## Sparse Quadrature in PC UQ

### Relevance
- Non-intrusive, sampling-based. UQ methods have general utility
  - Black box handling of computational codes
- Independent embarrassingly parallel runs
- Polynomial Chaos (PC) non-intrusive Galerkin methods
- Quadrature-based numerical evaluation of projection integrals
- Each quadrature point is a computational sample
- High-dimensional setting (e.g. large # uncertain inputs)
- Care is required to minimize # requisite samples
  - Efficient sparse quadrature methods

### Adaptive Sparse Quadrature and Collocation
- Avoid dense tensor product grid sampling
- Target sparse optimal set of points
- Use Leja sequences to greedily generate 1D points that are approximately optimal for weighted interpolation
- Non-isotropic, Adaptive

### Fault-Tolerant Quadrature
- Quadrature relies on availability of all samples
- Investigate alternative integration methods with missing quadrature evaluations
  - Quadrature reweighting
  - Polynomial regression
  - Gaussian process estimate of missing values
- Missing a single quadrature point reduces the quadrature formula accuracy (polynomial exactness) by a factor of two.

### Evaluation of quantum chemistry integrals
- Developing sparse quadrature techniques for integration arising in 2nd-order many-body perturbation theory (MP2)
- Enhancing sparse quadrature with spherical transformations
- BES partnership initiated with UIUC

## Random Fields

### Relevance
- Many applications involve uncertain inputs/outputs that have spatial or time dependence
- Such an uncertain function, represented probabilistically, is a random field/process.
  - It is a random variable at each space/time location
  - Generally with some correlation structure in space/time
  - An infinite-dimensional object
- The Karhunen Loeve expansion (KLE) provides an optimal representation of random fields, employing a (small) number of eigenmodes of its covariance function

### Ice Sheet Basal Boundary Layer
- We wish to quantify uncertainty in predictions of sea level rise from ice-sheet melting.
- Friction between an ice sheet and the land mass is the first order uncertainty effecting predictions of sea level rise.
- The friction is a random field which can be represented using a KLE.
- Current study involves inferring friction B(x,y) from field measurements of surface velocities
  - BER PISCEES partnership with UT

### Sea Surface Temperature
- We perform a KLE/PCA analysis of NOAA's sea surface temperature data for the past three decades.
- The figure to the right shows the magnitude of the first KL mode for the Fall months from 2000 – 2009.
- This data set has ~10^6 dimensions

## Compressed Sensing

### Relevance
- Many physical models have a large # of uncertain inputs
- UQ in this high-dimensional setting is a major computational challenge – too many samples and/or large # PC modes
- Yet physical models typically exhibit sparsity
  - A small number of inputs are important
  - Seek sparse PC representation on input space
    - Small number of dominant terms
- Compressed sensing (CS) is useful for discovering sparsity in high dimensional models
  - Identify terms that contribute most to model output variation
  - Ideal for when data is limited

### Basis selection
- Cardinality of total degree basis grows factorially with the number of uncertain inputs.
- Even for lower dimensional problems redundant basis terms can degrade accuracy
- To reduce redundancy and improve accuracy the PCE truncation can be chosen adaptively.

### Sparsity in Atmospheric Modeling
- QOI : time averaged profile of ozone concentration
- 95 dimensional input space
- Adaptive: start with first order terms, successively adding higher order terms
- 2nd-order approximation
  - 25-150 terms
  - Full 2nd-order: ~4500 terms
- BER ACES4GCM partnership

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**Sensitivity indices for ozone at six different altitudes. Each color represents a different input parameter: reactants e.g. CO**