Uncertainty Quantification Methodologies for Climate Model Data with Discontinuities

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SIAM Annual Meeting
Pittsburgh, PA
July 14, 2010

Uncertainties in Climate Modeling

- Uncertainty sources
  - Parameter uncertainty
    - Model parameters
    - Initial/boundary conditions
    - Model geometry/structure
  - Model/structural uncertainty
    - Unknown physics
    - Reduced order models
  - Scenario uncertainty
    - Policy restrictions
    - Technology improvement
  - Intrinsic variability
    - Stochastic physics
  - Numerical errors

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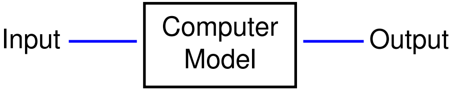
- Need UQ for...
  - Model validation
  - Confidence assessment
  - Optimal design
  - Data assimilation

UQ components and methods



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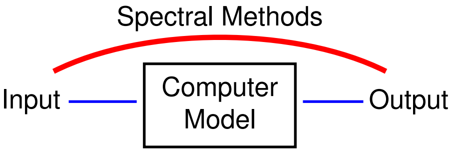

- Sensitivity analysis
  - Small parameter perturbations
- Predictability assessment
  - Larger parameter uncertainties

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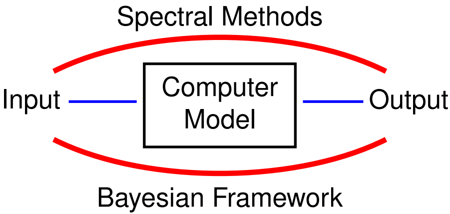

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- Parameter estimation
  - Inverse problems

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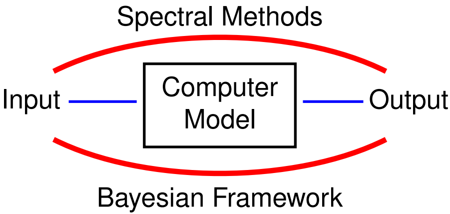

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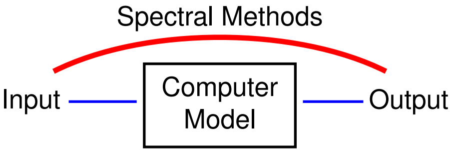

- Forward UQ methods
  - Direct (intrusive)
    - Derive new forward model
    - Intrusive Spectral Projection (ISP)
  - Sampling (non-intrusive)
    - Monte-Carlo, Quasi Monte-Carlo
    - Non-intrusive Spectral Projection (NISP)

Polynomial Chaos expansion represents any random variable as a polynomial of a standard random variable

- Truncated PCE: finite dimension n and order p

$$X(\boldsymbol{\lambda}(\boldsymbol{\eta})) \simeq \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\eta})$$

with the number of terms $P+1 = \frac{(n+p)!}{n!p!}$.

- $\boldsymbol{\eta} = (\eta_1, \cdots, \eta_n)$ standard i.i.d. r.v.
  Ψ_k standard orthogonal polynomials
  c_k spectral modes.
- Most common standard Polynomial-Variable pairs:
  (continuous) Gauss-Hermite, Legendre-Uniform,
  (discrete) Poisson-Charlier.

[Wiener, 1938; Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002; Le Maître & Knio, 2010]

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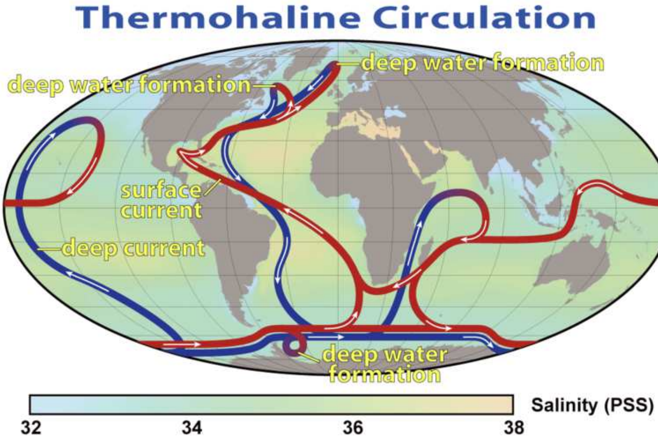
Meridional Overturning Circulation



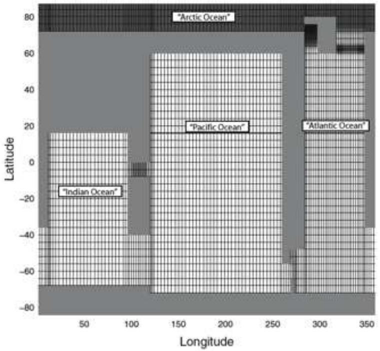
MOC transports heat from warm to cold regions

Webster et al - J. Environ. Syst. 31: 39-59, 2007

- Computational model
  - 3D Ocean general circulation model
  - Zonally-averaged atmospheric model
  - Thermodynamic sea-ice model
  - Simplified models for river runoff

- Input parameters
  - Rate of CO_2 increase (r)
  - Climate sensitivity (λ)

- Output observable
  - Overturning streamfunction (Z)



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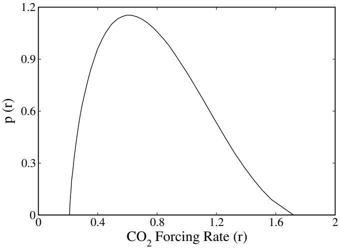

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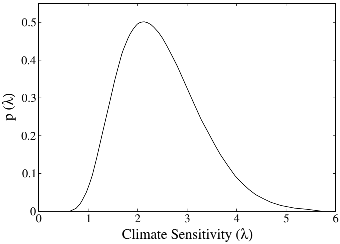

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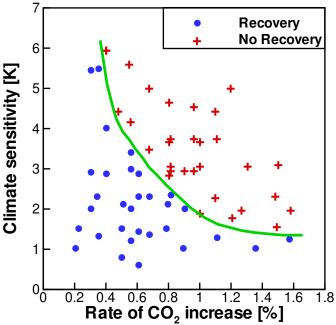

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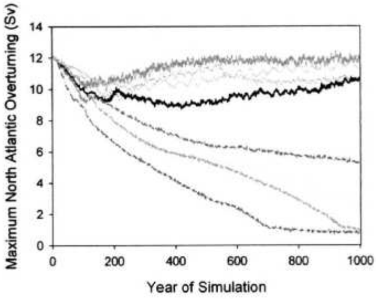

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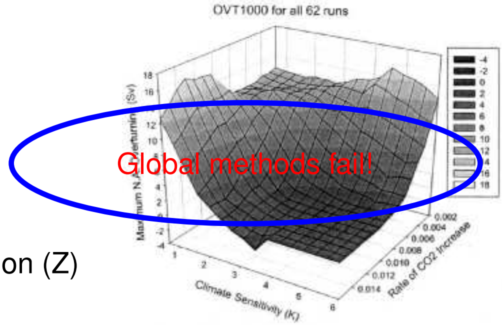


UQ & Discontinuities - Proposed Methodology

Our approach locates the discontinuity first so the domain can be subdivided into regions with smooth model response where spectral uncertainty quantification methods can be used

- Need to represent model output in a problem-independent fashion that takes into account the bifurcations
  - **Bayesian inference of the location of the discontinuity**
- Need to perform uncertainty quantification with only a limited set of sample points, due to the computational cost of the forward model
  - **Polynomial chaos representation via parameter domain mapping**

Bayesian Inference of the Location of Discontinuity

- Parameterize the discontinuity: $r \approx p_{\boldsymbol{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda)$

- Approximation model:

$$\mathcal{M}_{\boldsymbol{c}} \equiv g(\lambda, r) = m_L + (m_R - m_L)\frac{1 + \tanh\left(\alpha(r - p_{\boldsymbol{c}}(\lambda))\right)}{2}$$

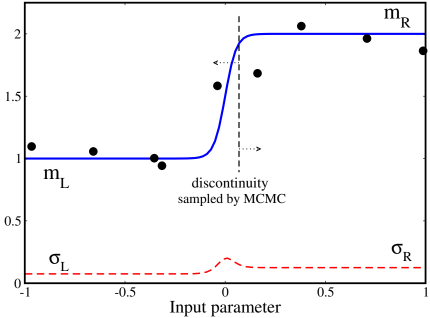
- Noise model postulated: $\sigma(\lambda, r)$
- Likelihood function:

$$\log P(\mathcal{D}|\mathcal{M}_{\boldsymbol{c}}) = \sum_{i=1}^{N} \log\left(P(z_i|\mathcal{M}_{\boldsymbol{c}})\right) = -\sum_{i=1}^{N} \frac{(z_i - g(\lambda, r))^2}{2\sigma(\lambda, r)^2}.$$

Bayesian Inference of the Location of Discontinuity

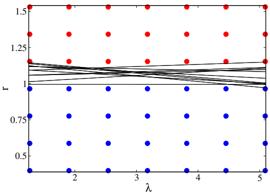
- Parameterize the discontinuity: $r \approx p_{\boldsymbol{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda)$

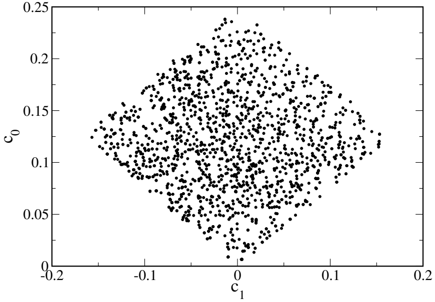
- Bayes' formula: $P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D})}$

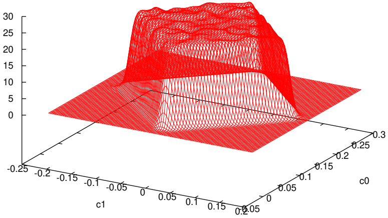


Highlights

- Any distribution of input points
- Generalizes to multiple dimensions
- Probabilistic representation







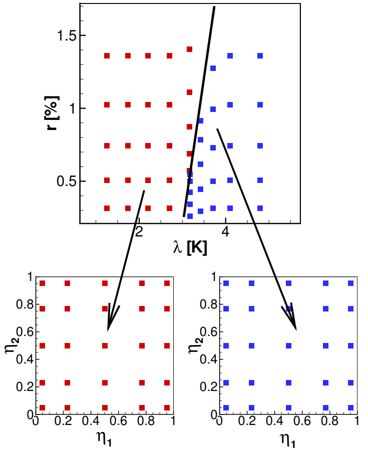
Discontinuity curve samples and their pdf

Parameter Domain Mapping

- Assume linear discontinuity
- Use Rosenblatt Transformation (RT) to map the pair of uncertain parameters (λ, r) to i.i.d. uniform random variables η_1 and η_2:

$$
\begin{aligned}
\lambda &= F_\lambda^{-1}(\eta_1), \\
r &= F_{r|\lambda}^{-1}(\eta_2|\eta_1)
\end{aligned}
$$

- Apply the RT mapping to both sides of the discontinuity



ROSENBLATT TRANSFORMATION: $(\lambda, r) \rightarrow (\eta_1, \eta_2)$

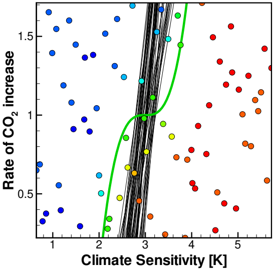
Inference of Discontinuity - 3^{rd} order polynomial

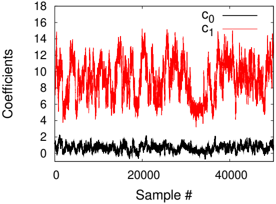
- Synthetic discontinuous data

$$z_i = (1 + \sigma\xi)\mathrm{erf}\left(\beta(r_i - \tilde{r}(\lambda_i))\right).$$

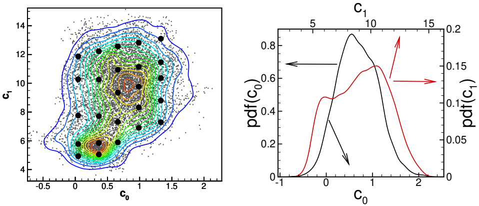
- Use straight lines to infer the discontinuity

$$\tilde{r}(\lambda) = c_0 + c_1\lambda.$$





MCMC samples



Joint and Marginal Posterior Distributions

PC expansion, averaged over discontinuity curves

- PC expansion for each discontinuity curve sample:

$$Z_{\boldsymbol{c}}^{L,R}(\lambda, r) = \tilde{Z}_{\boldsymbol{c}}(\eta_1, \eta_2) = \sum_{p=0}^{P} z_p \Psi_p^{(2)}(\eta_1, \eta_2)$$

- Model expansion depends on the parameter location:

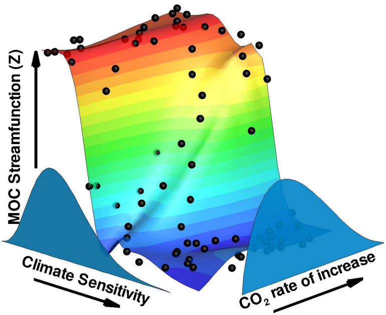
$$Z_{\boldsymbol{c}}(\lambda, r) = \begin{cases} Z_{\boldsymbol{c}}^{L}(\lambda, r) & \text{if } (\lambda, r) \in D_L \\ Z_{\boldsymbol{c}}^{R}(\lambda, r) & \text{if } (\lambda, r) \in D_R \end{cases}.$$

- Average over all PC expansions via RT:

$$\hat{Z}(\lambda, r) = \int_C p(\boldsymbol{c}) Z_{\boldsymbol{c}}(\lambda, r) d\boldsymbol{c} = \int_{[0,1]^{K+1}} Z_{R^{-1}(\vec{\eta})}(\lambda, r) d\vec{\eta}$$

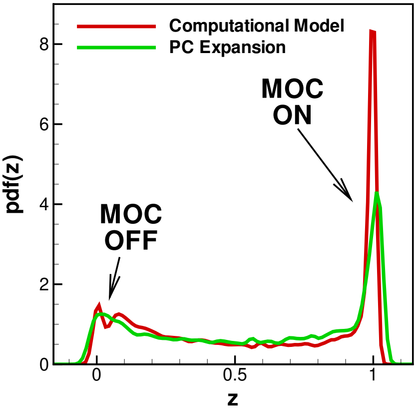
Discontinuous data represented well with the averaged PC

PCE IN (η_1, η_2) DOMAIN



Discontinuous data represented well with the averaged PC.

OUTPUT PDF



Resulting output PDF given input parameter joint PDF.

Summary

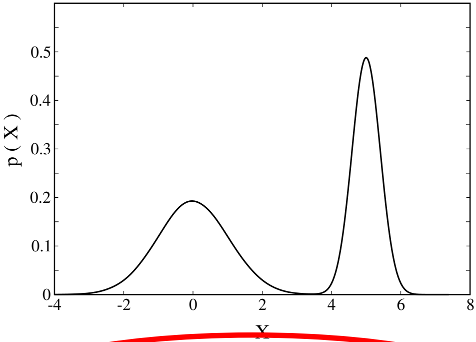
- A methodology for uncertainty quantification in climate models with limited data and discontinuities was proposed:
  - Bayesian approach to detect and parameterize the discontinuity as well as the uncertainty associated with it.
  - Rosenblatt transformation maps each of the irregular domains to rectangular ones where the application of the local spectral methods of uncertainty propagation is feasible.
- "Knowledge Discovery from Climate Data: Prediction, Extremes, and Impacts" Workshop Proceedings - 9th IEEE International Conference on Data Mining, 2009.
- Full paper in preparation.

Work in progress

- Bring in real climate model data.
- Still prohibitively many model runs required: possibly give up orthogonal projection in favor of Bayesian inference.
- Gaussian process emulation to implement uncertainties due to the lack of knowledge at non-sampled points.
- Experimental design: inform climate modelers on the optimal parameter sets to run simulations.

UQ methods are challenged by..

- Nonlinearities, Bifurcations, Bimodalities
- Tail regions
- Limited data
- Curse of dimensionality
- Intrinsic stochasticity



Smart domain decomposition

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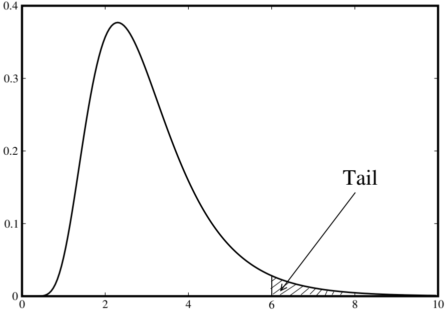

Custom spectral bases

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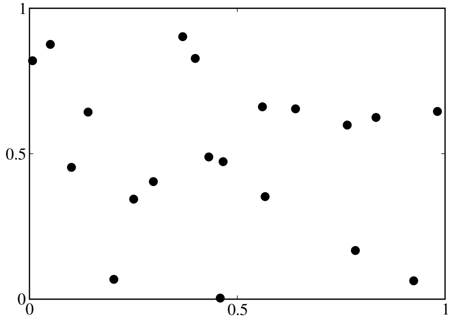

Bayesian approach, O'Hagan's work

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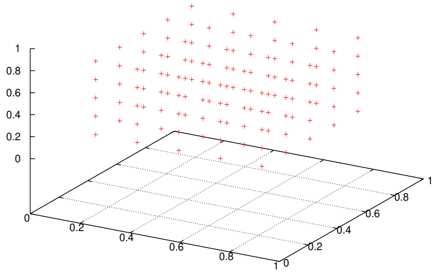

Sparse quadrature/cubature

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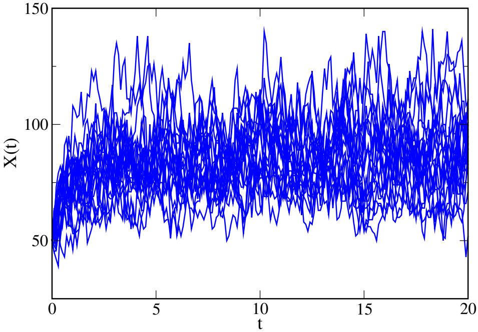

Work with moments, Bayesian?

Acknowledgements

- Sandia's internal
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Literature

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