Global Sensitivity Analysis (GSA)

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SENSITIVITY ANALYSIS

Sensitivity Analysis provides a means to quantify the relative importance of inputs to the variability in a system response or a model output.

$$\mathcal{Q} = f(\theta_1, \ldots, \theta_p)$$

- θ_i's are uncertain
- p can be large
- Higher the sensitivity index, more important is the input

Applications: Model verification, dimension reduction, model reliability, optimal experimental design

H_2/O_2 Reaction Kinetics

- Clean energy source for transportation, fuel cells
- Reaction Rate:

$$k_i(T) = A_i T^{n_i} \exp(-E_{a,i}/RT)$$

A_i: Pre-exponent $E_{a,i}$: Activation Energy

- Initial conditions: P_0, T_0, ϕ_0
- **Research Interests**: Uncertainty propagation, reduction, design
- GSA plays a critical role!

Reaction #	Reactants		Products
$\mathcal{R}_1$	$H + O_2$	$\rightleftharpoons$	$O + OH$
$\mathcal{R}_2$	$O + H_2$	$\rightleftharpoons$	$H + OH$
$\mathcal{R}_3$	$H_2 + OH$	$\rightleftharpoons$	$H_2O + H$
$\mathcal{R}_4$	$OH + OH$	$\rightleftharpoons$	$O + H_2O$
$\mathcal{R}_5$	$H_2 + M$	$\rightleftharpoons$	$H + H + M$
$\mathcal{R}_6$	$O + O + M$	$\rightleftharpoons$	$O_2 + M$
$\mathcal{R}_7$	$O + H + M$	$\rightleftharpoons$	$OH + M$
$\mathcal{R}_8$	$H + OH + M$	$\rightleftharpoons$	$H_2O + M$
$\mathcal{R}_9$	$H + O_2 + M$	$\rightleftharpoons$	$HO_2 + M$
$\mathcal{R}_{10}$	$HO_2 + H$	$\rightleftharpoons$	$H_2 + O_2$
$\mathcal{R}_{11}$	$HO_2 + H$	$\rightleftharpoons$	$OH + OH$
$\mathcal{R}_{12}$	$HO_2 + O$	$\rightleftharpoons$	$O_2 + OH$
$\mathcal{R}_{13}$	$HO_2 + OH$	$\rightleftharpoons$	$H_2O + O_2$
$\mathcal{R}_{14}$	$HO_2 + HO_2$	$\rightleftharpoons$	$H_2O_2 + O_2$
$\mathcal{R}_{15}$	$H_2O_2 + M$	$\rightleftharpoons$	$OH + OH + M$
$\mathcal{R}_{16}$	$H_2O_2 + H$	$\rightleftharpoons$	$H_2O + OH$
$\mathcal{R}_{17}$	$H_2O_2 + H$	$\rightleftharpoons$	$HO_2 + H_2$
$\mathcal{R}_{18}$	$H_2O_2 + O$	$\rightleftharpoons$	$OH + HO_2$
$\mathcal{R}_{19}$	$H_2O_2 + OH$	$\rightleftharpoons$	$HO_2 + H_2O$

[Yetter et al., 1991]

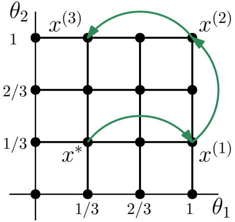
Local vs. Global

Local SA	Global SA
Deterministic Approach	Statistical Approach
Local behavior at a specific point	Considers the entire input domain
Input/Output Correlation, Perturbation method	Morris screening, Sobol' Sensitivity Indices

Estimation of Sensitivity Measures

- **Sampling-based**
  - Morris Screening: Trajectory-based sampling
  - Sobol' indices: Monte Carlo Sampling
- **Surrogate-based**
  - Polynomial Chaos Expansion (PCE)
- **Dimension reduction**: Reduced-space Surrogates
  - Derivative-based global sensitivity measures (DGSMs)
  - Active subspaces $\rightarrow$ Activity scores

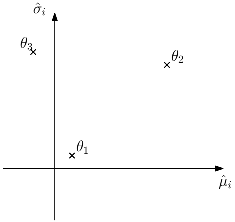
Morris Screening



- Trajectory-based sampling approach is adopted
- Elementary effect of θ_i at $\boldsymbol{x}^{(j)}$:

$$d_{\theta_i}(\boldsymbol{x}^{(j)}) = \frac{\mathcal{M}(x_1^{(j)},\ldots,x_i^{(j)}+\Delta,\ldots,x_m^{(j)})-\mathcal{M}(\boldsymbol{x}^{(j)})}{\Delta}$$

- Mean and variance of the distribution of $d_{\theta_i}(\boldsymbol{x}^{(j)})$ is examined



Analysis of Variance (ANOVA)

- Consider a square integrable function, $f(\boldsymbol{\theta})$; $\boldsymbol{\theta} : (\theta_1, \ldots, \theta_m)$ defined in a unit hypercube: $\Gamma = [0,1]^m$
- Split $\boldsymbol{\theta}$: $\{\theta_i, \boldsymbol{\theta}_{\sim \boldsymbol{i}}\}$ and decompose f as follows:

$$f = f_0 + f_1(\theta_i) + f_2(\boldsymbol{\theta}_{\boldsymbol{i}\sim}) + f_{12}(\theta_i, \boldsymbol{\theta}_{\boldsymbol{i}\sim})$$

  - f_i's are orthogonal, and $\int f_{\boldsymbol{i}} d\theta_{\boldsymbol{i}} = 0$
  - $f_0 = \int f(\boldsymbol{\theta}) d\boldsymbol{\theta}$
  - $f_1 = \int (f - f_0) d\boldsymbol{\theta}_{\sim \boldsymbol{i}}$
  - $f_2 = \int (f - f_0) d\theta_i$
  - f_{12} = remainder

Sobol' Sensitivity Indices

- Consider the variance of f:

$$\begin{aligned}\mathbb{V}(f) &= \int (f - f_0)^2 d\boldsymbol{\theta} = \int f^2 d\boldsymbol{\theta} - f_0^2 \\ &= \underbrace{\int f_1^2 d\boldsymbol{\theta}}_{\mathbb{V}(f_1)} + \underbrace{\int f_2^2 d\boldsymbol{\theta}}_{\mathbb{V}(f_2)} + \underbrace{\int f_{12}^2 d\boldsymbol{\theta}}_{\mathbb{V}(f_{12})}\end{aligned}$$

- **First-order** or **Main-effect** index (S_i):

$$S_i = \frac{\mathbb{V}(f_1)}{\mathbb{V}(f)} = \frac{\overbrace{\mathbb{V}\left(\mathbb{E}\left[f|\theta_i\right]\right)}^{\text{contribution due to } \theta_{\text{i}}}}{\mathbb{V}(f)}$$

- **Total-effect** index (S_{T_i}):

$$S_{T_i} = \frac{\mathbb{V}(f_1) + \mathbb{V}(f_{12})}{\mathbb{V}(f)} = \frac{\mathbb{V}(f) - \mathbb{V}(f_2)}{\mathbb{V}(f)} = 1 - \frac{\mathbb{V}(f_2)}{\mathbb{V}(f)} = 1 - \frac{\overbrace{\mathbb{V}\left(\mathbb{E}\left[f|\boldsymbol{\theta}_{\sim i}\right]\right)}^{\text{contribution due to } \boldsymbol{\theta}_{\sim i}}}{\mathbb{V}(f)}$$

Algorithm: Sobol' Indices

$$S_i = \frac{\mathbb{V}\left(\mathbb{E}[f|\theta_i]\right)}{\mathbb{V}(f)}$$

$$\mathbb{V}\left(\mathbb{E}[f|\theta_i]\right) = \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{A})_k f(\boldsymbol{B}_{\boldsymbol{A}}^{(i)})_k - f_0^2$$

[Sobol, 1990]

$$S_{T_i} = \frac{\mathbb{E}\left(\mathbb{V}[f|\theta_{\sim i}]\right)}{\mathbb{V}(f)} = 1 - \frac{\mathbb{V}\left(\mathbb{E}[f|\theta_{\sim i}]\right)}{\mathbb{V}(f)}$$

$$\mathbb{E}\left[\mathbb{V}(f|\theta_{\sim i}])\right] = \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{A})_k (f(\boldsymbol{A})_k - f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k)$$

[Sobol, 2007]

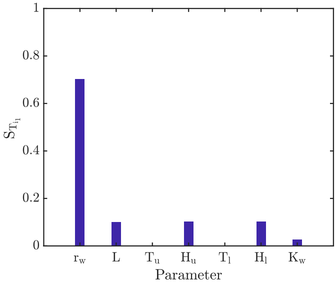
1. Normalize the parameters $\boldsymbol{\theta} \to \boldsymbol{\xi} \in [-1, 1]$
2. Construct matrices, $\boldsymbol{A}$ and $\boldsymbol{B}$ comprising $N \times m$ independent MC samples
3. Construct modified matrices, $\boldsymbol{B}_{\boldsymbol{A}}^{(i)}$ and $\boldsymbol{A}_{\boldsymbol{B}}^{(i)}$
4. Generate vectors: $f(\boldsymbol{A})$, $f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})$ and $f(\boldsymbol{B}_{\boldsymbol{A}}^{(i)})$ using the model response
5. Estimate S_i and S_{T_i}

The Borehole function

$$\mathcal{Q} = \frac{2\pi T_u(H_u - H_l)}{\ln(r/r_w)\left[1 + \dfrac{2LT_u}{\ln(r/r_w)r_w^2K_w} + \dfrac{T_u}{T_l}\right]}$$

$$\boldsymbol{\theta} = \begin{bmatrix} r_w & L & T_u & H_u & T_l & H_l & K_w \end{bmatrix}^T$$

Parameter	Distribution
Borehole radius, r_w (m)	$\mathcal{N}$(0.1,0.016)
Borehole length, L (m)	$\mathcal{U}$[1120,1680]
Transmissivity, T_u (m^2/yr)	$\mathcal{U}$[63070,115600]
Potentiometric head, H_u (m)	$\mathcal{U}$[990,1110]
Transmissivity, T_l (m^2/yr)	$\mathcal{U}$[63.1,116]
Potentiometric head, H_l (m)	$\mathcal{U}$[700,820]
Hydraulic conductivity, K_w (m/yr)	$\mathcal{U}$[9855,12045]



POLYNOMIAL CHAOS EXPANSION

$$\mathcal{Q}(\boldsymbol{\xi}) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

$$c_k = \frac{1}{\langle \Psi_k^2 \rangle} \langle \Psi_k, \mathcal{Q}(\boldsymbol{\xi}) \rangle$$

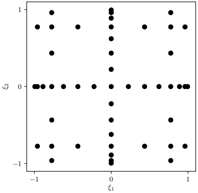
$$c_k = \arg\min \mathbb{E}\left[\left(\boldsymbol{c}^\top \Psi(\boldsymbol{\xi}) - G(\theta)\right)^2\right] + \lambda \|\boldsymbol{c}\|_1$$

Quadrature-based:

- Gauss Quadrature, Sparse grids
- Adaptive Pseudospectral Projection

Regression-based:

- Least angle regression
- Orthogonal Matching Pursuit



PCE-based Sobol' Indices

First-order Index

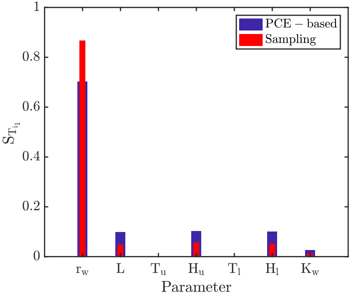
$$S_i = \frac{1}{\mathbb{V}(\mathcal{Q})} \sum_{k \in \mathcal{K}_{\mathcal{S}_i}} c_k^2 \langle \Psi_k^2 \rangle$$

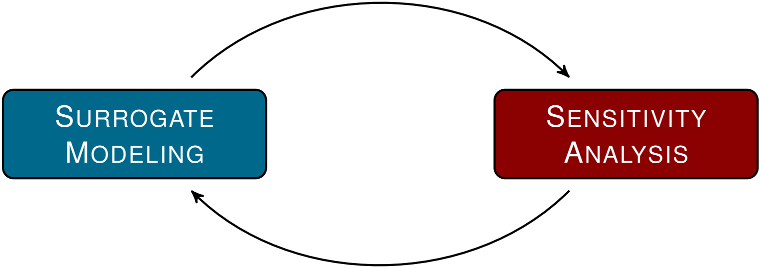
$\mathcal{K}_{\mathcal{S}_i}$: Contribution from only the i^{th} variable

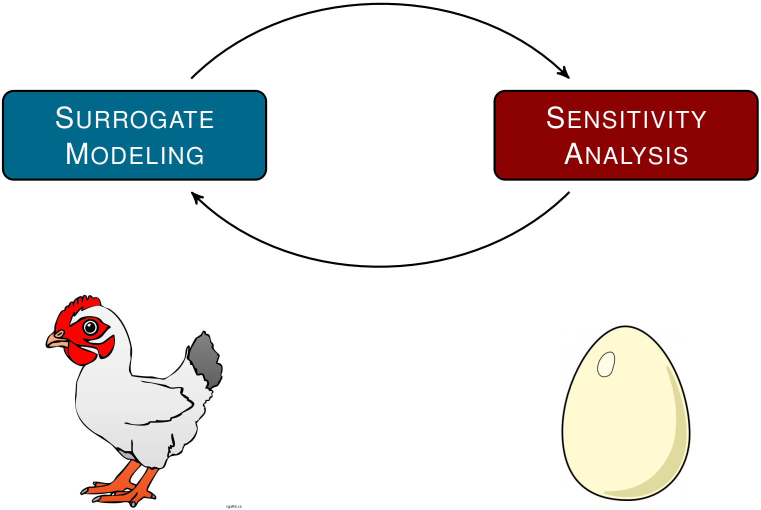
Total-effect Index

$$S_{T_i} = \frac{1}{\mathbb{V}(\mathcal{Q})} \sum_{k \in \mathcal{K}_{\mathcal{T}_i}} c_k^2 \langle \Psi_k^2 \rangle$$

$\mathcal{K}_{\mathcal{T}_i}$: Contribution from the i^{th} variable




Surrogate Modeling
Sensitivity Analysis


Surrogate Modeling
Sensitivity Analysis

Derivative-based Global Sensitivity Measures (DGSMs)

- DGSM for a parameter, θ_i:

$$\mu_i = \mathbb{E}\left[\left(\frac{\partial G(\boldsymbol{\theta})}{\partial \theta_i}\right)^2\right]$$

[Sobol' and Kucherenko, 2009]

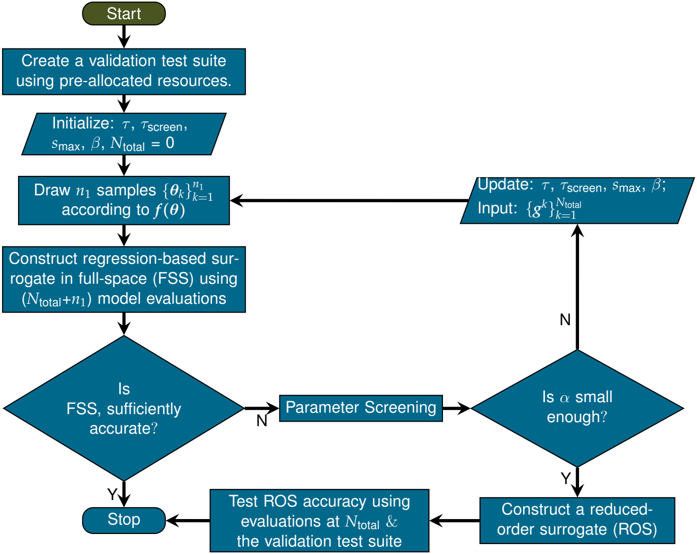
- Upper bound on $S_{T_{i_1}}$:

$$S_{T_i} \leq \frac{\mathcal{C}_i \mu_i}{\mathbb{V}(G)},\ \mathcal{C}_i\text{: Poincaré Constant}$$

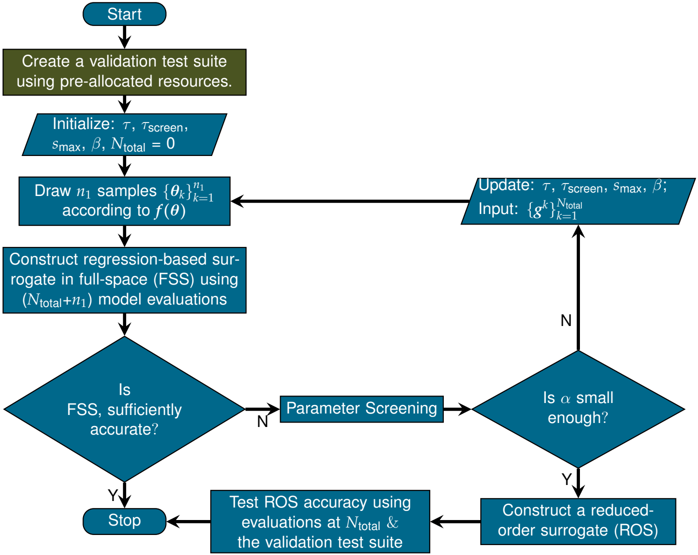
[Lamboni et al., 2013]

- Typically, fewer samples are needed to converge to the upper bound.
- **Limitation**: Need gradient information

Adaptive Surrogate Construction



ADAPTIVE SURROGATE CONSTRUCTION



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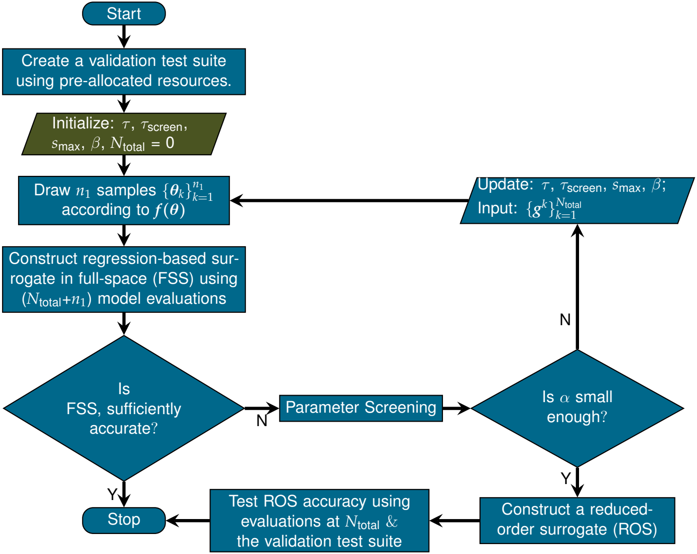

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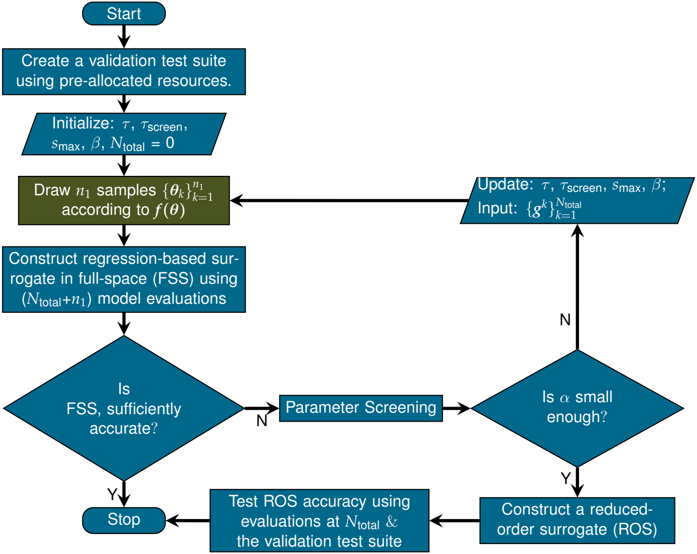

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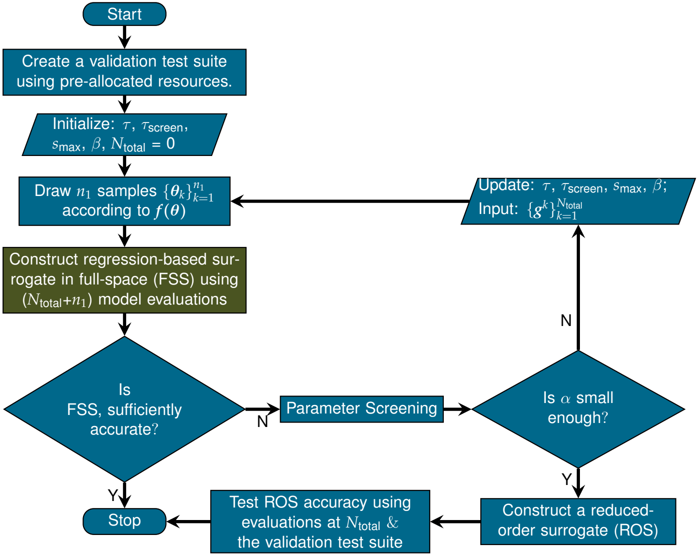

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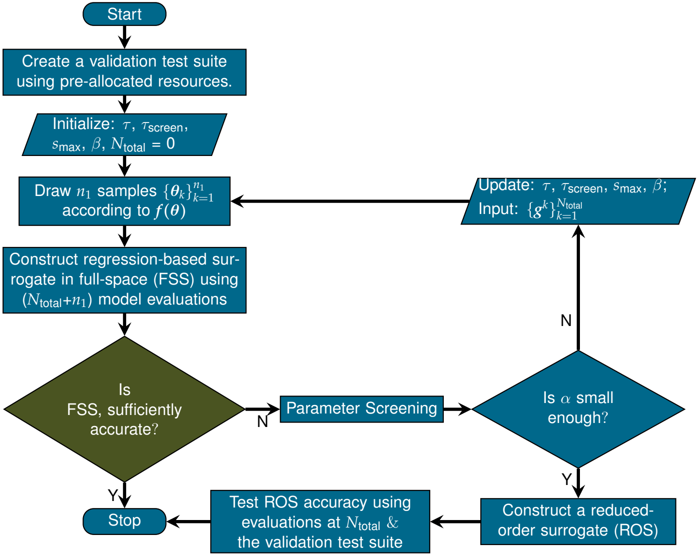

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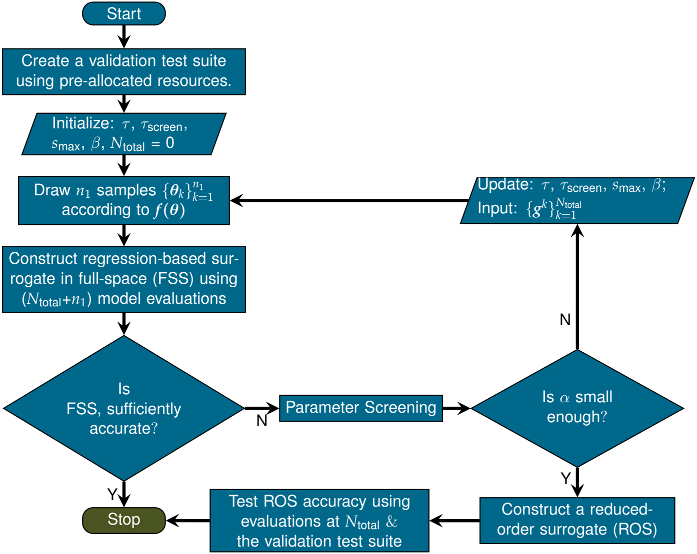

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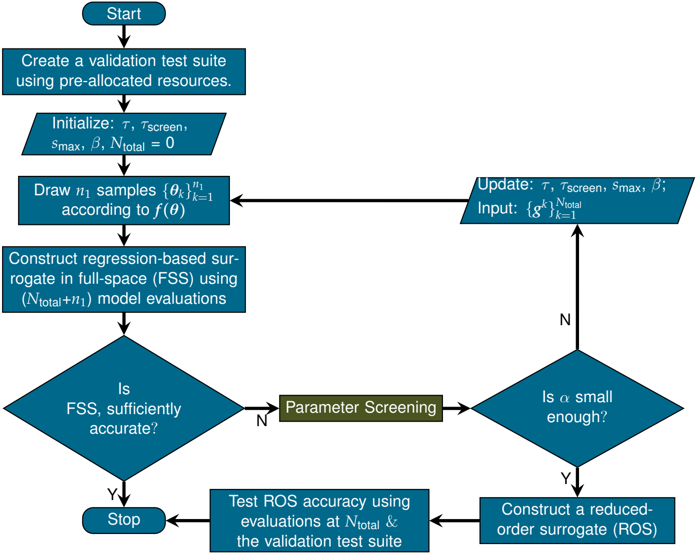

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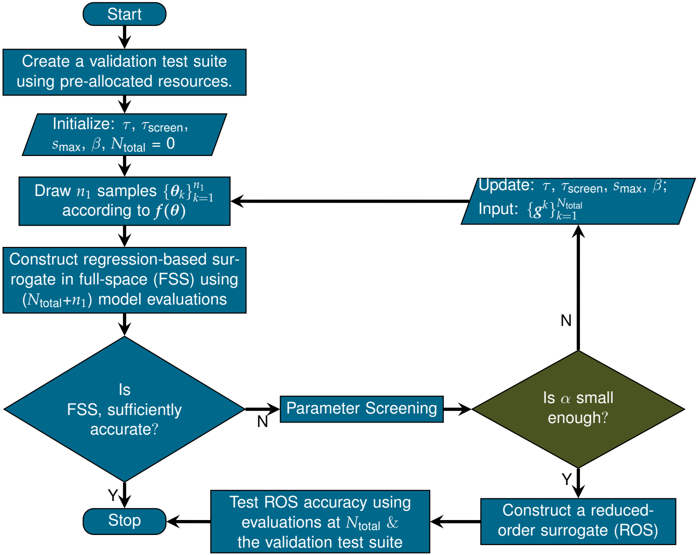

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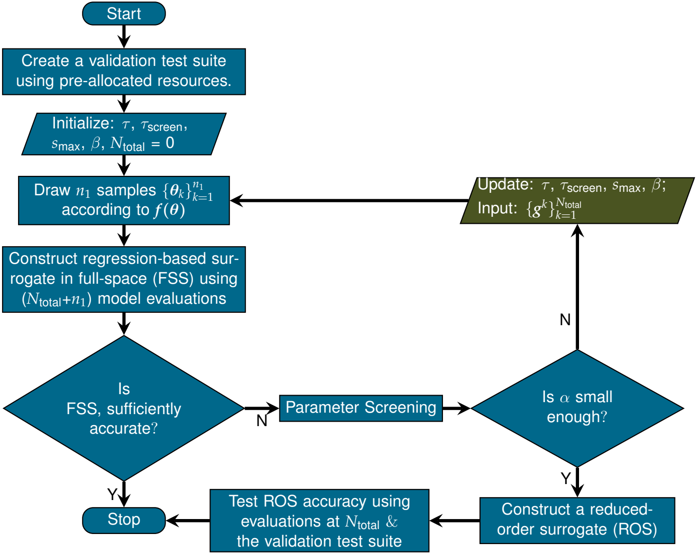

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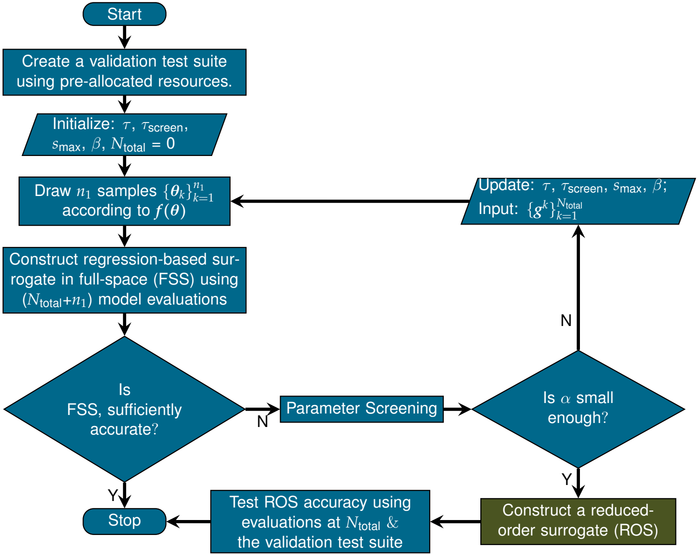

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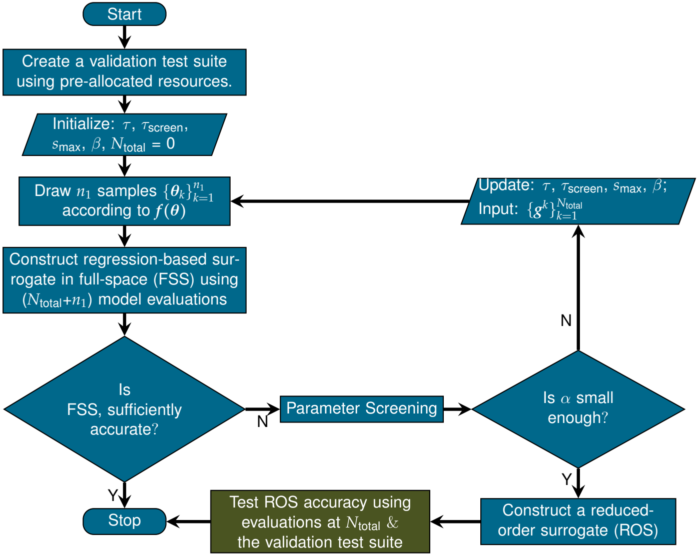

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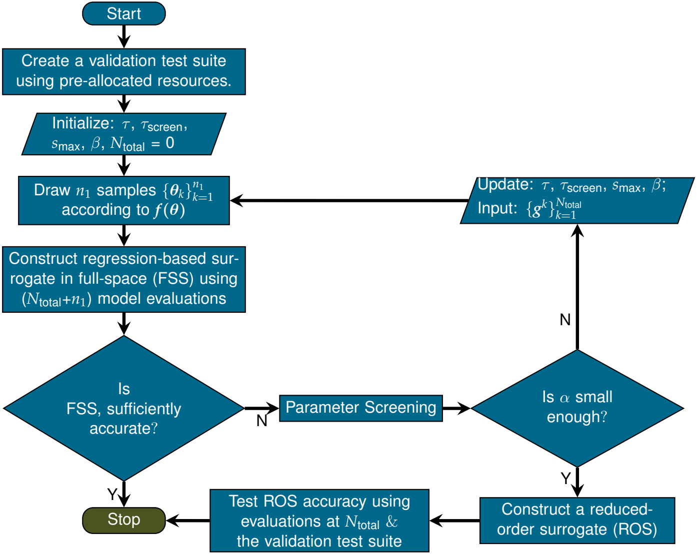
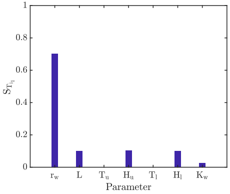
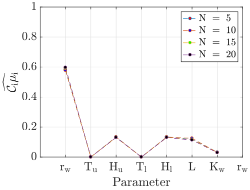


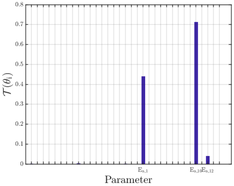
APPLICATIONS

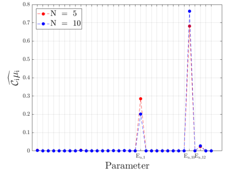
- Borehole function





- Chemical Kinetics: H_2/O_2 Reaction Mechanism





M. Vohra, A. Alexanderian, C.Safta, S. Mahadevan, *Journal of Scientific Computing*, 2019

Activity Scores

- Consider a positive semi-definite matrix, $\boldsymbol{C}$:

$$\boldsymbol{C} = \int_{\Omega} (\nabla_{\boldsymbol{\xi}} G)(\nabla_{\boldsymbol{\xi}} G)^{\top} dP_{\boldsymbol{\xi}}$$

- Eigenvalue decomposition of $\boldsymbol{C}$:

$$\boldsymbol{C} = \boldsymbol{W}\boldsymbol{\Lambda}\boldsymbol{W}^{\top}$$

- Partition the eigenspace:

$$\boldsymbol{W} = [\boldsymbol{W}_1 \ \boldsymbol{W}_2], \quad \boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_1 & \\ & \boldsymbol{\Lambda}_2. \end{bmatrix}$$

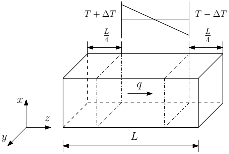
- Activity score for parameter, θ_i:

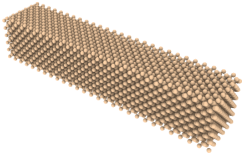
$$\nu_{i,p}(G) = \sum_{j=1}^{p} \lambda_j w_{i,j}^2$$

P. Constantine, P. Diaz, *Reliability Engineering and System Safety*, 2017

APPLICATIONS

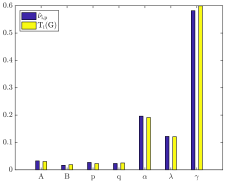
- Thermal transport in Si using Non-equilibrium Molecular Dynamics (NEMD)





SW Potential, $\Phi = \sum_{i,j(i<j)} \phi_2(A, B, p, q, \alpha) + \sum_{i,j,k(i<j<k)} \phi_3(\lambda, \gamma)$

- GSA of the SW parameters



M. Vohra, S. Mahadevan, *International Journal of Heat and Mass Transfer*, 2019

PROBABILITY MODELS: GSA

- Variance decomposition methods assume independence

$$S_{i_c} = \frac{\mathbb{V}_{\boldsymbol{\theta}_c}\left[\mathbb{E}[f|\boldsymbol{\theta}_c]\right]}{\mathbb{V}(f)}$$

$$S_{T_{i_c}} = 1 - \frac{\mathbb{V}_{\boldsymbol{\theta}_r}\left[\mathbb{E}[f|\boldsymbol{\theta}_r]\right]}{\mathbb{V}(f)}$$

$$\boldsymbol{\theta} : (\boldsymbol{\theta}_c, \boldsymbol{\theta}_r)$$

- Conditional expectation, $\mathbb{E}[f|\boldsymbol{\theta}_c]$:

$$\mathbb{E}[f|\boldsymbol{\theta}_c] = \int_{\Omega_f} f\, p(f|\boldsymbol{\theta}_c) df = \int_{\Omega_f} f \frac{p(\boldsymbol{\theta}_c, f)}{p(\boldsymbol{\theta}_c)} df$$

Probability Models: GSA

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PROBABILITY MODELS: GSA

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GAUSSIAN COPULA

$$p(\boldsymbol{\theta}_c, f) = \mathcal{C}\left(p_f \prod_{i=1}^{n(\boldsymbol{\theta}_c)} p_{\theta_i}\right)$$

GAUSSIAN MIXTURE MODEL

$$p(f|\boldsymbol{\theta}_c) = \sum_{i=1}^{n(\boldsymbol{\theta}_c)} \lambda_i(\boldsymbol{\theta}_c)\phi(f, \boldsymbol{\mu}_i, \Sigma_i)$$

Z. Hu, S. Mahadevan, *Reliability Engineering and System Safety*, 2019