Probabilistic Collocation Method (PCM) for modeling response of GEOS-Chem simulations to model parameter uncertainties

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GEOS-Chem Simulation of POPs

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The problem

Given the uncertainty of the parameters that affect the outcome of GEOS-Chem's benzo[a]pyrene simulations, what is the resulting uncertainty in Arctic mean total (gas- and particle-phase) atmospheric concentrations?
Uncertain parameters and PCM

Collocation points → Parameter values → CTM → PCE → Easy to sample polynomial
Testing

Test it out with an example from Pan et al.

$$\Delta F = S_0 (1-A_c) T^2 (1-R_s) \beta \delta$$

- Run through PCM scheme to get polynomial estimate
- Compare randomly sampled true function with randomly sampled estimate polynomial
Chemical parameters

- $K_{OA}$ octanol-air partition coefficient
- $K_{BC}$ black carbon-air partition coefficient
- $k_{OH}$ oxidation rate (by OH$^-$)
- $H^*$ Henry's Law constant
- $\Delta_H$ enthalpy of phase transfer (gas to OC)
- $\Delta_{Hw}$ enthalpy of phase transfer (gas to aqueous)
Parameter space
Parameter space
GEOS-Chem model runs

- Prescribed meteorology, emissions
- Benzo[a]pyrene is modeled “offline”
- For each run, parameters are set and a 1 year spin-up is performed, followed by 1 year of simulation
- 112 runs performed (28 + 84)
- Log of resulting concentrations is used
2nd order results
3\textsuperscript{rd} order results

![Graph showing the 3rd order results](image-url)
With lower parameter uncertainty
What it means

- PCM gives a reasonable result at low order, even for CTM simulations
- Even given large parameter uncertainty, Arctic concentrations likely in the $0.0003 - 0.01 \text{ ng}/\text{m}^3$ range
- More optimistically, $0.001 - 0.01 \text{ ng}/\text{m}^3$
What it doesn't mean

- Only includes model response to the given parameters
- Does not include uncertainty due to emissions
- Under the assumption that the chemistry is correct (complete)
Another option

- Regression-based surface response model
  - use most of the same procedure, but instead of solving a system of equations (n by n matrix) for the PCE coefficients, use singular value decomposition to get them (m>n by n matrix)
  - would provide a good comparison, as a “similar but different” method
  - currently under construction