Chair of Scientific Computing
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Efficient FUQ and SA of Time-Dependent Outputs in Hydrology Modeling

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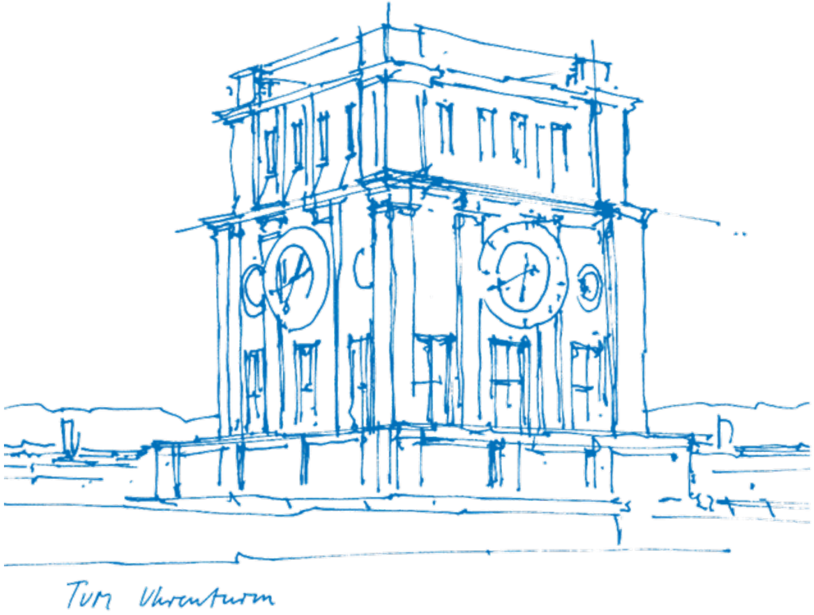
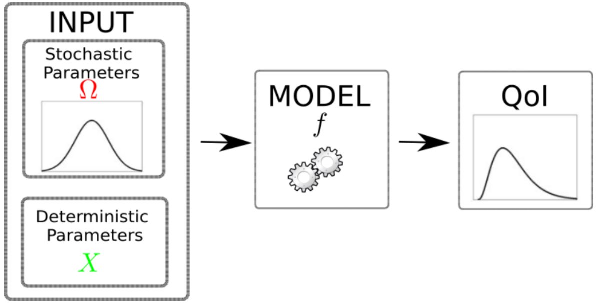


Problem Statement

- **Scientific Approach:** Experiment with different strategies for combining (spatially adaptive) Sparse Grids (SG) with Uncertainty Quantification (UQ) and Sensitivity Analysis (SA) algorithms
- **Final Goal:**
  Efficient and accurate UQ and SA of complex dynamical models (e.g., HBV-SASK hydrologic model [1])



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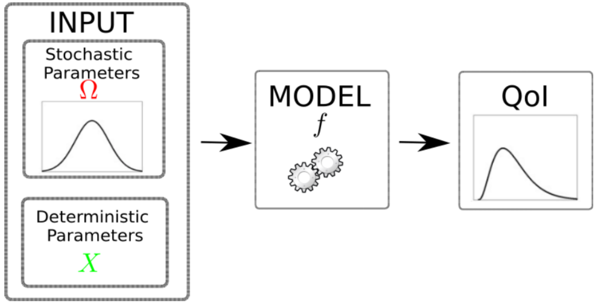


Impediments:

- High-dimensionality
- High execution times
- Possible discontinuities in the parameter space; anisotropic or decoupled parameters
- Time-dependent model output

Building Blocks

- **Sparse Grid (SG)**
  - Standard SG and Combination Technique
  - Spatially Adaptive SG (SparseSpACE Framework)
- **Non-intrusive UQ and SA**
  - Polynomial Chaos (PC) Approximation & Pseudo-spectral Approximation
  - Variance-based Sensitivity Analysis
  - Integrating SG into UQ: Exploring different combination approaches
- **UQ with SG for Time-dependent Models**
  - Karhunen–Loéve (KL) Expansion

Sparse Grids | UQ | SG & UQ for Time-dependent

Part I: Sparse Grids

Sparse Grid & Combination Technique

Combination Technique (CT) [4, 5]:

Efficient SG computation by linearly combining computations on cheap/coarser anisotropic full grids

For these full grids any conventional full grid solver can be applied

$$u_{\mathscr{I}}^{CT} = \sum_{\boldsymbol{l} \in \mathscr{I}} c(\boldsymbol{l})(\mathscr{U}^{l_1} \otimes, \ldots, \otimes \mathscr{U}^{l_d})(f); \quad \mathscr{I} = \{\boldsymbol{l} \in \mathbb{N}^d \mid \|\boldsymbol{l}\|_1 = l + d - 1\} \tag{1}$$

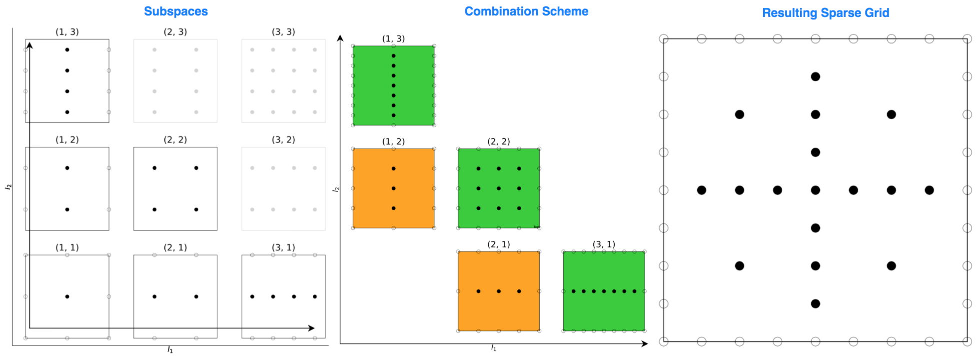


Abbildung: Combination technique represented via subspaces, grid components and the final resulting sparse grid; green component grids are added and orange ones are subtracted

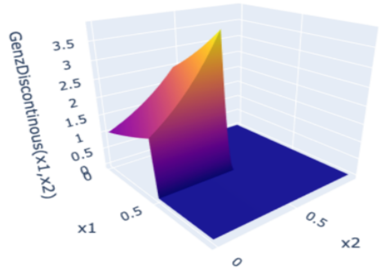
SparseSpACE Framework [Obersteiner and Bungartz, 2021]

CT with Spatial Adaptivity - Use rectilinear grids constructed via a tensor product of refined 1-D grids

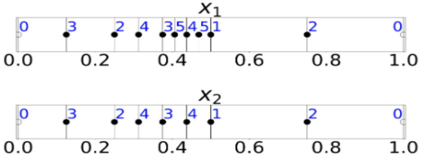
Key components:

- 1D Refinements define the adaptive process
  - A vector of points and levels $\boldsymbol{P}^k$ $\boldsymbol{L}^k$ for each dimension $k \in [d]$
- Global Combination Scheme:
  - Generate a global valid combination scheme from 1D refinements
  - Ceate the index set $\mathscr{I}$ and for each $\boldsymbol{l} \in \mathscr{I}$, perform mapping $\boldsymbol{P}^k, \boldsymbol{L}^k \Rightarrow \boldsymbol{P}^{k,\boldsymbol{l}}, \boldsymbol{L}^{k,\boldsymbol{l}})$
- Grid Construction:
  - Build the d-dimensional rectilinear grids via tensor construction
- **Compute approximation**
- Error Estimators:
  - Special error estimators guide the refinement process
- Note: Spatial adaptivity requires nested points

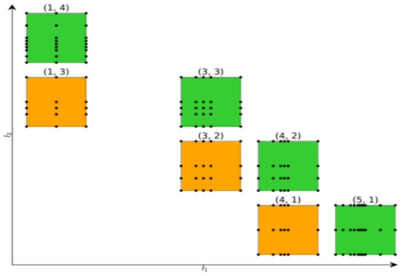
2D Genz Discon. Function



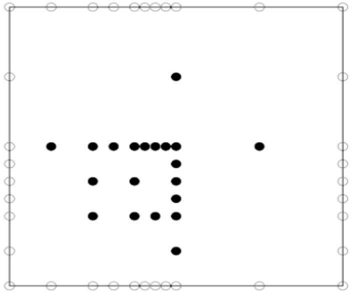
The output of Dimension-wise Spatial refinement



The resulting combination scheme



The resulting Sparse Grid



Part II: Uncertainty Quantification and Sensitivity Analysis

Polynomial Chaos Expansion (PCE) [6]

- approximate $f(t,\theta) : \mathbb{T} \times \Gamma \to \mathbb{R}$ by series of polynomials

$$f(t,\theta) \approx f_N(t,\theta) = \sum_{\boldsymbol{p}} c_{\boldsymbol{p}}(t)\Phi_{\boldsymbol{p}}(\theta) \quad (2)$$

- stochastic part - $\theta = (\theta_1, \theta_2, \ldots, \theta_d)^T; \theta : \Omega \to \Gamma$ and $\rho(\theta) = \prod_{k=1}^{d} \rho_k(\theta_k)$
- $\boldsymbol{p} = (p_1, \ldots, p_d)$ is a multi-index in $\mathscr{P}_P = \{\boldsymbol{p} \in \mathbb{N}^d : \sum_{k=1}^{d} p_k \leq P\}$,
- $\Phi_{\boldsymbol{p}}(\theta)$ are orthonormal multivariate polynomials constructed via a tensor product basis of the univariate polynomials $\Phi_{\boldsymbol{p}}(\theta) = \Phi_{p_1}(\theta_1) \cdot \ldots \cdot \Phi_{p_d}(\theta_d)$

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Pseudo-spectral (PS) approach - uses (full tensor) quadrature rule to calculate $c_{\boldsymbol{p}}$

$$c_{\boldsymbol{p}}(t) = \int_{\Omega} f(t,\theta)\Phi_{\boldsymbol{p}}(\theta)d\theta \approx \sum_{\boldsymbol{q}=1}^{\boldsymbol{Q}} f(t,\theta_{\boldsymbol{q}})\Phi_{\boldsymbol{p}}(\theta_{\boldsymbol{q}})\omega_{\boldsymbol{q}} \tag{3}$$

Total number of coefficients (total-degree basis): $N = \binom{P+d}{d}$
Total number of model evaluations: $\boldsymbol{Q} = \prod_{k=1}^{d} Q_k$; and it has to hold - $p_k = \text{floor}(DE(Q_k)/2)$ [7]

Post-processing & Sensitivity Analysis

Quantify uncertainty of f by computing, e.g.

$$\mathbb{E}[f] = \int_{\Omega} f(t,\theta)\rho(\theta)d\theta; \qquad \mathbb{V}[f] = \mathbb{E}[f^2] - (\mathbb{E}[f])^2 \tag{4}$$

Variance-based (Sobol) sensitivity analysis

$$S_i = \frac{\mathbb{V}(\mathbb{E}(f|\theta_i))}{\mathbb{V}(f)} = \frac{1 - \mathbb{E}(\mathbb{V}(f|\theta_i))}{\mathbb{V}(f)} \tag{5}$$

Use gPCE coeff. to approximate expectation and variance:

$$\mathbb{E}[f_N(t,\theta)] = c_0(t) \qquad \mathbb{V}[f_N(t,\theta)] = \sum_{position(\boldsymbol{p})=1}^{N-1} c_{\boldsymbol{p}}^2(t) \tag{6}$$

Use gPCE coeff. to compute Sobol' indices (SI)[2]:

$$S_i = \frac{\sum_{\boldsymbol{p}\in A_i} c_{\boldsymbol{p}}^2(t)}{\mathbb{V}[f_N(t,\theta)]}, \quad A_i = \{\boldsymbol{p} \in \mathscr{P}_P : \boldsymbol{p}_i \neq 0 \wedge \boldsymbol{p}_{j\neq i} = 0\} \tag{7}$$

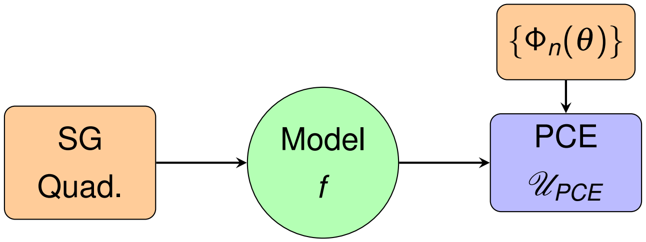
Part II: UQ with Sparse Grids

Sparse Grids & UQ

Multiple ways to combine PCE (i.e., PSP) and SG.

Almost all adaptive methods are applied exclusively to a single QoI.

Var 1: (Sparse) Quad. + (Truncated) Poly basis = PSP



The order of the polynomial basis and the half-exact set of the quadrature rule must match.

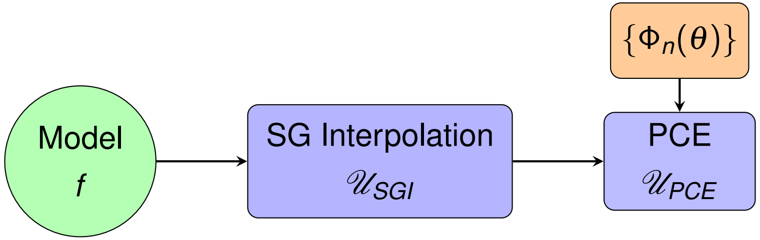
Truncation of the polynomial scheme.

Var 2: Sparse Interpolation Surrogate (i.e., f_{SGI}) + PSP

Var 3: Sparse PSP

Sparse Grids & UQ

Var 2: Sparse Interpolation Surrogate (i.e., f_{SGI}) + PSP

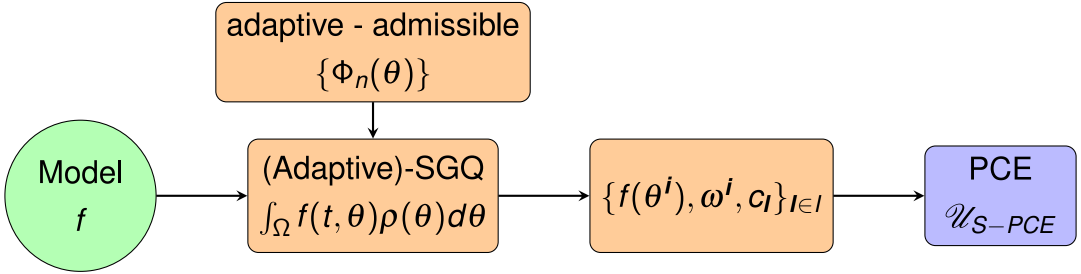


$$
\begin{aligned}
\hat{c}_{n,l}(t) &= \int_{\Omega} f_{\text{SGI}}(t,\theta)\Phi_n(\theta)\rho(\theta)d\theta \\
&= \int_{\Omega} \underbrace{\left(\sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i}\in\prod_{k=1}^{d}[|\boldsymbol{P}^{k,\boldsymbol{l}}|]} f(t,\theta^{\boldsymbol{i}})\Psi_{\boldsymbol{i}}(\theta)\right)}_{f_{\text{SGI}}} \Phi_n(\theta)d\theta \\
&= \sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i}\in\prod_{k=1}^{d}[|\boldsymbol{P}^{k,\boldsymbol{l}}|]} f(t,\theta^{\boldsymbol{i}}) \int_{\theta} \Psi_{\boldsymbol{i}}(\theta)\Phi_n(\theta)d\theta
\end{aligned} \tag{8}
$$

where $\Psi_{\boldsymbol{i}}(\theta)$ are basis functions of the SG scheme, $\Phi_n(\theta)$ are basis polynomials of the PCE, $n \in [N]$ is a scalar index of the gPCE coeff. $\hat{c}_n$, and $c_{\boldsymbol{l}}$ is a scalar coeff. streaming from CT.

Sparse Grids & UQ

Var 3: Sparse PCE

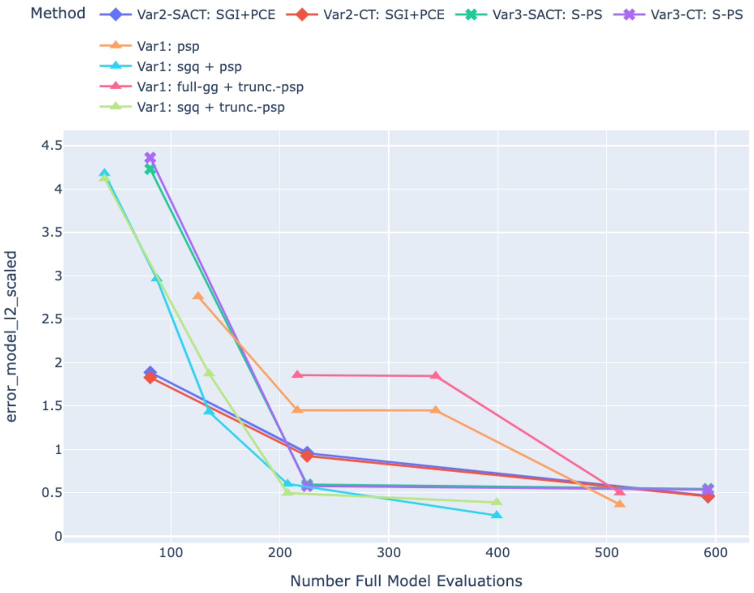


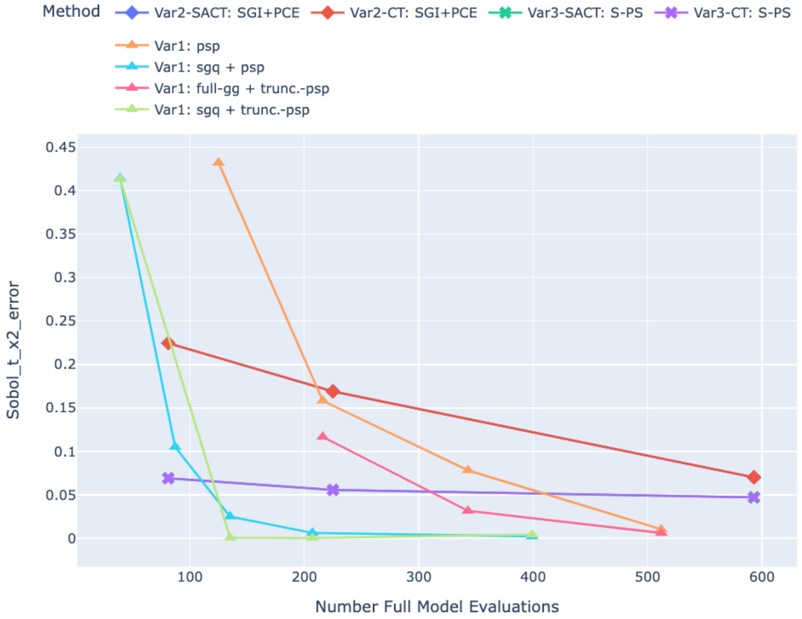
Not straightforward to combine with adaptive SG.
Extra precaution is needed when constructing a set of adaptive (admissible) orthogonal polynomials.
Practical implementation requires some tuning.

UQ & Sparse Grids - Benchmark convergence of different methods

Ishigami fun. (3D)

$$f_{\text{ishi}}(x) = sin(x_1) + a \cdot sin^2(x_2) + b \cdot x_3^4 \cdot sin(x_1)$$



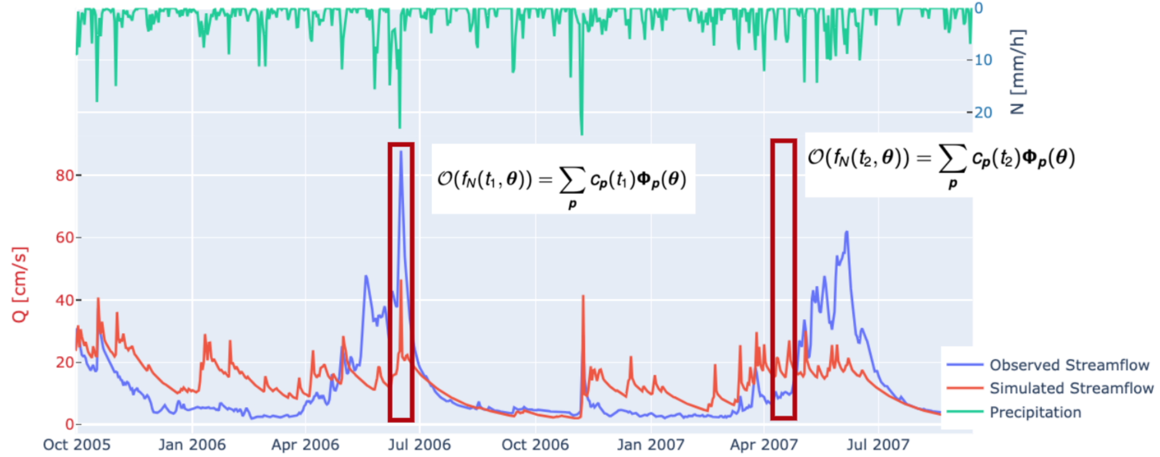


Part III: UQ for Time-dependent model outputs (with SG)

Time Dependent Analysis

Initial Strategy: Independent Time-Varying Analysis

- Assumes no correlation across time
- The number of Quantities of Interest (QoI) equals the number of time steps
- Most Sparse PCE algorithms consider **scalar** model responses
- Alternative approach: Summarize the entire time span using a goodness-of-fit metric and construct a single PCE surrogate based on it



Time Dependent Analysis

Improved Approach: Incorporate time dependency by representing the process f using Karhunen–Loéve (KL) Expansion.

$$f(t,\theta) \approx f_0(\theta) + \sum_{j=1}^{N_{KL}} \hat{f}_{KL}^{j}(\theta) e_j(t) \tag{9}$$

$$\tilde{\hat{f}}_{KL}^{j}(\theta) = \sum_{n=0}^{N_{pc}} c_n^j(t) \Phi_n(\theta); \qquad \text{Learn} \left\{ \left\{ c_n^j \right\}_{n=0}^{N_{pc}} \right\}_{j=1}^{N_{KL}} \text{using model evaluations} \left\{ f(t_m, \theta^i) \right\}_{i=1}^{N} \tag{10}$$

- Reduces the number of QoI to the number of KL terms
- Adaptivity - Jointly optimizes PC expansions for all KL expansion terms
- Still, the single adaptive solution for all KL terms may not be optimal (N_{PC} the same for all N_{KL} terms)

Generalized Sobol S.I [Alexanderian, et al., 2020]

$$\mathfrak{S}^i(f;t) = \frac{\int_0^T \mathbb{V}^i(f;t)dt}{\int_0^T \mathbb{V}(f;T)dt}; \qquad \text{computed via KL(+PCE) expansion} \mathfrak{S}^i(f;t) \approx \frac{\sum_{j=1}^{N_{KL}} \sum_{\boldsymbol{p} \in A_i} {c_{\boldsymbol{p}}^j}^2}{\sum_{j=1}^{N_{KL}} \lambda_j} \tag{11}$$

Time Dependent Analysis

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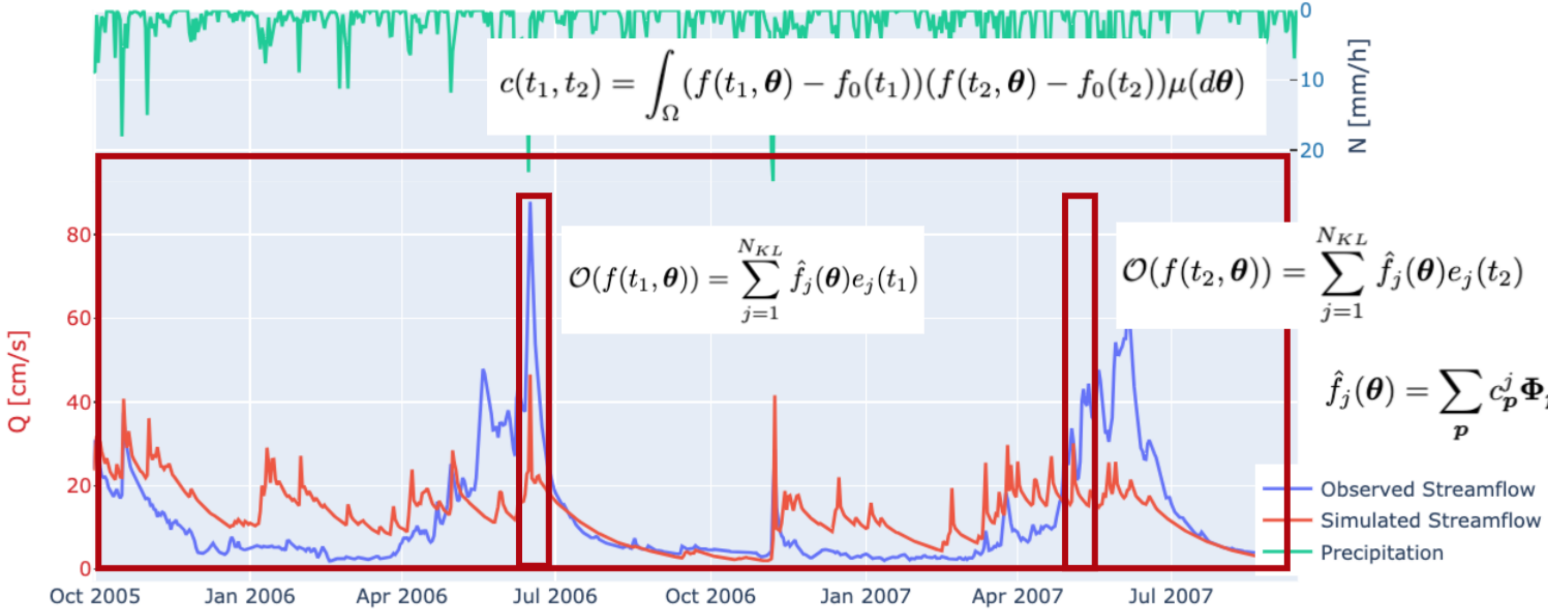


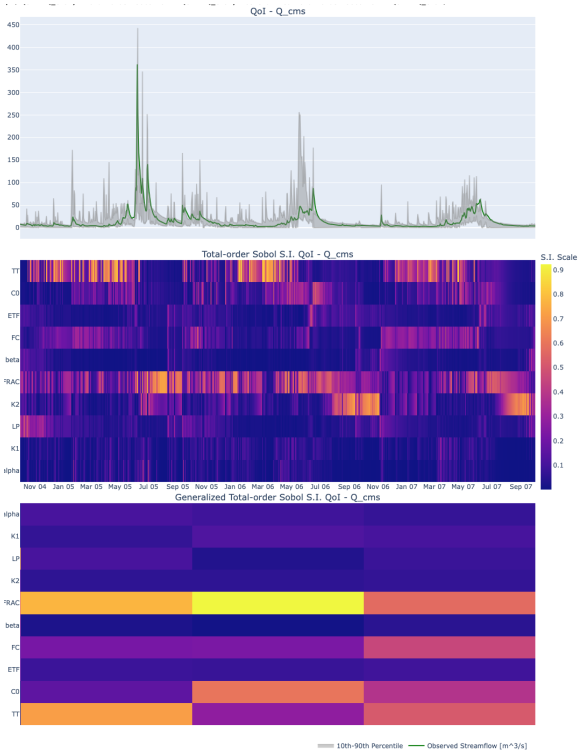
$$c(t_1, t_2) = \int_\Omega (f(t_1, \boldsymbol{\theta}) - f_0(t_1))(f(t_2, \boldsymbol{\theta}) - f_0(t_2))\mu(d\boldsymbol{\theta})$$

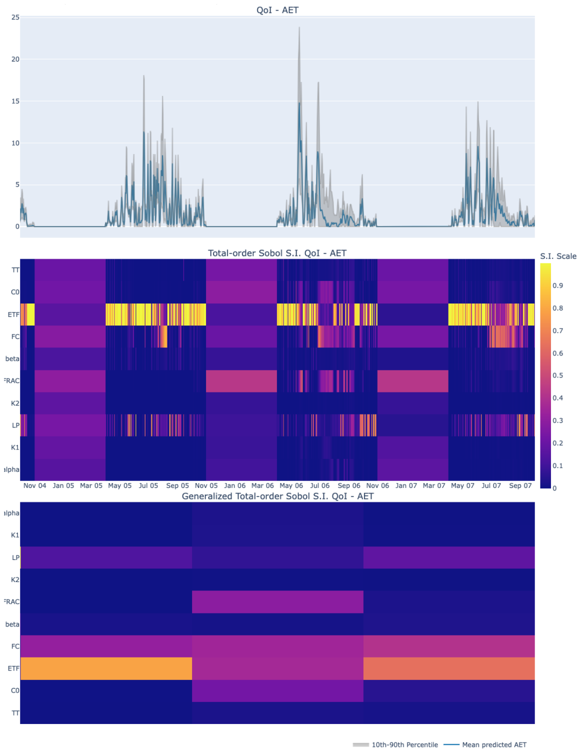
$$\mathcal{O}(f(t_1, \boldsymbol{\theta})) = \sum_{j=1}^{N_{KL}} \hat{f}_j(\boldsymbol{\theta}) e_j(t_1)$$

$$\mathcal{O}(f(t_2, \boldsymbol{\theta})) = \sum_{j=1}^{N_{KL}} \hat{f}_j(\boldsymbol{\theta}) e_j(t_2)$$

$$\hat{f}_j(\boldsymbol{\theta}) = \sum_{\boldsymbol{p}} c_{\boldsymbol{p}}^j \boldsymbol{\Phi}_{\boldsymbol{p}}(\boldsymbol{\theta})$$

Time Aggregated UQ & SA with Adaptive SG





Conclusion & Future Work

- **Novelty**
  - Combing Spatial Adaptivity with PS Approximation
  - Experiment with different ways to integrate SG & UQ algorithms
  - Extend adaptive UQ to time-dependent models using KL-based surrogates

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Ongoing work:

- **SpareSpACE**
  - Implement parallelization in SpareSpACE
  - Explore different grid/point choices (e.g., Leja) and basis functions (e.g., b-splines for interpolation)
- **Time-varying UQ & Sparse Grids**
  - Construct multiple surrogates as model behavior evolves
  - Use GSA to adaptively build higher-order PC bases

Thank You

Questions and Feedbacks

SparseSpACE

UQEF-Dynamic

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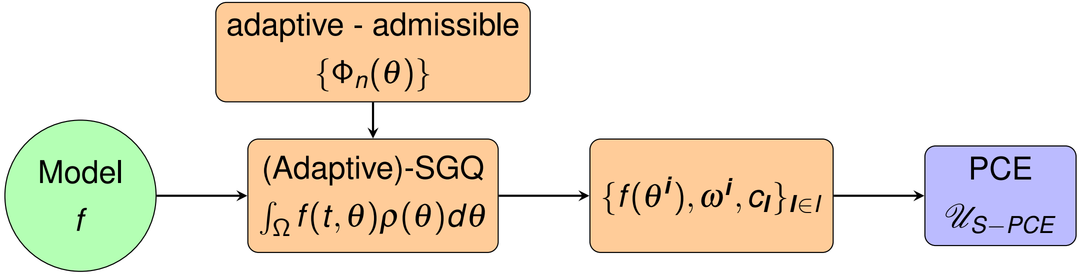
Sparse Grids & UQ

Var 3: Sparse PCE



$$\begin{aligned}\mathscr{U}_{S-PCE} &= \sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \mathscr{U}_{PCE} = \sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \sum_{n} \hat{c}_n \Phi_n(\theta) \\ &= \sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \sum_{n\in \mathrm{PCE}} \left| \sum_{\boldsymbol{i}\in \prod_{k=1}^{d} |\boldsymbol{P}^{k,\boldsymbol{l}}|} f(t,\theta^{\boldsymbol{i}})\Phi_n(\theta^{\boldsymbol{i}}) \int_\Omega \Psi_{\boldsymbol{i}}(\theta)\, d\theta \right| \Phi_n(\theta)\end{aligned} \tag{19}$$

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