Poster Blitz Session 1

Posters number 1 to 47

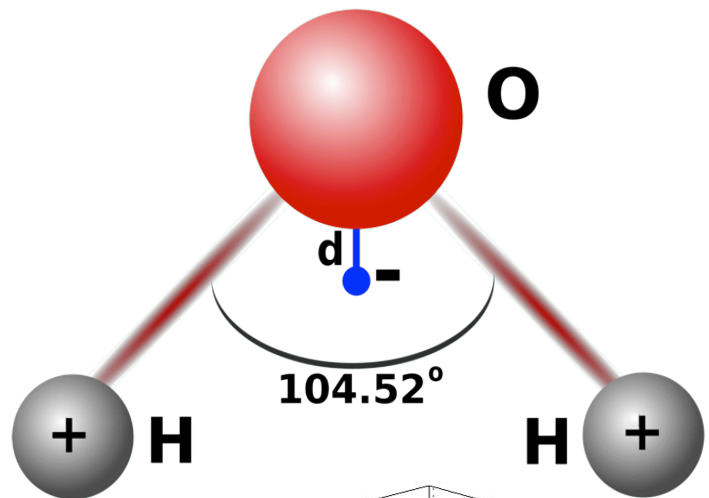
Regency Ballroom A

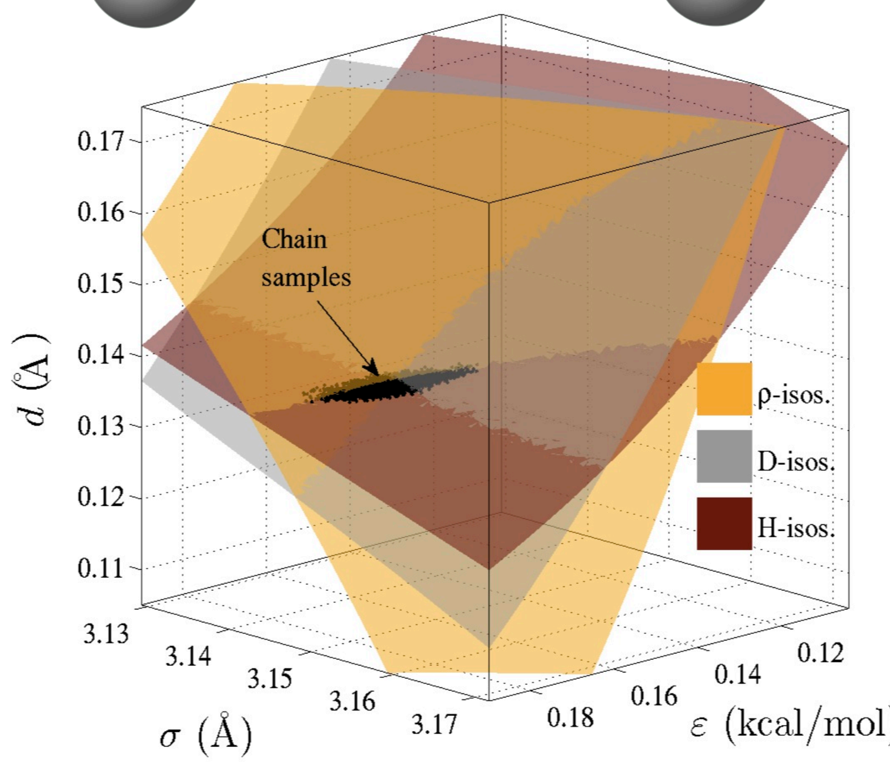
Poster 1 - Knio

Uncertainty Quantification in MD Simulations: Forward Propagation and Parameter Inference

O. Knio, F. Rizzi, H. Najm, B. Debusschere, K. Sargsyan, M. Salloum, H. Adalsteinsson

- We develop two approaches for propagating uncertainty in MD simulations, namely using
  - Non Intrusive Spectral Projection
  - Bayesian inference
- We demonstrate how the resulting Polynomial Chaos representations can be used as model surrogates in a Bayesian framework to infer atomistic force field parameters





Poster # 02

Emil Constantinescu & Mihai Anitescu, Argonne National Laboratory

Physics-based Covariance Models for Gaussian Processes with Multiple Outputs

Statistical Models for Petascale Spatiotemporal Data

- **Covariance structure has a chief role for UQ robustness**
- Many covariance models exist for single outputs, but few for multiple outputs
- Typically **ad hoc parametric models are considered** for modeling cross-correlations among fields
- Develop **analytical and numerical nonstationary** covariance models **compatible with underlying physical properties:**

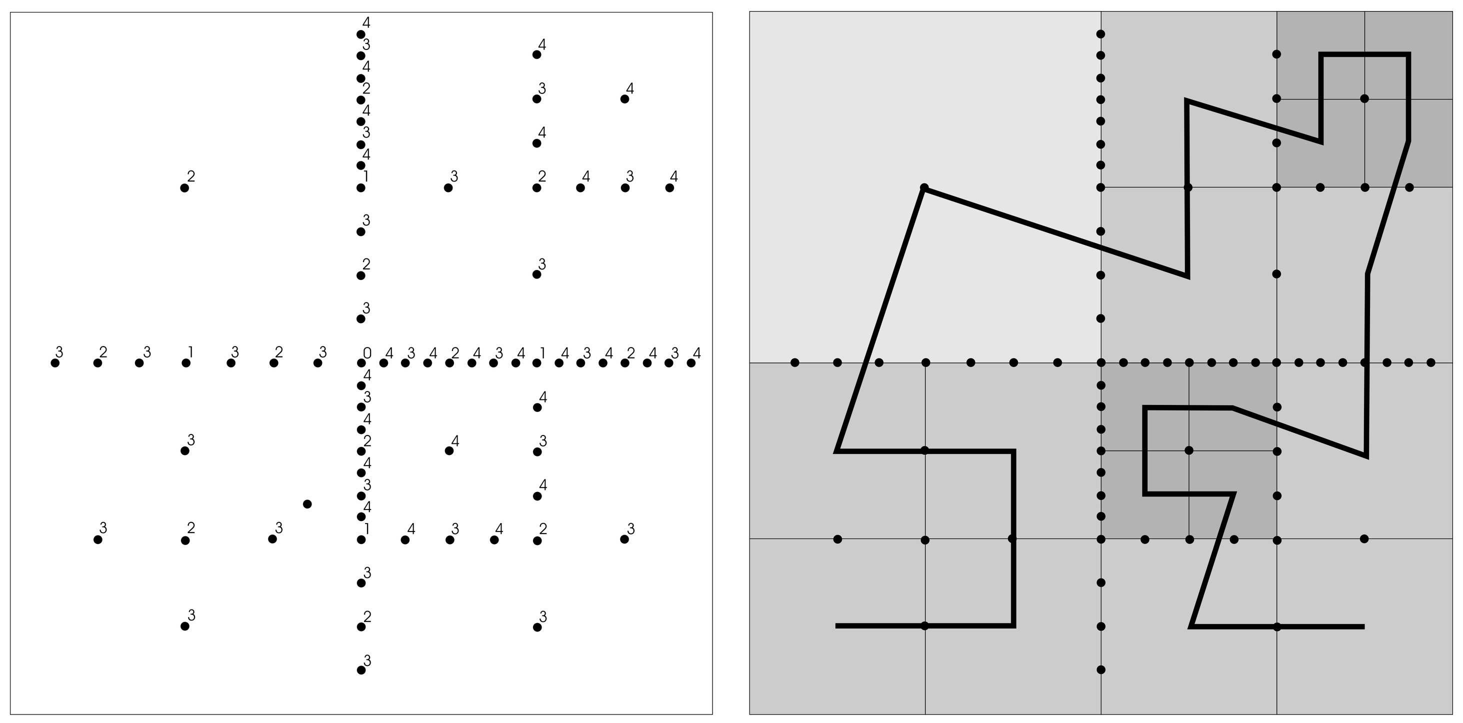
$$y_1 = f(y_1, y_2, \ldots, y_m) + \omega; \quad \text{e.g., } y_1 = \frac{\partial}{\partial x} y_2 \,, \ y_1 = \frac{\partial^2}{\partial x^2} y_2 \,, \ y_1 = y_2^2$$

- Applications: GP regression/kriging/co-kriging for spatial interpolation

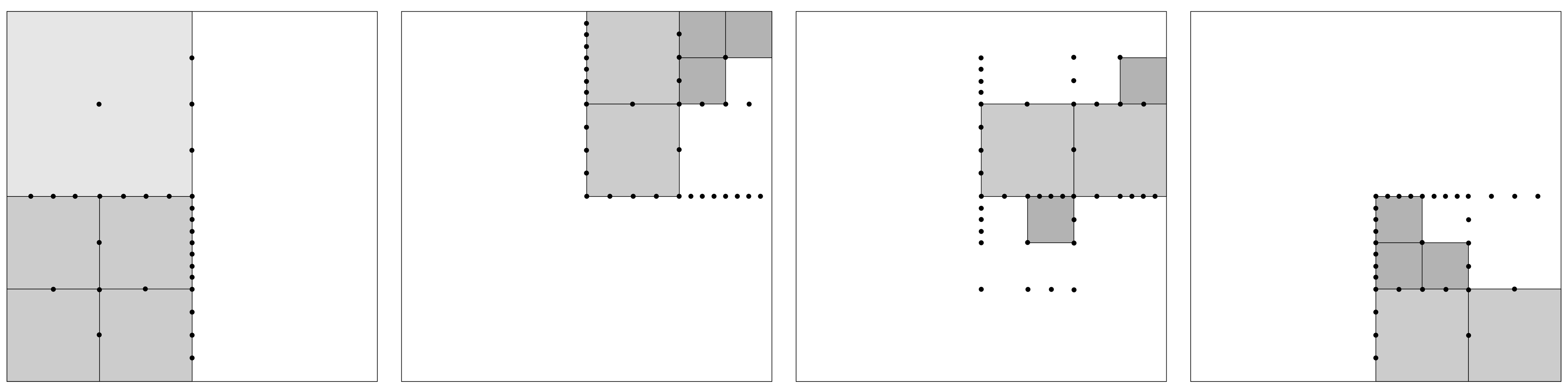
Extending adaptive sparse grids for stochastic collocation to hybrid architectures

Rick Archibald[1](archibaldrk@ornl.gov), Ralf Deiterding[1], Cory Hauck[1], John Jakeman[2], Dongbin Xiu[2]
[1]Computer Science and Mathematics Division, Oak Ridge National Laboratory, [2]Department of Mathematics, Purdue University

Parallelization



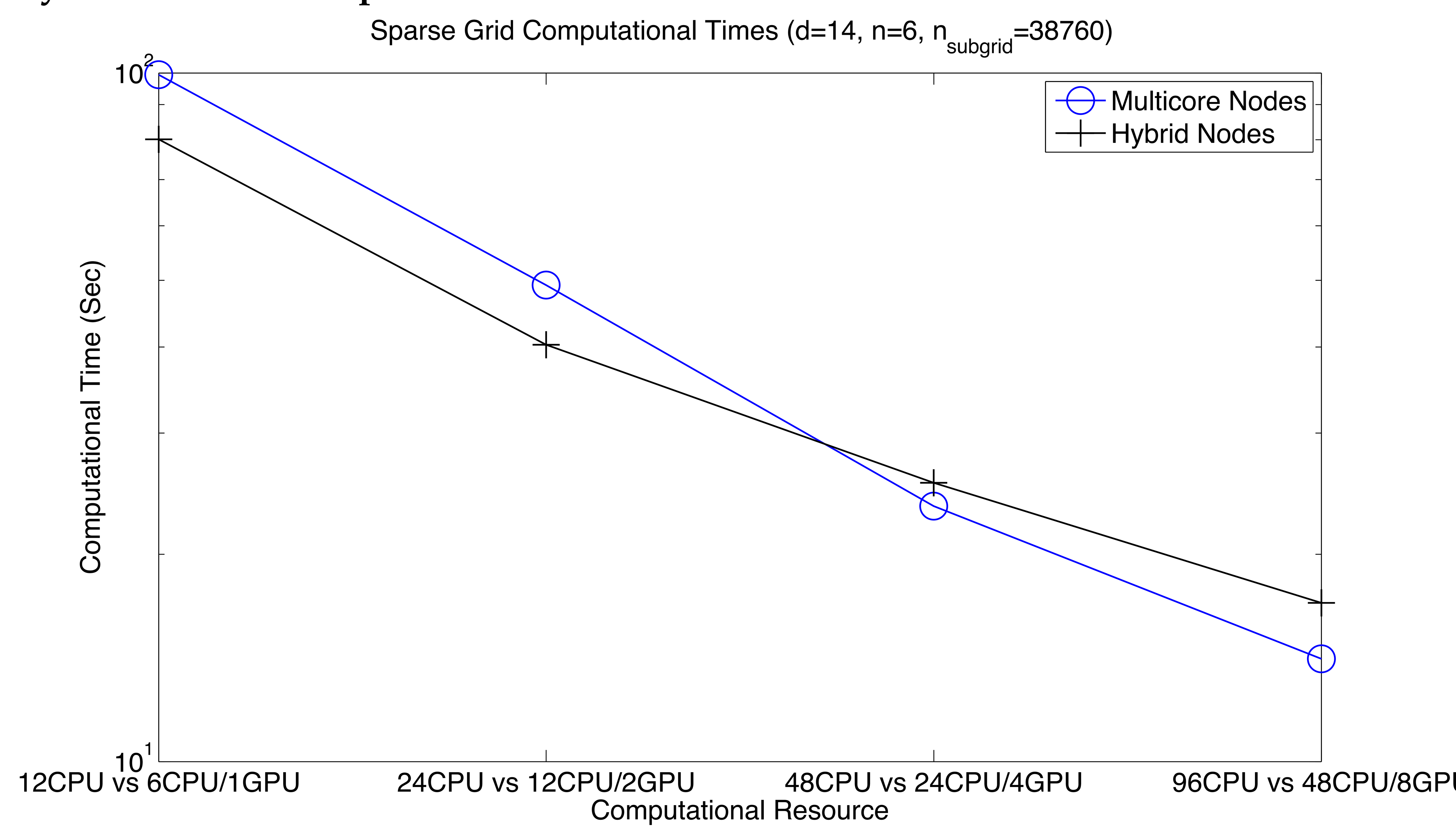
2D unbounded adapted sparse grid using 5 subspace levels. Left: each point indexed with subspace level used. Right: domains of the respective highest level and a generalized SFC used for decomposition.



Domain decomposition of above adaptive sparse grid to four nodes and/or thread blocks based on a generalized SFC.

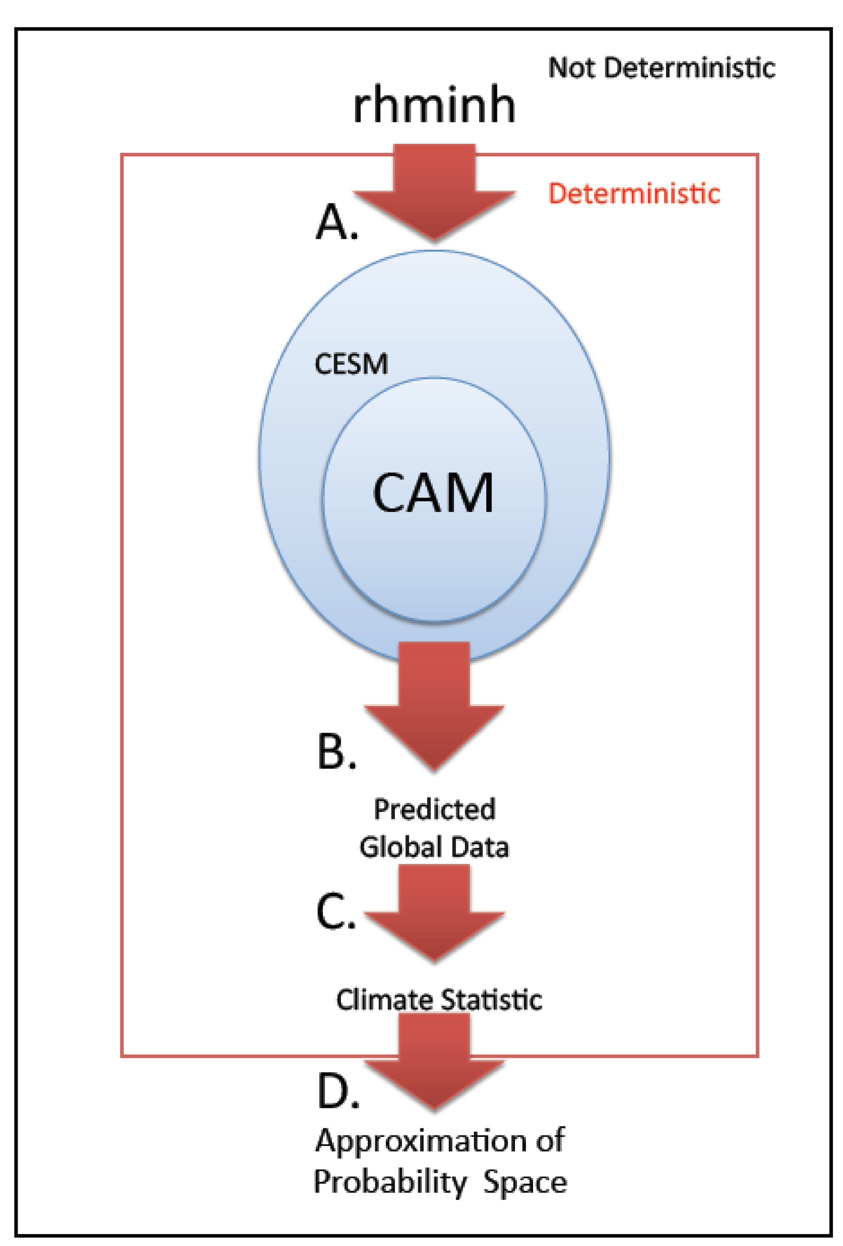
Hybridization

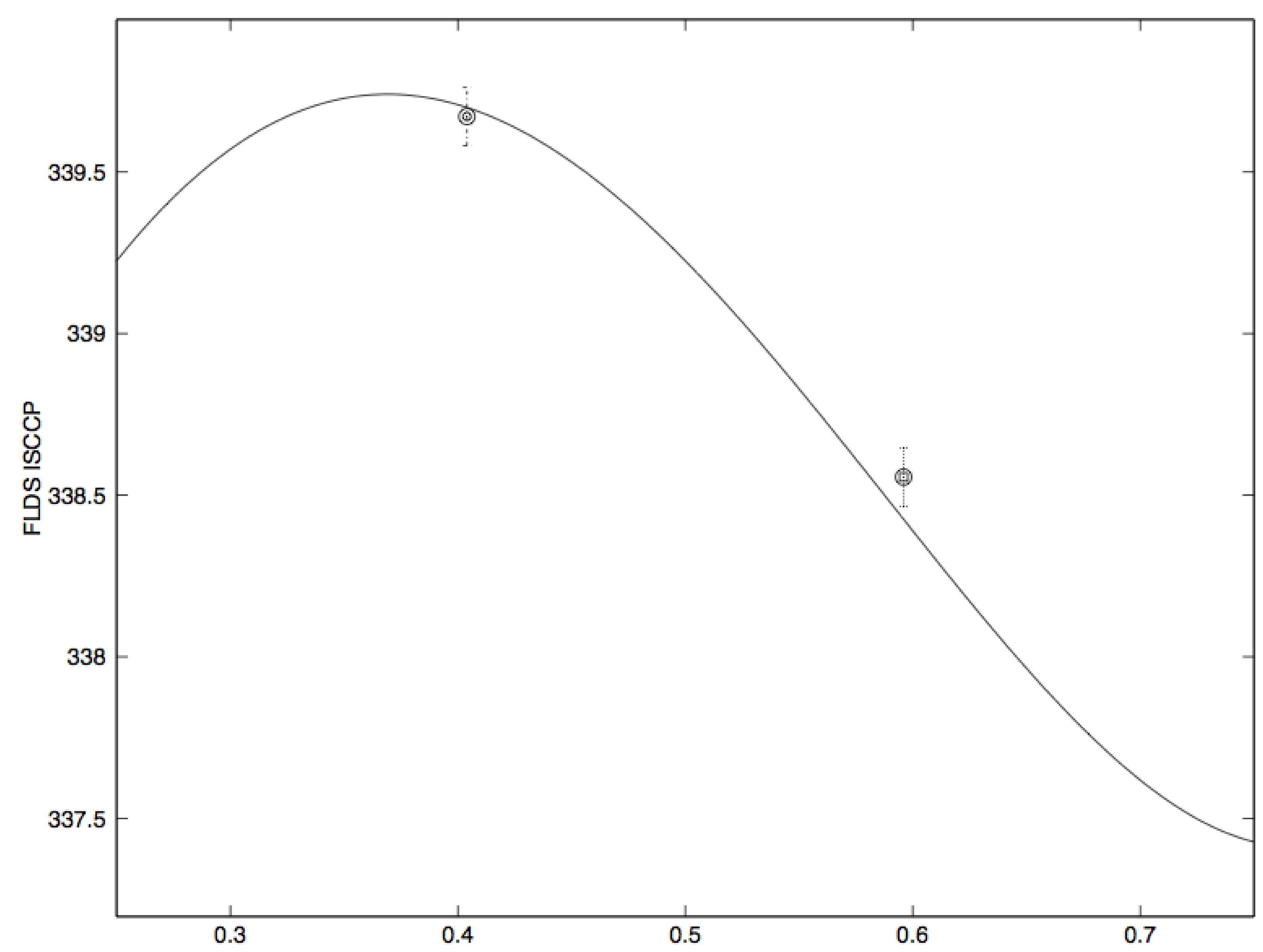
Strong scaling of sparse grid construction on the hybrid test cluster. MPI only vs. hybrid MPI/CUDA parallelization.



Application

We demonstrate how uncertainty error estimates can be derived from sparse grids to characterize parameter distributions in the community climate earth systems model (CESM). Left: Process for UQ in the CESM. Right: UQ error estimates of CESM statistics.





Poster #4: Conditional Value-at-Risk Based Approaches to Robust Network Flow, Connectivity and Design Problems

Baski Balasundaram, Oklahoma State University
Vladimir Boginski, University of Florida
Sergiy Butenko, Texas A&M University
Stan Uryasev, University of Florida

- **Objective**: Investigate models and algorithms for network flow, network design, and connectivity problems with the aim of obtaining robust solutions to the problems under uncertainty.
    - **Uncertainty**: Probabilistic arc failures- uniform random graphs, random graphs of given expected degree sequence
    - **Robustness (via Risk Aversion)**: By bounding or minimizing the conditional value-at-risk (CVaR) of an appropriately designed loss function, which quantifies losses as a function of decisions made under uncertainty
    - **Problems**: Minimum cost flows, shortest paths, minimum spanning *k*-cores, and low-diameter cluster detection
    - **Features**: Use of the quantitative risk measure CVaR in network optimization; Focus on uncertainty in network structure as opposed to costs and capacities

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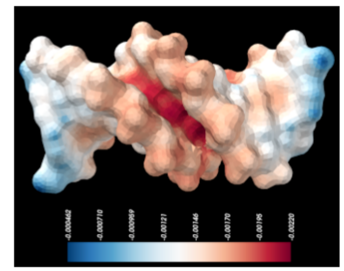
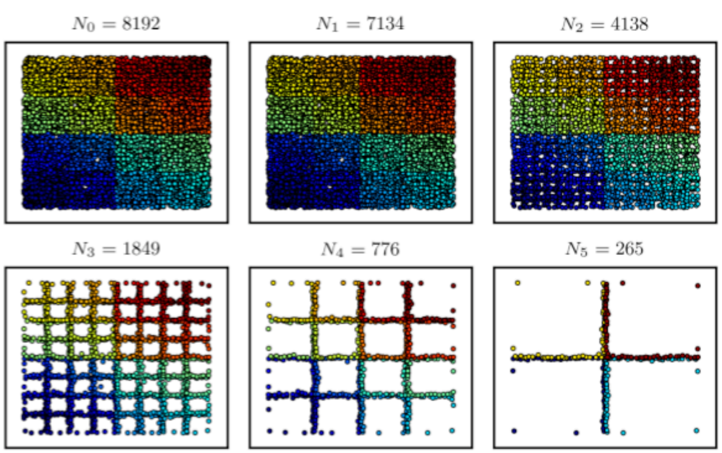
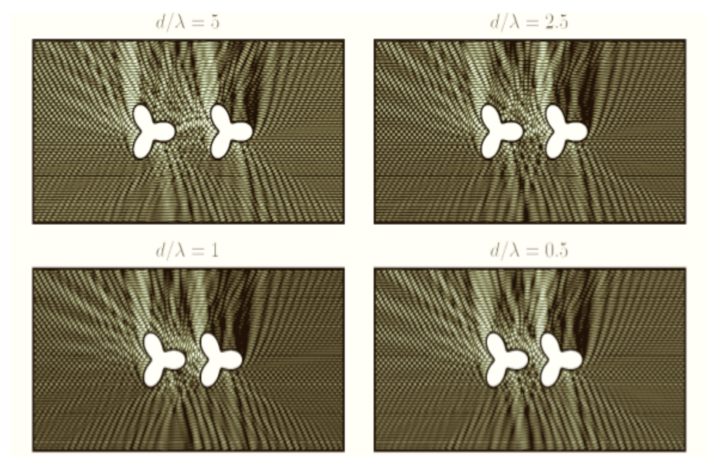
Poster 5: Kenneth L. Ho and *Leslie Greengard*
Courant Institute, NYU

A fast direct solver for structured matrices

- Multilevel matrix compression (non-oscillatory integral equations in 3D): extension of Martinsson/Rokhlin algorithm
- Efficient storage, fast matrix-vector multiplication, fast inverse
- Factorization cost is currently O(N) in 2D and O($N^{3/2}$) in 3D
- Application of inverse is O(N) in 2D and O(N log N) in 3D
- Closely related to *HSS matrices* (Chandrasekaran/Gu et al.), *H-matrices* (Hackbusch et al.)

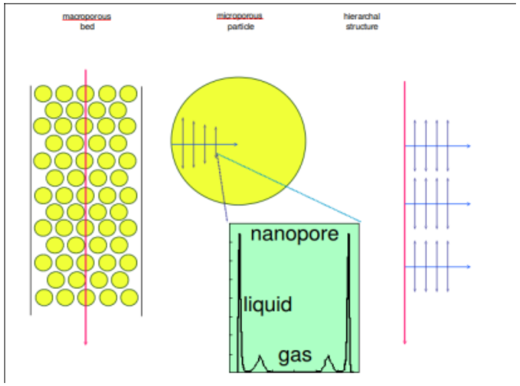




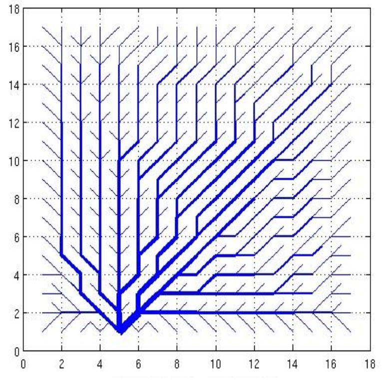


Poster Number 6, Stephen G. Nash
Complex Hierarchical Optimization Algorithms for the Design of Nanoporous Materials

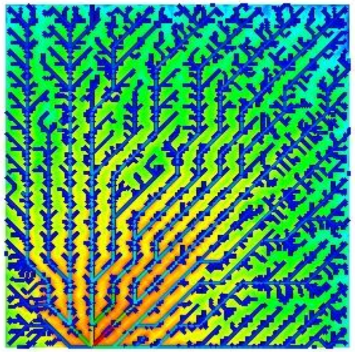
- **Objectives**
  - Formulate and solve multi-scale optimization problems for energy storage applications
  - Develop multi-scale models for optimizing the internal structure of nanoporous materials
    - Allow different physics at different scales
    - Derive methods to communicate between scales
  - Create a general multi-grid optimization algorithm to solve such problems on high-performance computers



Transport Model



Network Approximation



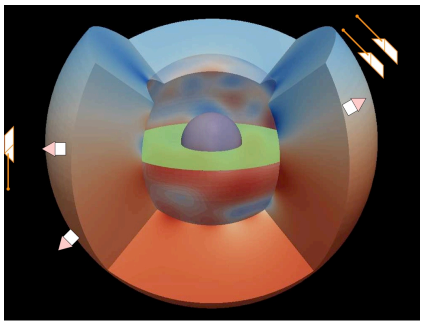
Optimization Model

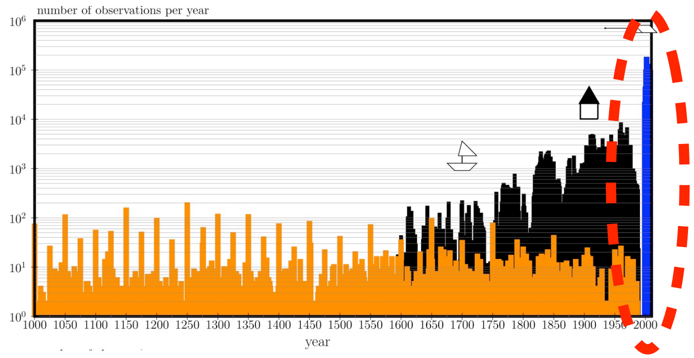
Implicit Sampling with Application to Filtering and Data Assimilation

Ethan Atkins*°, Alexandre J. Chorin*°, Matthias Morzfeld°, Xuemin Tu‡

° Lawrence Berkeley National Laboratory, ‡ Department of Mathematics, University of Kansas, * Department of Mathematics, University of California, Berkeley

Data Assimilation:
Use data to update the forecasts of numerical models





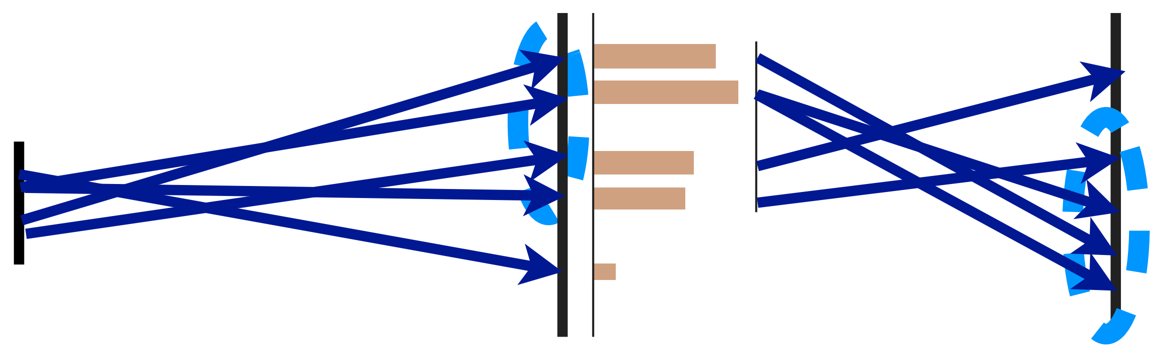
Sequential Monte Carlo

- Tool for nonlinear, non-Gaussian data assimilation
- Relies on efficient sampling of large dimensional probability densities

Implicit Sampling

- Sequential Monte Carlo method
- Uses available data to sample high probability region of the target pdf and avoids regions of low probability

Implicit sampling algorithms find
high probability samples by solving algebraic equations



64. Jinghe ZHANG

Adaptive Kalman Filtering for Robust Power System State Tracking

THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

Kalman Filters (KF) in Power System State Estimation

Applying Kalman filters to the dynamic state estimation of modern power grid is promising, however there are challenges such as:

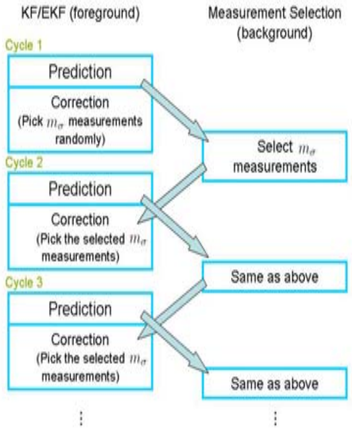
- **Computational burden with large-scale data processing**
- **Unknown system dynamics and false measurements**

Our Solution: LoDiM

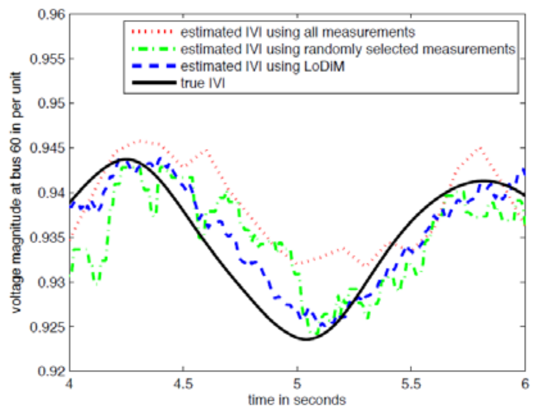
- When the measurement data to be processed is massive, calculating the **Kalman gain** is expensive
- A background-running **measurement selection procedure** analyzes the error covariance matrix per cycle using PCA, then create a "ranking vector" for all measurements
- LoDiM selects only **a subset of measurements** per cycle with most "value" --- largest **sensitivity-to-uncertainty** ratio

Our Solution: AKF with InNoVa

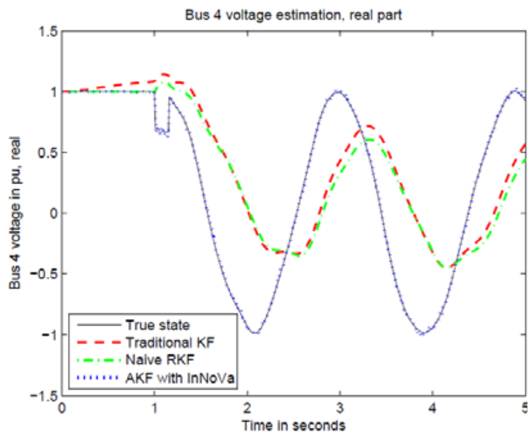
- Estimates using traditional KF can deviate from truth fast when facing unknown system dynamics and/or false measurements
- AKF with InNoVa employs a **normalized a priori innovation test** and a **normalized a posteriori innovation test**, to adjust process/measurement noise cov. separately on the fly
- These tests help **separating the process and measurement factors** when facing terrible estimations



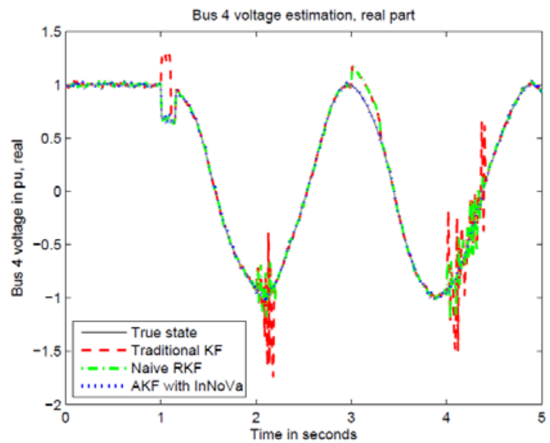
LoDiM Structure



LoDiM Performance



Performance with wrong modeling and a mulfunctioned device



Performance with several noise interfered devices

Multigrid methods in PDE constrained optimization

- Abstract problem formulation:

$$\begin{cases} \text{minimize} & J(y,u) = \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + R(u,y), \\ \text{subj. to} & u \in U_{ad} \subset U, \quad y \in Y_{ad} \subset Y, \\ & e(y,u) = 0\ . \end{cases} \tag{1}$$

- Goal: Develop optimal order preconditioners for linear systems arising in the solution process of (1).
- We extend methods and analysis from unconstrained, linear PDEs to the following model problems:
  - **A.** Nonlinear PDE constraints: semilinear elliptic equations (optimal order).
  - **B.** Control constraints: 1. interior point methods; 2. semi-smooth Newton methods (suboptimal).
  - **C.** Problems constrained by fluid flow: Stokes equations (optimal order).

A High Order Spectral Deferred Correction Method in CAM-HOMME

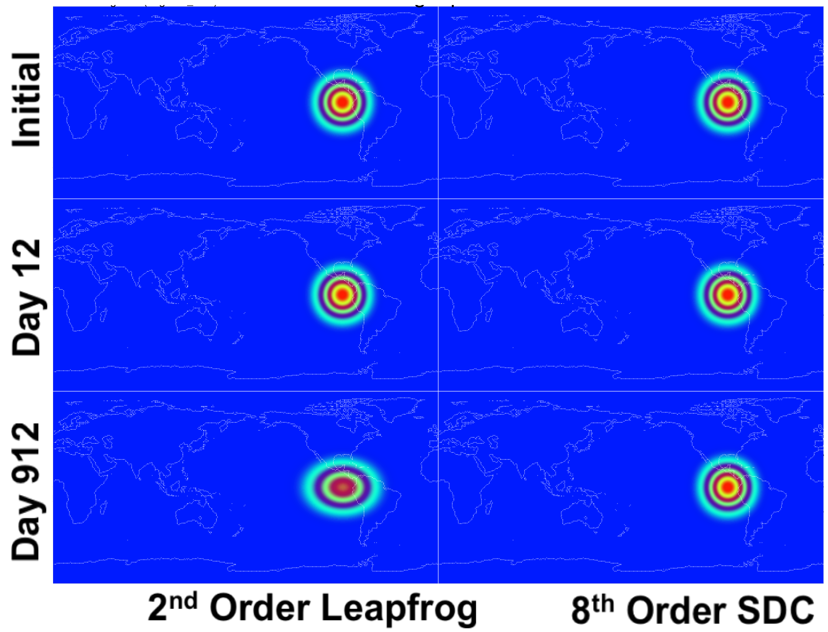
J. Jia, J. Hill, G. Fann, K. Evans (ORNL), M. Taylor (SNL)

Objectives

- **Accurate and efficient time integrations in testbed climate simulations**
- **Accurate long time simulations of physical systems where error accumulation is an issue**
- **Use generic solver interface to test new algorithms**

Accomplishments

- **Developed and demonstrated new mathematical method and algorithms for high accuracy simulations in time up to 8th order**
  - Highest Runge-Kutta is of 6th order
  - Exceeds the Fully Implicit Jacobian-Free Newton-Krylov method
  - Scalable variants of deferred correction methods
- **Passed shallow water test cases in the climate dynamics spectral element core of HOMME**



Accurate time-dependent simulations computes

- *Accurate flow fields*
- *Conserves mass and energy*
- *Topological and geometric features*

After 12 simulation days, both the existing explicit leapfrog (left) and the new spectral deferred correction (SDC) (right) time methods preserve the shape of a Gaussian bell as it is advected around a sphere. For climate length simulation times ~2.5 years, the improved temporal accuracy of the SDC method is evident by the preservation of the Gaussian shape compared to the leapfrog method.

11. Misun Min and Paul Fischer (Mathematics and Computer Science Division, ANL)

Scaling PDE Solvers to Exascale

NekCEM, NekLBM, Nek5000: Scalable Software based on Spectral-Element Discretizations for Electromagnetics and Fluids

- Peta- and exascale simulations are driven by scale disparity: small scales λ interacting with scales $L \gg \lambda$
- Dispersion errors accumulate linearly with time:

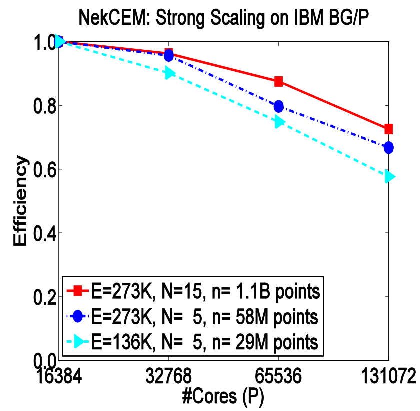
  $\varepsilon_t \sim$ |correct speed - numerical speed|$*t$

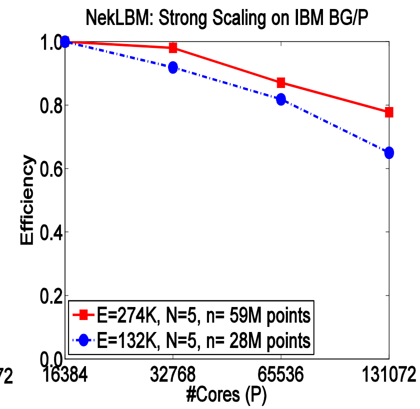
  $\rightarrow \varepsilon_{\text{final}} \sim$ |numerical dispersion error|$*t_{\text{final}}$

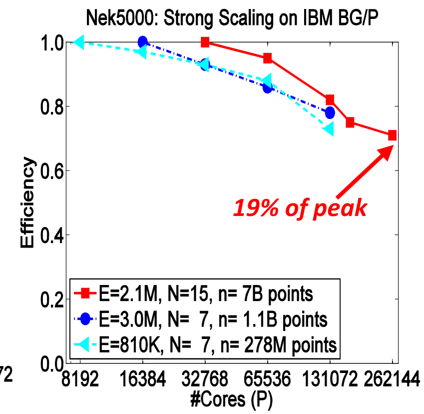
  $\sim$ |numerical dispersion error|$*(L/\lambda)$
- For final error $\varepsilon_{\text{final}} < 1$, require:

  |numerical dispersion error| $\sim (\lambda/L)\varepsilon_{\text{final}} \sim O(h^N) \ll 1$

  h: grid spacing, N: approximation order
- Well-implemented, high-order discretizations efficiently deliver small dispersion errors, yielding an ***order -of-magnitude*** savings in computational cost (Kreiss & Oliger 72, Gottlieb et al. 07)

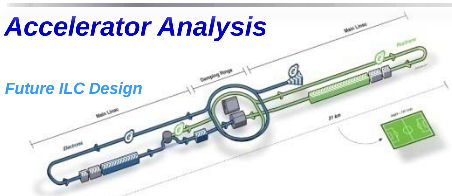




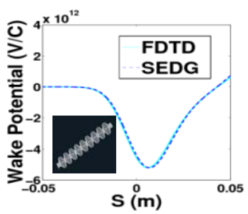


Accelerator Analysis

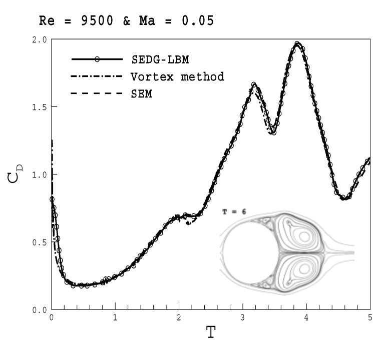
Future ILC Design



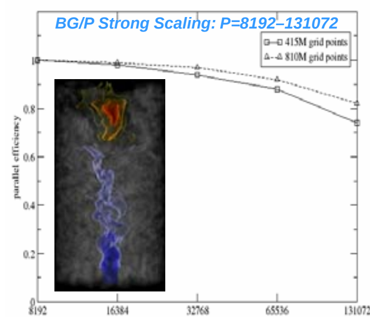
TESLA cavity



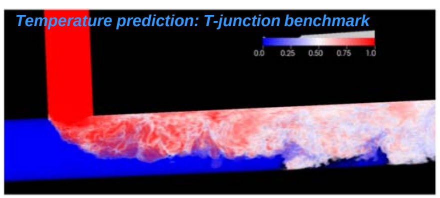
Lattice Boltzmann Method

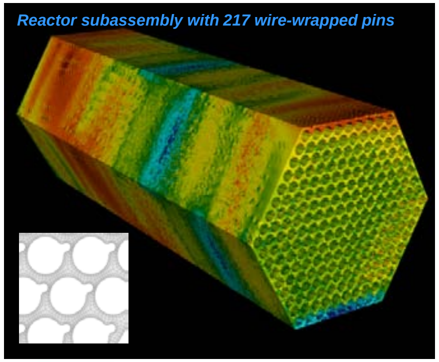


Turbulent Combustion

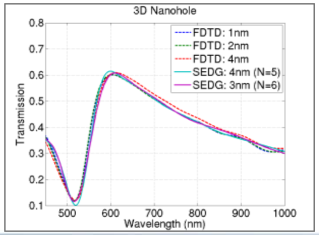


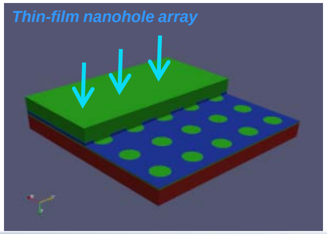
Nuclear Reactor Modeling



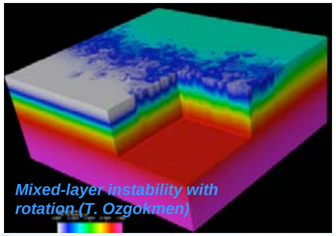


Nanophotonics





Ocean Modeling



Multiscale Nonlinear Characterization of Highly Entangled Polymers

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[b]Department of Applied Science, University of California, Davis, CA 95616

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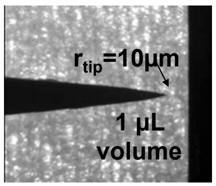
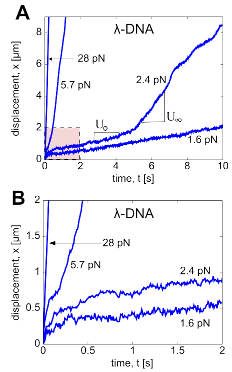
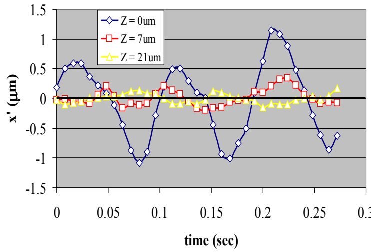
Micron scale experiments

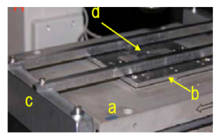




The experimental signature is an acceleration phase which is captured by the RP model simulations making the phenomenon tunable.

Millimeter scale experiments





There is no observable signature of nonlinearity, except FFT of passive tracers. With RP model simulations of finite depth layers in oscillatory strain we develop metrics of nonlinearity and determine depth of nonlinear penetration.

•Conservation of momentum

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = \frac{1}{\mathrm{Re}}\nabla\cdot(-p\mathbf{I}+\boldsymbol{\tau})$$

Mitran et al. JNNFM 154 (2008)
Lindley et al. JNNFM 156 (2009)

•Variables

$$p = p(y,t), \quad v_x = v_x(y,t), \quad v_y = 0, \quad v_z = 0$$

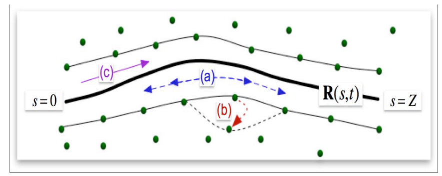
$$X(y,t) = \int_0^t v_x(y,t')dt' + X(y,0)$$

Rolie Poly Model

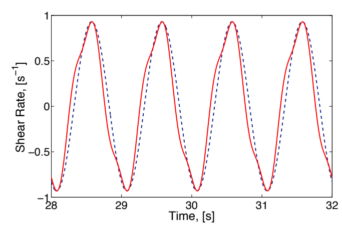
Likhtman et al. JNNFM 114 (2003)
Teixeira et al. Macromolecules 40 (2007)
Cribb,Vasquez, Forest, et al. Preprint

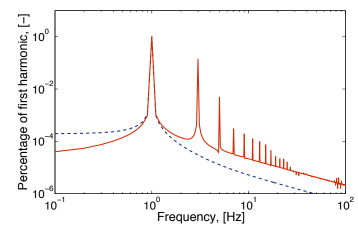
$$\frac{\boldsymbol{\tau}}{G_0} = \int_0^Z \left\langle \frac{\partial R_\alpha}{\partial s}\frac{\partial R_\beta}{\partial s}\right\rangle ds$$

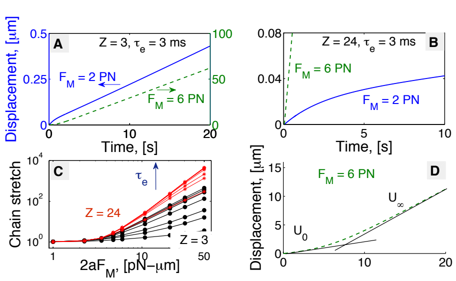
$$\lambda\overset{\nabla}{\boldsymbol{\tau}} = \eta_p\dot{\gamma} - \boldsymbol{\tau} - \frac{2}{\lambda_R}\left(1-\frac{1}{\sqrt{\mathrm{tr}(\boldsymbol{\tau})/3+1}}\right)\left[\boldsymbol{\tau}+\mathbf{I}+\beta\,\boldsymbol{\tau}\,\sqrt{\mathrm{tr}(\boldsymbol{\tau})/3+1}\right]$$

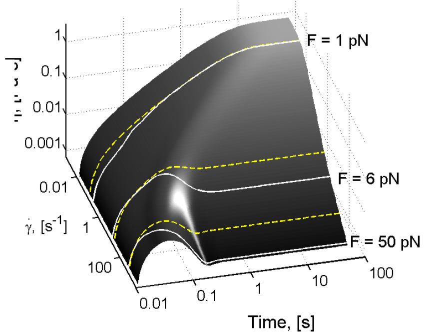


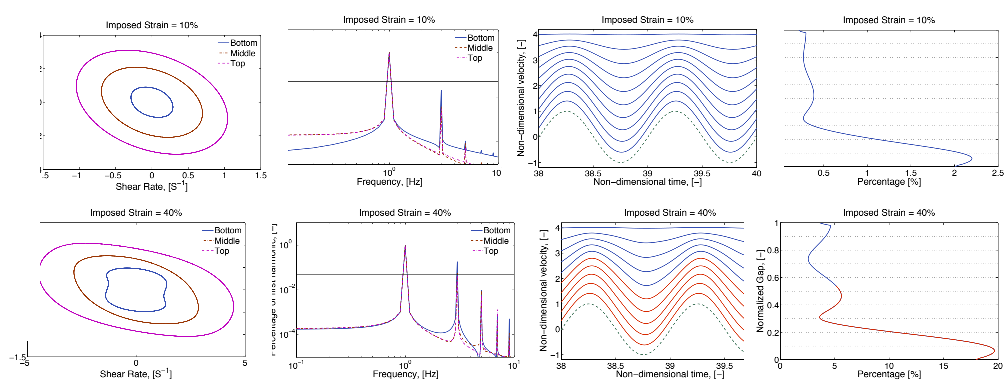
a) Reptation
b) Convective constraint release
c) Retraction











Fast Alternating Direction Augmented Lagrangian Methods for Solving Convex Optimization Problems

DOE Grant #: DE-FG02-08ER-25856

P.I. Donald Goldfarb†, Co P.I. Garud Iyengar†

† Department of Industrial Engineering and Operations Research, Columbia University

Stable Principal Component Pursuit

- The problem

$$\min_{X,Y \in \mathbb{R}^{m \times n}} \|X\|_* + \rho\|Y\|_1 \quad s.t. \ \|X + Y - M\|_F \le \delta.$$

- Split X, i.e. solve

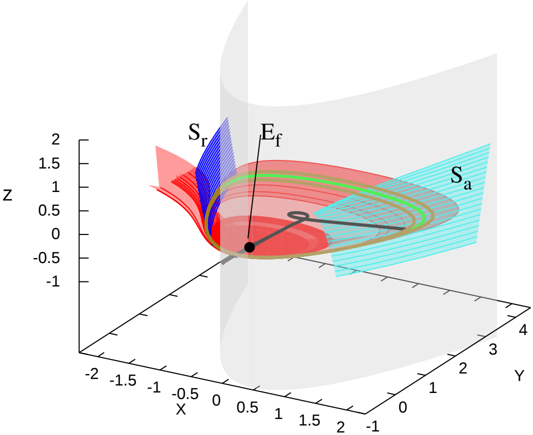
$$\begin{aligned}\min_{X,Y,Z \in \mathbb{R}^{m \times n}} \ & \|X\|_* + \rho\|Y\|_1 \\ s.t. \ & X = Z, \\ & \|Z + Y - M\|_F \le \delta.\end{aligned}$$

- Solve by the Alternating Direction Augmented Lagrangian (ADAL) method
- 15M variables, 5M linear constraints
- CPU time: 2.67 minutes (laptop)
- Fast (low complexity) algorithms: ϵ-optimal solution in $O(\frac{1}{\epsilon})$ iterations

Numerical Analysis of of Multiple Time Scale Dynamical Systems

Poster 14: John Guckenheimer

- Singular Hopf bifurcation analysis (Philipp Meerkamp)
- Normal forms of dynamic Hopf bifurcation (Hinke Osinga)
- MMOs of BZ reaction (Chris Scheper)
- Smooth multivariate interpolation



Steven Hofmeyr, Poster 16

Modeling Interventions in Complex Networks

- Malware spread on complex networks difficult to predict
- Effect of proposed security policies/interventions unclear
- Investigate using agent-based modeling and mathematical analysis
- Some results
  - Impact of different ISP-level interventions on spread of malware across the Internet
  - Impact of different search provider interventions on the spread of drive-by-downloads

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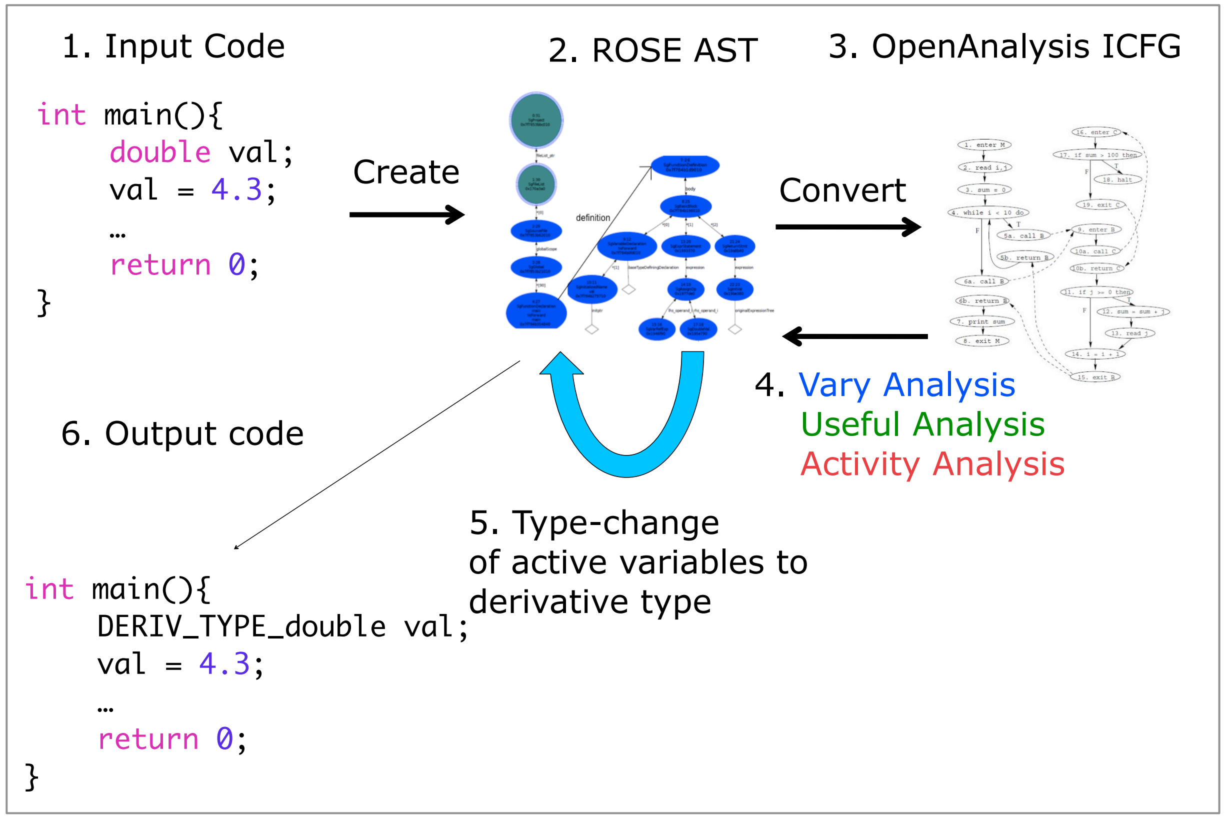
Poster 17, Sri Hari Krishna Narayanan

Identifying Active Variables to Improve the Performance of Operator Overloading Automatic Differentiation

- Operator overloading automatic differentiation can be inefficient.
- Overestimating the number of active variables exacerbates the situation.
- This tool performs active variable detection and automatic type change.
- Tested with Sacado.

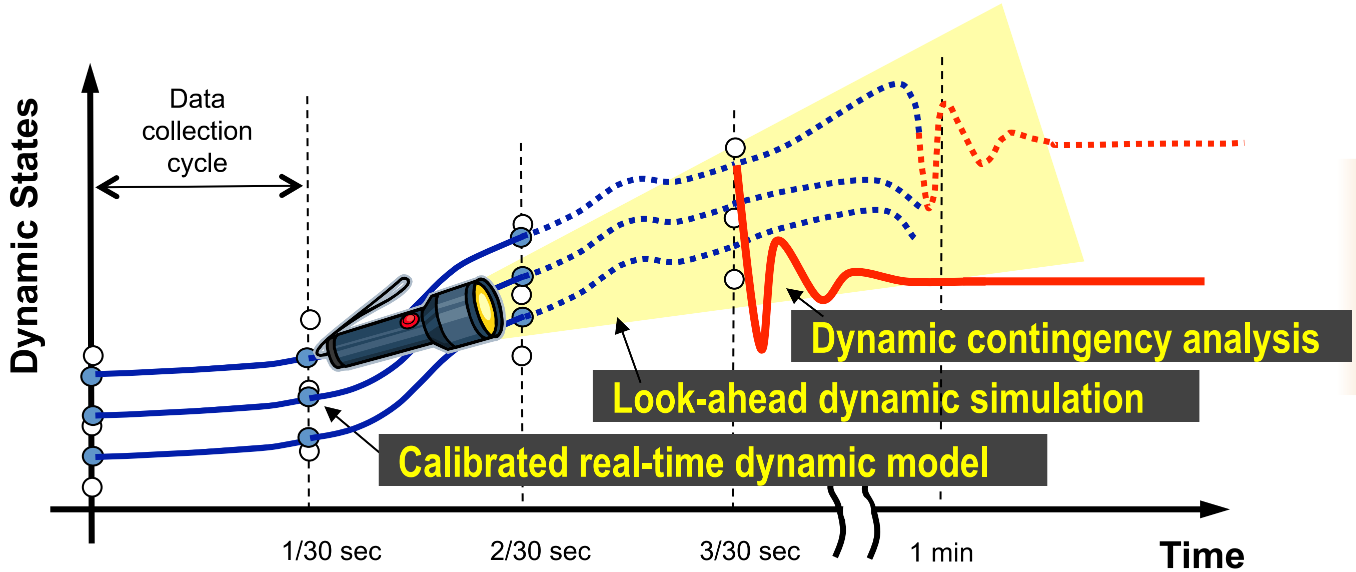
```
DERIV_TYPE operator* (const DERIV_TYPE &other)
{
   this->val = this->val() * other.val();
   this->dx = this->val() * other.dx() +
              other->val() * this->dx();
   return *this;
}
```



Fusing Models and Data for a Dynamic Paradigm of Power Grid Operations

Henry Huang, PNNL

- **National Driver**: Clean and Efficient Power Grid as well as being affordable, reliable, and secure. ➔ Grid Evolution Meeting Information Revolution

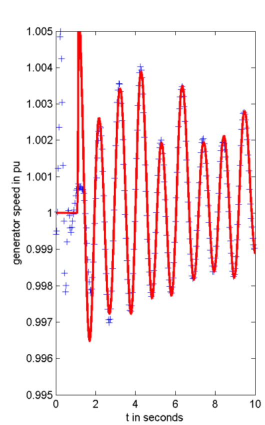


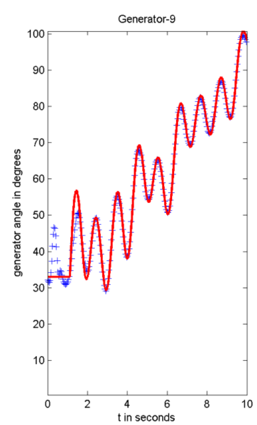
Better Reliability

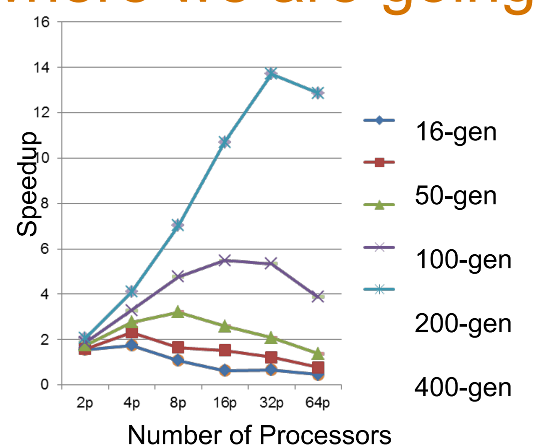
Clean Energy Integration

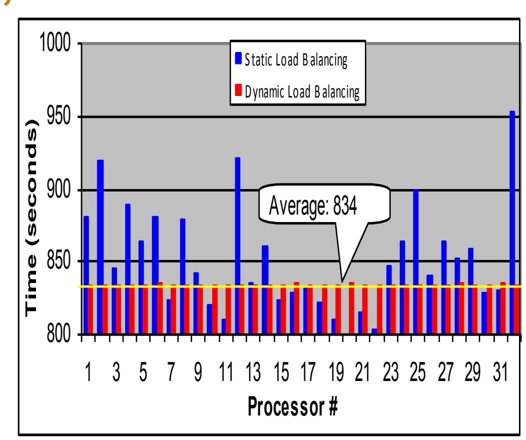
Better Asset Utilization

know where we are, where we are going, and what-ifs



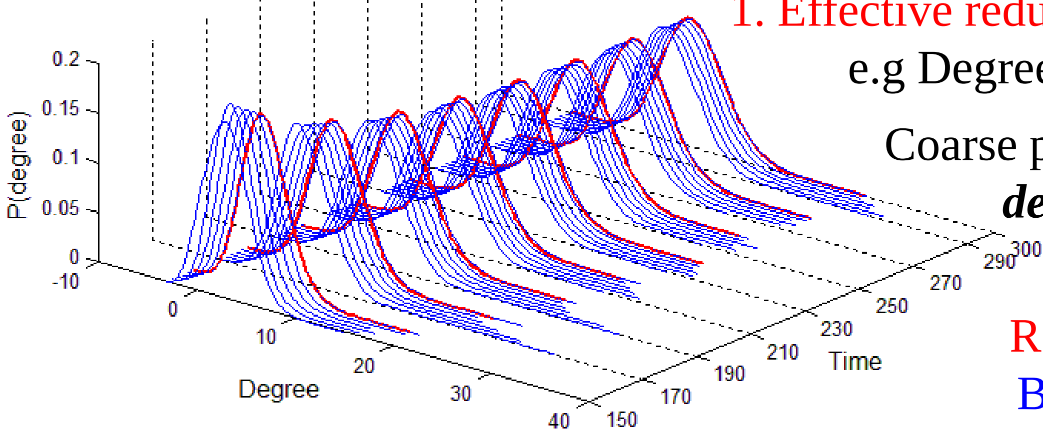






19. Yannis Kevrekidis & coworkers, Princeton U.

Coarse-graining the dynamics of (and on) evolving graphs: *Algorithms and Computation*



1. Effective reduced models for network evolution:

e.g Degree distribution evolves smoothly in time.

Coarse projective integration using ***degree distribution*** as the coarse variable

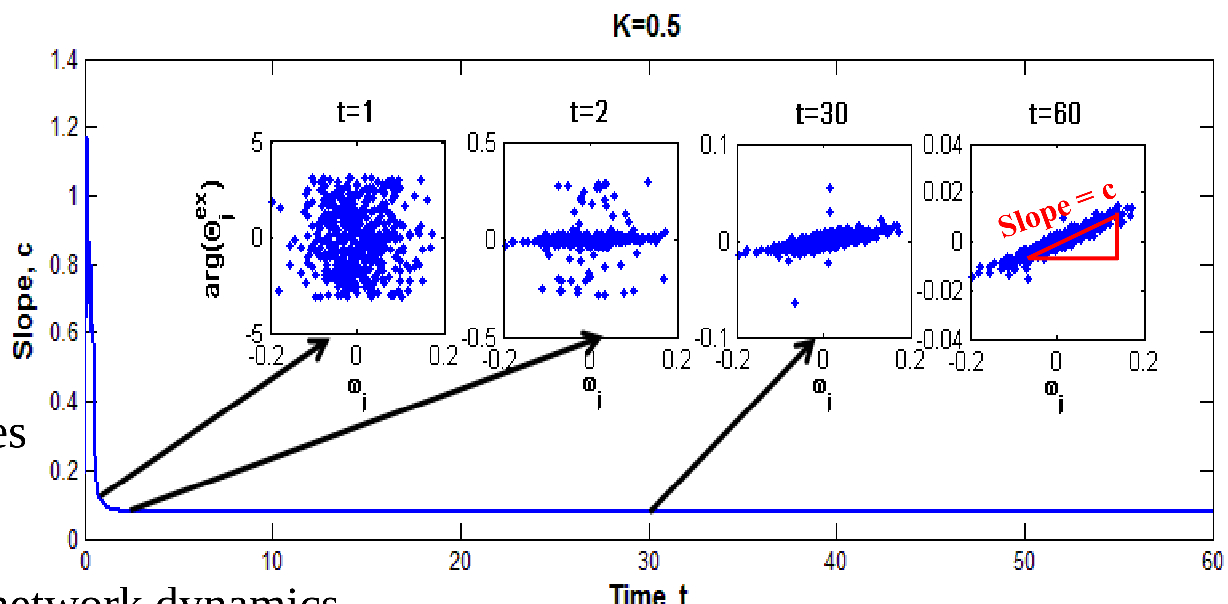
Red – Snapshots of direct simulation

Blue - Coarse Projective Integration

2. Heterogeneity and Coarse-Graining

Portions of the network state correlate strongly with heterogeneity.

Idea: Link with UQ techniques (like Polynomial Chaos) to parameterize the effect of heterogeneity in network dynamics.



Parallelization Challenges for Scenario-Based Decomposition of Stochastic Programs

- Your hosts: Jean-Paul Watson (Sandia/NM) and David Woodruff (UC Davis)
  - With support from: Roger Wets (UC Davis)

- Motivating observation:
  - Parallelizing scenario-based decomposition algorithms is conceptually easy
  - But as is usual in practice, the devil is in the many details

- You should care about this talk if:
  - You want to solve real, large-scale stochastic programs
    - Especially of the mixed-integer and non-linear varieties

- Some keywords you will hear us mention frequently should you stop by:
  - Scenario bundling, asynchronous decomposition, Progressive Hedging
  - Pyomo, PySP, Coopr, Pyro, Python, and open-source software

Mathematical analysis for the peridynamic continuum theory (poster 21)

- Peridynamic continuum theory is nonlocal
  - Interaction is nonlocal and not just due to contact
- Differential operators are replaced by integral operators
- Deformation allowed to be discontinuous
  - Nonlocal balance of angular and linear momentum
  - Nonlocal balance of energy (diffusion)
  - Nonlocal, nonlinear conservation laws
- Nonlocal vector calculus enables well-posedness of the equations (for linear materials)
- Qiang Du (PSU), Max Gunzburger (FSU), *Rich Lehoucq* (SNL)

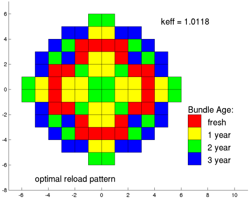
A New Toolkit for Nonlinear Optimization

Nonlinear Optimization:

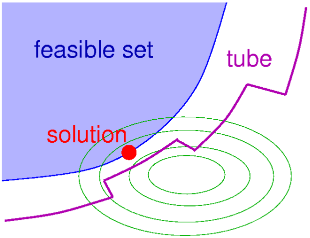
$$\text{minimize } f(x) \quad \text{subject to } c(x) \geq 0$$

Reactor core reloading

AC power flow models



xTiNO: C++ extensible toolkit for nonlinear optimization



Globalization Strategies:

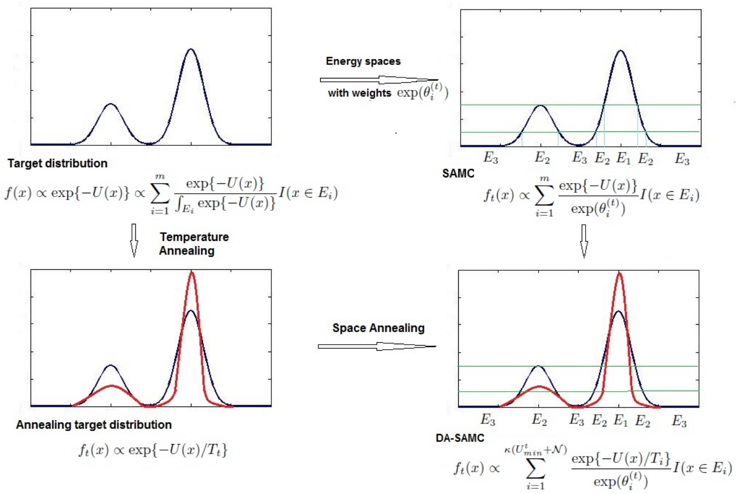
- traditional penalty function
- nonmonotone filter or tube

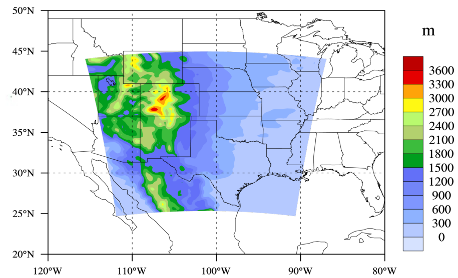
Step Computation:

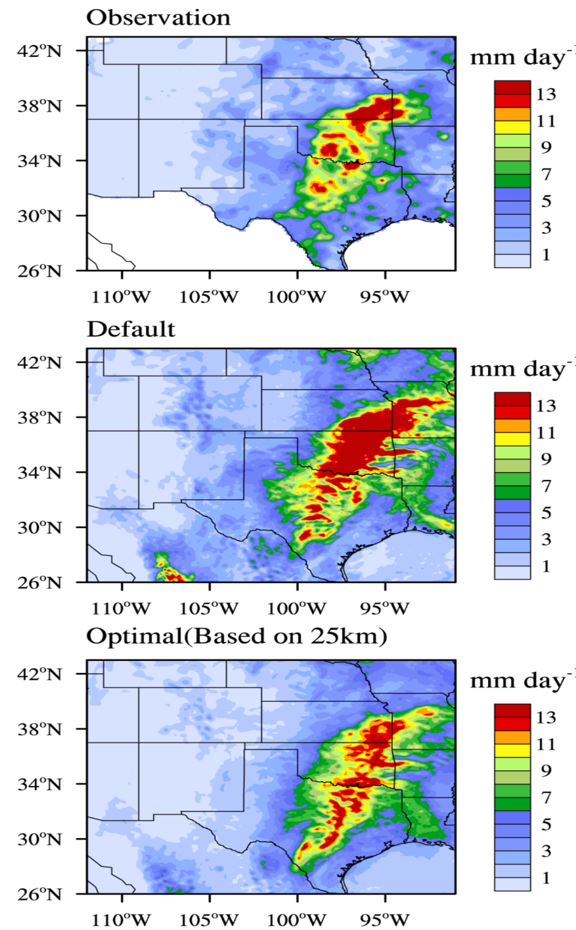
- SQP, SLQP, ... SQQP
- novel augmented Lagrangian

Optimal Parameter and Uncertainty Estimation for Climate Model Prediction using Multi-Level Dual-Annealing Stochastic Approximation Monte Carlo Algorithm

Guang Lin, Yichen Cheng, Ben Yang, Yun Qian, L. Ruby Leung
Pacific Northwest National Laboratory



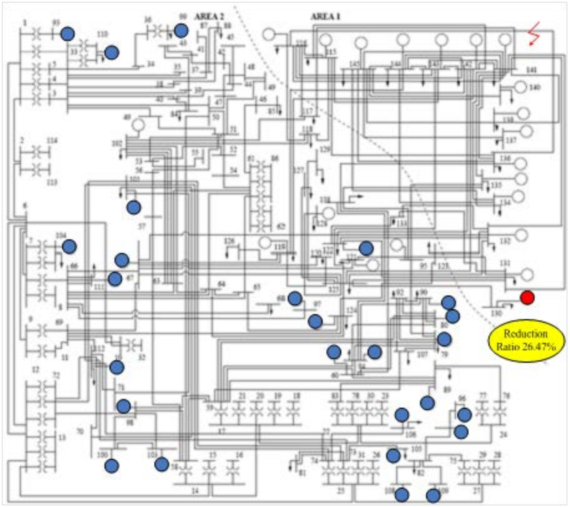




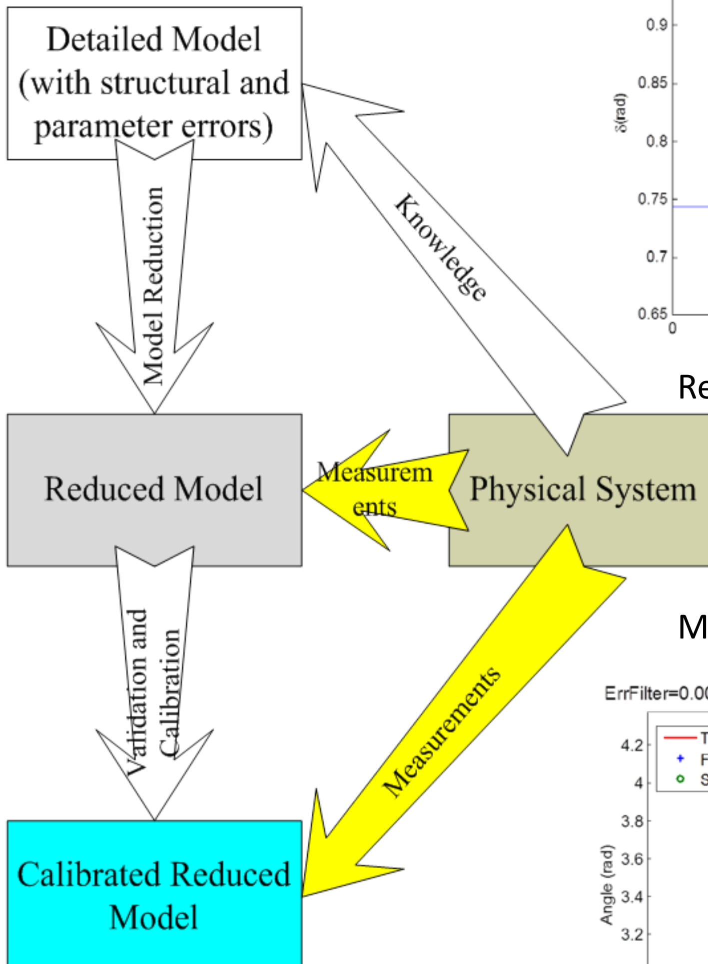
- Multi-level DA-SAMC algorithm can:
  - greatly speedup the convergence of Bayesian model parameter calibration and dramatically reduce the number of ensemble runs;
  - The proposed method is a scare-aware model parameter calibration method;
  - The multi-level dual-annealing SAMC method can guarantee to find the global optimal parameter estimation and avoid local trapping

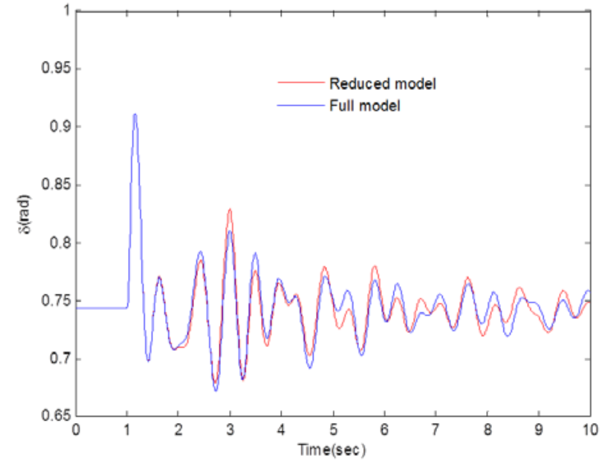
#24 – Shuai Lu and Ning Zhou

Real-time Dynamic Model Reduction and Calibration for Electric Power Systems



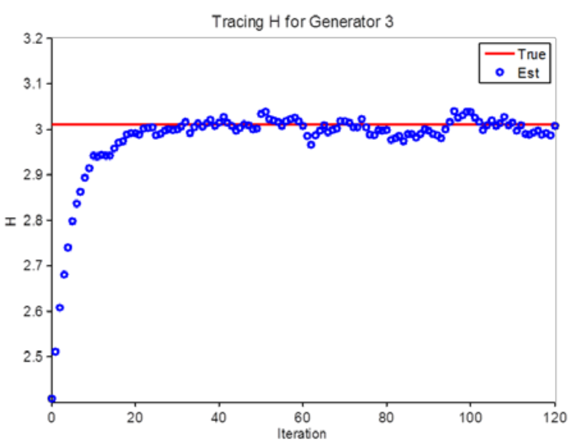
50 machine system



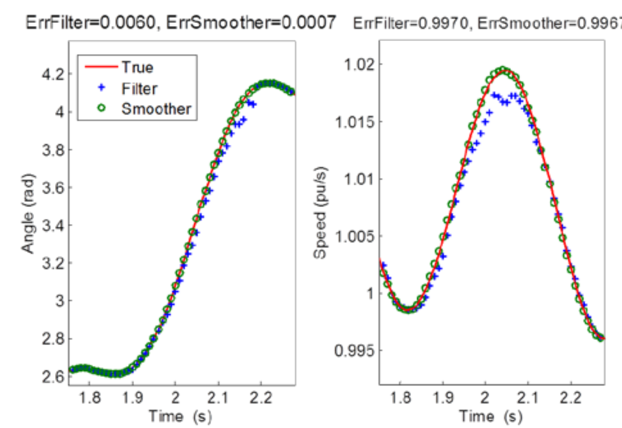


Reduced model matches full model

Calibration using particle filter



Model response after calibration



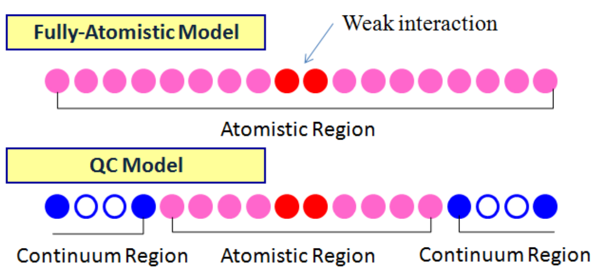
Pacific Northwest
NATIONAL LABORATORY

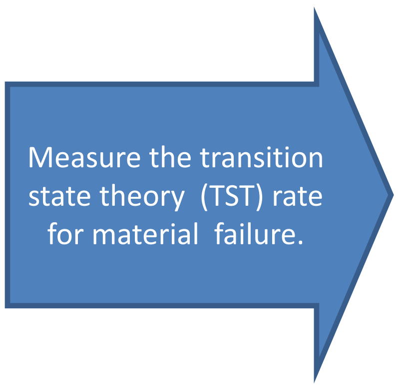
Predictive Simulation and Design of Materials by Quasicontinuum and Accelerated Dynamics Methods

Mitchell Luskin, Ellad Tadmor, Woo Kyun Kim, Brian Van Koten, University of Minnesota
Arthur Voter, Danny Perez, Los Alamos National Laboratory

Objectives

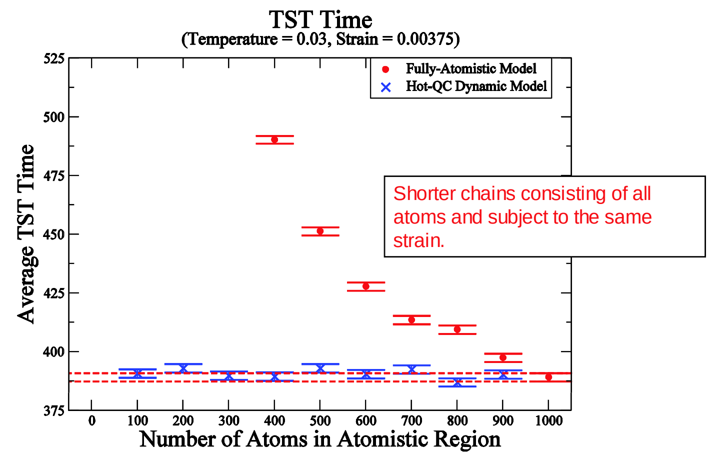
- Develop a simulation-method, **hyper-QC**, extending spatial and temporal scales:
  - *Couple hot-QC with hyperdynamics to accelerate infrequent events.*
  - *Develop the mathematical foundations for atomistic-to-continuum coupling, accelerated dynamics, and hyper-QC methods.*

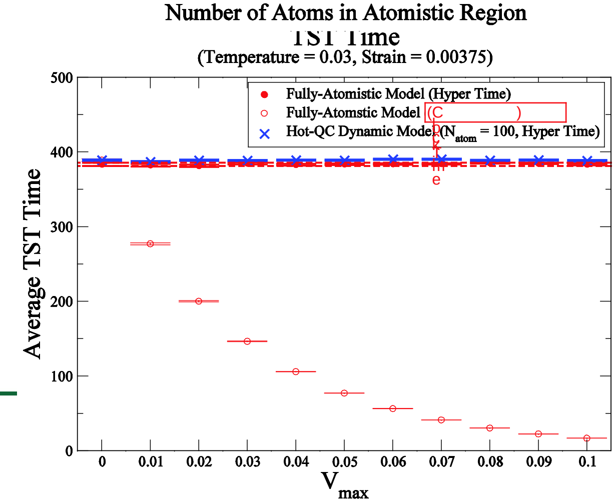




Impact

- *Make it possible to simulate models closer to real experimental systems both in length and time scales.*
- *Observe and predict deformation mechanisms which the conventional methods may not be able to capture, such as thermally-activated defect nucleation in the vicinity of a crack tip during crack corrosion.*





Accomplishments

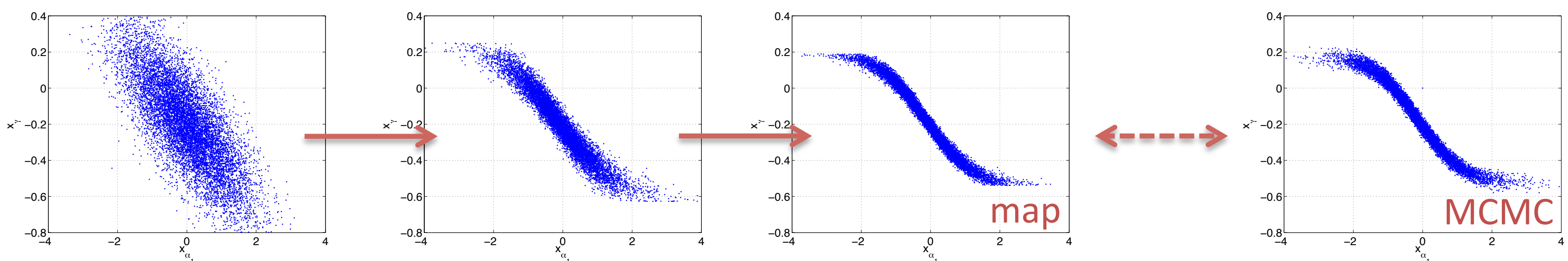
- Developed, analyzed, and tested a quasicontinuum energy with **optimal complexity** for materials with defects.
- Developed a **mathematical analysis** of the parallel replica accelerated dynamics method.
- Numerical experiments demonstrate that hyper-QC can reproduce the original TST time with both a **smaller number of atoms** and **shorter simulation times**.

U.S. DEPARTMENT OF ENERGY | Office of Science

26. Bayesian inference with optimal maps

Youssef Marzouk, MIT

- A new approach to Bayesian inference, based on optimal transport
- **Key ideas:**
  - Seek a map that *pushes forward* the prior measure to the posterior measure
  - Map constructed through solution of an optimization problem
  - Yields, e.g., polynomial chaos representation of the posterior
- **Computational advantages:**
  - Clear convergence criterion, unlike Markov chain Monte Carlo (MCMC)
  - Generate arbitrary numbers of *independent* posterior samples
  - Posterior normalization constant computed "for free" (model selection)
  - Optimization algorithms exploit gradient information; embarrassingly parallel



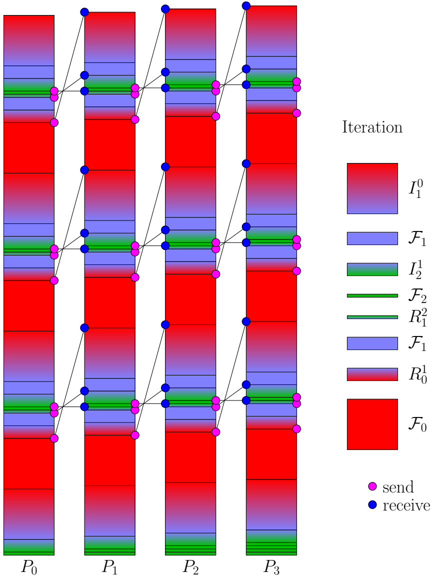
- **Demonstration** via parameter inference in nonlinear ODEs and large-scale statistical inverse problems, in hundreds of dimensions

Poster 27, Michael Minion and Matthew Emmett
Toward Efficient Parallel in Time Methods for PDEs

The *Parallel Full Approximate Scheme in Space and Time* (PFASST) algorithm for time parallelization is presented.

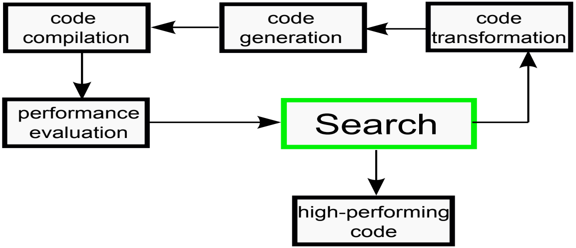
PFASST iteratively improves a provisional solution using a deferred correction scheme. Further efficiency is gained by using a heirarchy of space/time grids and the multi-grid full approximation scheme to transfer information between the discretizations.

The diagram depicts the correction sweeps of a 3-level V-cycle PFASST run.



Poster number: 28; Presenter: Prasanna Balaprakash

Model-Based Optimization Algorithms for Empirical Performance Tuning



Number of code variants to evaluate grows exponentially with the parameters

Goal

Design, implement, and analyze efficient numerical optimization algorithms

Contributions

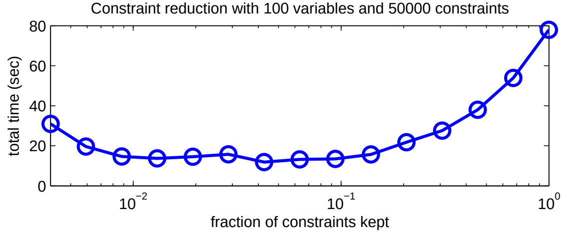
- Formulated the search in tuning as a mathematical optimization problem
- Developed SPAPT test suite for benchmarking optimization algorithms
- Designing model-based derivative-free algorithm for performance tuning

Infeasible Constraint-Reduced Methods for Quadratic and Semidefinite Optimization

S. Park, M.Y. He, D.P. O'Leary, and A.L. Tits

[DOE Grant DESC0002218]

- Constraint Reduction:
  - With unbalanced problems (many more inequality constraints than variables), cost per iteration of interior-point methods is large (large linear system must be solved).
  - Constraint reduction selects a small subset of constraints at each iteration.
- Two New Contributions this Year:
  - Polynomial Complexity (Sungwoo Park). For semidefinite optimization, which includes linear and convex quadratic as special cases.
  - Major speedup on practical problems (MYH and Sungwoo Park). On linear, convex quadratic, and semidefinite optimization problems.



Coupling Methods for Multiscale Simulations and Adaptive Modeling

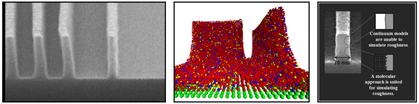
J.T. Oden, **S. Prudhomme**, and P. Seleson

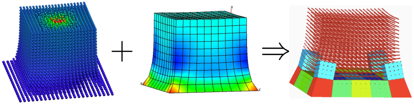
Institute for Computational Engineering and Sciences
The University of Texas at Austin, Austin, TX 78712

In collaboration with H. Ben Dhia (Ecole Centrale Paris, France), L. Chamoin (ENS Cachan, France) and L. Demkowicz, G. Rodin, P. Rossky, G. Willson, . . . , K. Farrell, and E. Wright (UT Austin)

Development of multiscale approaches for coupling concurrent models that describe phenomena spanning different spatial scales.

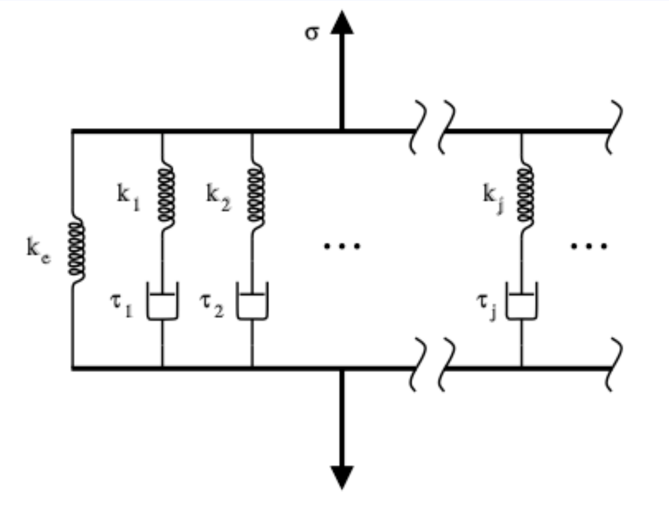
- a new averaging operator for coupling models;
- a new adaptive method based on optimal control to adapt the position of the coupling zone in order to reduce modeling errors with respect to QoI;
- an approach for statistical calibration and validation of coarse-grained/continuum models.

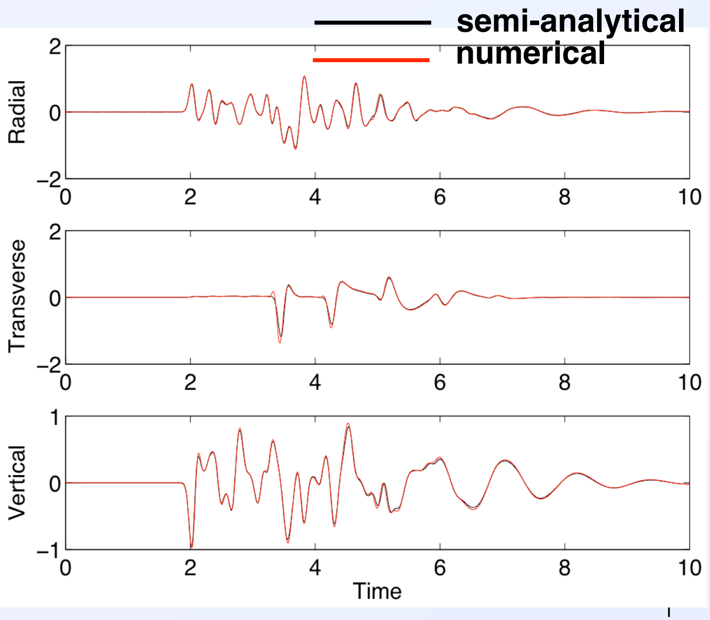




Poster # 32 presented by Anders Petersson

- A generalized Maxwell material is used to approximate a visco-elastic constant-Q absorption band solid in the time-domain.
  - **Sufficient conditions on the material properties through an energy estimate.**
- Memory variables are based on the history of the displacement (instead of the strain).
  - **3 dependent variables instead of 6 per mechanism**
  - **Enables a discrete energy estimate**
- The visco-elastic modeling is part of WPP version 2.1.
  - **Parallel open source code for 3-D seismic wave propagation**



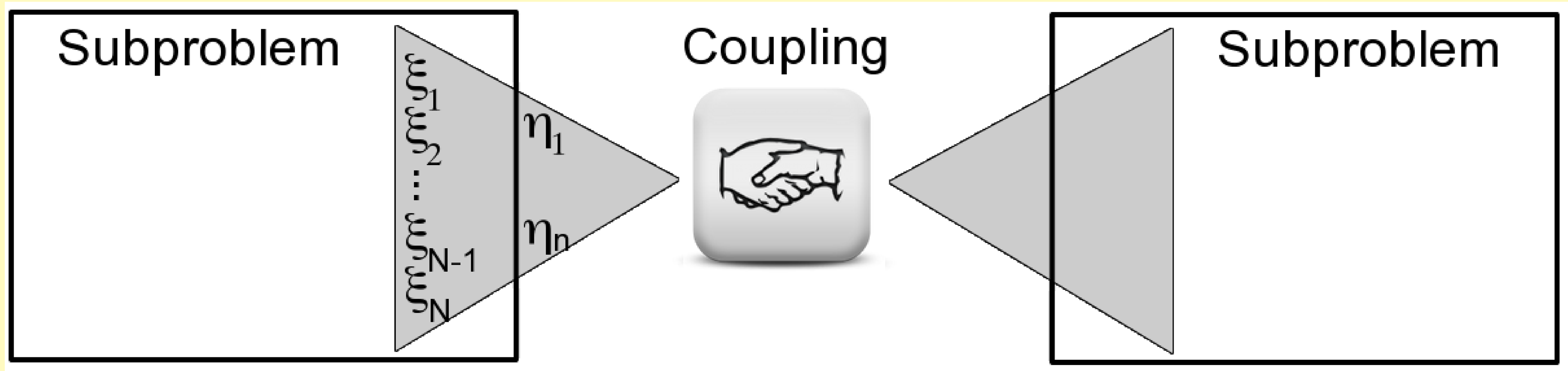


Dimension Reduction and Measure Transformation in Stochastic Simulations of Coupled Systems

{Maarten Arnst, Roger Ghanem} @USC.edu
{Eric Phipps, John Red-Horse} @Sandia.gov

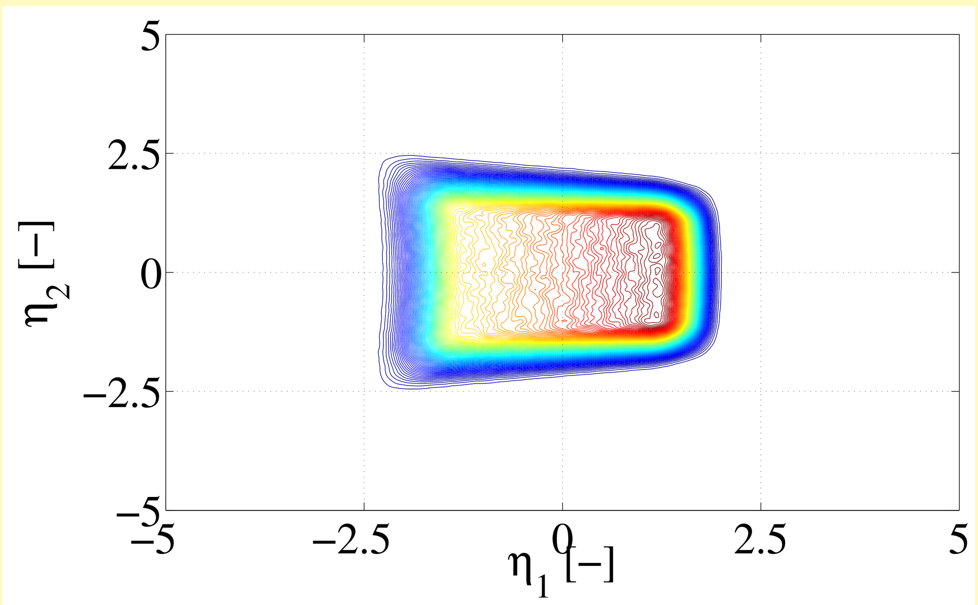
Objectives & Challenges

- Develop UQ for coupled models in Nuclear Reactor Technology.
- Adapt measure of approximation at every handshaking.
- Mitigate mixing of uncertainty at handshaking.
- Develop multiscale quadrature rules.



Interface Variables

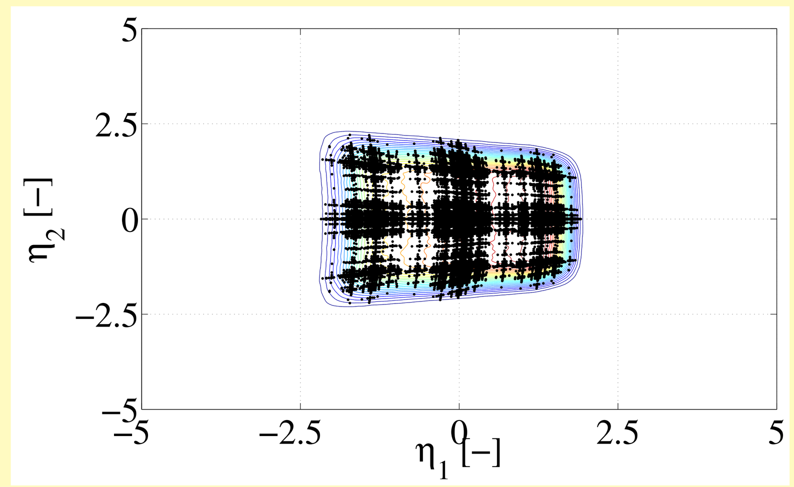
The output from Model I is reduced using Karhunen-Loeve expansion. The joint PDF of the dominant KL variables is estimated and a corresponding orthogonal polynomials constructed.



Joint Probability Density of Interface Random Variables.

Multiscale Quadrature

Numerical quadrature in Model II can be developed relative to new measure:



Quadrature points relative to initial measure.

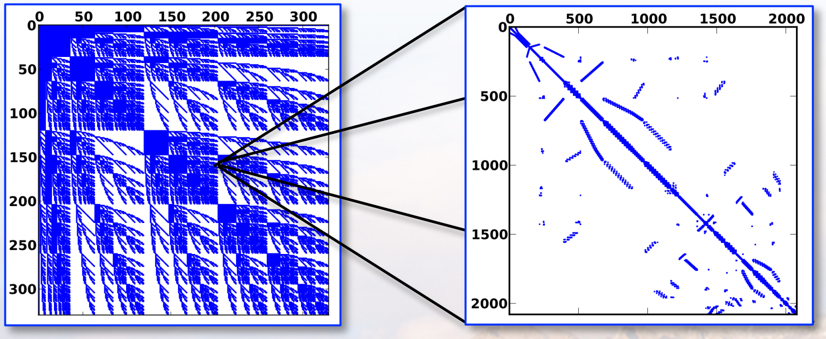
Quadrature points relative to adapted measure.

Embedded Stochastic Galerkin Projection and Solver Methods via Template-based Generic Programming

$$F_i(u_0, \ldots, u_{P_{SG}}) \equiv \frac{1}{\langle \Psi_i^2 \rangle} \int_\Gamma f(\hat{u}(x), x)\Psi_i(x)\rho(x)dx = 0, \; i = 0, \ldots, P_{SG}$$

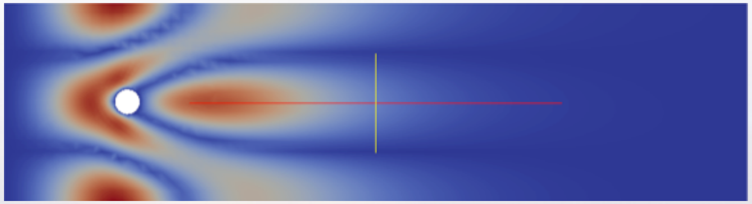
```
#include "Stokhos_Sacado.hpp"

template <class ScalarType>
inline ScalarType simple_function(const ScalarType& u) {
  return 1.0/(std::pow(std::log(u),2.0) + 1.0);
}
```



Stochastic sparsity

Spatial sparsity



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Robustness of Cyber-Physical Network Infrastructures: A Game Theoretic Approach

Nagi Rao — Oak Ridge National Laboratory; **David Yau, Chris Ma** — Purdue University
Fei He, Jun Zhuang — State University of New York, Buffalo

Problem Space: Operation of infrastructures for cyber services, such as network connectivity and computing capacity, requires the continued functioning of:

(i) *cyber components* such as computers, routers and switches, and
(ii) *physical components* such as fiber routes, cooling and power systems.

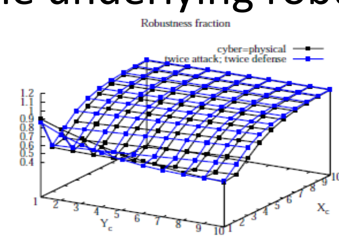
Our Approach: We present systematic analysis and design methods for achieving robustness of cyber infrastructures based on two game-theoretic models that capture different levels of detail.

When the utility functions of the attacker and provider consist of sums of individual cost and system terms, Nash Equilibrium is deterministic, and is polynomial-time computable under uniform costs.

Applications: We apply these results to design and reinforce:

(i) UltraScienceNet network infrastructure, and
(ii) models of cloud and high-performance computing infrastructures
   – solution characterized by the same underlying robustness function

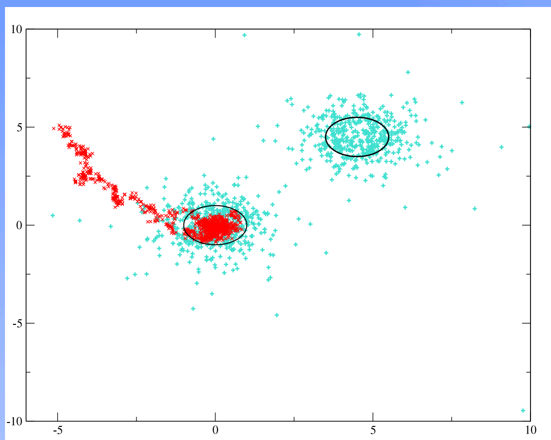
$$f_R\left(n_c, n_p, x_c, x_p, y_c, y_p\right)$$



(c) $x_p = 2x_c$ and $y_p = 2y_c$

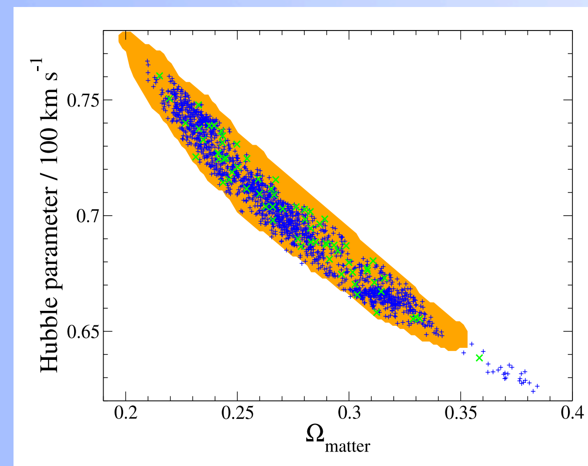
Oak Ridge National Laboratory
U. S. Department of Energy

Poster 36 – Scott Daniel (University of Washington)



Red points are sampled by MCMC

Blue points are sampled by our algorithm



Orange region is marginalized MCMC constraint after **640,000** points sampled.

Blue points are derived from our algorithm after **40,000** samples.

Monte Carlo Markov chains find parameter constraints by integrating over the entire high-likelihood region.

We present an alternative algorithm which selectively seeks out the boundary of the confidence limit.

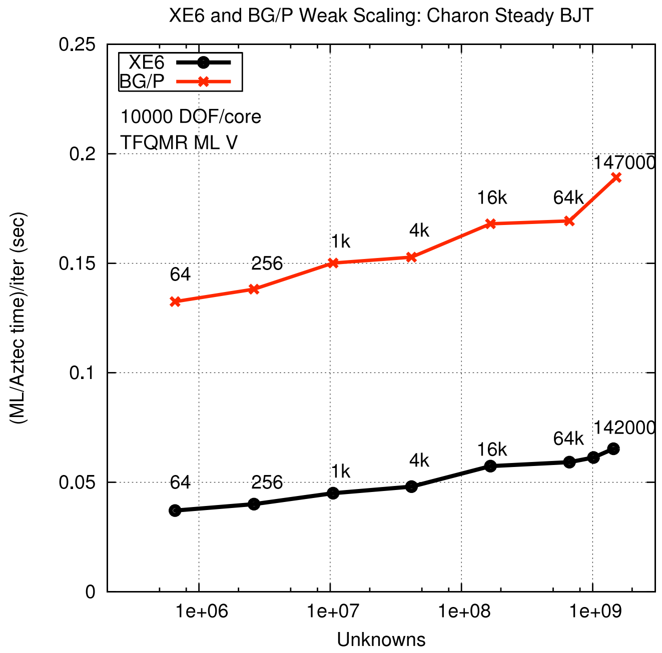
We test our algorithm on the CMB measurements in the WMAP 7 year data release. Our derived constraints are comparable to those of MCMC, but more efficient

Poster #37 Paul Lin, Sandia National Labs

Large-Scale Parallel Performance of Algebraic Multigrid Preconditioners for Multiphysics Systems

- FEM fully implicit Newton-Krylov with AMG preconditioner
  - Resistive MHD
  - Semiconductor drift-diffusion

- Large-scale machines: BG/P, Cray XE6
  - Comparison of 3 aggregation schemes
  - Efficiency of multigrid preconditioner; can be ~400X faster than 1-level preconditioner
  - Drift-diffusion weak scaling on IBM BG/P and Cray XE6: problem scaled over 1B DOF on 140,000 cores



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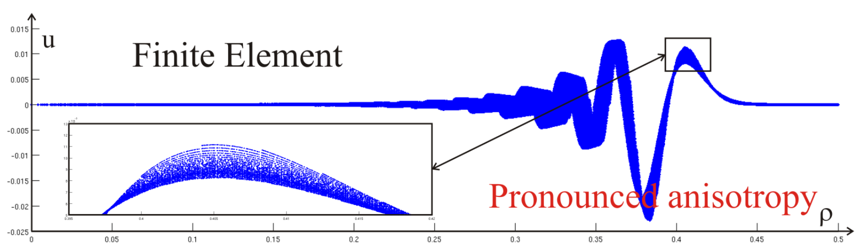
M-Adaptation. K.Lipnikov, V.Gyrya, M.Manzini, M.Shashkov, D.Svyatskiy

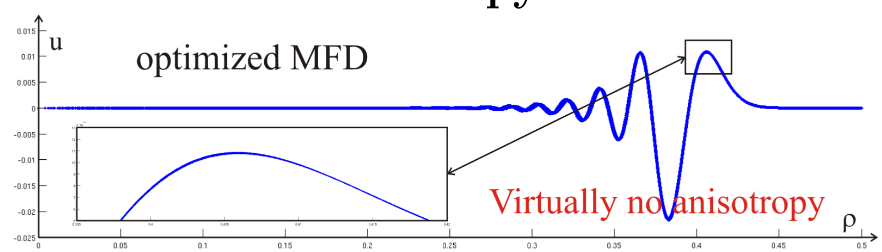
- The mimetic finite difference (MFD) method results in a parameterized family of methods with equivalent properties, such as accuracy and stencil size.
- The objective of m-adaptation is to select a proper method from the MFD family for a given problem and criteria.

Example 1. Acoustic problem on a cubic mesh.

method	DOF	Accuracy	Stencil	# parameters / cell
FEM	N^3	2nd	27	0
MFD	N^3	2nd	27	10

Criterion: minimization of numerical anisotropy.

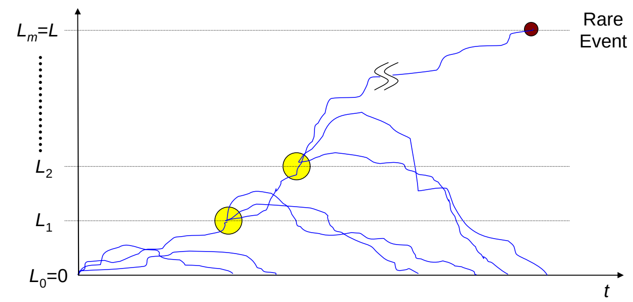




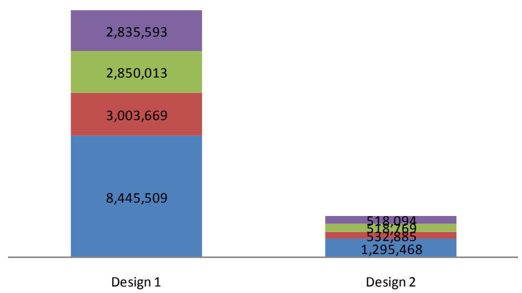
Example 2. Monotone discretization for Darcy's flow (see the poster).

Rare-event Splitting for Efficient Simulation of Cascading Blackouts

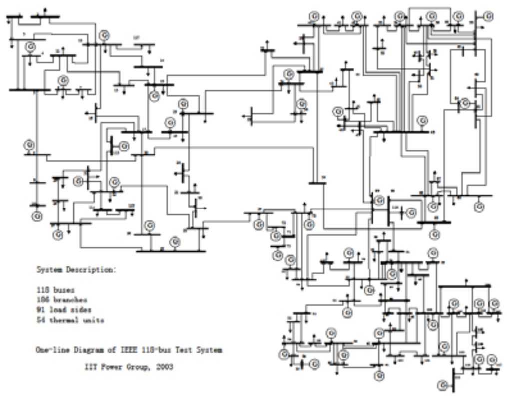
- Poster 39, John Shortle
- Splitting may be a useful technique when rarity of events prohibits standard simulation



- Methodological contribution: Allocation of computing budget among alternate design and levels



- Applied contribution: Application to improve simulation efficiency for cascading blackouts.



40. Daniel B. Szyld (with Fei Xue), Temple University

Analytical and Experimental Results for Inexact Methods for Linear and Nonlinear Eigenvalue Problems

For Generalized Eigenvalue Problems

$$Ax = \lambda Bx,$$

with Rayleigh Quotient Iteration (or single-vector Jacobi-Davidson) one solves, at the ith iteration, linear systems of the form

$$(A - \sigma^{(i)} B) y^{(i)} = B x^{(i)}.$$

Several issues are discussed, among them:

The linear systems can be solved inexactly with a fixed small tolerance (but not necessarily too small) and achieve the same local rate of convergence as if it were solved exactly (cubic for Hermitian matrices, quadratic for non-Hermitian).

A Collision-Based Hybrid Method for Multiscale, Linear Transport

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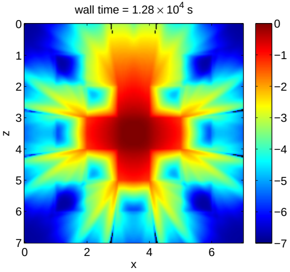
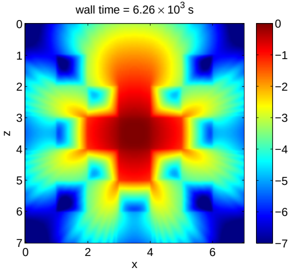


(a) S_8



(b) FLD-S_{36} Hybrid

Hybrid Uncertainty Quantification Methods for Multi-species Reactive Transport

- **Issue: how to embed UQ methods in a multi-physics code**
  - when physics modules are developed somewhat independently from one another
  - when sometimes commercial or open source modules are incorporated
  - UQ methods are in various stages of maturity for different modules
- **One solution: hybrid uncertainty quantification methods**
  - use divide-and-conquer strategies
  - yet propagate “global” uncertainties/sensitivities
  - massive concurrency and heterogeneity
  - many applied math and computer sciene research issues
- **This poster:**
  - results of initial investigation with application to a multi-species reactive transport problem

Geometric Multiscale Dictionaries for Large Data Sets

William K. Allard Guangliang Chen Mauro Maggioni
Duke University

Data sets are often modeled as point clouds in $\mathbb{R}^D$, for D large, while the data has some interesting low-dimensional structure, for example that of a d-dimensional manifold $\mathcal{M}$, with $d \ll D$. When $\mathcal{M}$ lies in a low-dimensional linear subspace one may use SVD to efficiently encode the data. When $\mathcal{M}$ is nonlinear, there are no "explicit" constructions of dictionaries that achieve a similar efficiency. We construct data-dependent multiscale dictionaries that aim at efficient encoding and manipulating of the data. Their construction is fast, and so are the algorithms to map data points to dictionary coefficients and vice versa. In addition, data points are guaranteed to have a sparse representation in terms of the dictionary. We think of dictionaries as the analogue of wavelets, but for approximating point clouds rather than functions.

Parallel kinetic Monte Carlo simulations: algorithms and numerical analysis

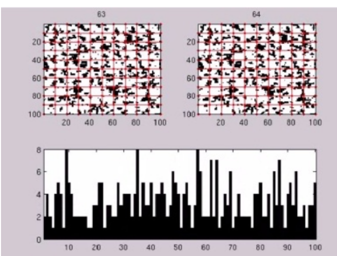
M.A Katsoulakis, P. Plechac and D. G. Vlachos

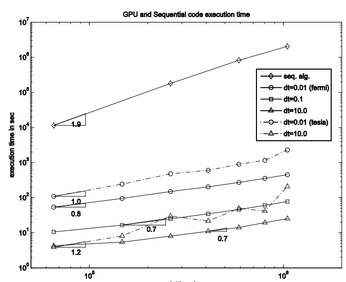
Science Objectives

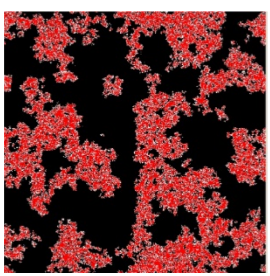
- Strategy: Parallel lattice kinetic Monte Carlo
- Driver: *Partially asynchronous kMC*
- Objectives:
  - *Simulate* complex chemical kinetics on surfaces
  - *Predict* dynamic formation
  - *Develop* portable parallel kMC programming environment
- Impact: Simulations at engineering scales of microns
  Unified mathematical framework for parallel kMC

Results: Catalytic kinetics on novel structures

- ❖**GPU/multicore acceleration of MC simulations**
- ❖**Mathematical framework for parallel lattice kinetic MC**
- ❖**Numerical and statistical consistency**
- ❖**Rigorous error analysis of parallel approximations**
- ❖**Load balancing**
- ❖**Efficient massively parallel random number generators**

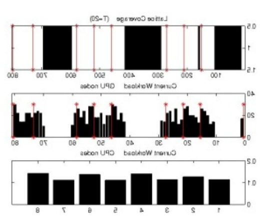






Performance on GPUs

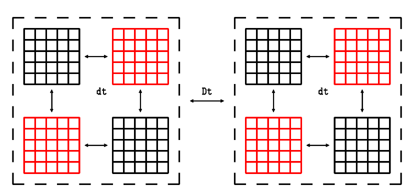
CO-oxidation on Pt, ZGB model

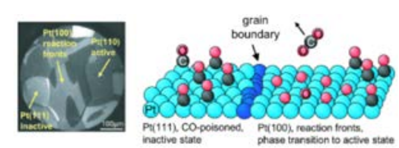


Dynamic load balancing

New Algorithms and Methods

- ❖**Fractional time-step approx. of Markov jump process**
- ❖**Partially asynchronous parallel kMC**
- ❖ **Deterministic and randomized processor schedules**
- ❖**Dynamic load balancing as Monge-Kantorovich transport**
- ❖**Error quantification for mesoscopic observables**





DE-SC0001340

Poster #45: Homer Walker, Worcester Polytechnic Institute

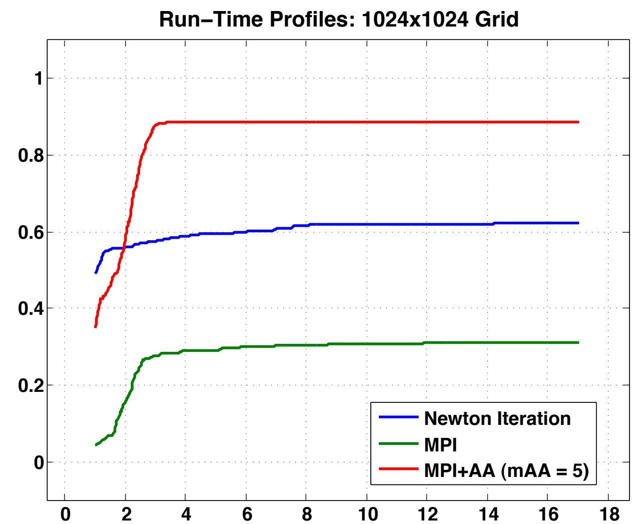
Anderson Acceleration: Theory and Applications

- **Fixed point iterations** occur often.
  - Application-specific forms, advantages.
  - Convergence often slow, in doubt.

- **Anderson acceleration** may help.

- **Theory**: "essentially equivalent" to GMRES on linear problems, implications for stationary iterations, numerical and implementational issues.

- **Applications**
  - **Illustrative**: EM algorithm, domain decomposition.
  - **Serious study**: Picard iteration for variably saturated flow (w/ Woodward, Yang, Lott).



Performance profiles for a Newton-GMRES-backtracking method, a modified Picard iteration, and the modified Picard iteration with Anderson acceleration on 408 test cases of a variably saturated flow problem.

Multiscale discretizations for multiphase porous media flow coupled with geomechanics

Poroelastic Model Problem

Geomechanics:

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{f} \qquad \mathbf{u} = \text{displacement}$$

$$\boldsymbol{\sigma} = \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} + 2\mu \boldsymbol{\epsilon} - \alpha p \mathbf{I} \qquad \boldsymbol{\epsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$$

Single phase flow:

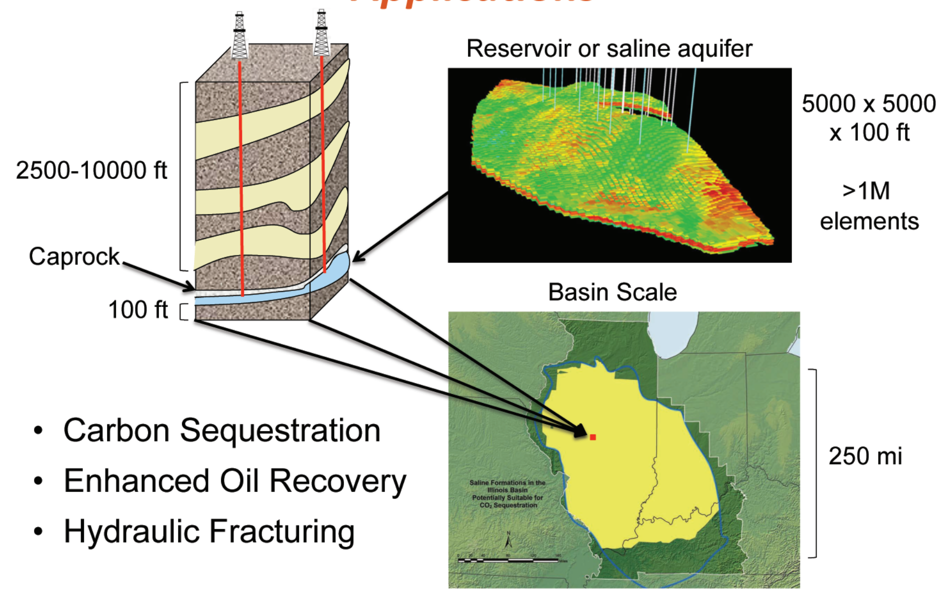
$$\frac{\partial}{\partial t}(c_o p + \alpha \nabla \cdot \mathbf{u}) + \nabla \cdot \mathbf{z} = q \qquad p = \text{pore pressure}$$

$$\mathbf{z} = -\mathbf{K}(\nabla p - \rho \mathbf{g}) \qquad \mathbf{z} = \text{fluid velocity.}$$

$$\Omega_p = \text{poroelastic region}$$

$$\Omega_e = \text{elastic region} \quad (\alpha = 0)$$

Applications

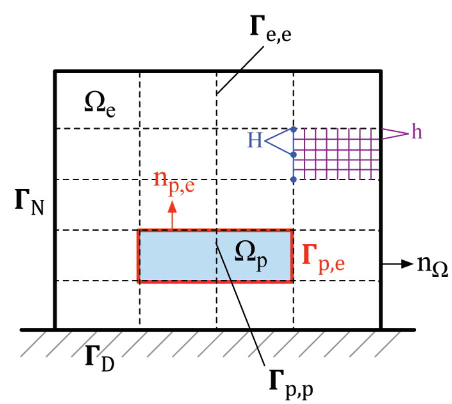


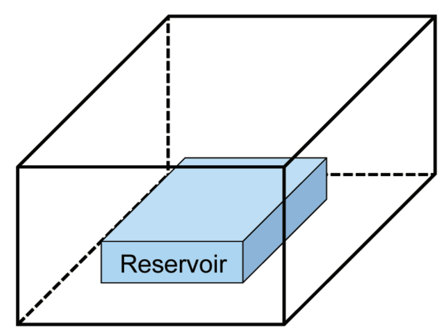
- Carbon Sequestration
- Enhanced Oil Recovery
- Hydraulic Fracturing

Modeling Goals

- Locally conservative discretization
- Capable of handling rough geometry
- Multi-scale and multi-physics
- Parallel algorithms
- Domain decomposition
- Efficient solvers
- Rigorous error estimates

Multiscale Mortar Modeling Methodology





U.S. DEPARTMENT OF ENERGY | Office of Science

Ivan Yotov, University of Pittsburgh
Mary F. Wheeler, University of Texas at Austin

Poster #47, Jieqiu Chen

Globally Solving Nonconvex Quadratic Programming
via Completely Positive Programming

- Problem: Nonconvex quadratic programming problem
  - many applications in science, engineering and business
  - fundamental, NP-hard
- Approach: a combination of
  - finite branch and bound method
  - strong semidefinite relaxations derived from completely positive programming
- Results: a global QP solver
  - competitive with state-of-the-art global solvers and more robust
  - MATLAB and YALMIP interface