Efficient FUQ and SA with Spatially Adaptive SG

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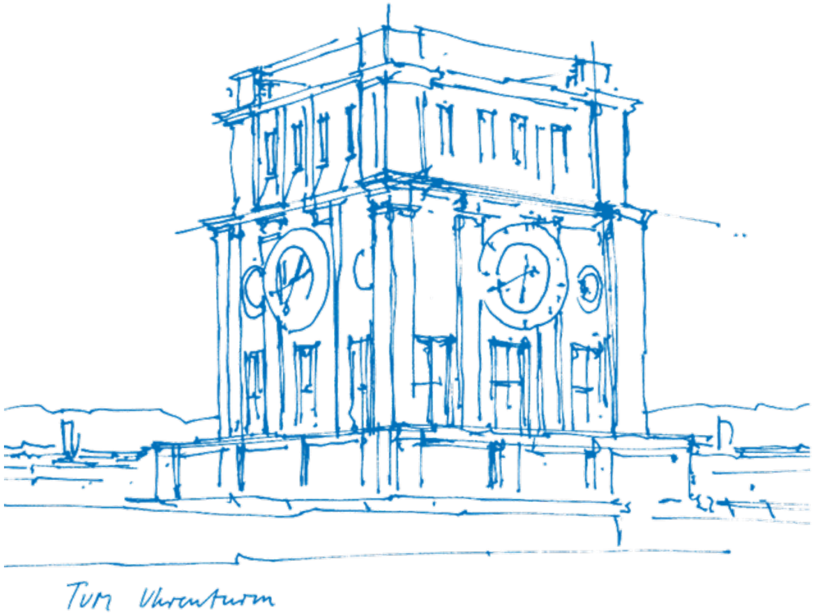
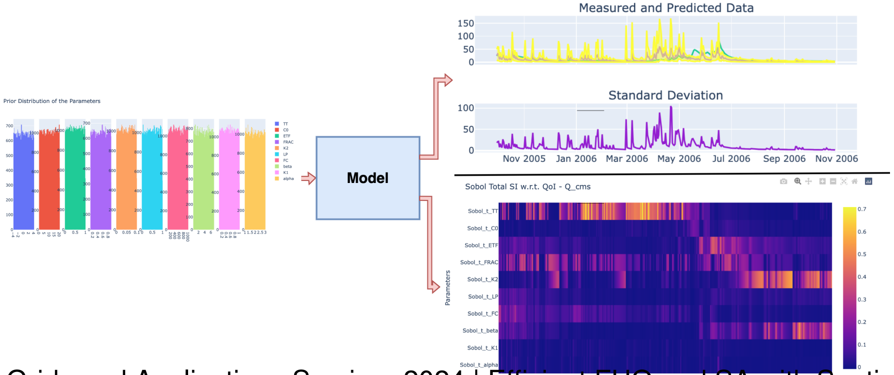


Motivation

- **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 UQ and SA of complex dynamical models (e.g., HBV-SASK hydrologic model [1]) by utilizing (adaptive) Sparse Grids
- **Impediments:**
  - High-dimensionality
  - High (model) execution time
  - Model as a black box
  - Possible discontinuities in the parameter space; anisotropic or decoupled parameters
  - Output of the model - time signal



UQ:

$$\mathbb{E}[\mathcal{O}(f)] := \int_{\Gamma} \mathcal{O}(f)(t, \boldsymbol{\theta})\rho(\boldsymbol{\theta})d\boldsymbol{\theta}$$

$$Var[\mathcal{O}(f)] := \mathbb{E}[\mathcal{O}(f)^2] - (\mathbb{E}[\mathcal{O}(f)])^2$$

Variance-based SA [Sobol 2001]:

$$S_j := \frac{Var[f] - \mathbb{E}_{\theta_j}[Var_{\boldsymbol{\theta}_{\sim j}}[f|\theta_j]]}{Var[f]}$$

Building Blocks

- **Sparse Grid (SG)**
  - Standard SG and Combination Technique
  - Spatially Adaptive SG
  - SparseSpACE Framework
- **Non-intrusive UQ and SA**
- **UQ with SG**
  - Different variant
  - Initial results
- **UQ with SG for Time-dependent models**
  - Initial results
  - Future works

Sparse Grid

Main problem: With high-dimensional problems the number of grid points in a regular grid increases exponentially

Sparse Grids Idea [4]: Selecting points that contribute most to the solution given certain smoothness criteria
[⇒] Reduction of point numbers from $\mathcal{O}(N^d)$ to $\mathcal{O}(Nlog(N)^{d-1})$

Sparse Grids can be constructed in various ways:

- hierarchization, combination technique, adaptivity...
- different basis functions (e.g., linear hat, Lagrange poly, b-splines etc.)
- or the point positions/ grid types (e.g., equidistant grids, Clenshaw-Curtis, Leja)

Sparse Grid & Combination Technique

Combination Technique (CT) [5]:

Efficient SG computation by linearly combining computations on cheap/coarser anisotropic full grids (e.g., component grids)

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

$$u_{\mathscr{I}}^{CT} = \sum_{\boldsymbol{l}\in\mathscr{I}} c_{\boldsymbol{l}} u_{\boldsymbol{l}}^d = \sum_{\boldsymbol{l}\in\mathscr{I}} \sum_{\boldsymbol{l}\leq\boldsymbol{i}\leq\boldsymbol{l}+1, \boldsymbol{i}\in\mathscr{I}} (-1)^{\|\boldsymbol{i}-\boldsymbol{l}\|_1} u_{\boldsymbol{l}}^d, \quad \mathscr{I} = \{\boldsymbol{l}\in\mathbb{N}^d \mid \|\boldsymbol{l}\|_1 = l+d-1\} \tag{1}$$

$c_{\boldsymbol{l}}$ scalar coefficients streaming from the combinatorics of the difference formulation

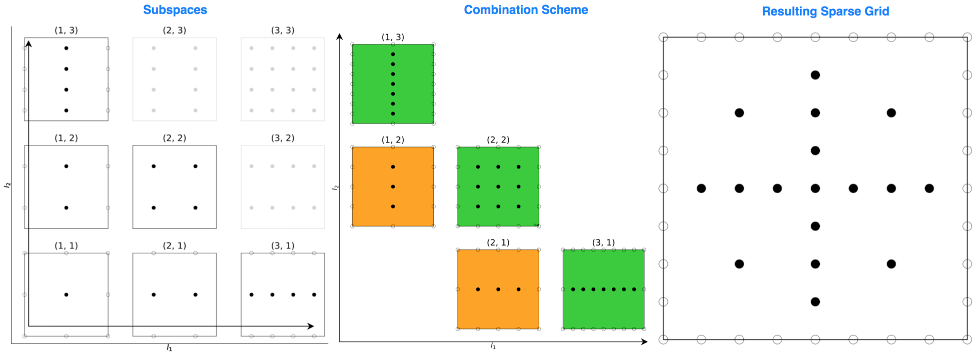


Abbildung: Combination technique represented via subspaces, grid components and the final resulting sparse grid; green component grids are added and orange ones are subtracted

Spatially Adaptive Sparse Grid

General assumptions of standard SG - similar contribution of all dimensions to the result and an overall smoothness throughout the domain

- **Dimension Adaptivity** [6, 7] - different dimensions or interactions between them contribute in different magnitudes to the solution; adjusting the index set in CT
- **Spatial Adaptivity** - often different resolutions are required at different parts of the domain; do not add full subspaces but only specific points to the SG
  - **Drawback:** Standard CT offers no spatial adaptivity
  - **CT with Spatial Adaptivity** - use rectilinear grids constructed via a tensor product of refined 1-D grids [2]

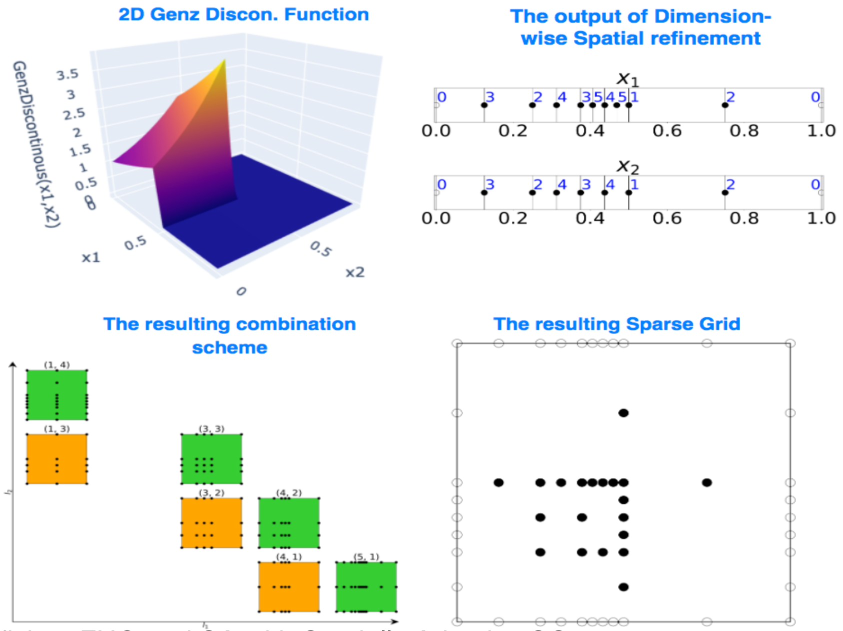
Spatially Adaptive Sparse Grid

Combination Technique with Dimension-Wise Refinement [2]

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

Key components:

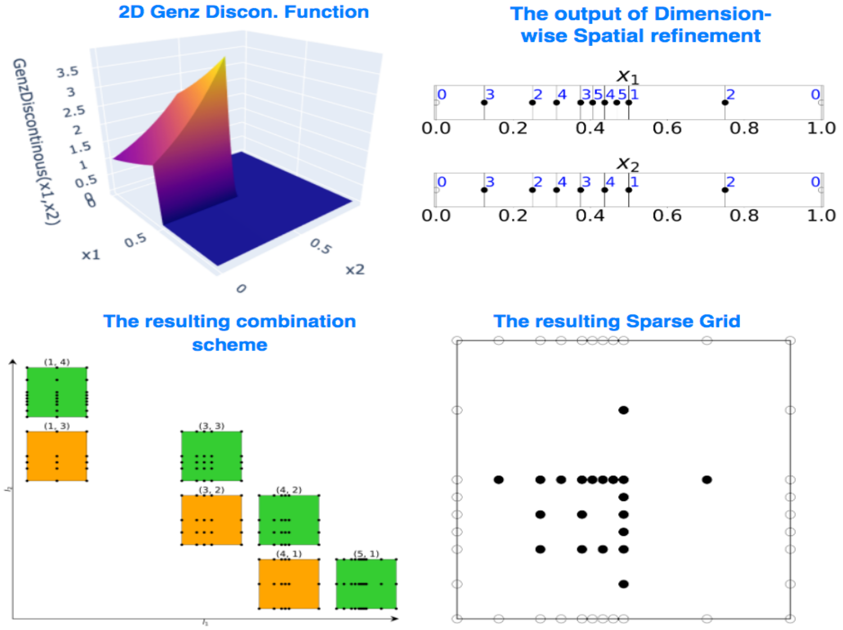
- 1D refinements define the adaptive process
- Creating a global valid combination scheme from 1D refinements
- Special error estimators guide the refinement
- Data structure and tree rebalancing for better performance
- SparseSpACE Framework
  https://github.com/obersteiner/sparseSpACE



Spatially Adaptive SG CT & SparseSpACE Framework

Key components:

- Step 1: 1D refinements define the adaptive process
  - look at every child in a grid and refine based on error approximation
  - error estimator
    - compute for each leaf node $p \in \boldsymbol{P}^k$, for each dim. $k \in [d]$ over all grids
    - for grid $\boldsymbol{l}$ error estimate $\varepsilon_p^{k,\boldsymbol{l}}$ is 1D surplus value weighted by the volume of the respective basis function
    - $\varepsilon_p^k = \sum_{\boldsymbol{l} \in I} |c_{\boldsymbol{l}} \cdot \varepsilon_p^{k,\boldsymbol{l}}|$
    - refine every point p with error estimate $|\varepsilon_p^k| \geq \gamma \cdot \varepsilon^{\max}$ (e.g., $\gamma = 0.5$)
    - global error - $\varepsilon = \sum_{k=1}^{d} \sum_{j=1}^{|\boldsymbol{P}^k|} |\varepsilon_j^k|$
  - output [$\Rightarrow$] vector $\boldsymbol{P}^k$ of points and respective point levels $\boldsymbol{L}^k$ for each dimension $k \in [d]$



Spatially Adaptive SG CT & SparseSpACE Framework

Key components:

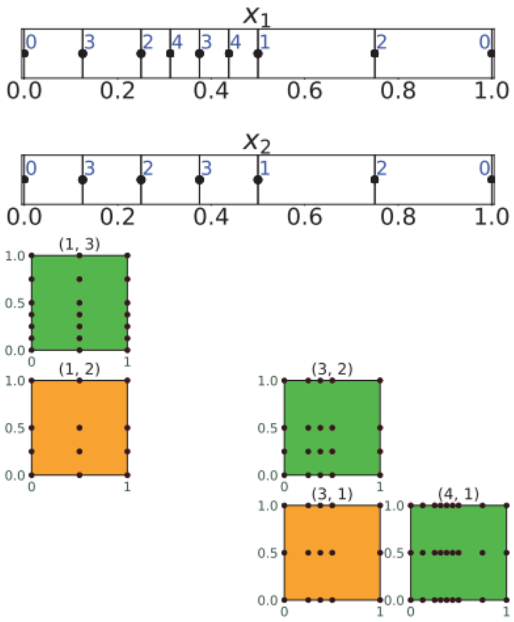
- Step 1: 1D refinements define the adaptive process
- Step 2: Creating a global valid combination scheme from 1D refinements
  - Step 2.1: create the index set based on the maximum levels $\boldsymbol{l}^{max}$ per dimension; where $l_k^{max} = max(\boldsymbol{L}^k)$

$$I = \{\boldsymbol{l} \in \mathbb{N}^d \mid \|\boldsymbol{l}\|_1 \leq max(\boldsymbol{l}^{max}) + d - 1, l_i \leq l_i^{max} \\ \vee (l_i = l_i^{max}, l_k = 1, k \in [d]/i)\} \qquad (2)$$

  - Step 2.2: define set of points $\boldsymbol{P}^{k,\boldsymbol{l}} \subseteq \boldsymbol{P}^k$ for each level vector $\boldsymbol{l}$ (i.e., $\boldsymbol{P}^k, \boldsymbol{L}^k \Rightarrow \boldsymbol{P}^{k,\boldsymbol{l}}, \boldsymbol{L}^{k,\boldsymbol{l}}$)
  - Ensure validity of combination scheme

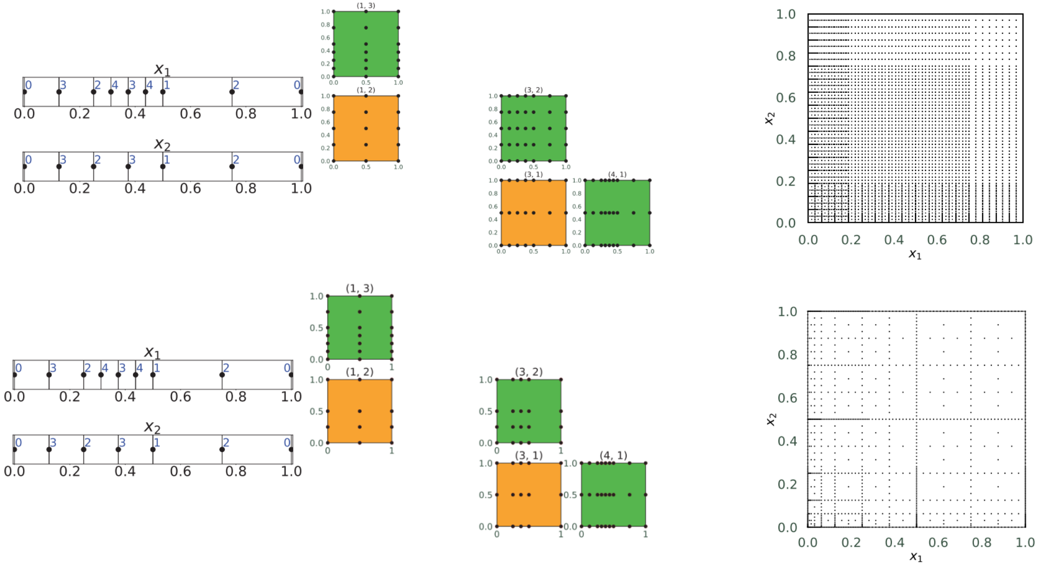
$$\boldsymbol{P}^{k,\boldsymbol{i}} \subseteq \boldsymbol{P}^{k,\boldsymbol{j}} \quad \text{for} \quad \boldsymbol{i}, \boldsymbol{j} \in I, k \in [d], \boldsymbol{j} \geq \boldsymbol{i} \qquad (3)$$

$$\boldsymbol{P}^{k,\boldsymbol{i}} = \boldsymbol{P}^{k,\boldsymbol{j}} \quad \text{for} \quad \boldsymbol{i}, \boldsymbol{j} \in I, k \in [d], i_k = j_k \qquad (4)$$



SparseSpACE Framework - creating component grids

Comparison of two strategies for creating component grids in SparseSpACE



Spatially Adaptive SG CT & SparseSpACE Framework

Complete algorithm:

- iterate over all component grids and calculate the 1D grid points for level vector $\boldsymbol{l} \in I$ (i.e., $\boldsymbol{P}^k, \boldsymbol{L}^k \Rightarrow \boldsymbol{P}^{k,\boldsymbol{l}}, \boldsymbol{L}^{k,\boldsymbol{l}}$)
- build via tensor construction the d-dimensional rectilinear grids
- **compute approximation** (e.g., interpolation or quadrature integration)
- compute error estimates for all leaf points
- refine every point $\varepsilon_p^{k,\boldsymbol{l}}$ with error estimate $|\varepsilon_p^k| \geq \gamma \cdot \varepsilon^{\max}$ (e.g., $\gamma = 0.5$)
- perform tree rebalancing for each dimension (update $\boldsymbol{P}^k, \boldsymbol{L}^k$)
- continue until tol. reached or max. num. of model evaluations

- **Example of the final approximation**

  (e.g., integration via quadrature approximation)

$$u_{\mathscr{I}}^{SCT} = \sum_{\boldsymbol{l} \in \mathscr{I}} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i} \in \prod_{k=1}^{d} [|\boldsymbol{P}^{k,\boldsymbol{l}}|]} \left(f(\theta^{\boldsymbol{i}}) \int_{\theta \in \Omega} \Psi_{\boldsymbol{i}}(\theta) d\theta \right) \quad (5)$$

  (e.g., interpolation)

$$u_I^{sct} = \sum_{\boldsymbol{l} \in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i} \in \prod_{k=1}^{d} [|\boldsymbol{P}^{k,\boldsymbol{l}}|]} \left(f(\theta^{\boldsymbol{i}}) \Psi_{\boldsymbol{i}}(\theta) \right) \quad (6)$$

- $\Psi_{\boldsymbol{i}}(\theta)$ are corresponding basis function assigned to point $\theta^{\boldsymbol{i}}$ with $\theta_k^{\boldsymbol{i}} = P_{i_k}^{k,\boldsymbol{l}}$

Non-intrusive Uncertainty Quantification

General Polynomial Chaos Expansion (gPCE) [8] of $f(t,\theta) : \mathbb{T} \times \Gamma \to \mathbb{R}$, reads:

$$f(t,\theta) \approx f_N(t,\theta) = \sum_{\boldsymbol{p}} c_{\boldsymbol{p}}(t)\Phi_{\boldsymbol{p}}(\theta) = \sum_{\boldsymbol{p}} < f(t,\theta), \Phi_{\boldsymbol{p}}(\theta) >_{\rho(\theta)} \Phi_{\boldsymbol{p}}(\theta) \tag{7}$$

- stochastic part - $\theta = (\theta_1, \theta_2, \dots, \theta_d)^T; \theta : \Omega \to \Gamma$ and $\rho(\theta) = \prod_{k=1}^{d} \rho_k(\theta_k)$
- $\boldsymbol{p} = (p_1, \dots, p_d)$ 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 projection (PSP) - uses (full tensor) quadrature rule to approximate the coefficients of the gPCE

$$c_{\boldsymbol{p}}(t) = \mathbb{E}[f(t,\theta)\Phi_{\boldsymbol{p}}(\theta)] \approx \hat{c}_{\boldsymbol{p}}(t) = \sum_{\boldsymbol{q}=1}^{\boldsymbol{Q}} f(t,\theta^{\boldsymbol{q}})\Phi_{\boldsymbol{p}}(\theta^{\boldsymbol{q}})\omega^{\boldsymbol{q}} \quad (8)$$

Total number of coefficients: $N = \binom{P+d}{d}$

Total number of model evaluations: $\boldsymbol{Q} = \prod_{k=1}^{d} Q_k$; and it has to hold - $p_k = \text{floor}(DE(Q_k)/2)$ [9]

Non-intrusive Uncertainty Quantification
Post-processing & Sensitivity Analysis

Quantify uncertainty of f (or $\mathscr{O}(f)$) by computing, e.g.

$$E[f] = \int_\Gamma f(t,\theta)\rho(\theta)d\theta; \qquad Var[f] = E[f^2] - (E[f])^2 \tag{9}$$

Variance-based (Sobol) sensitivity analysis

$$S_k^T = \frac{Var(f) - Var(E(f|\theta_{-k}))}{Var(f)} = \frac{E(Var(f|\theta_{-k}))}{Var(f)} \tag{10}$$

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Use gPCE coeff. to approximate expectation and variance:

$$\mathbb{E}[f_N(t,\theta)] = c_0(t) \qquad Var[f_N(t,\theta)] = \sum_{position(\boldsymbol{p})=1}^{N-1} c_{\boldsymbol{p}}^2(t) \tag{11}$$

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

$$S_k^T = \frac{\sum_{\boldsymbol{p}\in A_k} c_{\boldsymbol{p}}^2(t)}{Var[f_N(t,\theta)]}, \quad A_k = \{\boldsymbol{p} \in \mathscr{P}_P \wedge \boldsymbol{p}_k \neq 0\} \tag{12}$$

UQ & Sparse Grids I

Multiple ways how to combine the gPCE (i.e., PSP) and SG.
So far SparseSpACE framework & UQ - adaptive SG integration quadrature rule used for computing integrals in $E[\mathscr{O}(f)]$ and $Var[\mathscr{O}(f)]$

Var 1: Sparse Quadrature (i.e., Sparse PSP)

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

UQ & Sparse Grids II

Multiple ways how to combine the gPCE (i.e., PSP) and SG

Var 1: Sparse Quadrature (i.e., Sparse PSP)

$$
\begin{aligned}
\hat{c}_{n,I}(t) &= \sum_{\boldsymbol{l} \in I} c_{\boldsymbol{l}} \cdot S^{\boldsymbol{k}}_{\boldsymbol{l},n} \\
&= \sum_{\boldsymbol{l} \in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i} \in \prod_{k=1}^{d} [|\boldsymbol{P}^{k,\boldsymbol{l}}|]} \left(f(t, F^{-1}(\theta^{\boldsymbol{i}})) \Phi_n(F^{-1}(\theta^{\boldsymbol{i}})) \int_{\theta \in [0,1]^{\boldsymbol{d}}} \Psi_{\boldsymbol{i}}(\theta) d\theta \right) \\
&= \sum_{\boldsymbol{l} \in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i} \in \prod_{k=1}^{d} [|\boldsymbol{P}^{k,\boldsymbol{l}}|]} \left(f(t, F^{-1}(\theta^{\boldsymbol{i}})) \Phi_n(F^{-1}(\theta^{\boldsymbol{i}})) \omega^{\boldsymbol{i}} \right)
\end{aligned}
\tag{13}
$$

Problem with spatially adaptive approach - single adaptive SG integration rule needed for all the integrals $\hat{c}_{n,I}$

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

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; $F^{-1} : [0,1]^{\boldsymbol{d}} \to \Gamma$ is an isoprobabilistic transformation of the variables in the probability space.

UQ & Sparse Grids III

Multiple ways how to combine the gPCE (i.e., PSP) and SG

Var 1: Sparse Quadrature (i.e., Sparse PSP)

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

$$
\begin{aligned}
\hat{c}_{n,I}(t) &= \int_{\theta\in\Gamma} f_{\mathrm{SGI}}(t,\theta)\Phi_n(\theta)\rho(\theta)d\theta \\
&= \int_{\theta\in[0,1]^{\boldsymbol{d}}} \underbrace{\left(\sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i}\in\prod_{k=1}^{d}[|\boldsymbol{P}^{k,\boldsymbol{l}}|]} f(t,F^{-1}(\theta^{\boldsymbol{i}}))\Psi_{\boldsymbol{i}}(\theta)\right)}_{f_{\mathrm{SGI}}} \Phi_n(F^{-1}(\theta))d\theta \\
&= \sum_{\boldsymbol{l}\in I} c_{\boldsymbol{l}} \cdot \sum_{\boldsymbol{i}\in\prod_{k=1}^{d}[|\boldsymbol{P}^{k,\boldsymbol{l}}|]} f(t,F^{-1}(\theta^{\boldsymbol{i}})) \int_{\theta\in[0,1]^{\boldsymbol{d}}} \Psi_{\boldsymbol{i}}(\theta)\Phi_n(F^{-1}(\theta))d\theta
\end{aligned}
\tag{14}
$$

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UQ & Sparse Grids - Initial Results

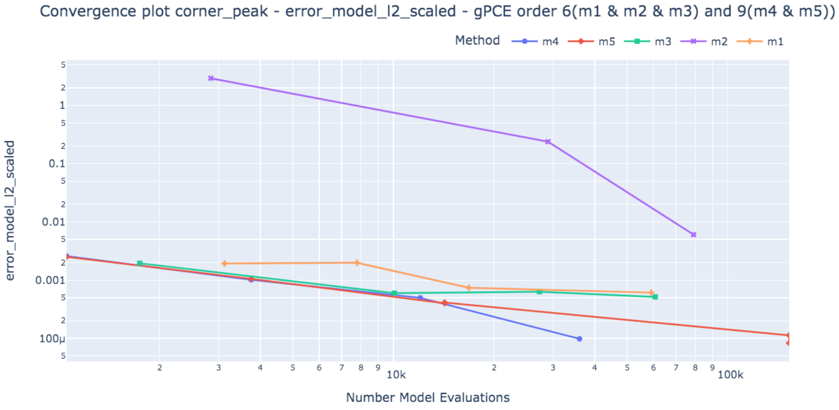
Variant	Method	Interpolation method (SGI)	quadrature method	gPCE
Var 1	m1	no	Full Gauss-Legendre	yes
	m2	no	(Sparse) Clenshaw-Curtis	yes
	m3	no	(Sparse) delayed Kronrod-Patterson[3]	yes
Var 2	m4	(piecewise linear) standard CT	Gauss-Legendre (high order) or analytical computation	yes
	m5	(piecewise linear) spatially adaptive CT	Gauss-Legendre (high order) or analytical computation	yes

Step 1: Benchmark Convergence of different methods

- **Surrogate construction:** SG-(gPCE) of **Genz function (5D)** and **Ishigami function (3D)**

$$f_{\text{corner}}(x) = \left(1 + \sum_{i=1}^{d} i \cdot x_i\right)^{-d-1} ; f_{\text{ishi}}(x) = sin(x_1) + a \cdot sin^2(x_2) + b \cdot x_3^4 \cdot sin(x_1)$$

- Practicalities:
  - linear basis functions
  - experiment with or without boundary points
  - using trapezoidal grid for sparse interpolation (m_4 & m_5)
  - refine up to 10% points with the largest surplus
- Convergence results as expected
- For simple cases, building an intermediate SG surrogate is not beneficial time-wise



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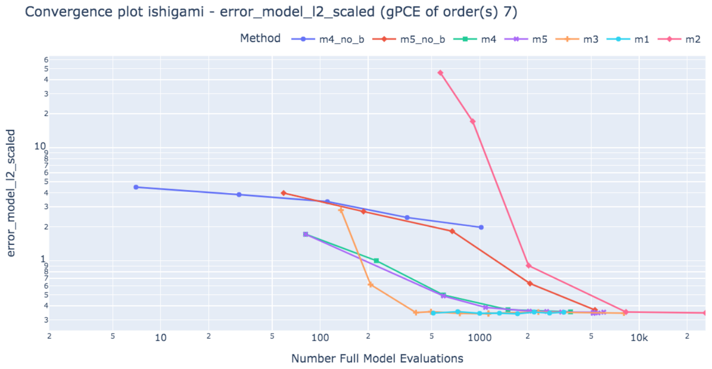
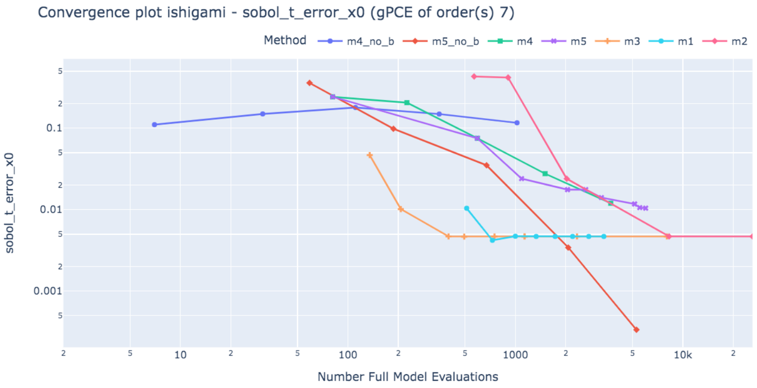
Step 1: Benchmark Convergence of different methods

- **UQ & SA: Ishigami fun. (3D)** - analytical values for S.I. available

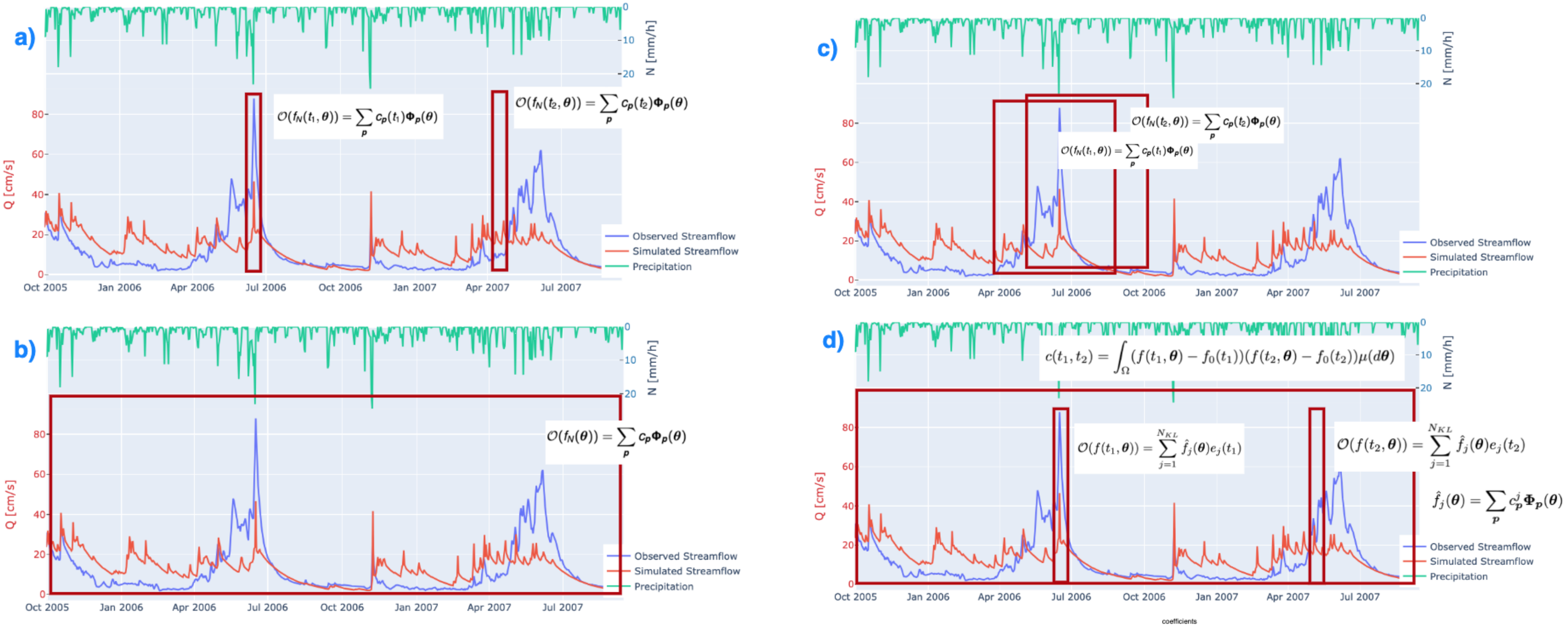




Time Dependent Analysis

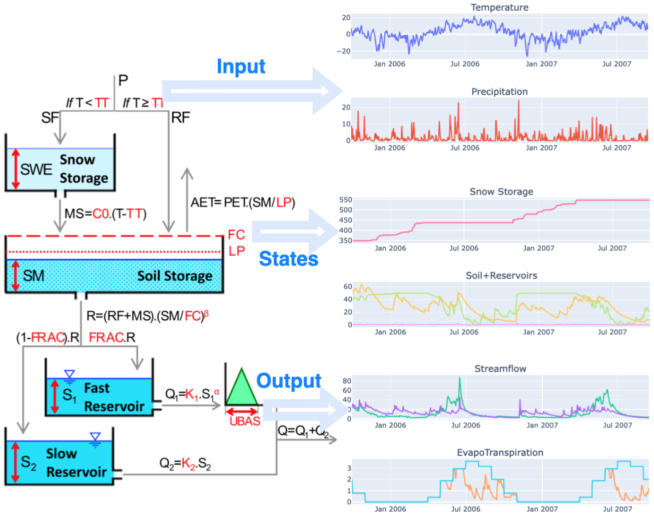
Different strategies: • a) Time-varying analysis; • b) Time-aggregated analysis; • c) Sliding-window analysis

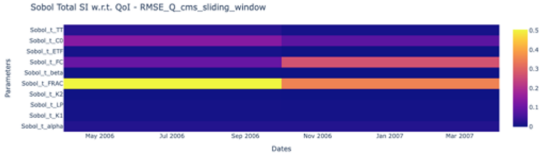
• d) Karhunen–Loéve (KL) expansion based intermediate surrogate

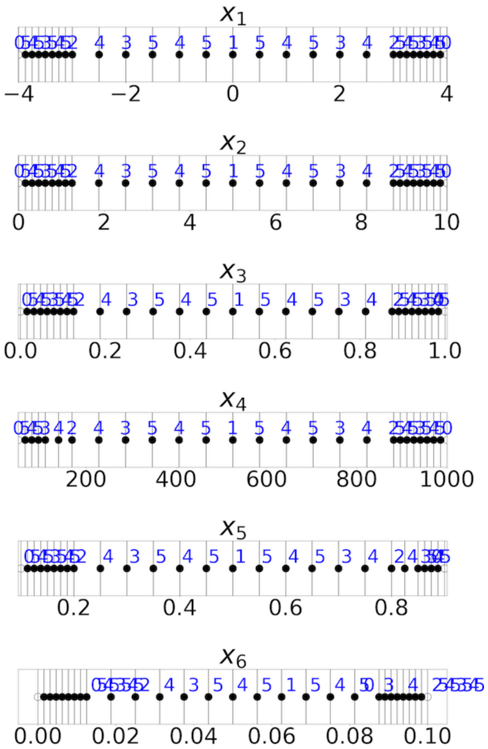


Time Aggregated UQ & SA with Adaptive SG

- **First Results - Time-aggregated:** Building a single (adpative) SG interpolation approximation of the data-misfit function (e.g., RMSE) for a certain time period;
- using it to learn gPCE surrogate of data-misfit function and derive Sobol S.I.
- convenient for identifying annual variability
- possible to use it as a surrogate model for efficient calibration instead of a full model







Future Work

- **SpareSpACE**
  - Introduce Parallelization in SpareSpACE (i.e., in parallel execution of a model for all the points in a single component grid)
  - Experiment with different grids/points (e.g., Leja) and basis functions (e.g., b-splines for interpolation)
- **Time-varying UQ & Sparse Grids**
  - Continue developing the KL intermediate surrogate and apply adaptive SG as needed

Thank You!

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SparseSpACE Framework - creating component grids

Strategies for creating component grids out of 1D refinements:

- **Strategy 1** Add all points $p_j \in \boldsymbol{P}^k$ to $\boldsymbol{P}^{k,\boldsymbol{l}}$ for which $L_j^k \leq l_k$ for a component grid with level $\boldsymbol{l}$.

$$\boldsymbol{P}^{k,\boldsymbol{l}} = \{P_j^k \in \boldsymbol{P}^k \mid L_j^k \leq l_k\} \tag{15}$$

- **Strategy 2** Introduce the value c_j^k that should delay the level increase for dimension k.

$$\boldsymbol{P}^{k,\boldsymbol{l}} = \{P_j^k \in \boldsymbol{P}^k \mid L_j^k \leq l_k - c_j^k\}; \quad c_j^k = l_k^{\max} - D_j^k \tag{16}$$

  where D_j^k is the maximum of the levels of the hierarchical descendants of point P_j^k in the hierarchical tree.

- **Strategy 3** Control $0 \geq \hat{c}_j^k \leq c_j^k$; i.e., guarantees that leaves of $\boldsymbol{P}^k$ are added if we are at the level vector with the maximum level in dimension k