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Sparse Quadrature in PC UQ

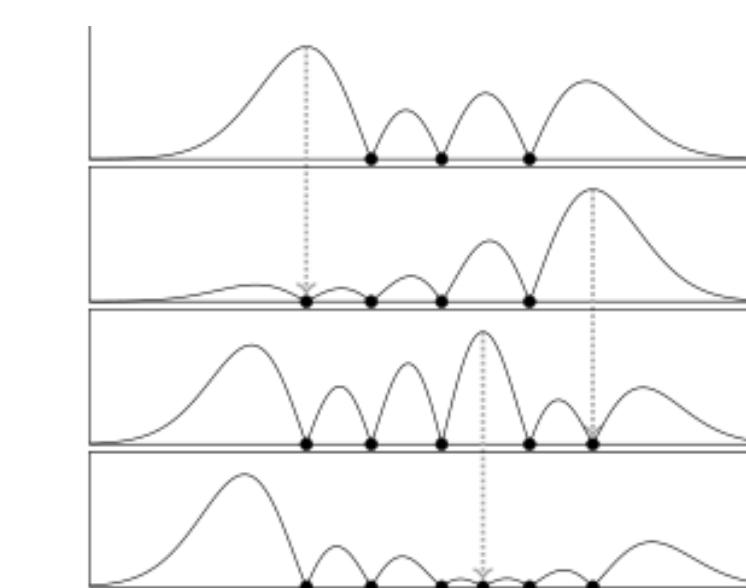
Relevance

- 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

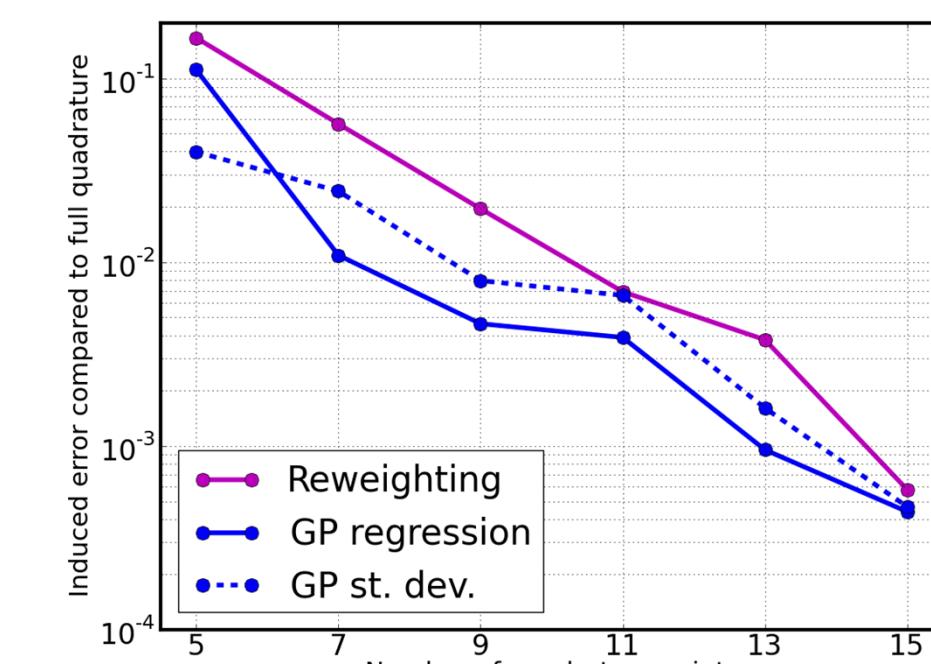
Adaptive Sparse Quadrature and Collocation

- 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

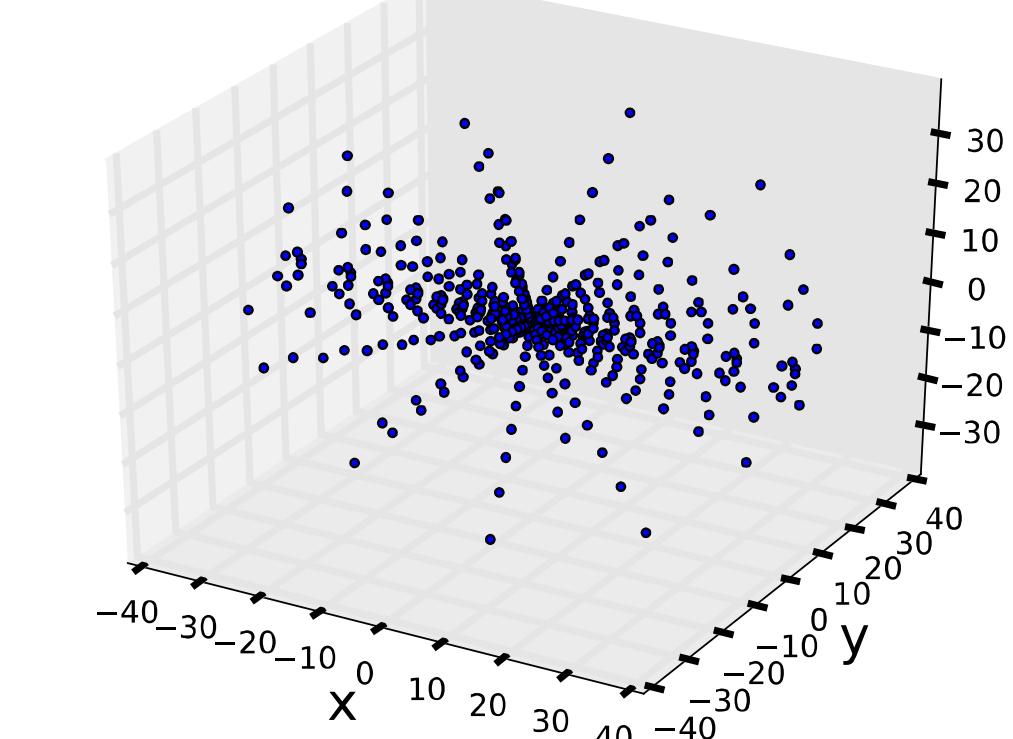
- Quadrature relies on availability of all samples
- Investigate alternative integration methods with missing quadrature evaluations
 - Quadrature reweighting
 - Polynomial regression
 - Gaussian process estimate of missing values
- Missing a single quadrature point reduces the quadrature formula accuracy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



GP regression estimates the missing values with a similar accuracy as re-weighting, but also provides error-bars on the final answer

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



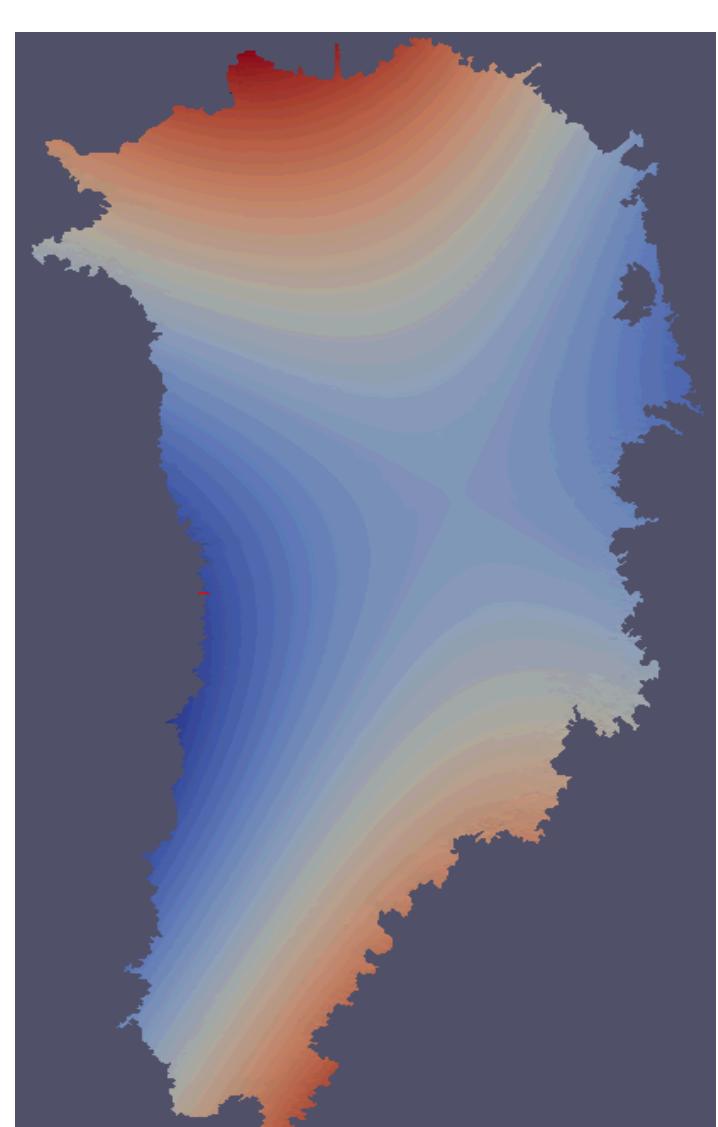
Random Fields

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

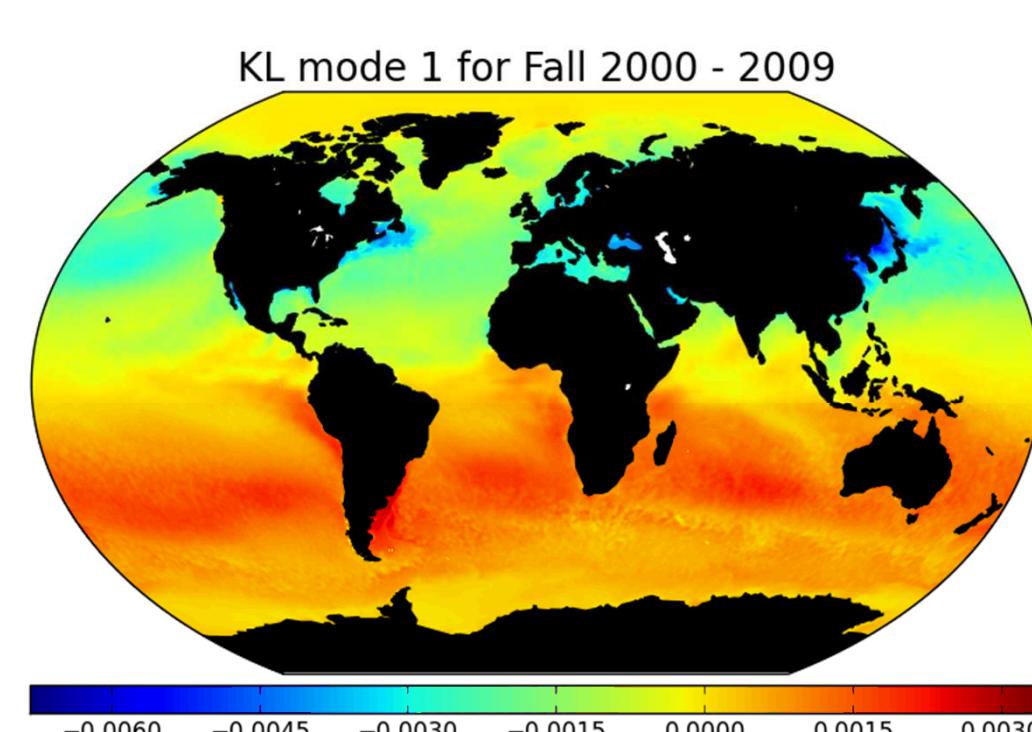
Ice Sheet Basal Boundary Layer

- 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 $\sim 10^6$ dimensions



Bayesian PCA

- Uncertain KLE given limited # of samples; Bayesian framework
- Compute principal directions of maximum variance
- Produce error bounds on the principal modes themselves
- The figure shows PCA modes in solid colored lines overlaid with the uncertainty: shaded regions.

More samples, less uncertainty

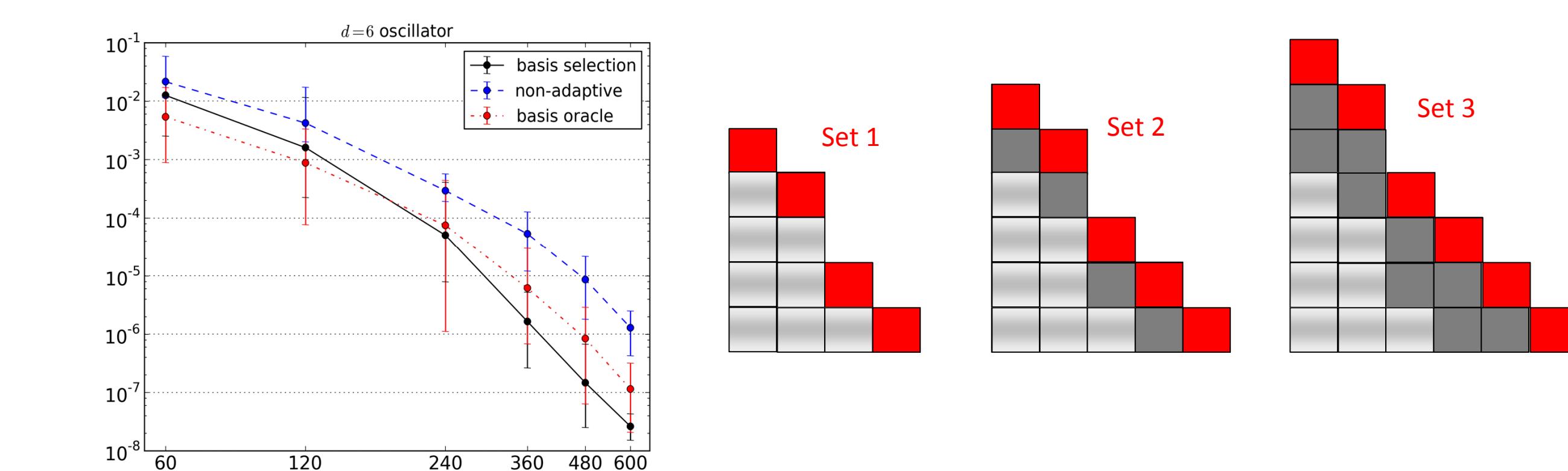
Compressed Sensing

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

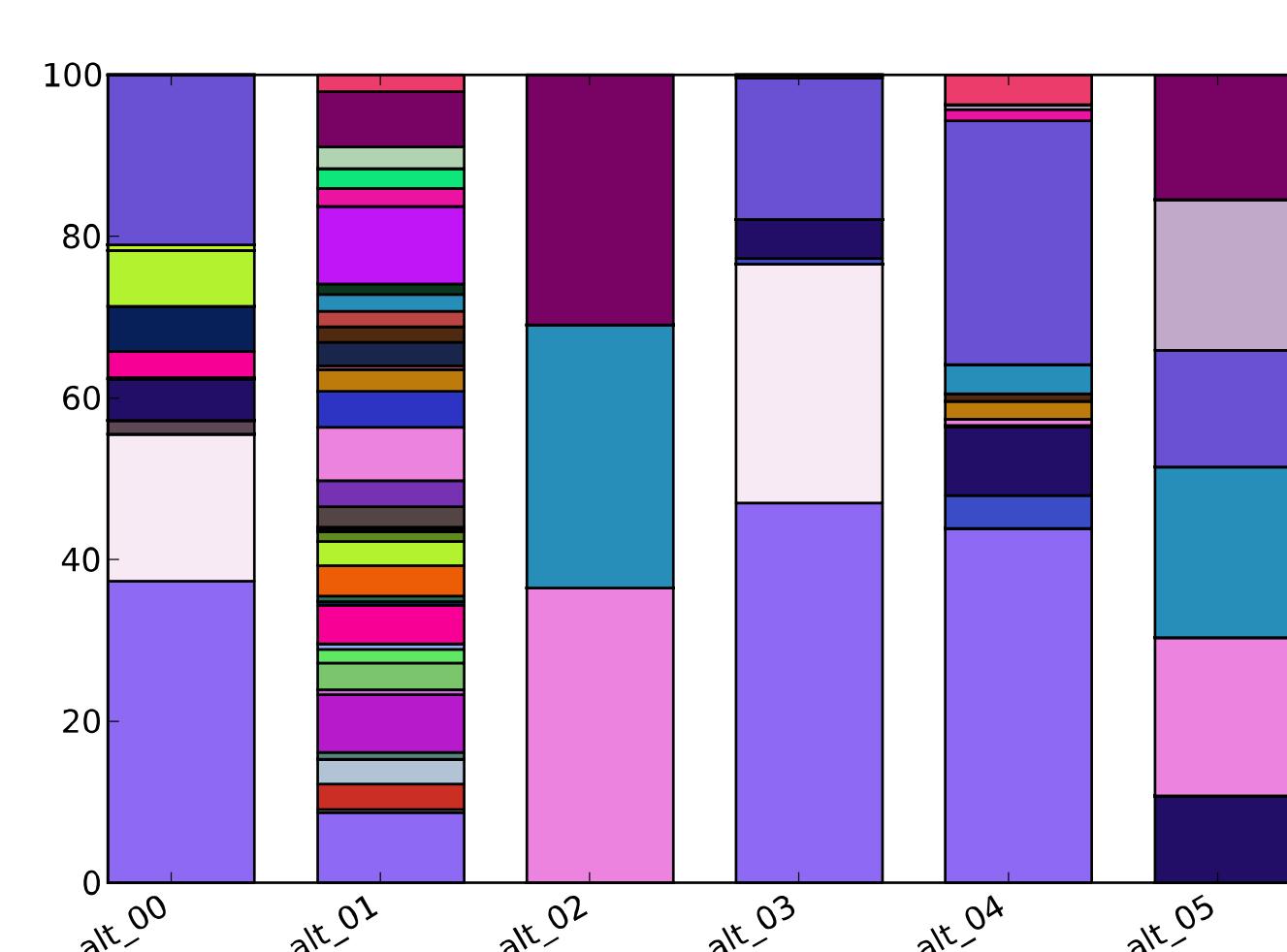
Basis selection

- 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

- Liquid cloud fraction models in CLUBB
- 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 Earth-system partnership



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