Advanced Methods for Uncertainty Quantification in Tail Regions of Climate Model Predictions

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Uncertainty Quantification Challenges in Complex Models

- Limited number of model simulations
- Extended parameter range with 'low' probabilities

Conventional methods for uncertainty quantification are generally challenged in the "tails" of probability distributions. This is specifically an issue for many climate observables since extensive sampling to obtain a reasonable accuracy in tail regions is especially costly in climate models. Moreover, the accuracy of spectral representations of uncertainty is weighted in favor of more probable ranges of the underlying basis variable, which, in conventional bases does not particularly target tail regions. Therefore, what is ideally desired is a methodology that requires only a limited number of full computational model evaluations while remaining accurate enough in the tail region.

To develop such a methodology, we explore the use of surrogate models based on non-intrusive Polynomial Chaos expansions and Galerkin projection. We consider non-conventional and custom basis functions, orthogonal with respect to probability distributions that exhibit fat-tailed regions. We illustrate how the use of non-conventional basis functions, and surrogate model analysis, improves the accuracy of the spectral expansions in the tail regions. Finally, we also demonstrate these methodologies using precipitation data from CCSM simulations.

Polynomial Chaos Expansions and Galerkin Projection

To propagate input parameter distributions to output observable distributions, Polynomial Chaos (PC) spectral expansions are used; see Ghanem and Spanos, "Stochastic Finite Elements: A Spectral Approach" ,1991.

Interpret input parameter γ as a random variable, and a climate forward model $f(\cdot)$.
PC expansion for the output observable $Z = f(\gamma)$

$$Z = \sum_{k=0}^{K} Z_k \Psi_k(\xi)$$

with standard polynomials $\Psi_k(\cdot)$ of independent, standard random variables ξ, orthogonal w.r.t. pdf $p_\xi(\xi)$, i.e.

$$\langle \Psi_i(\xi)\Psi_j(\xi)\rangle \equiv \int \Psi_i(\xi)\Psi_j(\xi)p_\xi(\xi)d\xi = \delta_{ij}\langle \Psi_i(\xi)^2\rangle$$

Conventional PCs are LU (Legendre polynomials of Uniform r.v.) or GH (Hermite polynomials of Normal r.v.).

Galerkin (orthogonal) projection

$$Z_k = \frac{\langle f(\gamma(\xi))\Psi_k(\xi)\rangle}{\langle \Psi_k^2(\xi)\rangle}$$

is weighted-L_2 optimal, i.e. it minimizes

$$\int \left| f(\gamma(\xi)) - \sum_{k=0}^{K} Z_k\Psi_k(\xi)\right|^2 p_\xi(\xi)d\xi$$

with respect to pdf $p_\xi(\xi)$ that controls the pointwise error, i.e., the larger $p_\xi(\xi)$, the smaller the pointwise error

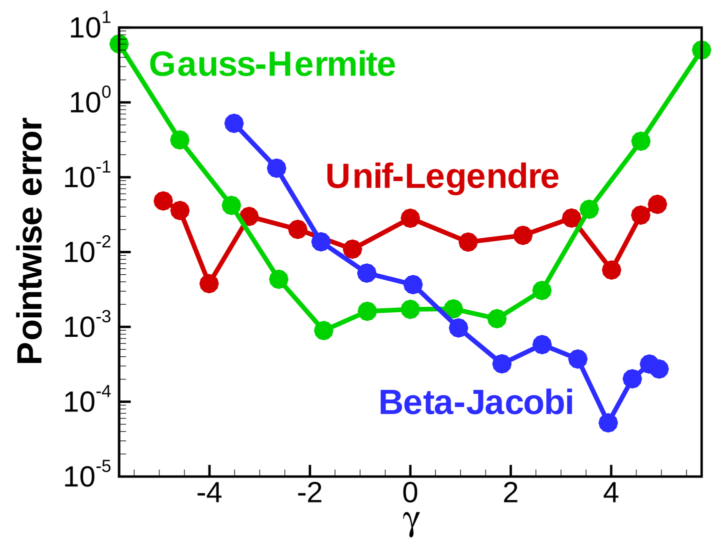
$$\text{err}(\xi) = \left| f(\gamma(\xi)) - \sum_{k=0}^{K} Z_k\Psi_k(\xi)\right|$$

Non-conventional and Custom Basis Functions

Non-conventional bases

Consider a synthetic forward model $f(\cdot)$ and assume input parameter $\gamma = \gamma_0 + \gamma_1\xi$. Non-conventional, Jacobi-Beta PC (i.e., ξ is a Beta r.v. and $\Psi_k(\xi)$ are Jacobi polynomials) may be more accurate in certain regions of interest given the choice of $p_\xi(\xi)$. Pointwise error is

- LU : independent of position
- GH : worse in "tails", away from the origin
- JB : small in desired region, i.e. it is controllable!

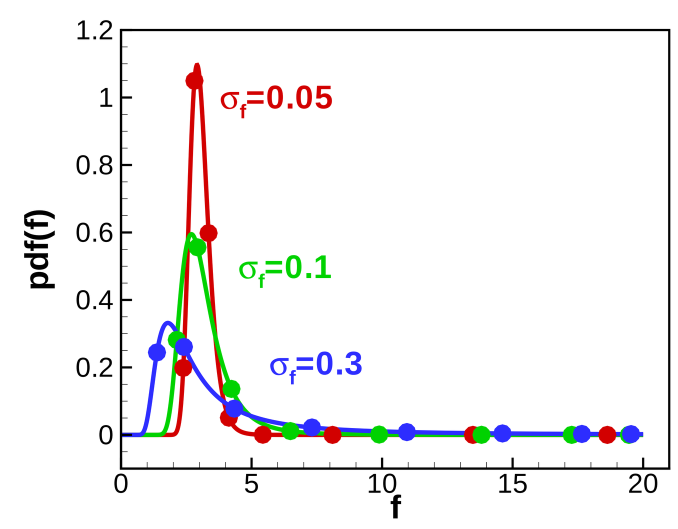


Custom bases

For general, non-standard input parameter γ, the output can be expanded in terms of custom polynomials that are orthogonal with respect to the basis pdf $p_\gamma(\gamma)$ to get near-optimal pointwise error.

The orthogonal polynomials $\Phi_k(\gamma)$'s are generated using the Stieltjes procedure; see W. Gautschi, "On generating orthogonal polynomials" SIAM J. Sct. Stat. Comput. 3, 289-317, 1982.

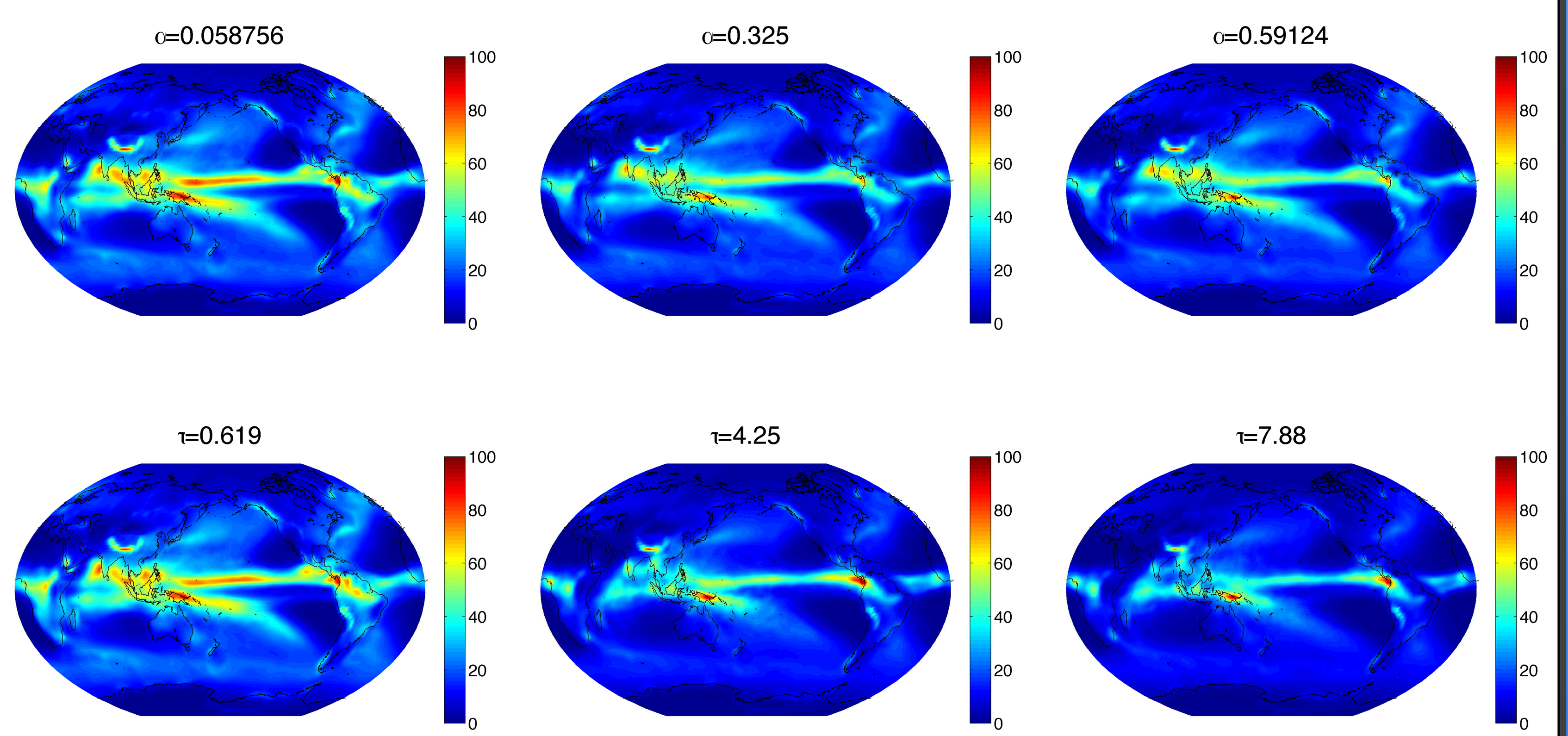
- Quadrature points' distribution for polynomials orthogonal w.r.t. truncated log-normal pdf.



Climate Simulations at Quadrature Point Locations for Input Parameters

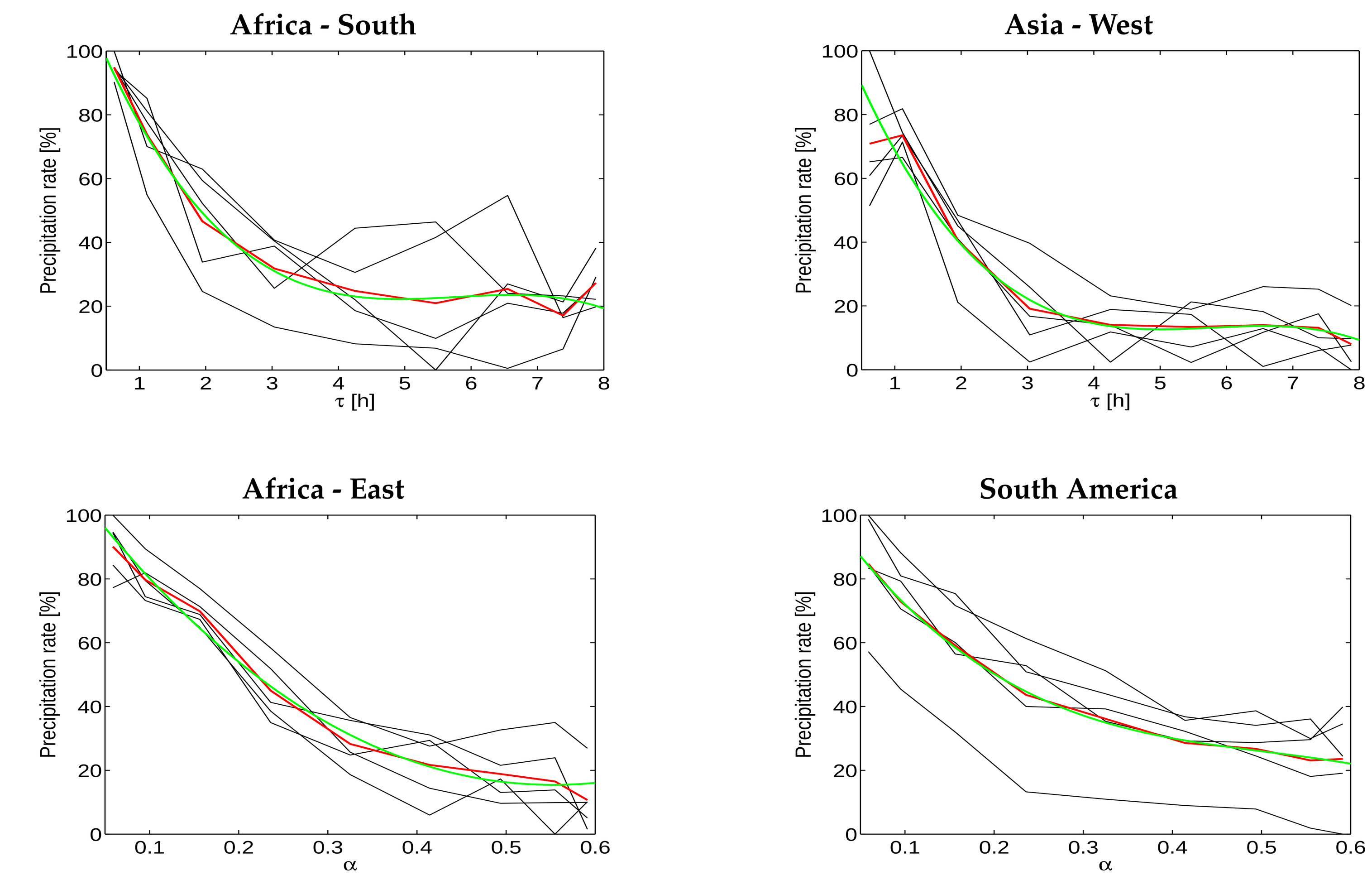
Parameters:

- α [%] - initial cloud downward flux; $\alpha \in [0.05, 0.6]$
- τ [h] - consumption rate of CAPE; $\tau \in [0.5, 8]$



precipitation rate (normalized) - 10 year averages
(*data courtesy of Mike Levy & Mark Taylor, Sandia National Labs*)

Surrogate Models for Precipitation Data



- Black lines - 2 year averages; Red lines - 10 year averages; Green lines - 3rd-order PC expansions.

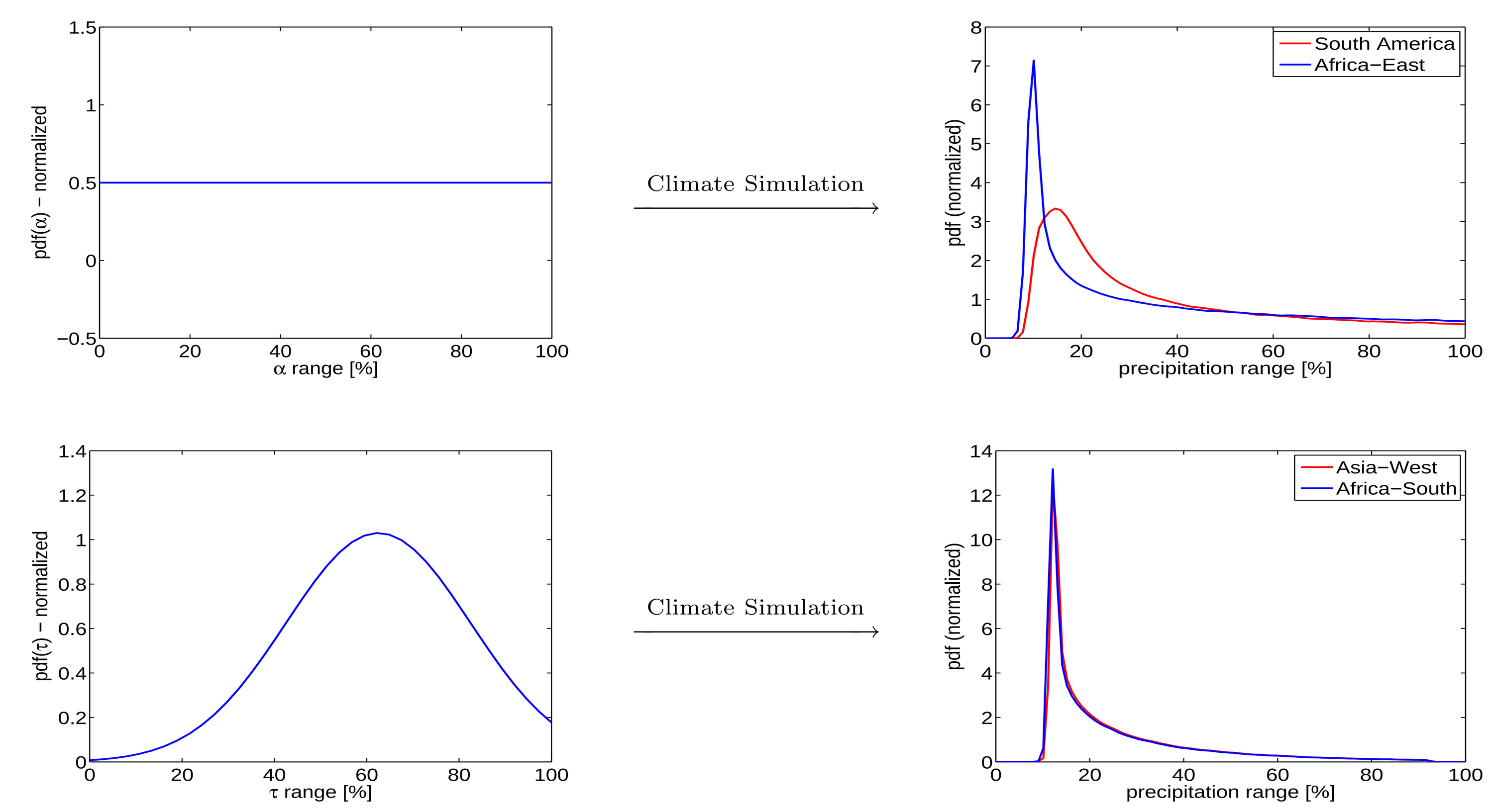
Accuracy of "Tail" Probabilities Based on Standard and Custom PC basis Surrogates

- Surrogate models are constructed based on both conventional PC basis (e.g. Hermite polynomials) and custom PC basis - orthogonal w.r.t. pdf's that exhibit "fat" tails.
- Compute the probability that average precipitation exceeds a certain amount:

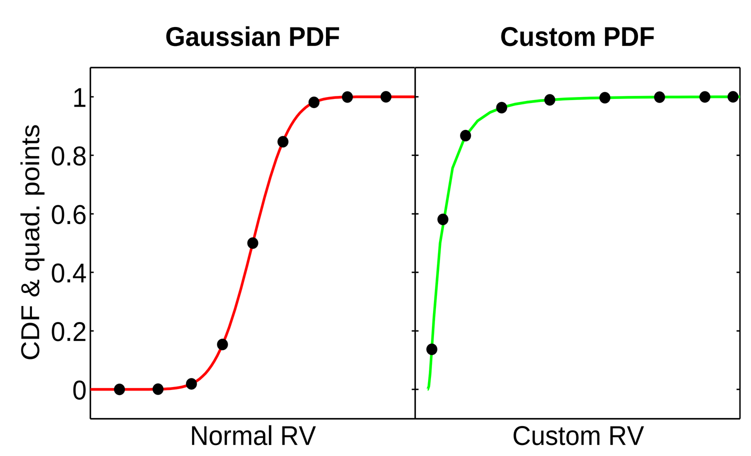
$$P(precip. > p_r) = \int_{\alpha: f(\alpha)>p_r} \text{pdf}(\alpha)d\alpha$$

- Compute the probabilities based on PC expansions with the "exact" values (using the models above).

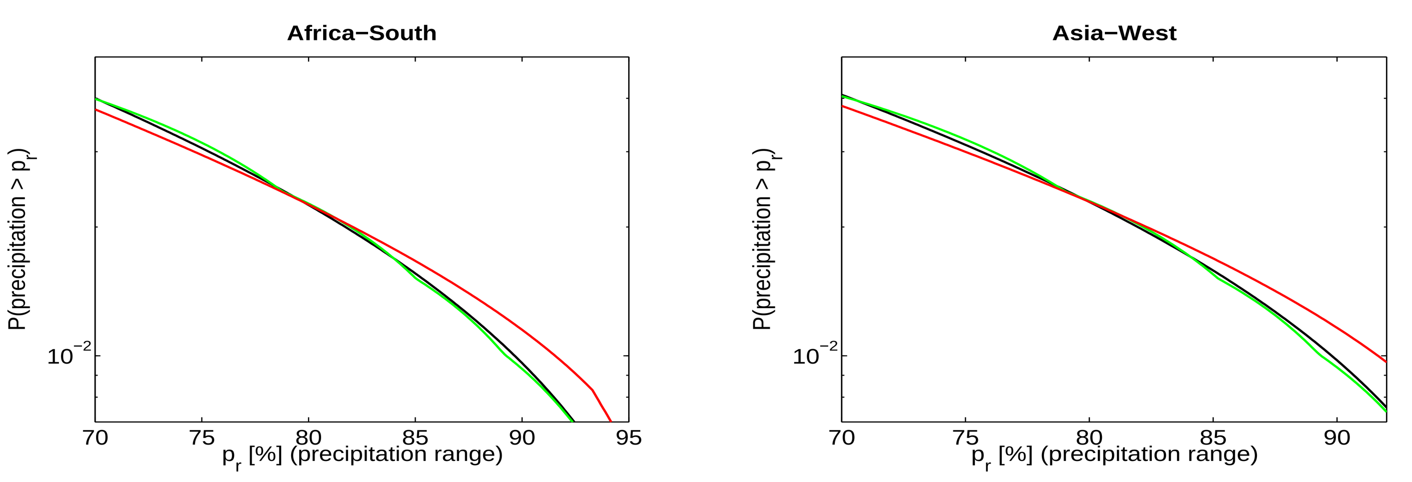
PDF's of Climate Observables



"Tail" Probabilities



- Custom PDF is based on a truncated log-normal distribution
- The set of quadrature points corresponding to the custom PDF have a better coverage of the distribution's tail compared to the set corresponding to a Gaussian PDF.



- Black lines - "Exact" values; Red lines - Hermite PC basis (9th order); Green lines - Custom PC basis (9th order).

Summary and Future Work

- Custom PC bases provide increased accuracy over standard PC's in low-probability regions.
- Extend this methodology to multi-dimensional parameter dependencies.
- Develop surrogate models as mixed PC expansions: accurate both near the mean as well as in the tail regions.

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