Algorithmic Developments for UQ in Extreme Scale Simulations

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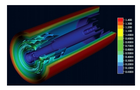
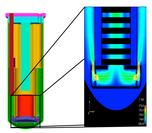
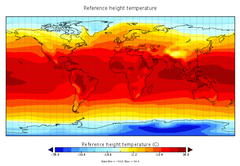
QUEST algorithmic developments focus on key challenges in extreme scale computing



- High Dimensionality
  - Gradient-enhanced interpolants
  - Local error estimation with hierarchical value/gradient surpluses
  - Compressive sensing for sparsity detection
- Data characterization:
  - Data-Free Inference to handle missing data
  - Random field representations
- Predictive model calibration:
  - Subgrid model upscaling

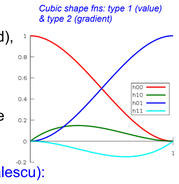




Gradient-enhanced interpolants: global h-refinement

Dimension-adaptive h-refinement for SC:

- *Local spline interpolants:* linear Lagrange (value-based), cubic Hermite (gradient-enhanced)
- *Global grids:* iso/aniso tensor, iso/aniso/generalized sparse
- *h-refinement:* uniform, adaptive, goal-oriented adaptive
- *Basis formulations:* nodal, hierarchical



Multivariate tensor product to arbitrary derivative order (Lalescu):

$$s^{(n)}(x_1, x_2, \ldots, x_D) = \sum_{l_1,\ldots,l_D=0}^{m} \sum_{i_1,\ldots,i_D=0,1} f^{(l_1,\ldots,l_D)}(i_1,\ldots,i_D) \prod_{k=1}^{D} \alpha_{i_k}^{(n,l_k)}(x_k)$$

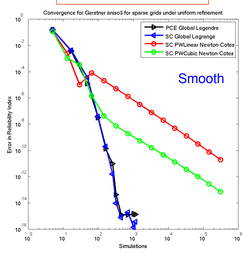
$$f = \sum_{i=1}^{N} f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3)$$

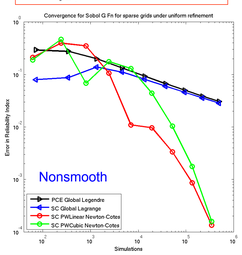
$$\mu = \sum_{i=1}^{N} f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)}$$

and similar for higher-order moments

$$f(\mathbf{x}) = \exp\left(-10x_1^2 - 5x_2^2\right)$$

$$f(\mathbf{x}) = 2\prod_{j=1}^{5} \frac{|4x_j - 2| + a_j}{1 + a_j}; \quad a = [0,1,2,4,8]$$



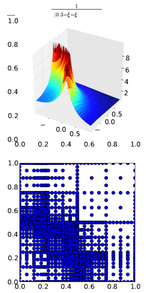


Local Error Estimation with Hierarchical Value/Gradient Surpluses

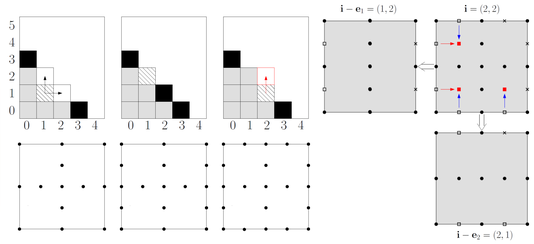
Hierarchical basis:

- *Improved precision* in QoI (mean and higher order moments) increments
- Surpluses provide error estimates for *local refinement* using local/global hierarchical interpolants
- New QoI error indicators naturally leverage *both value and gradient surpluses*

$$\Delta\Sigma_{ij} = \Delta E[R_i R_j] - \mu_{R_i}\,\Delta E[R_j] - \mu_{R_j}\,\Delta E[R_i] - \Delta E[R_i]\Delta E[R_j]$$

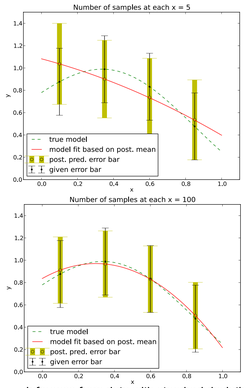


From J. Jakeman, July 2010



Data-Free Inference (DFI)

- Inputs often specified incompletely in the literature
  - Mean and confidence interval provided, but no covariance. Original data missing.
  - Data specified as mean and standard deviation, but number of samples missing
- Overall output uncertainty depends strongly on joint distribution of input parameters
- DFI infers joint distribution of parameters based on available information
  - Pool family of posteriors that are consistent with given information [Berry *et al.*, JCP, 2012]
- Application to
  - Inference of chemical kinetics
  - Inference from data products (processed raw data)

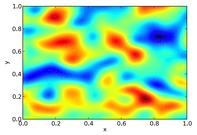


Inference from data with standard deviations but unknown number of samples

Random Field Characterization

- Random fields are conveniently represented with Karhunen-Loève Expansions (KLEs)
  - Enables dimensionality reduction
- KLEs require a covariance matrix
  - Sample covariance matrix requires large ensemble of realizations before eigenfunctions are smooth
  - Sometimes very few samples are available
- Ongoing work on estimation of covariance matrices from few realizations

$$F(x,\theta) = \langle F(x,\theta)\rangle_\theta + \sum_{k=1}^{\infty} \sqrt{\lambda_k} f_k(x) \xi_k$$



2D Gaussian Process realization

Stochastic Expansions on Unstructured Grids: Compressive Sensing

$$\mathbf{\Phi c} = \mathbf{y} \qquad (1)$$

where the elements of the measurement matrix are given by

$$\Phi_{ij} = \Phi_j(\boldsymbol{\xi}^{(i)}), \quad i = 1,\ldots,N,\ j = 1,\ldots,P$$

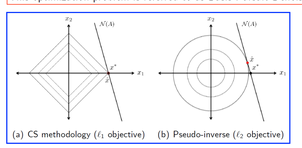
When $N \ll P$ (1) is ill-posed and additional constraints must be introduced to find a unique solution. The traditional way of estimating c is to find the minimum norm solution, which is the optimal set of coefficients

$$\mathbf{c} = \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{\Phi c} - \mathbf{y}\|_2^2$$

If the solution is sparse we can do better by seeking a solution

$$\mathbf{c} = \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{c}\|_1 \quad \text{such that} \quad \|\mathbf{\Phi c} - \mathbf{y}\|_2 \le \varepsilon \qquad (2)$$

This optimization problem is referred to as Basis Pursuit Denoising

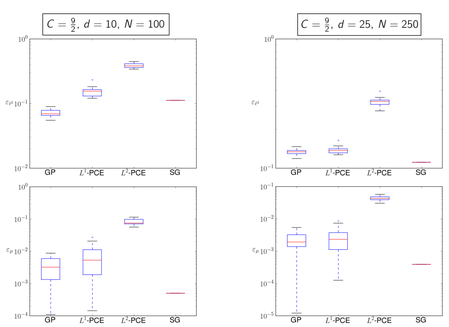


Courtesy of G. Tang (Stanford)

Solvers:

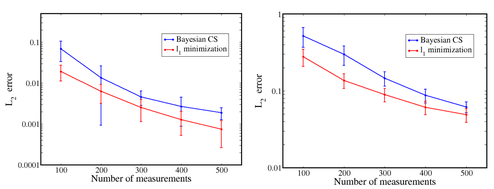
- l_0 denoising with Orthogonal Matching Pursuit
- l_1 Basis Pursuit with Linear Programming solvers
- l_1 Basis Pursuit Denoising with Interior Point solvers

$$f_{OS}(\mathbf{x}) = \cos\left(-\sum_{i=1}^{d} c_i x_i\right), \quad \mathbf{x} \in [0,1]^d \qquad c_i = \frac{\left(i - \frac{1}{2}\right)}{d}\frac{C}{W} \qquad \sum_{i=1}^{d} c_i = C$$



- With high-dimensional input, spectral representations require too many terms, therefore building sparse bases is important.
- Borrowing from the machine learning community, applying sparse learning methods to polynomial bases.
  - Evaluated and/or extended various Compressive Sensing (CS) and Bayesian Compressive Sensing (BCS) approaches
  - Analyzed the dependence of performance on the effective dimensionality (sparsity) of the model and the number of model simulations available.
  - K-folds cross validation is applied to determine the polynomial degree and tolerance ε that produce a PCE that generalizes well to new data [Doostan *et al.*, JCP 2011]
  - An iterative BCS methodology developed and applied to Community Land Model (CLM) in the context of CSSEF (Climate Science for a Sustainable Energy Future).
- Future directions:
  - Adjoint-enhanced CS
  - Least interpolation

Comparison of l_1-minimization CS and BCS algorithms



BCS/CS comparison for 5d, order 10(left) and 10d, order 5(right) Genz corner-peak functions

- CS generally lead to smaller errors
- BCS runs faster with the default settings and stores only relevant bases
- BCS computes uncertainty estimates enabling a posterior predictive distribution

- Dimensionality reduction by using hierarchical priors

$$p(c_k|\sigma_k^2) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{c_k^2}{2\sigma_k^2}} \qquad p(\sigma_k^2|\alpha) = \frac{\alpha}{2} e^{-\frac{\alpha\sigma_k^2}{2}}$$

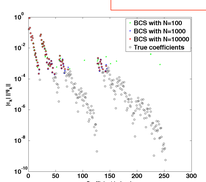
- The parameter α can be further modeled hierarchically, or fixed.
- Evidence maximization dictates values for $\sigma_k^2, \alpha, \sigma^2$ and allows exact Bayesian solution

$$\boldsymbol{c} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

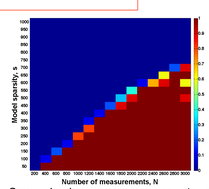
with

$$\boldsymbol{\mu} = \sigma^{-2}\boldsymbol{\Sigma}\boldsymbol{P}^T\boldsymbol{u} \qquad \boldsymbol{\Sigma} = \sigma^2(\boldsymbol{P}^T\boldsymbol{P} + \operatorname{diag}(\sigma^2/\sigma_k^2))^{-1}$$

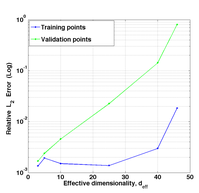
$$f = \cos\left(2\pi e + \sum_{i=1}^{d} a_i x_i\right) \qquad a_i = \frac{1}{i^2}$$

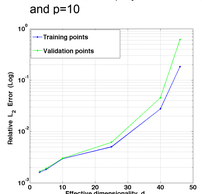


The coefficient recovery for a 5-dimensional Genz oscillatory function up to total order 5. True coefficients are computed by a high-level sparse quadrature.



Sparse basis recovery success rate, out of 10 replicas, vs. the number of measurements and the model sparsity, i.e. the number of non-zero polynomial coefficients in a polynomial model of d=5 and p=10





Relative L2 error measures for both training and validation datasets as the effective dimensionality increases, for three different values of the number of measurements, N = 1000 (left), N = 5000 (right) for d = 50. Effective dimensionality is the number of dimensions that contain 95% of the total sum of a_i's.

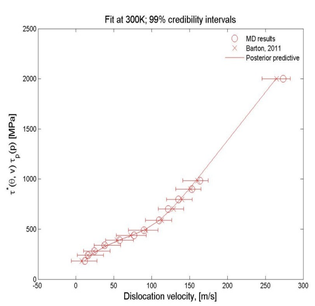
Predictive Model Calibration

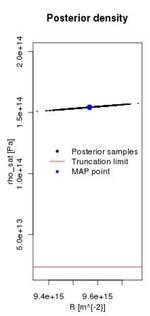
- Multiscale-Multiphysics simulations often rely on subgrid models, based on
  - First principles or other higher-fidelity simulations
  - Observational data
- To asses predictive fidelity of overall simulation, need to
  - Properly calibrate subgrid models
  - Propagate uncertainty in subgrid models across scales (upscaling)

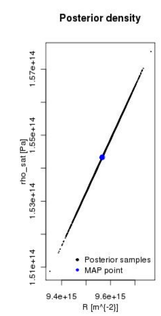
- Application to ParaDiS
  - a LLNL dislocation density (DD) model
  - used to create "sub-grid" models of crystal dislocation dynamics for use in continuum codes (ALE3D)
- Inputs:
  - Dislocation velocity model, by upscaling MD experiments
  - Various operational conditions (P, T, strain rate etc)
- Output
  - Simple ODE models, fitted to ParaDiS simulation of dislocation density and stress-strain evolution

- Analyses done only for Ta
- MD -> DD upscaling [Big source of uncertainty, for Ta]
  - Fitted the dislocation density model to MD simulation data, using MCMC
  - Forward UQ propagation shows significant spread in dislocation density predictions
    - A big source of input uncertainty
- DD -> continuum upscaling [Smaller source of uncertainty, for Ta]
  - ODE models fits ParaDiS outputs very well
    - Posterior distribution of model parameters estimated

- Left: MD -> DD upscaling (uncertainty in model predictions)
- Right: Posterior distribution of DD -> Continuum upscaling model







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