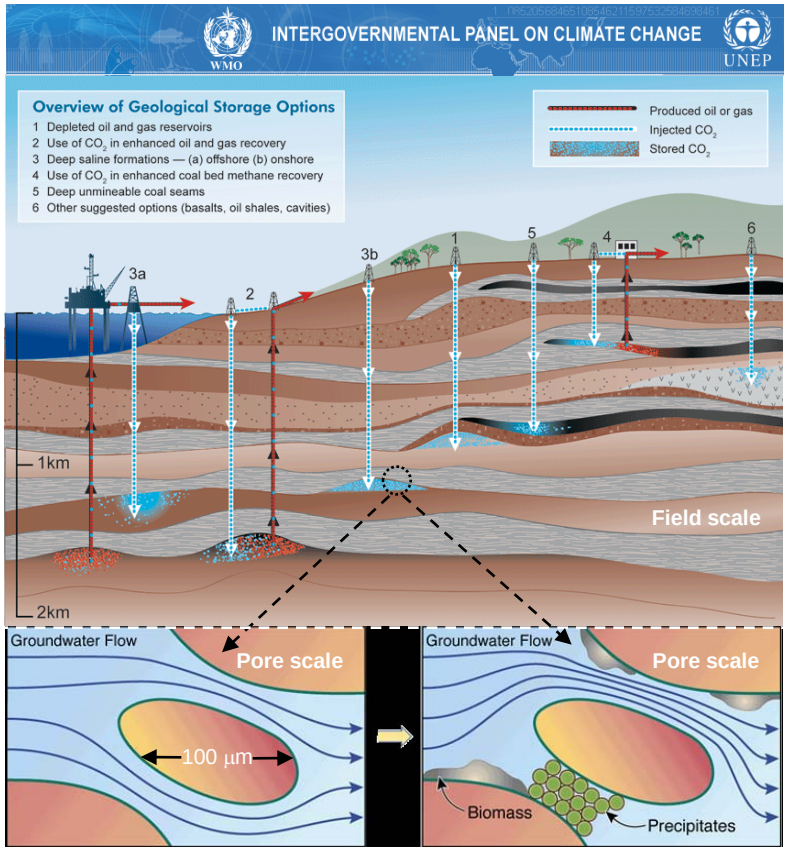


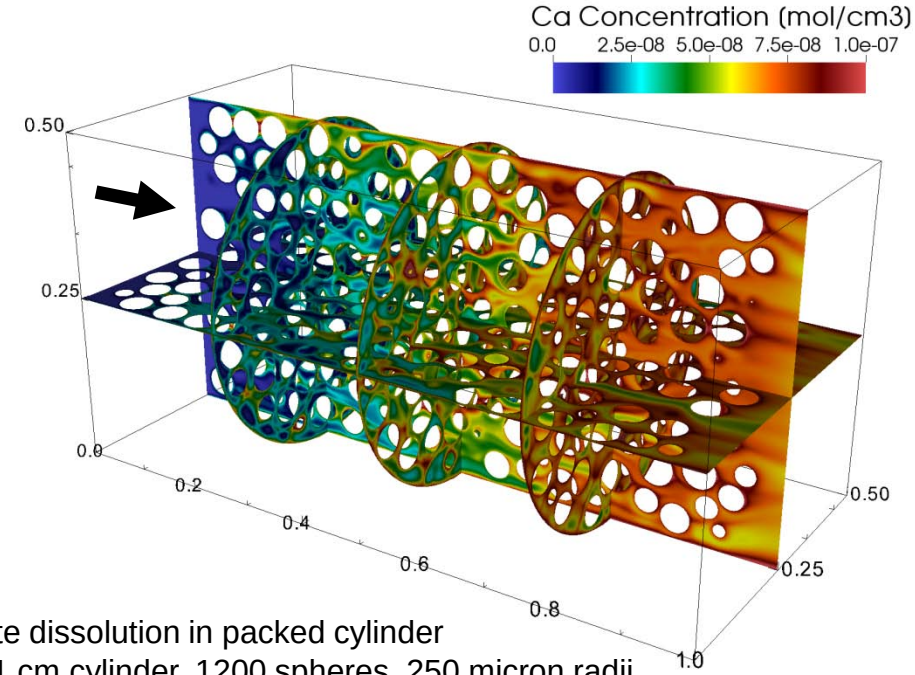
Yulong Xing, Oak Ridge National Laboratory

# #58 An Adaptive Embedded Boundary Method for Pore Scale Reactive Transport

"World's largest pore scale reactive transport simulation"

David Trebotich, Sergi Molins, Carl Steefel, Chaopeng Shen and Greg Miller

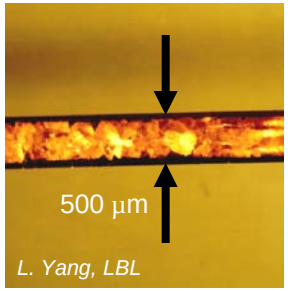



Calcite dissolution in packed cylinder

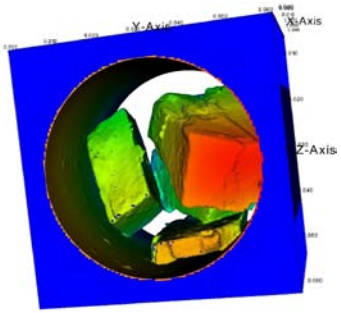
- 1 cm cylinder, 1200 spheres, 250 micron radii
- 5 components, 9 complexation reactions, influent pH=5
- 33.5 million grid points, < 20 micron grid resolution
- 1024 cores, 0.6 GB per core, scalable to 65K cores

**Direct Numerical Simulation From Image Data**



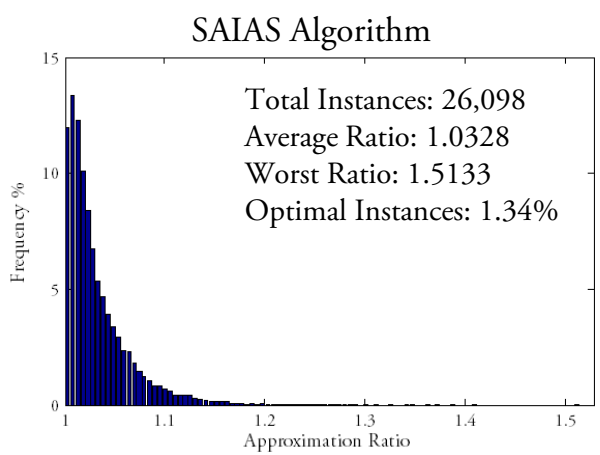

Experiment to XMT imagery

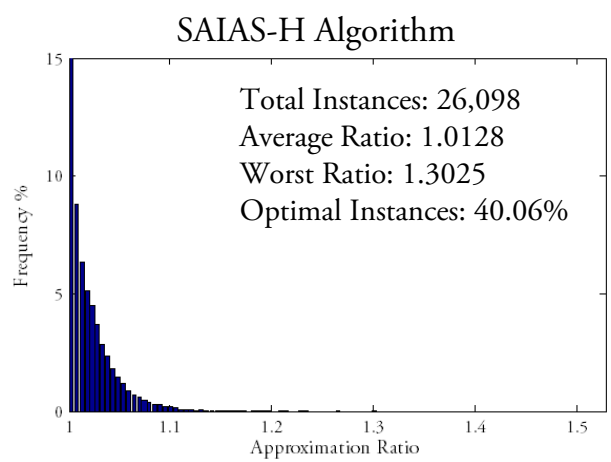
Image data to pore scale RT simulation (pressure data in a section)



# We propose a new methodology for incorporating speed and energy costs into scheduling problems

- Our algorithms compute a *O(1)*-approximation for weighted completion time and weighted tardiness for very general energy cost functions.
- Experimental results show that the algorithms perform very close to optimal:




- Extensions: online and multiple parallel machines.
- Algorithms can also be used with other speed-related costs: maintenance, wear & tear, etc.

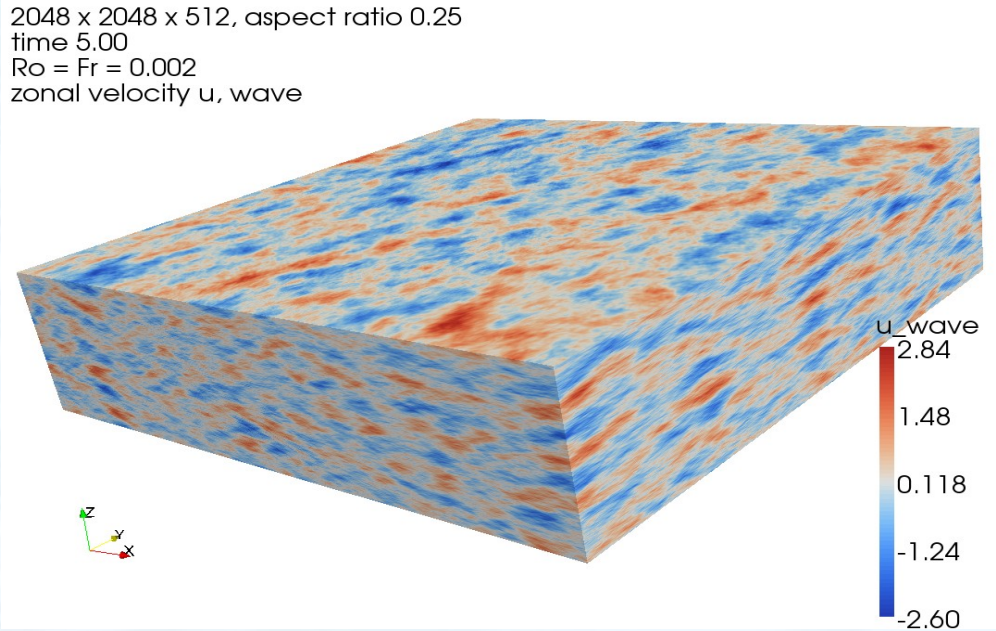
IEOR Department
Columbia University

DE-FG02-08ER25856: Algorithms for Mathematical Programming with emphasis on bi-level models
Rodrigo A. Carrasco, Garud Iyengar, Cliff Stein

# Poster # 61

Susan Kurien (LANL)
Leslie Smith (U. Wisconsin, Madison)

Characterize layer formation in small aspect-ratio rotating and stratified flows




- 2048 x 2048 x 512 gridpoints
- Rossby = Froude = 0.002
- time-resolved fastest waves
- 15M core hours (BG/P, Argonne)

- How does layer thickness change as aspect-ratio decreases?
- What is the relative fraction of energy in fast wave-modes?

Poster #62: Michael Parks

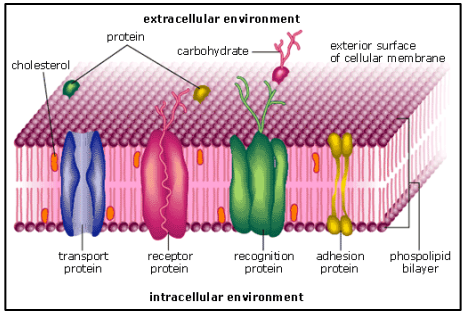
# Enabling Tools for Extreme Scale Computation of Nanoscale Fluids

- ❑ Fluid density functional theories enable modeling and simulation of a wide range of applications
- ❑ Minimize free energy functional with Newton-Krylov
- ❑ Use Sandia's *Tramonto* package for complex fluid systems, built upon *Trilinos* software components
- ❑ Increased performance by reducing memory bandwidth and size usage
- ❑ Stop by my poster to see:

(1) Mixed-precision, precision-neutral, and high precision solvers leveraging the *Tpetra* solver stack (templated C++)

(2) Robust mixed-precision solvers via least-squares methods that shield user from details of computation

(3) Block Krylov recycling solver with superior convergence properties due to block formulation and information reuse from previous linear solves




Tramonto

Trilinos

SAND2011-7515P

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Multiscale approach for network compression-friendly ordering

## Problem

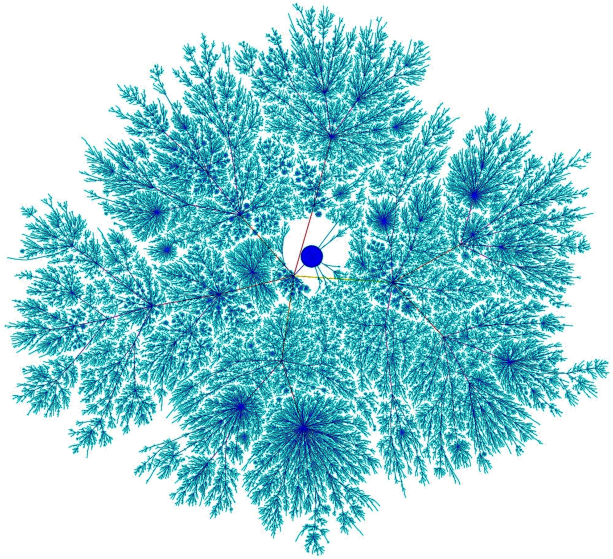
*Find a compressed representation of a network.*

Many modern networks/graphs/matrices

- are huge and noisy
- are structurally different at different resolutions
- describe data collected in parallel

With the growth of the networks we need

- to store the network efficiently
- to have an extremely fast access to network elements (nodes, links, non-zero entries, etc)



A network from a web crawl, 138263 nodes, 193251 edges.

## Results

*We find better ordering → better compression → faster performance.*

# Poster 64: Out-of-core algorithms for dense matrix factorization on GPGPU

Ed D'Azevedo

- General Purpose Graphics Processing Unit (GPGPU) achieves high performance on dense matrix operations
- GPU accelerator on supercomputer to consumer game video card (< $200)
- Largest problem size may be limited to the amount of device memory on GPGPU
- Idea: adapt out-of-core algorithm to factor 10 GB matrix on CPU host using only 1 GB device memory
- Cholesky factorization (DPOTRF) using only 1 GB (out of 5 GB) on Tesla M2050

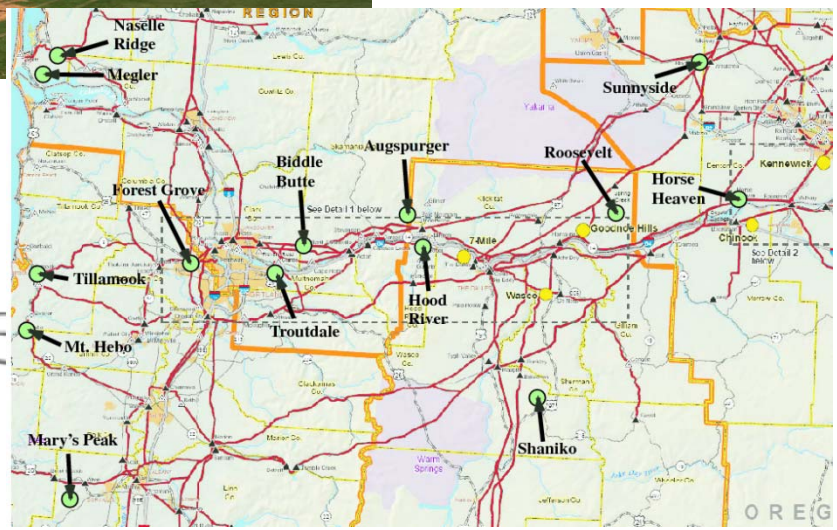
| | MAGMA 1.0 | Out-of-core algorithm |
|---|---|---|
| N=25,000 | 266 Gflops/s | 246 Gflops/s |
| N=35,000 | Out of memory | 263 Gflops/s |

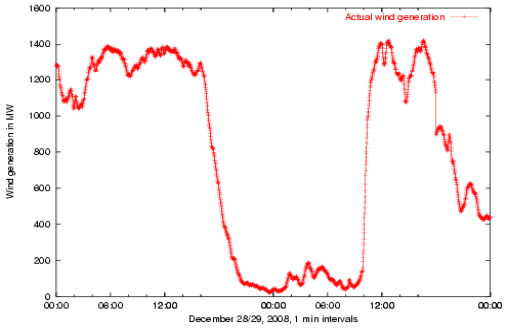
U.S. DEPARTMENT OF ENERGY
Office of Science

OAK RIDGE National Laboratory

# 65: Chandrika Kamath (LLNL)

## Real-time Analysis of Streaming Data from Sensors

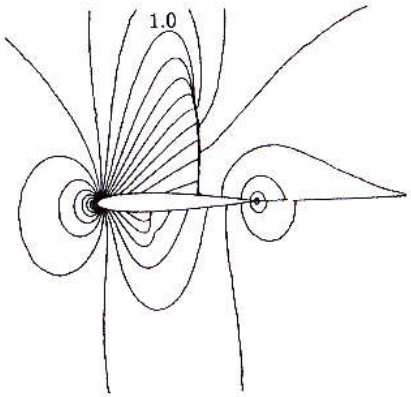


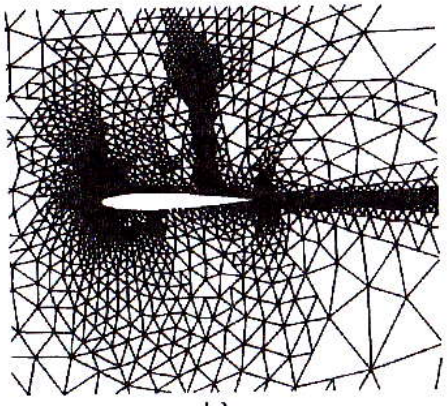



- Can we adaptively reduce noise in the sensor data?
- Which data streams are important?
- How do we incorporate the spatial distribution of sensors into the predictive models?

# Allen M. Tesdall, Poster 66
# High resolution solutions for shock formation

Shock waves form generically in solutions of transonic flow problems. An example: transonic flow over an airfoil



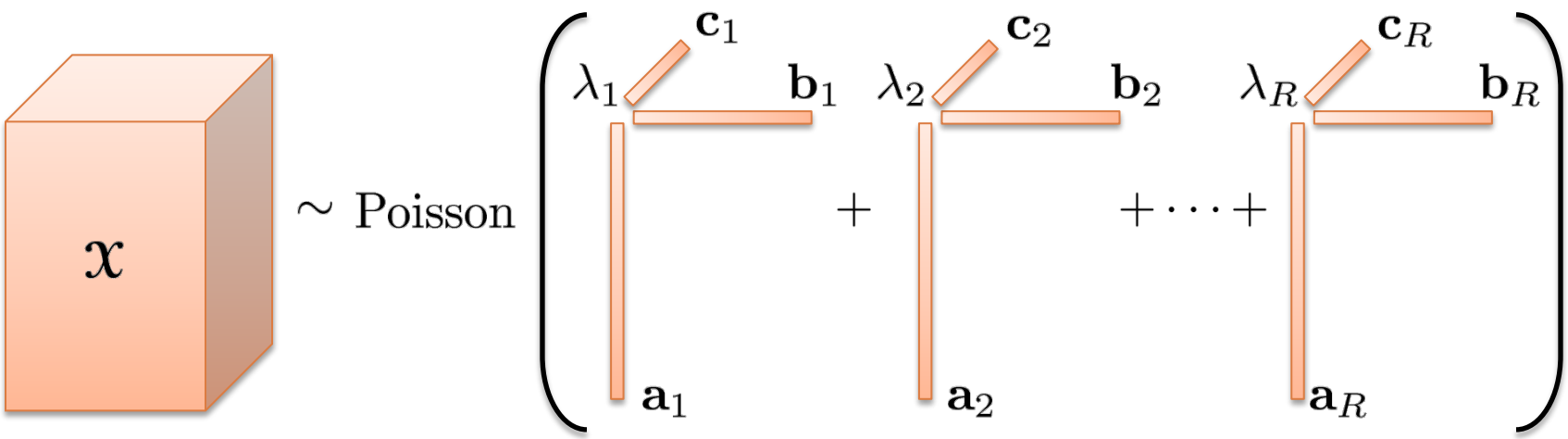
Where does the shock form?

- Whether a shock forms on the sonic line or inside the supersonic region is an open question.
- We numerically solve this problem and others, and find that the shock forms inside the supersonic region, and very close to, but not at, the sonic line.

Poster 67: Tamara G. Kolda

# Tensors Factorizations for Sparse Data

We propose that **sparse count data** is better modeled as a Poisson distribution than Gaussian:




Data

Model: $\mathcal{M}(i,j,k) \equiv \sum_r \lambda_r \, \mathbf{a}_r(i) \, \mathbf{b}_r(j) \, \mathbf{c}_r(k)$

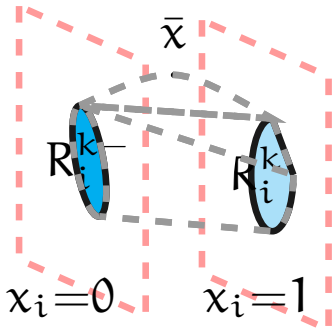
Such an assumption yields the following objective function (negative of the log likelihood) for fitting observed data:

$$\min_{\mathcal{M}} \sum_{ijk} \mathcal{M}_{ijk} - \mathcal{X}_{ijk} \log \mathcal{M}_{ijk}$$

*Joint work with Eric C. Chi, Rice Univ. & UCLA*

# Effective Disjunctive Cuts for Convex MINLPs

- Disjunctive cutting planes are a tremendously effective tool for solving mixed integer *linear* programs
- Used in all state-of-the-art software packages



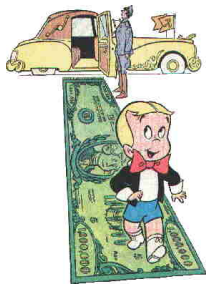

It's only half bull

## Our Team's Quest

Develop computationally effective methodology for disjunctive cutting planes in (convex) mixed integer nonlinear programs

## Does it Work?

- First use of disjunctive cutting planes on practically-sized convex MINLP instances
- Cuts are very strong: Tremendous speedups on many instances, including portfolio optimization



# An adaptive high-order minimum action method

Xiaoliang Wan, LSU

## Stochastic Model:

$$\frac{\partial}{\partial t}u(x,t) = Gu(x,t) + \sqrt{\varepsilon}\,\dot{W}(x,t)$$

$\dot{W}$ is space-time white noise.

$\varepsilon$ is a small positive number.

## Problem Description:

- *A transition from one state in the phase space to another one always has a positive probability. How can we quantify this probability? How does the transition occur?*
- *When $\varepsilon$ is small, the transition probability will be also small, direct sampling method will not be affordable, especially when we consider a large-scale problem, such as Navier-Stokes equations.*

## A General Numerical Strategy:

$$u^* = \min_{\substack{\text{all possible} \\ \text{transition paths}}} S_T(u)$$

*hp* FEM discretization in both time and space

Adaptive time mesh consistent with dynamics

Scalable parallel optimization algorithm

Large deviation theory for the transition probability

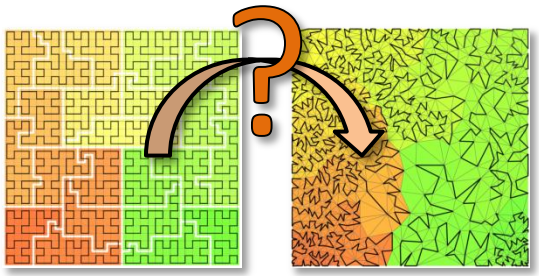
## Applications:

chemical reactions, bi-stable genetic toggle switch, nucleation events during phase transitions, regime changes in climate, subcritical bifurcations, etc.

# Reducing Data Movement using Cache-Oblivious Layouts

Peter Lindstrom
Lawrence Livermore National Laboratory

#70



## Effective caching, streaming require good ***data locality***

- ***Space-filling curve*** layouts are ideal for structured grids
- ... but don't do well on unstructured & non-geometric data

## We have developed a ***cache-oblivious locality measure***

- Applicable to any data set modeled as an ***affinity graph***
- Optimal unstructured grid layouts are qualitatively "space-filling"
  - Hamiltonian, hierarchical, unbiased, scale-free, ...

$$\mu_0 = \left( \prod_{ij \in E} |\varphi(i) - \varphi(j)| \right)^{1/|E|}$$

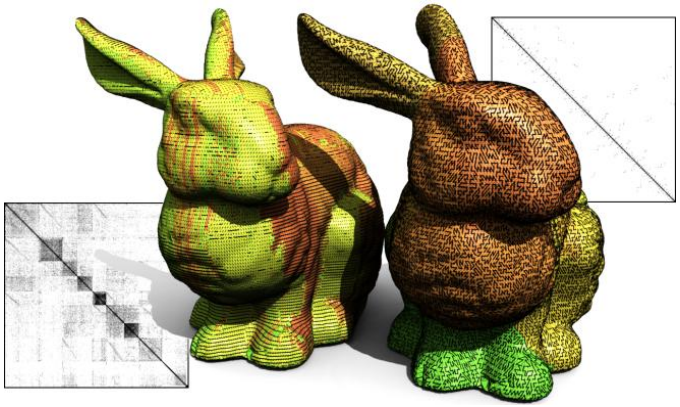
$$= \exp\left( \frac{1}{|E|} \sum_{ij \in E} \log |\varphi(i) - \varphi(j)| \right)$$

## Linear ordering problem is NP-hard

- ... but good ***multilevel heuristics*** exist: see poster #63 for details

## Applications abound

- Sparse matrix ordering
- "Instant" graph partitioning & load balancing
- Databases, GIS, image processing, clustering, GPU rendering, graph drawing, ...
- Web graph compression



This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Poster 71, Danny Perez, LANL

# Generalizations of the Parallel Replica Dynamics method for long-timescale atomistic simulations

- Parallel Replica Dynamics is a method to parallelize molecular dynamics simulation *in the time domain*. This enables atomistic simulations of nanoscale systems over long timescales (>μs), as long as they evolve through a sequence of rare, activated events.

- We discuss a recent mathematical analysis of the method where we quantify the underlying approximation. We show that this approximation can be made arbitrarily good.

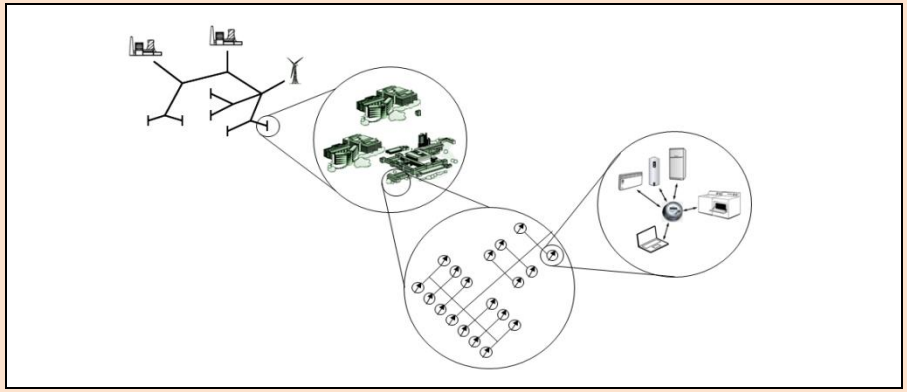
- Through the same analysis, we show that the method can be generalized to handle arbitrary partitions of configuration space instead of the conventional definition. When chosen properly, this can significantly improve the efficiency of the method.

- We show how this leads to a generalization of the method that can handle both diffusive, as well as activated, rare events.

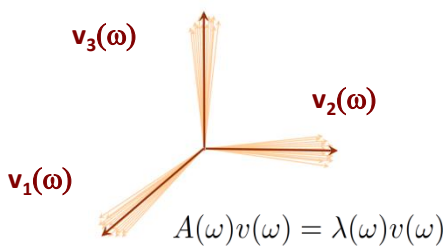
72. Hadi Meidani

# Random transitions and eigenvalues for modeling demand and stability for the Smart Grid

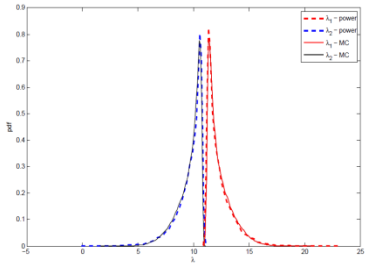
Hadi Meidani, Roger Ghanem



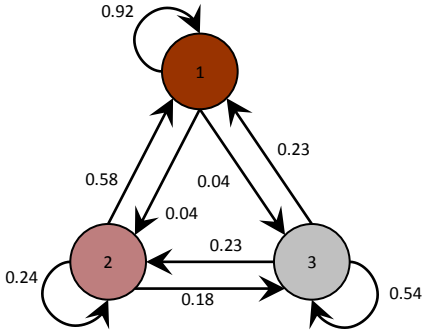
## Random eigenvalue analysis

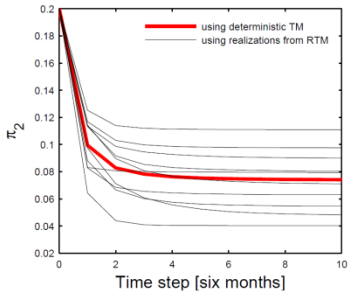



$$A(\omega)v(\omega) = \lambda(\omega)v(\omega)$$

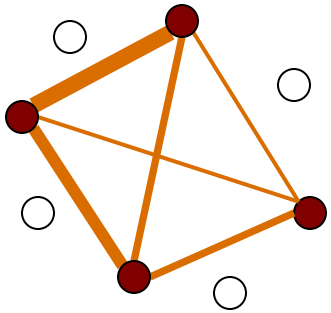


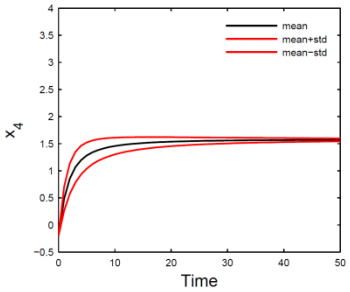
## Markov chains with random transitions




## Synchronization in random networks





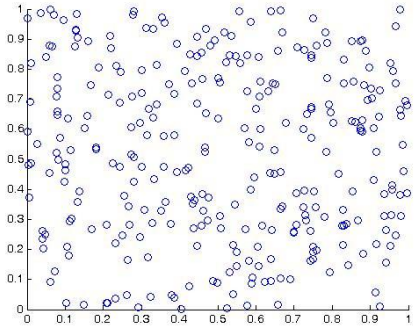
# Sparse Grid Scenario Generation and Interior Algorithms for Stochastic Optimization in a Parallel Computing Environment:

Sanjay Mehrotra, Northwestern University

Award: DE-FG02-10ER26037; SC0005102

## Scenario Generation

### STATUS QUO



**Uncertainty are generated using Monte-Carlo and Quasi-MC Methods**

## Optimization Algorithms

two-stage convex optimization problem

$$\min \; c^T x + \sum_{k=1}^{K} \bar{\eta}^k(x) \;\text{ s.t. } x \in G \cap L$$

$$\bar{\eta}^k(x) := \min \; (d^k)^T y^k \;\text{ s.t. } y^k \in G^k \cap L^k(x),$$

$G$ and $G^k, k = 1, \ldots, K$ are compact convex sets

$L := \{x \mid Ax = b\}$, and

and $L^k(x) := \{y^k \mid Q^k y^k = q^k + T^k x\}$

**Current Algorithms Require Extensive Formulation of the Two-Stage Problem**

## ACHIEVEMENTS:

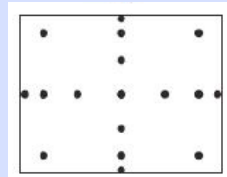
### Scenario Generation Methods:

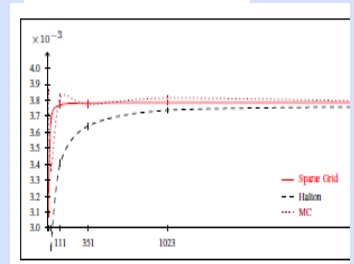
- Convergence Analysis of Sparse Grid Scenario Generation Methods in Optimization framework showing similar convergence properties as those for the integration problems.
- Developed an optimization based approach to generate moment matching cubature formulae by solving semi-infinite linear programs.

### Interior Decomposition Algorithms:

- Developed a primal-interior decomposition algorithm for two-stage convex programs admitting self-concordant barriers that decomposes the second stage problem.
- Analysis shows that the order of the number of inner iterations of this algorithm is same as that for primal-interior algorithm applied to the extensive formulation.

## Scenarios are More Structured and give better performance






Number of scenarios in a 6-dimensional stochastic problem.

**Sparse Grid Methods give** two to three orders of m**agnitude Scenario (time) reduction** when compared with Monte-Carlo, Quasi-Monte Carlo and Full Grid Methods for smooth problems

**Semi-infinite linear programming** approach allows generation of cubature formulae with non-negative weights for any distribution function.

## Polynomial Convergence in decomposition Framework

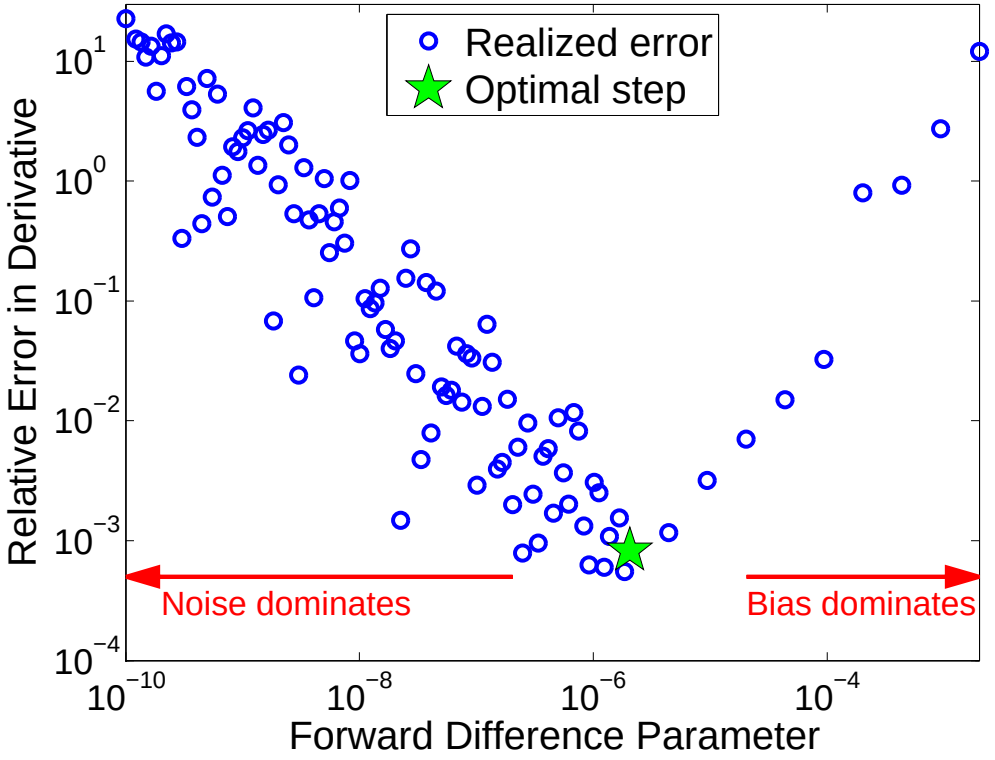
**Interior decomposition algorithm** allows adaptive scenario addition and distributed computations.

**Improved Scenario Generation in Stochastic Optimization; Polynomial Convergence of Interior Decomposition Algorithms**

Poster 74 - Stefan Wild

# Optimal Derivatives of Noisy Simulations

## How should difference parameter $h$ be chosen in $\frac{f(t+h)-f(t)}{h}$?



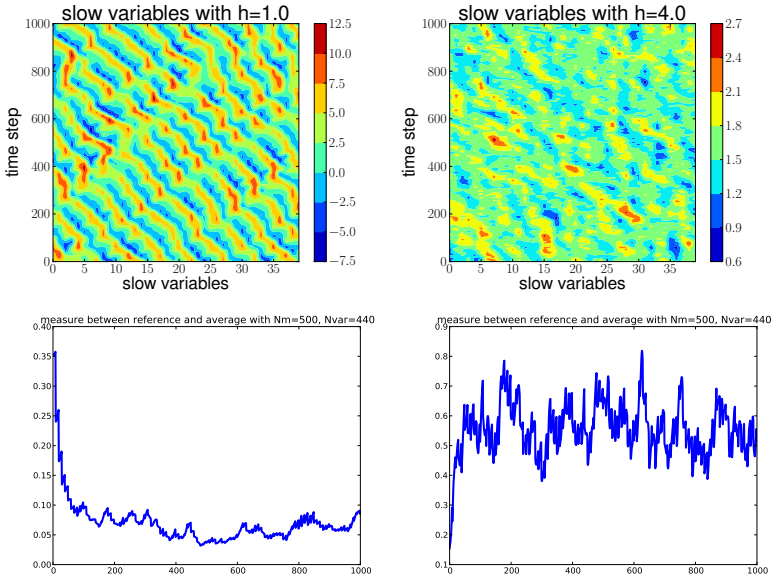

Choose $h = h_{\text{opt}}$ based on the noise in $f$

- Provably optimal: $\mathcal{E}(h_{\text{opt}}) \leq \gamma \min_{h \leq h_U} \mathcal{E}(h)$
- Inexpensive: Noise estimate and 2-4 $f$ evaluations

# Data Assimilation in Multiscale Systems

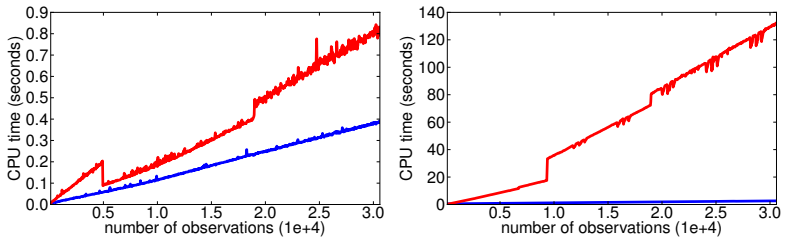
Humberto C. Godinez, Balu Nadiga, J. David Moulton
Los Alamos National Laboratory

## Part I: Ensemble Data Assimilation for Strongly Coupled Systems



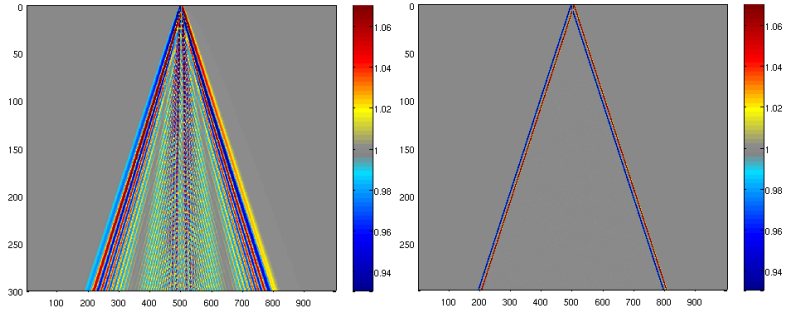

## Part II: An Efficient Matrix-Free EnKF Algorithm

Matrix-free implementation of EnKF using a Sherman-Morrison linear solver to efficiently assimilate large data sets.

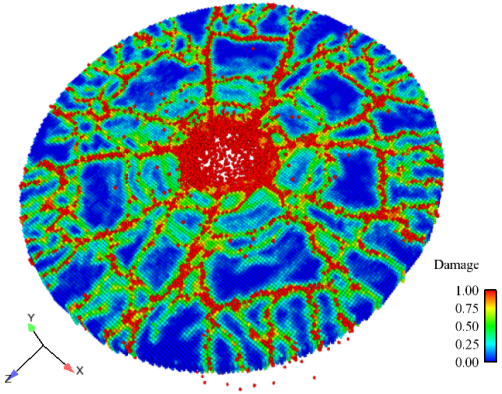


# 77. Pablo Seleson

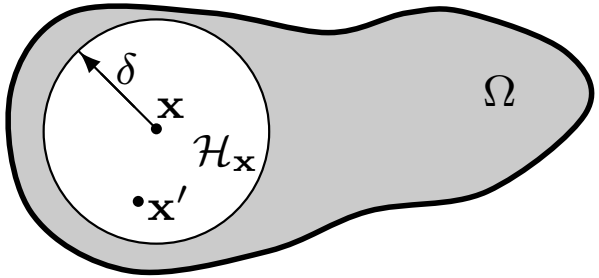
# Peridynamics as a Multiscale Material Model



$$\rho\ddot{\mathbf{u}} = \int_{\mathcal{H}_{\mathbf{x}}} \boldsymbol{\kappa}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \mathrm{d}V_{\mathbf{x}'} + \mathbf{b}$$



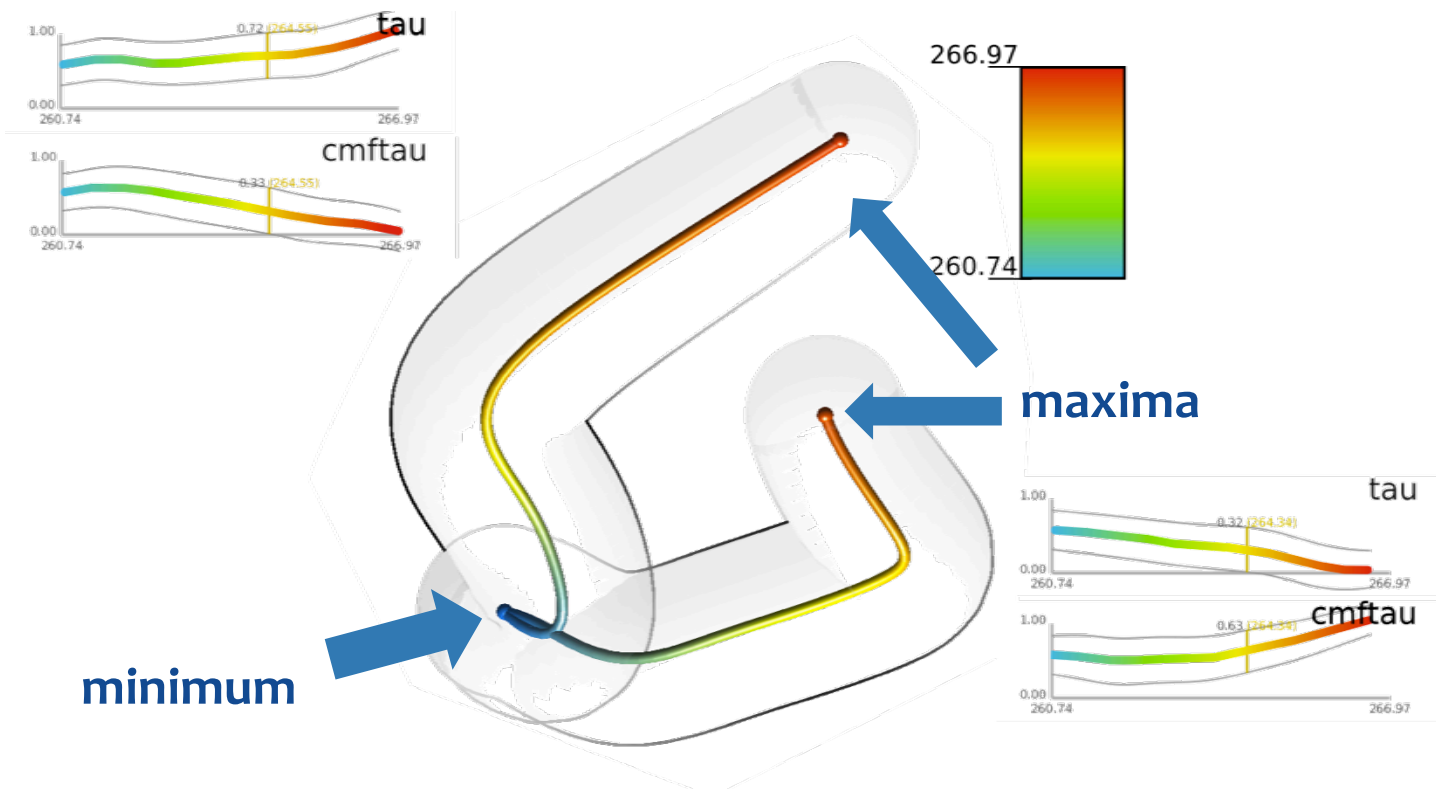

- Nonlocal
- Continuum
- Length scale
- Fracture



# Poster #78 – Peer-Timo Bremer

## Analysis and Exploration of High Dimensional Functions for UQ

- Topological analysis of high-dimensional functions provides new insights into parameter dependencies within simulation ensembles

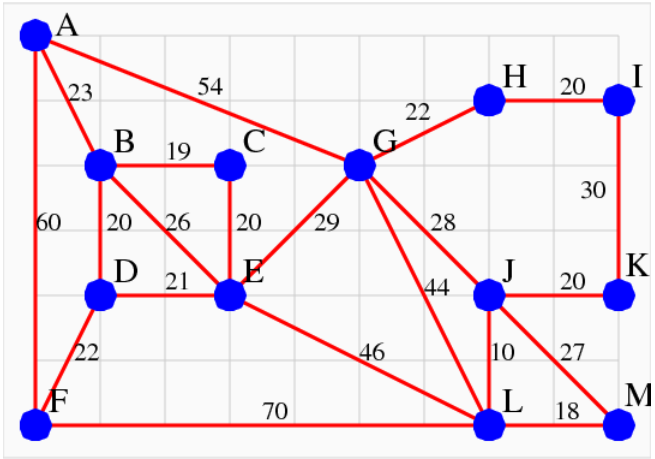



**Average Clear Sky Flux in a 21-dimensional CAM ensemble**

# Approximating a 2-edge-connected subgraph problem

- New algorithm for computing a minimum-cost 2-connected subgraph; cost reduction for multi-edges.
  - Special case of buy-at-bulk network design with protection, used actively for designing optical communication networks. Network must function if an edge fails.
  - Provable 5/3-approximation (best previous bound = 2)
  - First tree-based formulation and new analysis techniques involving multiple convex decompositions

A 2-connected graph




If any edge is broken, all nodes remain connected

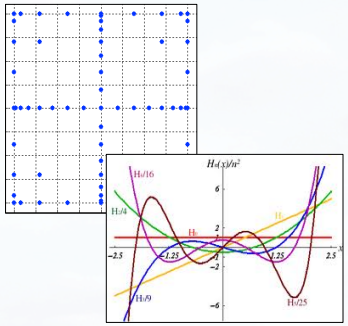
Figure from: http://people.sc.fsu.edu/~jburkardt/latex/asa_2011_graphs_homework/

# Poster 80: Tim Wildey

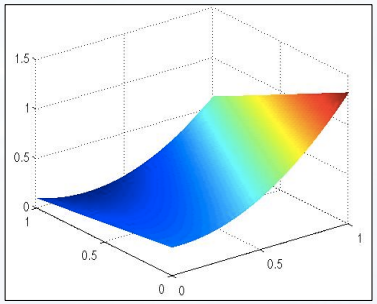
# A Posteriori Error Analysis of Stochastic Differential Equations Using Polynomial Chaos Approximations

***Mathematical and Computational Tools for Predictive Simulation of Complex Coupled Systems Under Uncertainty***

Paul Constantine, Eric Phipps and Tim Wildey: Sandia National Laboratories, Albuquerque, NM 87123
Troy Butler and Clint Dawson: The University of Texas at Austin, Austin, TX 78723



**Model:**
$u = M(\lambda)$



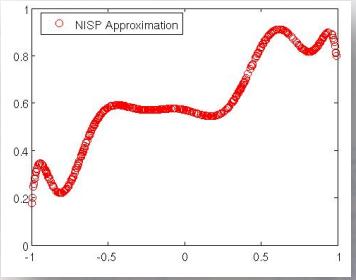
Do we trust surrogate models to compute statistical properties given (virtually) unlimited samples?

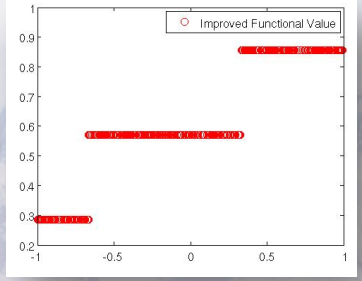
The goal is to estimate the error in samples of a quantity of interest computed from a polynomial chaos (PC) approximation.

## Accurate Error Estimates

| $\lambda$ | Std Err Est $u(x^{\{5\}}, t)$ | PC Err Est $u(x^{\{5\}}, t)$ | Ratio |
|---|---|---|---|
| 0.50 | 0.22660 | 0.22667 | 1.00032 |
| 0.75 | 0.19693 | 0.19694 | 1.00006 |
| 1.00 | 0.17823 | 0.17823 | 1.00000 |
| 1.25 | 0.16520 | 0.16519 | 0.99996 |
| 1.50 | 0.15550 | 0.15548 | 0.99983 |

## Improved Linear Functionals

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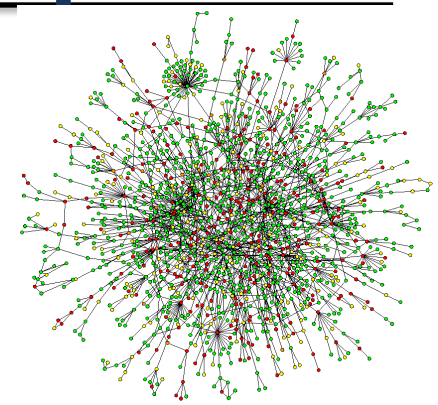
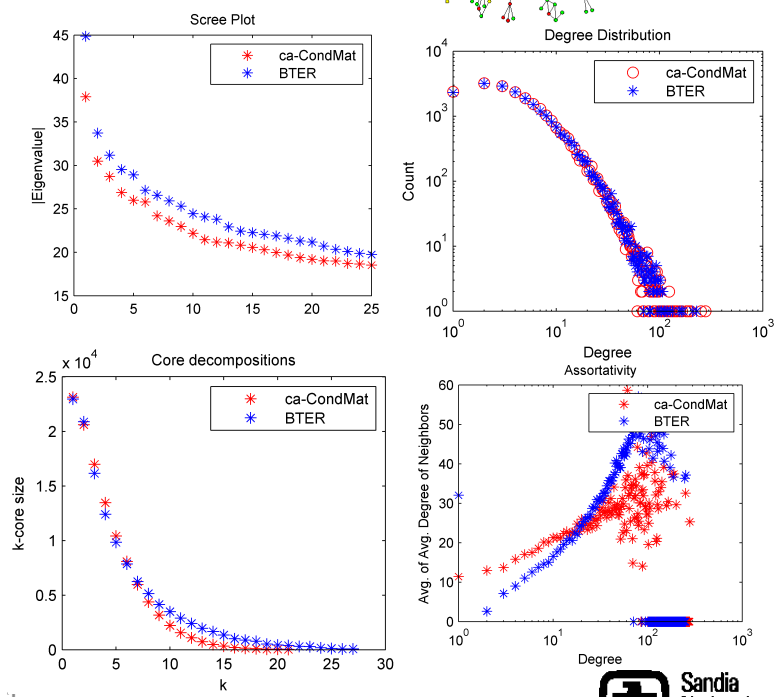
# Models for Generating Large Realistic Graphs

- **Goal:** Create models that can describe and generate realistic networks at the large scale.
- **Challenge:** We have to design both the descriptors and the methods to generate graphs from these descriptors.
- **Approach:** Use observations on real data as input to theoretically sound analysis.
- **Status:**
  - Analysis and improvements on the Graph500 benchmark
  - A new model, BTER, that produces accurate approximations for large class of graphs

$f(x) =$






Contact: Ali Pinar, Sandia Natl. Labs



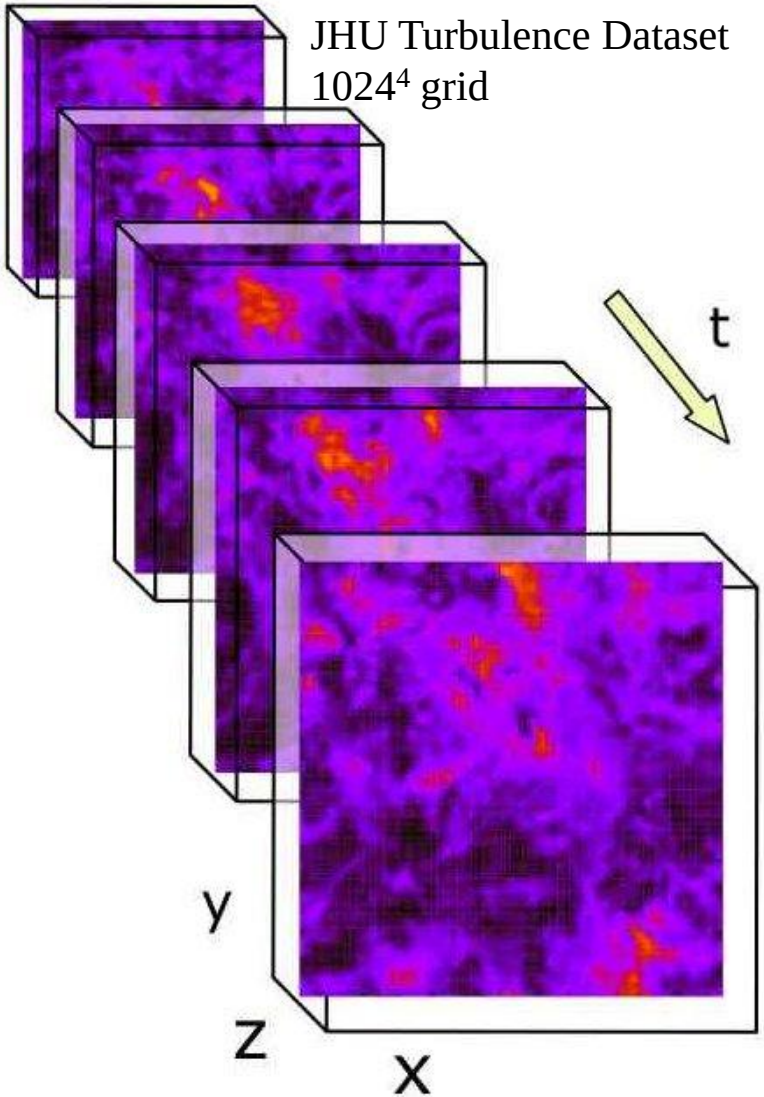
Sandia National Laboratories

83 – Jeff Schneider

# Machine Learning to Recognize Phenomena in Large Scale Simulations

Given a petabyte of simulation data

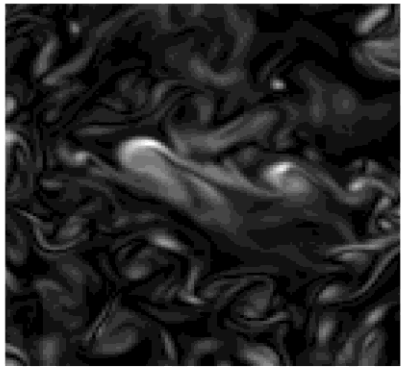
- what interesting happened?
- how often did it happen? when? where?




APPROACH

- Treat nearby grid points as a group
- Propose Support Distribution Machine for groups (distributions) of data points
- Use SDM to find anomalies, classify phenomena, cluster results

Sample result:



Identified a "sheet" of vortices

Carnegie Mellon

## On stochastic gradient and subgradient methods with adaptive steplength sequences

- Consider the convex stochastic optimization problem given by

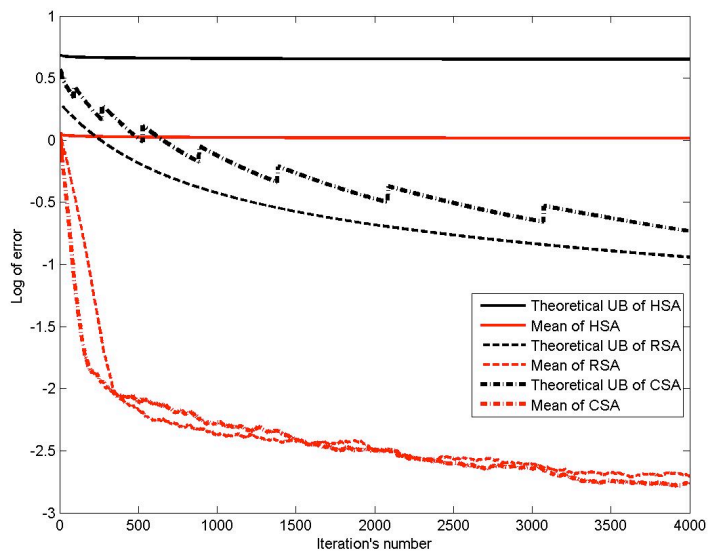
$$\min_{x \in K} \quad \mathbb{E}[f(x;\xi(\omega))].$$

- A stochastic approximation scheme: $x_{k+1} := \Pi_K(x_k - \gamma_k \nabla f(x_k;\xi_k)), \quad k \geq 1.$
- If $\sum_{k=0}^{\infty} \gamma_k^2 < \infty$ and $\sum_{k=0}^{\infty} \gamma_k = \infty$, the $x_k \to x^*$ almost surely.

### Challenge

Standard choices of $\gamma_k = 1/k$ can be VERY poor; are there adaptive rules?

- Two adaptive steplength rules with a.s. convergence guarantees
- Extensions to nonsmooth regimes




Joint work with A. Nedić and F. Yousefian

# 85 - Mikhail J. Shashkov

# ReALE - Reconnection-Based Multimaterial Arbitrary Lagrangian-Eulerian Method

**Mikhail J. Shashkov**

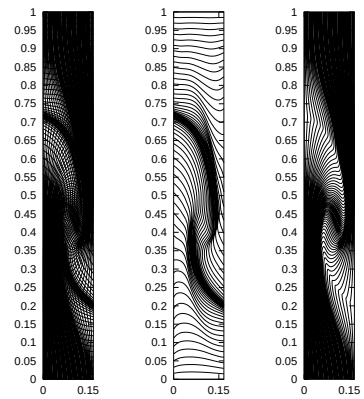
**X-Computational Physics Division, Methods & Algorithms Group, Los Alamos National Laboratory**

## Conventional ALE Methods

- **Explicit Lagrangian (solving Lagrangian equations) phase — grid is moving with fluid**
- **Rezone phase — changing the mesh (improving geometrical quality, smoothing, adaptation) — mesh movement**
- **Remap phase (conservative interpolation) — remapping flow parameters from Lagrangian grid to rezoned mesh**

## Limitation of ALE

## Fixed Connectivity




## ReALE - Reconnection-based ALE

- **Lagrangian phase**
  **General polygonal meshes**
- **Rezone phase**
  **Allows mesh reconnection**
- **Remap phase**
  **Remapping from one polygonal mesh to another**

# *The Devil is in the Details*

Poster 86: Chi-Wang Shu, Brown University

# Positivity-preserving High-Order Runge-Kutta Discontinuous Galerkin Schemes

- A general framework with a simple local limiter to enforce maximum principle or positivity retaining uniform high order accuracy (with rigorous proof).
- Works in multi-dimensions on arbitrary triangulations.
- Maximum principle: scalar nonlinear conservation laws, incompressible flows in two-dimensional vorticity-streamfunction formulation, and passive convection in incompressible fields.
- Positivity-preserving: Euler equations of compressible flow (density and pressure), shallow water equations (water height).

Poster #87 Peng Wang

# PDF Methods for Uncertainty Quantification in Hyperbolic Conservation Laws

- While standard techniques for uncertainty quantification typically yield only system state's mean and variance, the proposed approach leads to its full probabilistic description.
- The shape of the probabilistic density function (PDF) changes with time, varying between the known initial and steady-state distributions. This makes reliance on assumed PDFs problematic.
- PDF methods provide a computationally efficient means for uncertainty quantification.

# High Performance Embedded Hybrid Methodology for Uncertainty Quantification in Multi-physics Problems

Charles Tong - LLNL
Barry Lee - PNNL
Akshay Mittal, Gianluca Iaccarino - Stanford

## Intrusive/Non-Intrusive Coupling - Example

**We use the following test problem to illustrate a forward uncertainty propagation method.**

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - Ku;\ \ 0 \le x \le 1;\ \ 0 \le t \le T$$

$$u(0,t) = u(1,t) = 0, t \ge 0$$

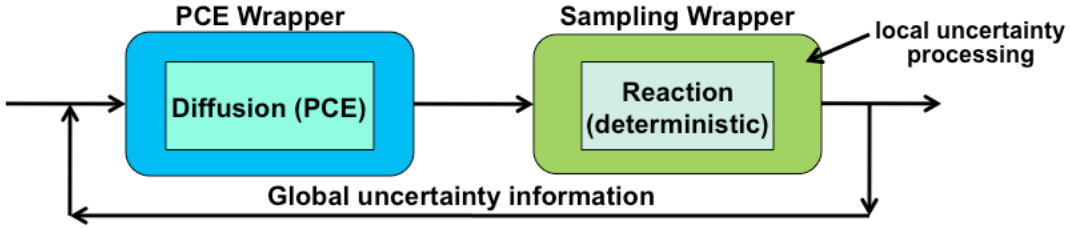
$$u(x,0) = f(x), 0 \le x \le 1$$

- D and K are second order random variables
- D = [0.0001, 0.001] with uniform distribution
- K = [0.1, 0.5] with uniform distribution
- time-step = 0.01
- Track root-mean-squared errors at T=2

- Operator splitting scheme: (n = time step)
  - diffusion module: PCE (polynomial chaos)
  - reaction module: sampling

$$\begin{bmatrix} \frac{\partial u}{\partial t} - D\frac{\partial^2}{\partial x^2} & 0 \\ \text{I.C.} & \frac{\partial u}{\partial t} + K \end{bmatrix} \begin{bmatrix} u_D^{n+1/2} \\ u_R^{n+1} \end{bmatrix}$$

- Global uncertainty representation: PCE
- Global uncertainty managed by software framework




| PCE Order | Pure PCE rms error | Pure PCE Time (s) | Hybrid rms error | Hybrid Time (s) |
|---|---|---|---|---|
| 1 | 4.9e-4 | 8.0 | 7.8e-3 | 10.5 |
| 2 | 5.7e-4 | 10.5 | 4.8e-5 | 14.5 |
| 3 | 5.7e-4 | 13.5 | 4.0e-5 | 23.5 |
| 4 | 5.7e-4 | 16.5 | 8.9e-5 | 29.5 |
| 5 | 5.7e-4 | 20.5 | 8.6e-5 | 40.0 |
| 6 | 5.7e-4 | 25.5 | 8.7e-5 | 46.0 |

**Discussions:**

- The hybrid method attains smaller errors than the pure PCE method when p is sufficiently large. This may be due to the use of analytic solution.
- The higher accuracy can be attained for pure PCE with smaller time step.
- Hybrid methods take longer, but
  - Pure PCE may need smaller time step
  - Multi-species problem will need special ODE solvers (the reason for operator splitting)
  - Some more code optimization may be possible (in the non-intrusive module)

# POSTER 89: Construction and Properties of Coarse Discretization Spaces by AMGe

**Panayot S. Vassilevski, CASC, LLNL**

**Abstract:** Several approaches to construct AMG coarse finite element discretization spaces are presented based on element agglomeration AMG (or AMGe) as well as smoothed aggregation AMG (or SA AMG). The spaces can be used both for building multilevel iterative methods as well as upscaling (discretization) tool. This is illustrated on diffusion equation with large jumps in coefficient in primal and mixed formulation.

**Convergent Multigrid implies "approximation property" of coarse spaces.**

**Hence, "use coarsening techniques from AMG to construct coarse spaces with guaranteed approximation property".**

**We use specialized, "element-based" AMG (or AMGe) techniques applied to :**

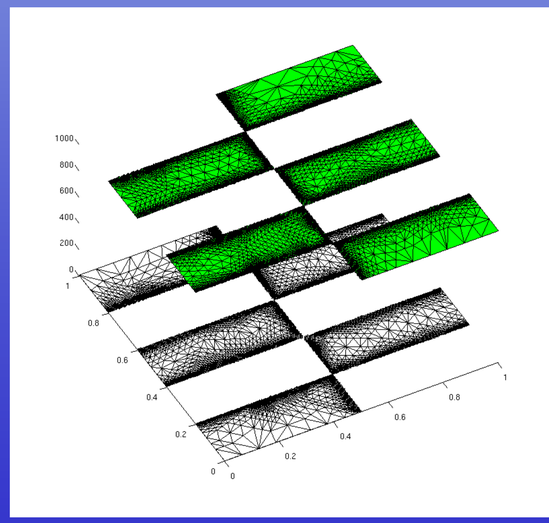
Diffusion equation with coefficient not resolved by a coarse grid

$$-div(k(x)\nabla p(x)) = f(x) \text{ in } \Omega;\ p(x) = g(x) \text{ on } \partial\Omega.$$

Mixed form: Find u and $p$ such that:

$$(k^{-1}\mathrm{u}, v) + (p, div\, v) = 0, \qquad \text{for all } v \in H(div, \Omega),$$

$$(div\, \mathrm{u}, q) \qquad = -(f, q), \text{ for all } q \in L_2(\Omega).$$

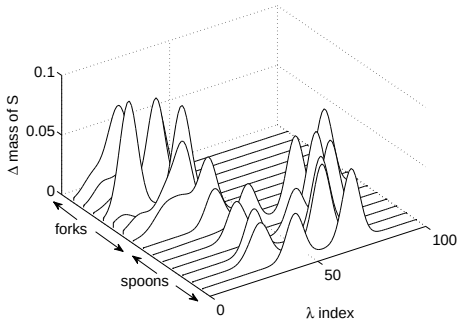


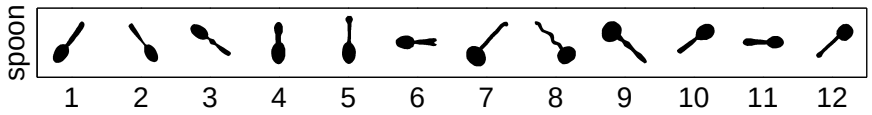
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

# Poster #90 – Tom Asaki
# Geometric Signatures for Fast Shape Processing

Keith Clawson, Sharif Ibrahim, Heather Van Dyke, Tom Asaki, Kevin Vixie

## Scale Sensitive Signatures



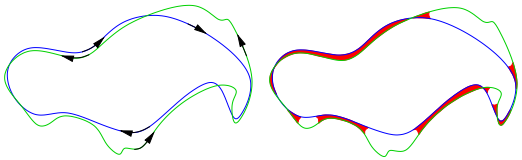



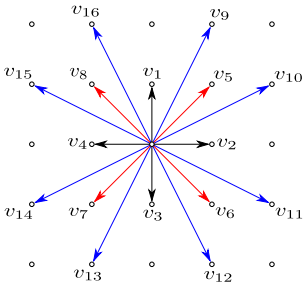

## Flat Norm Surrogate Signatures

disk convolution, heat kernel, erosion

## Flat Norm Decomposition

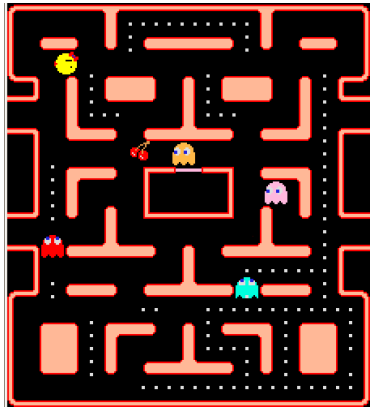
$$\mathbf{F}(\lambda) = M(T - \partial S) + \lambda M(S)$$






## Streaming Video

parallelization
GPU implementation
algorithms
novel surrogates



# INTERPOLATING PARAMETERIZED SIMULATION RESULTS

**Paul G. Constantine**

**Stanford University/Sandia National Labs**

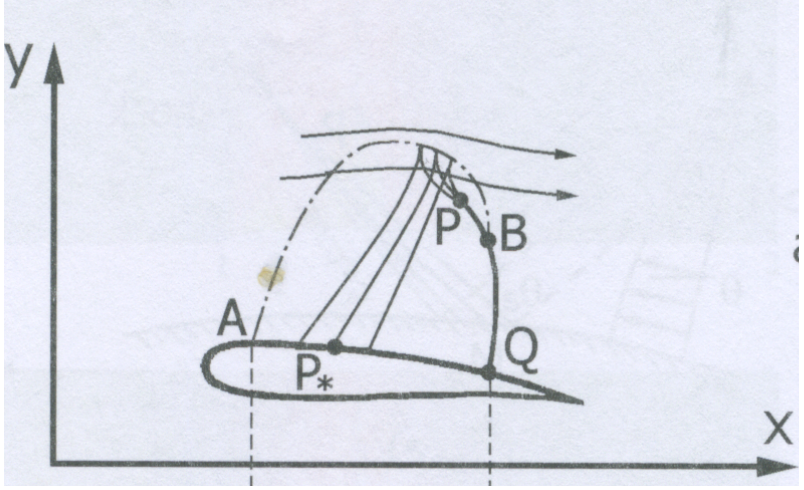
With:
David Gleich (Purdue), Qiqi Wang (MIT)

***Exascale computing needs exascale data management!***

Keywords: model reduction, uncertainty quantification, MapReduce

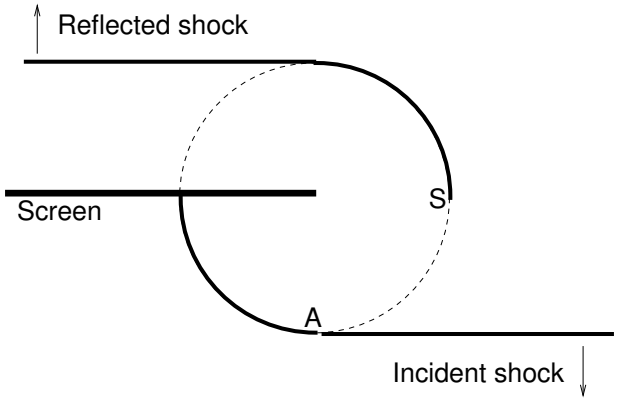
## Can It Happen?

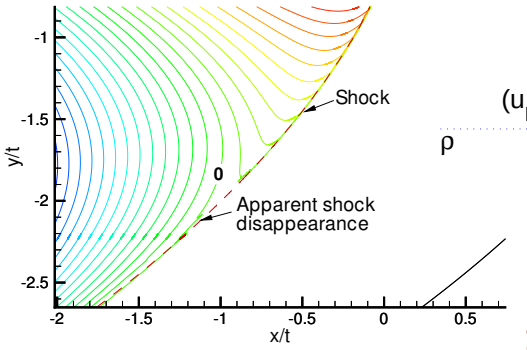
### Alexander Kuz'min: No

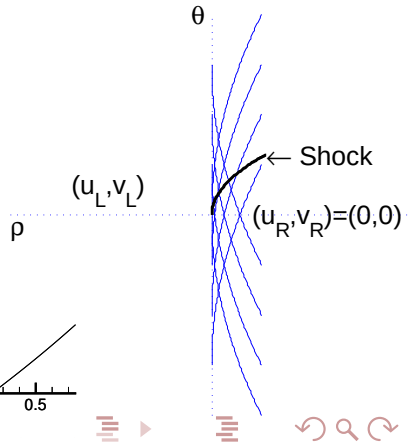



Objective
Give general proof that shocks cannot form at sonic line

### John Hunter - Allen Tesdall: Yes



# A Computational Studay of the Optimization Problem in High-Order Entropy-Based Moment Closures for Linear Transport

Graham Alldredge, Cory Hauck, Dianne O'Leary, and André L. Tits

[DOE Grant DESC0001862. PIs: Cory Hauck, D.P. O'Leary, and A.L. Tits]

- Entropy-based Moment Closures: Reduced, parallelizable model with attractive theoretical properites.
- Optimization challenges:
  - Solution needed at each point on a space-time mesh.
  - Hessian of objective function becomes singular near the realizable boundary
- Our solutions:
  - A kinetic solver which preserves realizability
  - Adaptive quadrature
  - Iterative change of polynomial basis
  - Regularization method for hardest problems

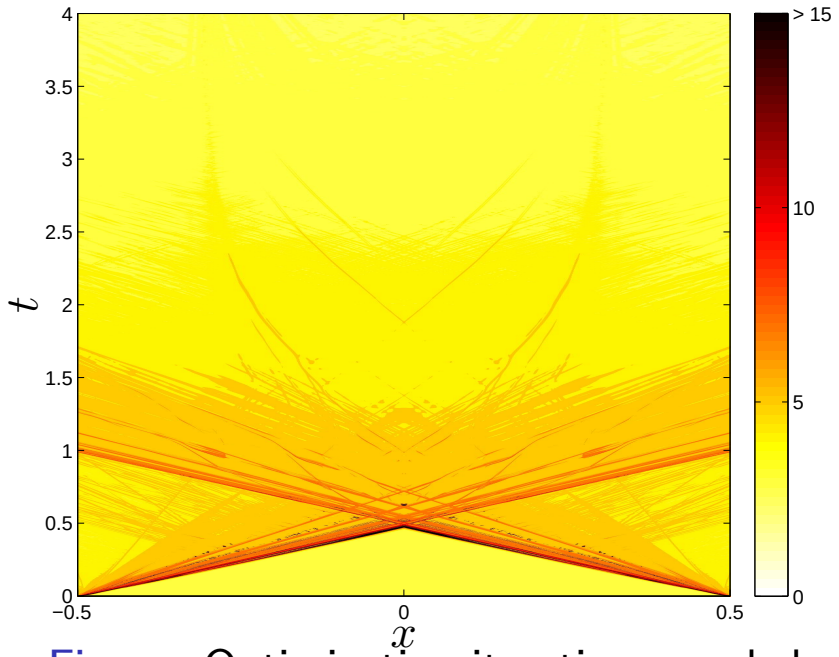



Figure: Optimization iterations needed for a sixteen-moment problem.

# A Scalable Numerical Approach to MHD Systems

Jinchao Xu, Penn State, xu@math.psu.edu, http://www.math.psu.edu/xu/

$$\begin{aligned} u_t + (u\cdot\nabla)u\,(= Du/Dt) - \mu\Delta u + \nabla p - (\nabla\times B)\times B &= 0, \quad \operatorname{div} u = 0, \\ B_t - \nabla\times(u\times B)\,(= \delta B/\delta t) + \eta\nabla\times(\nabla\times B) &= 0, \quad \operatorname{div} B = 0. \end{aligned}$$

Observation: Both convective terms are derivatives along flow trajectories:

$$\frac{\delta B}{\delta t} = \lim_{k\to 0}\frac{B(x,t) - F^{-1}B(y(x,t-k,t),t-k)}{k} = \frac{\partial B}{\partial t} - \nabla\times(u\times B).$$

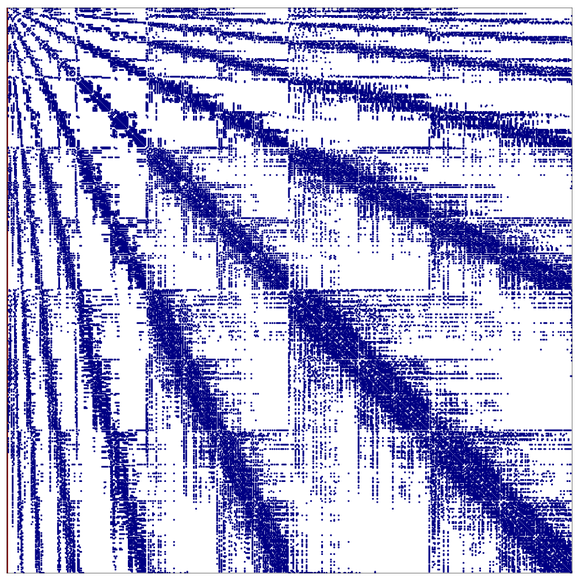
Eulerian-Lagrangian Method (ELM) $\Rightarrow$

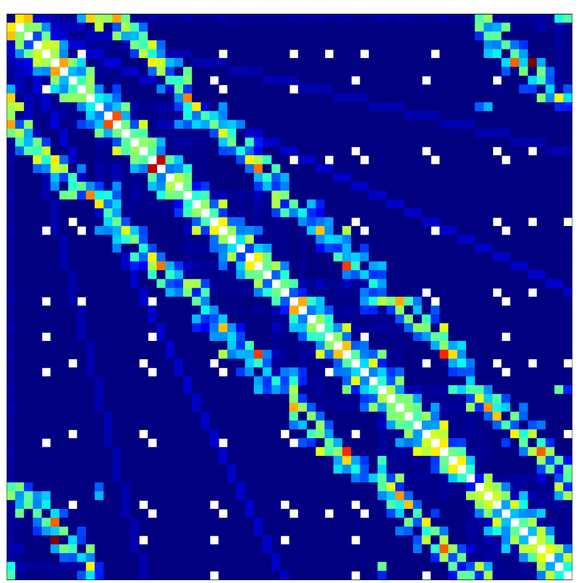
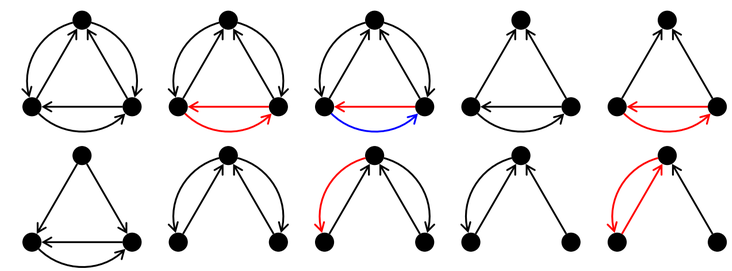
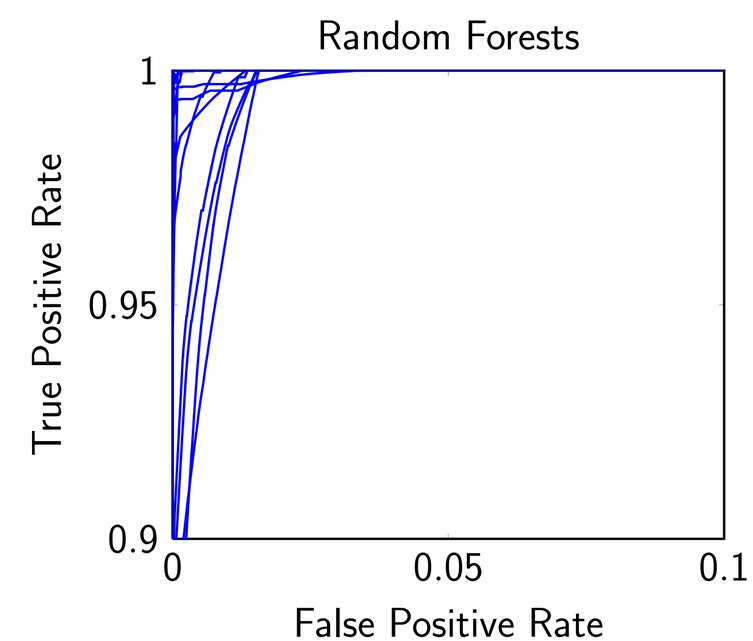
$$\begin{pmatrix} A_1 & N \\ 0 & A_2 \end{pmatrix}\begin{pmatrix} ((u,p)^T) \\ B \end{pmatrix} = \begin{pmatrix} ((f,0)^T) \\ g \end{pmatrix}. \quad (1)$$

$$A_1 = \begin{pmatrix} -\mu\Delta + k^{-1}I & (\operatorname{div})^* \\ \operatorname{div} & 0 \end{pmatrix}, A_2 = \eta\operatorname{curl}\operatorname{curl} + k^{-1}I, N(B) = (\nabla\times B)\times B.$$

- Scalable AMG and HX methods for (1) on unstructured grids;
- Appropriate numerical (exact) quadratures for ELM;
- Preliminary numerical examples;

# Classifying Distributed Computation





- Hypothesis: **distributed scientific computations exhibit well-structured communications**
- Task: **Infer the algorithm underlying observed communication patterns**
- Impacts: **security, performance analysis, algorithm replacement**
- Topics: **graph theory, network theory, machine learning**