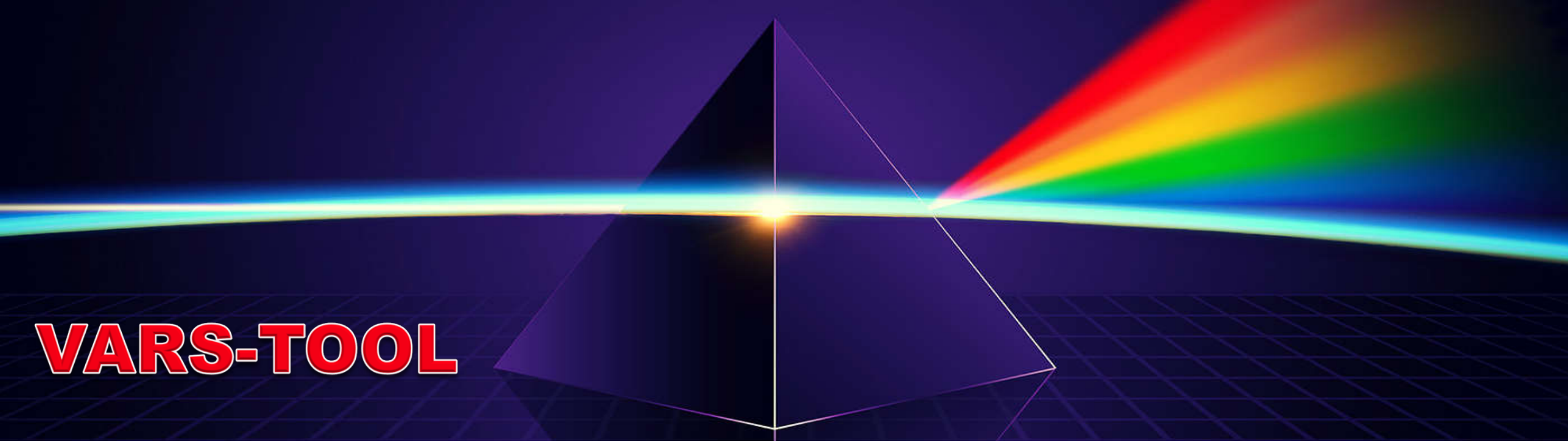

A Toolbox for Comprehensive, Efficient, and Robust Sensitivity and Uncertainty Analysis

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Global Water Futures Annual Science Meeting, June 6, 2018

UNIVERSITY OF SASKATCHEWAN
Global Institute for Water Security
USASK.CA/WATER

GLOBAL WATER FUTURES
SOLUTIONS TO WATER THREATS IN AN ERA OF GLOBAL CHANGE

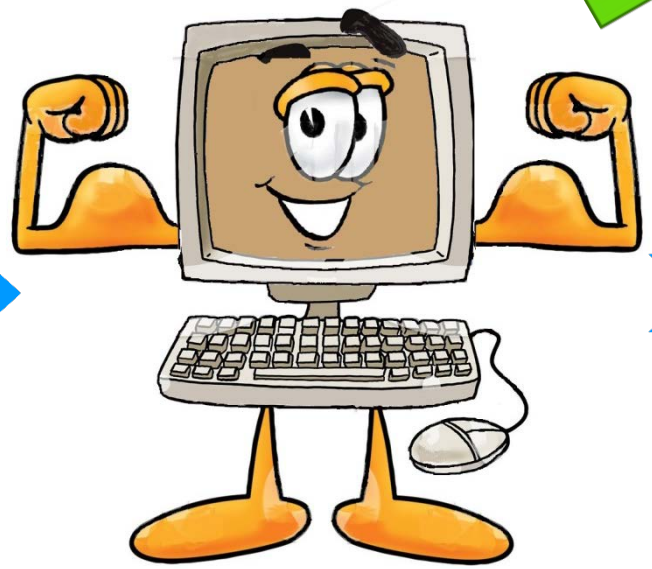
Integrated Modelling Program for Canada
Global Water Futures

Earth and Environmental Systems Models

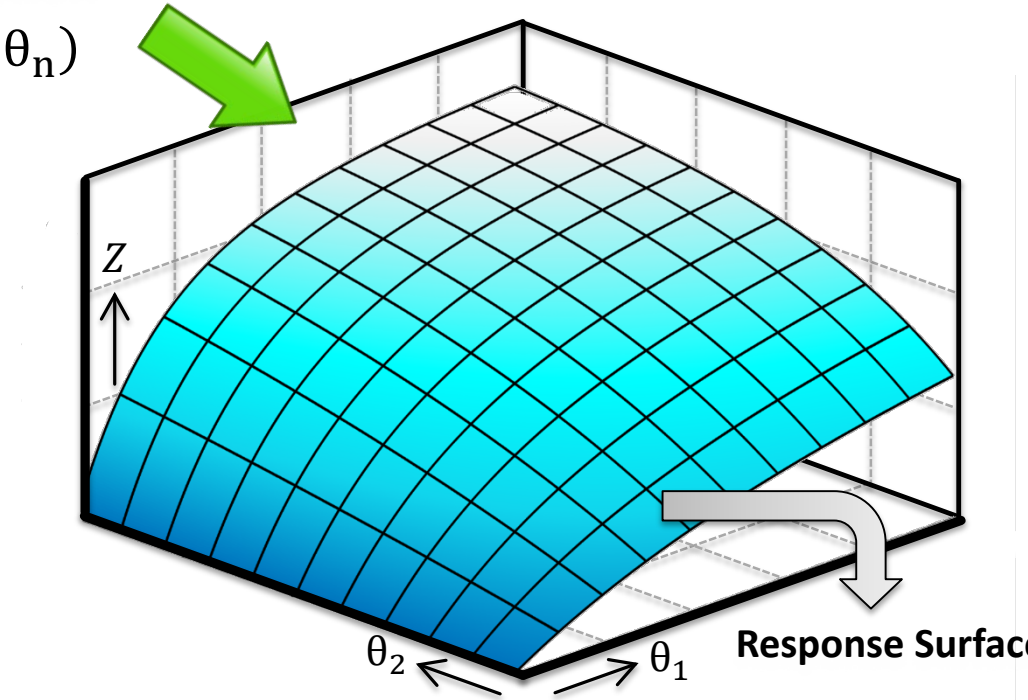
Response Function

$$Z = f(\theta_1, \ldots, \theta_n)$$

Parameters, Forcings, boundary conditions



One or multiple responses or metrics



- Continue to grow in complexity with our ever-growing understanding of underlying system processes, their heterogeneity, and feedback mechanisms.

- This growth in complexity results in Large, computationally intensive models with many “uncertain” parameters and factors whose effects on model behavior need to be characterized and understood.

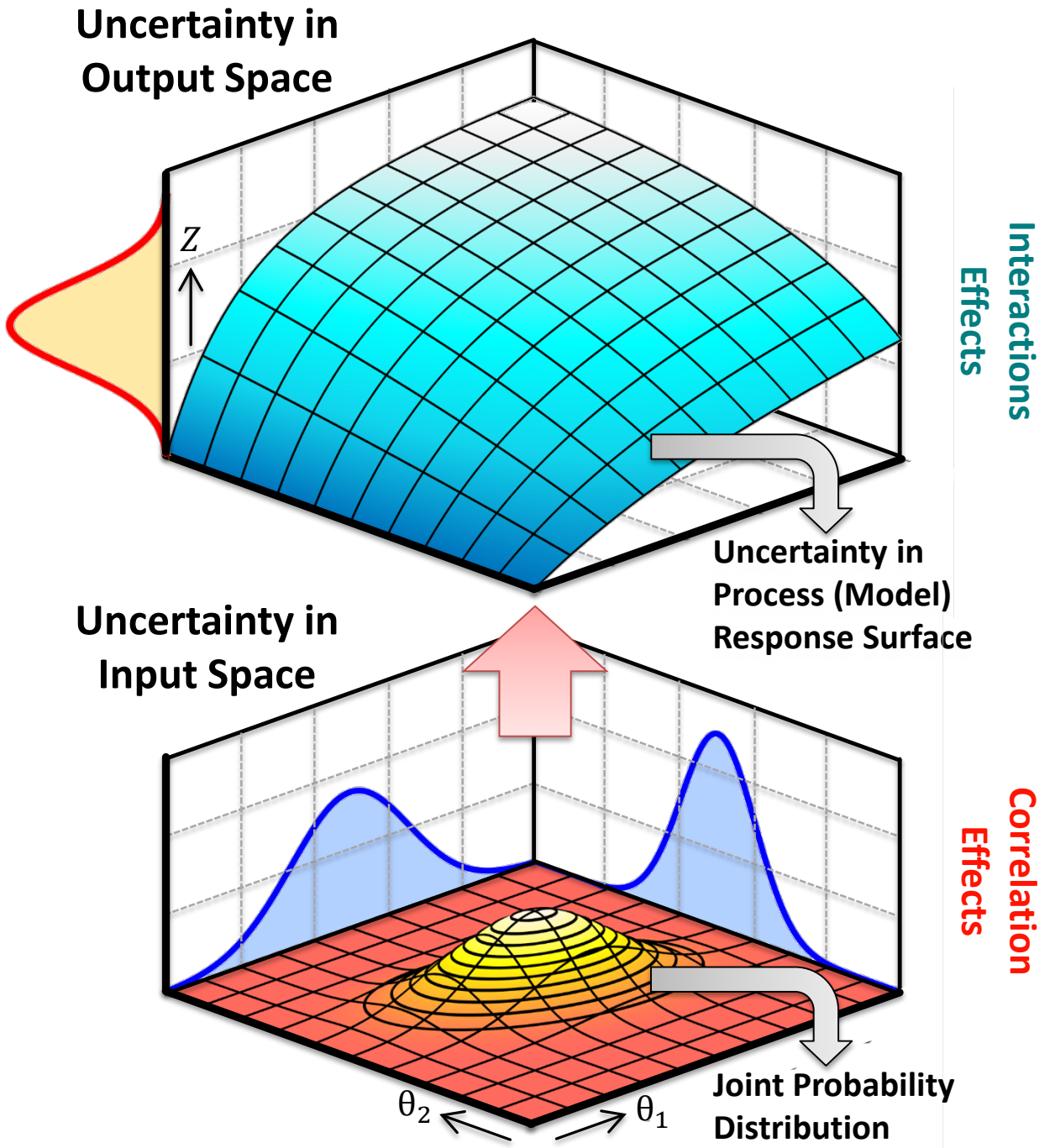
Approaches to Uncertainty Analysis

(1) Forward-Problem Approach

propagates assumptions on uncertainties in inputs and other system properties through the model to obtain some understanding on uncertainties in model predictions.

(2) Inverse-Problem Approach

uses information in the mismatch between model predictions and data to identify “good” values for the model “parameters”, and to characterize their posterior uncertainty.



Approaches to Uncertainty Analysis

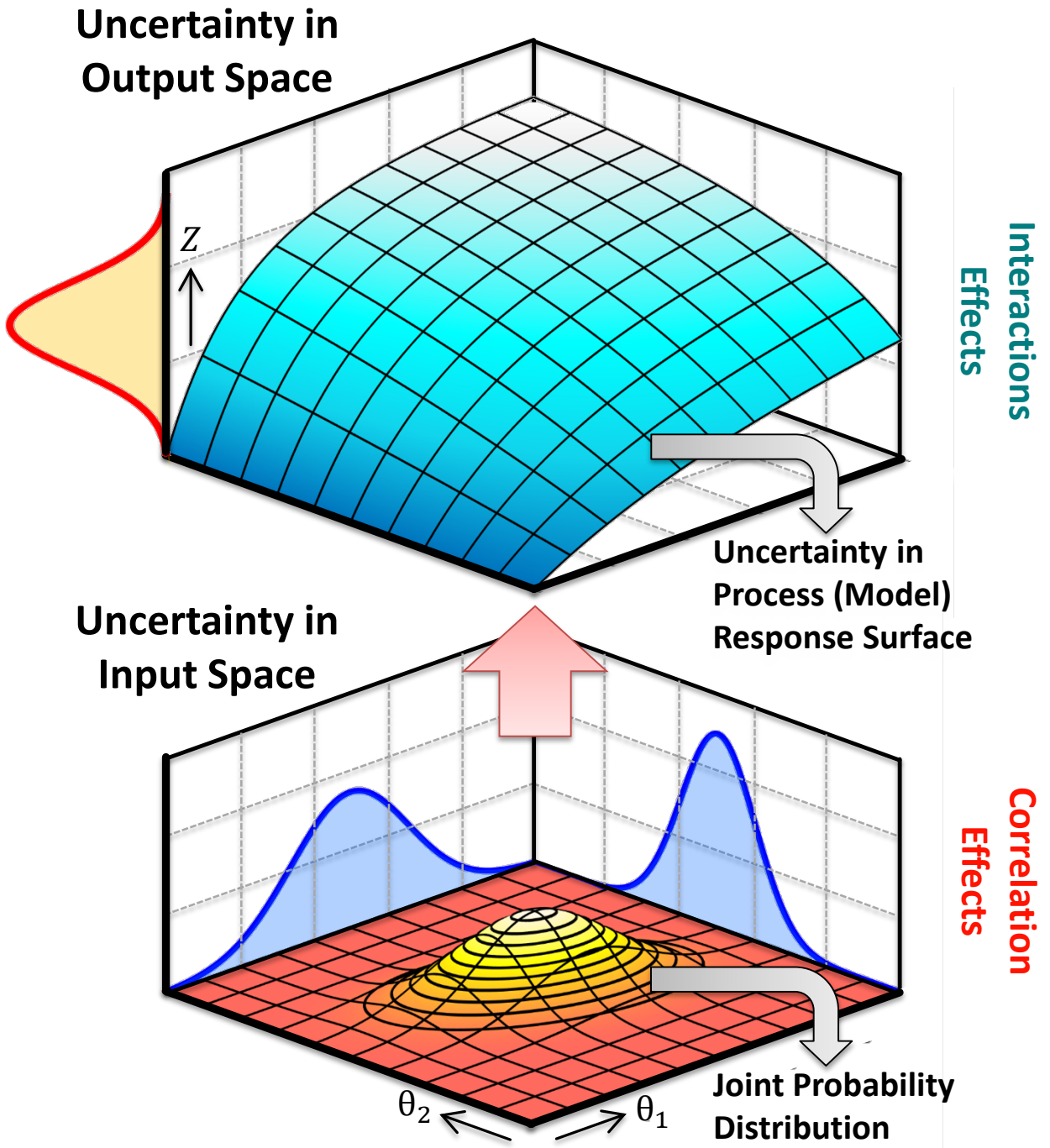
(3) Sensitivity Analysis Approach

attributes the uncertainty in a model prediction to the uncertainties in inputs, and seeks to answer the critical question:

when does uncertainty matter?

illuminates the controls on model behavior, thereby characterizing the dominant controls on predictive uncertainty.

guides research towards reducing the uncertainties that matter, as it points to the most important aspects of the problem.



What is VARS-TOOL?

A comprehensive, multi-approach, multi-algorithm software toolbox for sensitivity analysis of any computer simulation model, including Earth and environmental systems models.

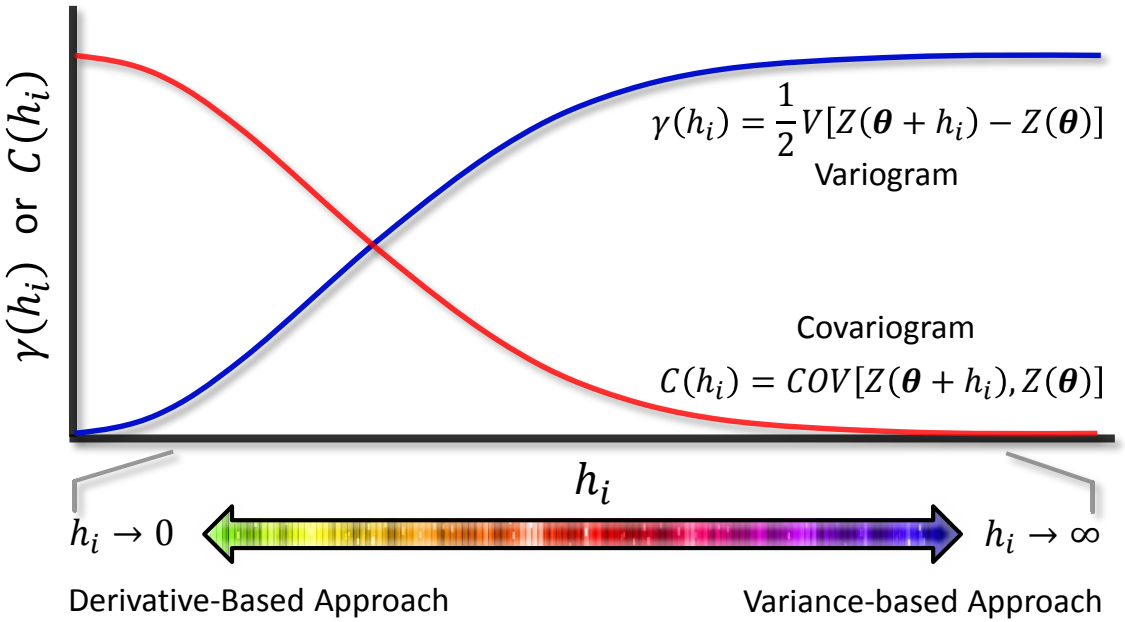
> Razavi, S., Sheikholeslami, R., Gupta, H., Haghnegahdar, A., *VARS-TOOL: A Toolbox for Comprehensive, Efficient, and Robust Sensitivity and Uncertainty Analysis*, submitted to Environmental Modelling & Software.

Important Features:

- Multi-Method Approach to Sensitivity Analysis
- Sensitivity Analysis of Dynamical Systems Models (NEW)
- Various Sampling Strategies, e.g., Progressive Latin Hypercube Sampling (NEW)
- Handling High-Dimensional Problems: A Grouping Solution to Curse of Dimensionality (NEW)
- Characterizing Confidence, Convergence, and Robustness
- Reporting and Visualization: Monitoring Stability and Convergence (NEW)
- Handling Model Crashes via Model Emulation (NEW)
- Interface with Any Computer Model and Linkage to OSTRICH toolkit (NEW)
- A Comprehensive Test Bed for Training and Research (NEW)

Multi-Method Approach to Sensitivity Analysis

VARS-TOOL is home to the novel "Variogram Analysis of Response Surfaces" or VARS framework, which can be seen as a "unifying theory" for SA and encompasses the pre-existing, widely used derivative-based and variance-based methods as special/limiting cases.



Summary Derivations:

If $h_i \to 0 \Rightarrow$

$$\gamma(h_i) \propto V\left[\frac{dZ}{d\theta_i}\right] \propto E\left[\left(\frac{dZ}{d\theta_i}\right)^2\right]$$

"Elementary Effects" based Metrics of Morris

If $h_i \to \infty \Rightarrow \gamma(h_i) = V(Z)$

Variance of Response Surface

$$S_i^{TO} = \frac{\gamma(h_i) + E\left[C_{\boldsymbol{\theta}_{\sim i}}(h_i)\right]}{V(Z)}$$

"Total-Order Effects" of Sobol'

References:

Razavi, S., and H. V. Gupta, (2015), *What do we mean by sensitivity analysis? The need for comprehensive characterization of "global" sensitivity in Earth and Environmental systems models*, Water Resources Research.

Razavi, S., and Gupta, H. V., (2016), *A new framework for comprehensive, robust, and efficient global sensitivity analysis: 1. Theory*, Water Resources Research.

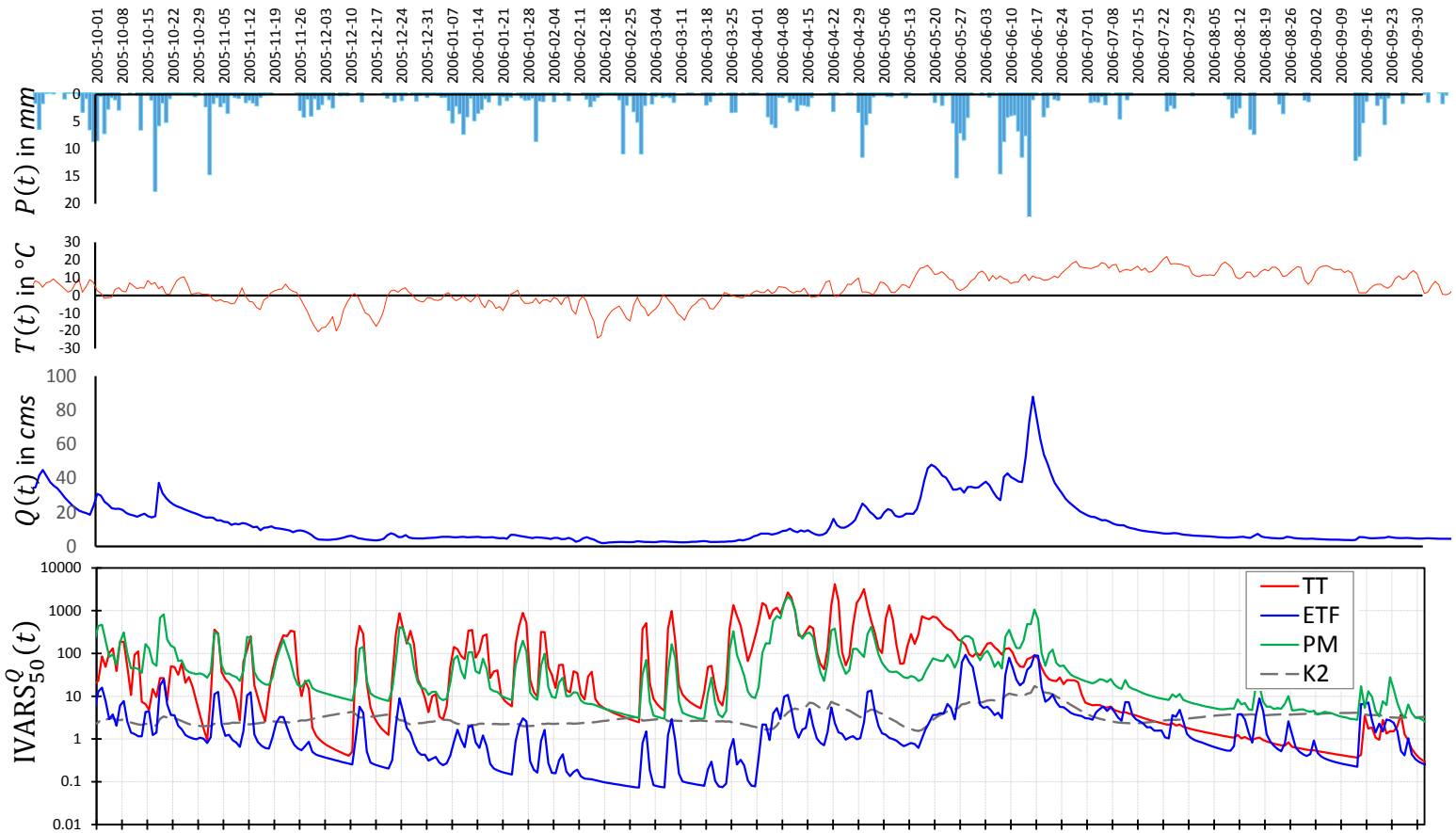
Razavi, S., and Gupta, H. V., (2016), *A new framework for comprehensive, robust, and efficient global sensitivity analysis: 2. Application*, Water Resources Research.

VARS-TOOL includes other derivative-based (Morris), variance-based (Sobol'), and Monte-Carlo Filtering methods.

Sensitivity Analysis of Dynamical Systems Models

- Most approaches to SA of Earth systems models ignore or, at best, do not adequately account for the dynamical nature of such models. These approaches handle problems with only a single response.

- VARS-TOOL includes "Generalized Global Sensitivity Matrix" approach to account for models' the dynamical nature and generate:



- **"Time-varying" sensitivity indices:** time series that reveals time-dependent sensitivities of model responses to factors.
- **"Time-aggregate" sensitivity indices:** summary statistics that aggregate the dynamical sensitivity information.

References:

Razavi, S., Gupta, H., *A General Approach to Multi-Method Sensitivity Analysis of Dynamical Systems Models*, submitted to Environmental Modelling & Software.

Gupta, H.V., and Razavi, S., *Rethinking the Fundamental Basis of Sensitivity Analysis for Dynamical Earth Systems Models*, submitted to Water Resources Research.

http://vars-tool.com/

VARS-TOOL: A Toolbox for Comprehensive, Efficient, and Robust Sensitivity and Uncertainty Analysis

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Submitted to Environmental Modelling & Software
Manuscript 5/17/2018

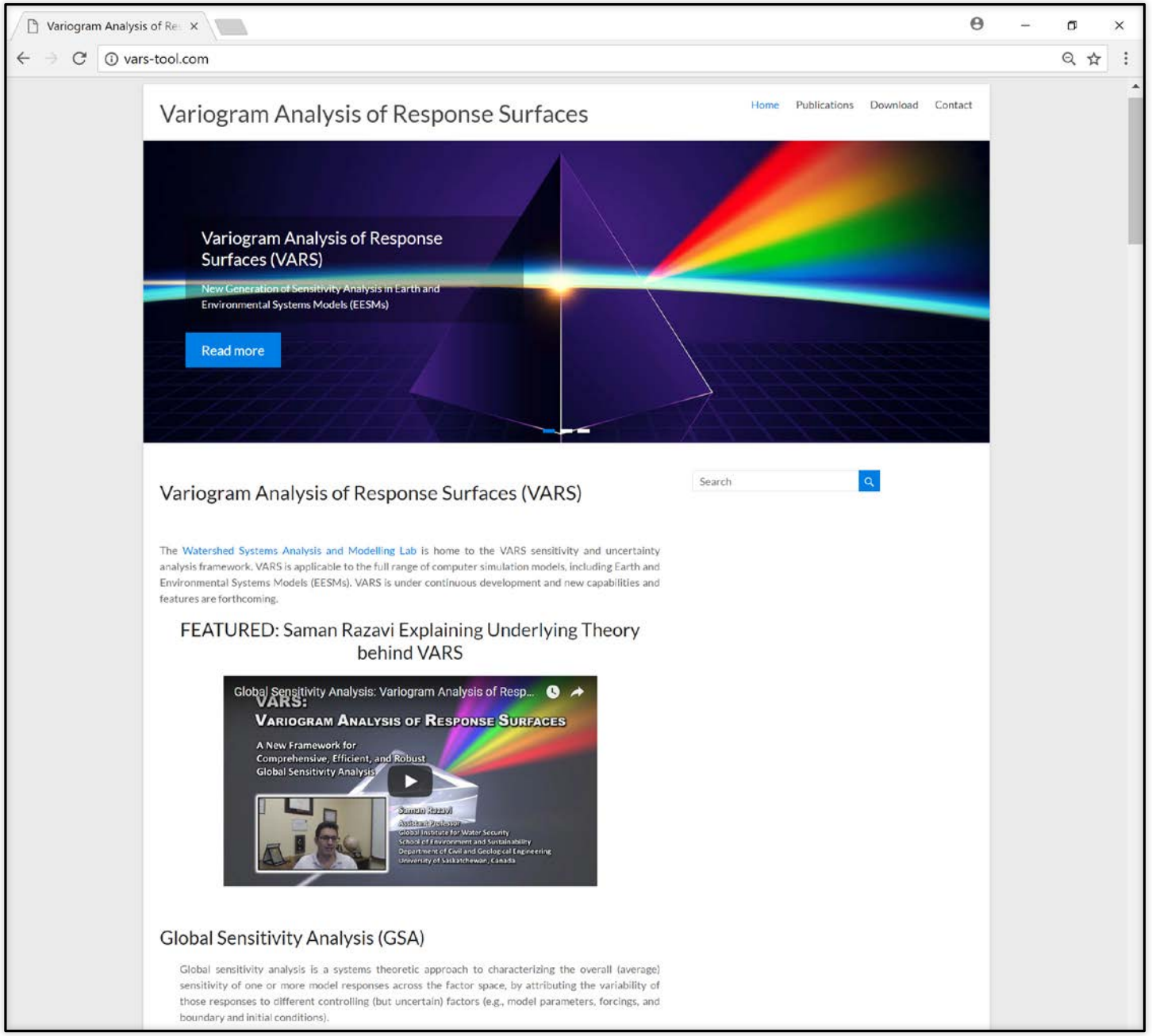
Abstract (150 Words MAX LIMIT):

VARS-TOOL is a software toolbox for sensitivity and uncertainty analysis of computer simulation models. Developed primarily around the powerful "*Variogram Analysis of Response Surfaces*" framework, VARS-TOOL provides a comprehensive suite of algorithms for global sensitivity analysis (GSA), including the methods of Morris and Sobol'. It also incorporates a set of highly efficient sampling techniques, such as Progressive Latin Hypercube Sampling (PLHS), that help to reduce costs while maximizing robustness and rapid convergence to stable sensitivity estimates. Special features of VARS-TOOL include (1) tools for analysis of dynamical systems, (2) factor grouping for dealing with high-dimensional problems, (3) visualization tools for monitoring stability and convergence, (4) model emulation for handling model failures, and (5) an interface that allows working with any model in any programming language and operating system. As a test bed for training and research, VARS-TOOL provides a set of mathematical test functions and the (dynamical) HBV-SASK hydrologic model.

Keywords: global sensitivity analysis, uncertainty analysis, variogram analysis of response surface (VARS), Sobol', Morris, progressive Latin hypercube sampling (PLHS), dynamical systems models, sensitivity indices, performance metrics

Highlights (3 to 5 bullet points; maximum 85 characters, including spaces, per bullet point):

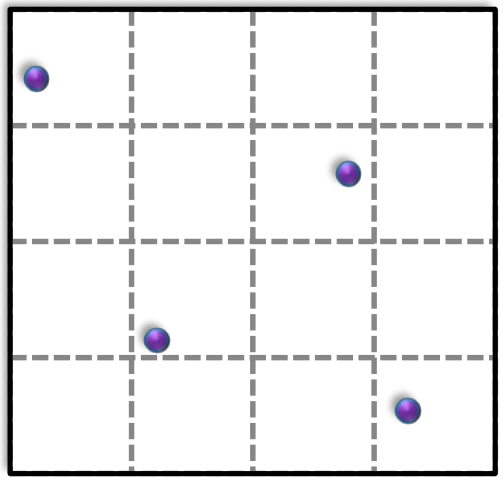
- Introduces a next-generation toolbox for sensitivity and uncertainty analysis
- Provides a multi-method approach that unifies different theories and strategies
- Accounts for dynamical properties of Earth and environmental systems models
- Provides various sampling strategies including progressive Latin hypercube sampling
- Facilitates handling of high-dimensional models with hundreds of uncertain factors



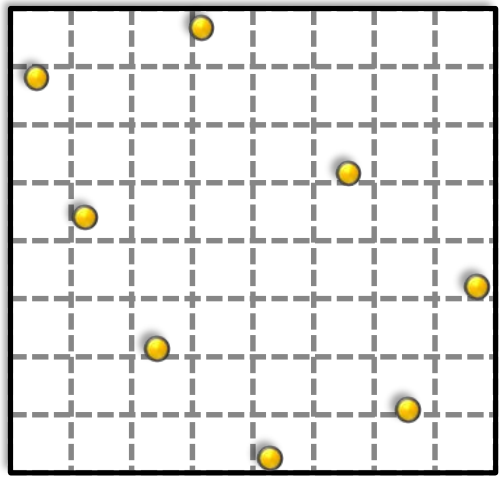
Sampling Strategies

- Sampling strategies are necessary fundamental components of any algorithm for sensitivity and uncertainty analysis of computer simulation models.
- VARS-TOOL includes a variety of sampling strategies, including Latin Hypercube Sampling (LHS), Symmetric LHS, Progressive LHS (PLHS), Halton and Sobol Sequences, STAR, etc.
- PLHS sequentially generates sample points while progressively preserving important distributional properties (Latin hypercube, space-filling, etc.), as the sample size grows.

Progressive Sample Size = 4, 8, 12, ...



#1



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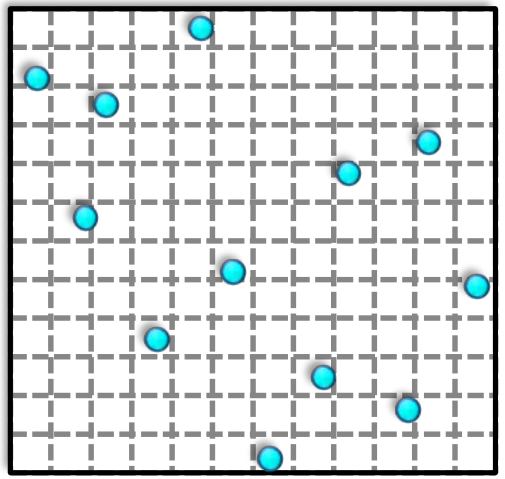
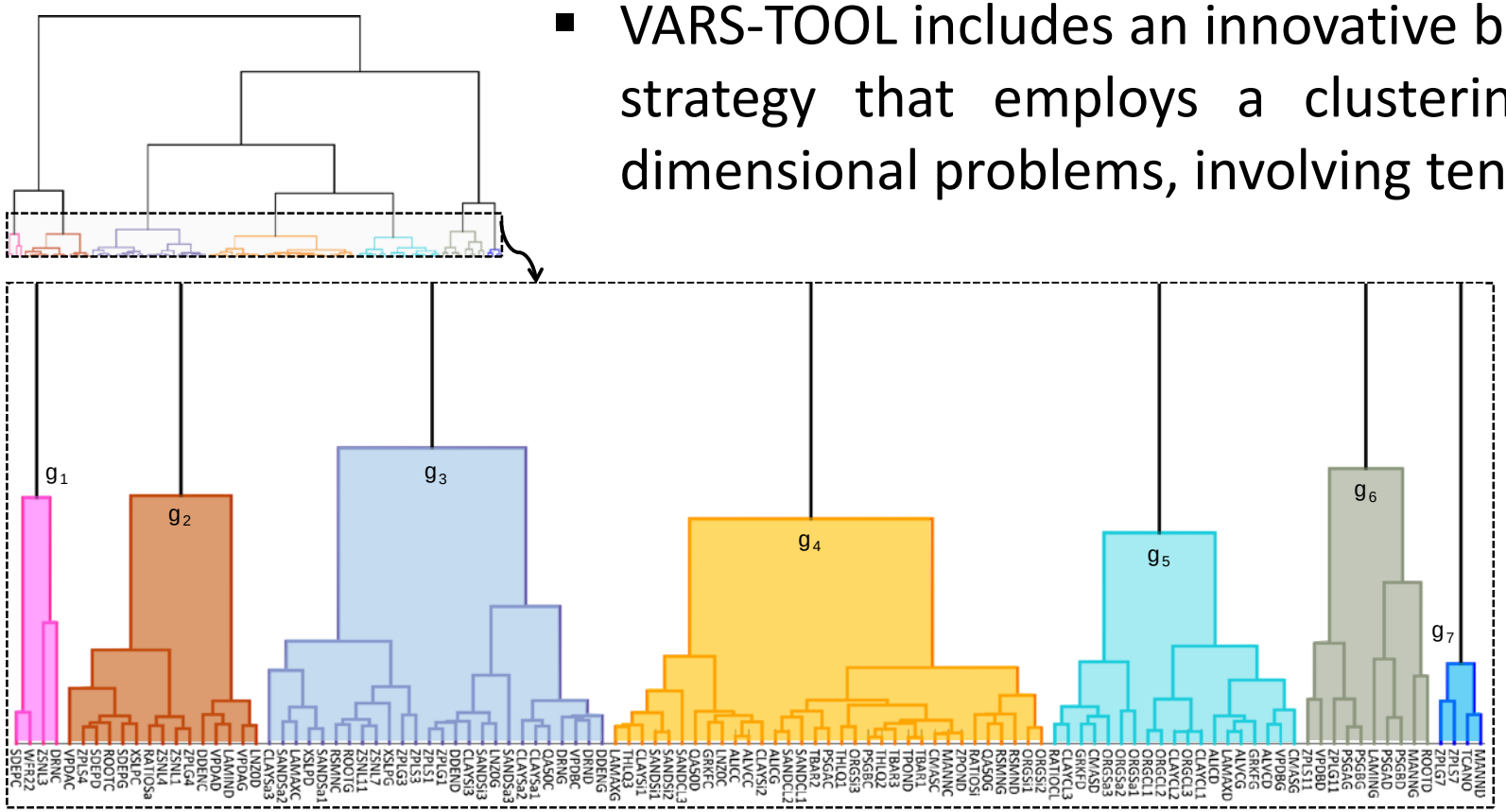


#1 + #2 + #3

References:
Sheikholeslami, R., and Razavi, S., (2017), *Progressive Latin Hypercube Sampling: An efficient approach for robust sampling-based analysis of environmental models*, Environmental Modelling & Software.

Handling High-Dimensional Problems

- Approximately, 70 percent of GSA applications in the environmental modelling literature focused on models with less than 20 parameters, suggesting GSA is paradoxically under-utilized where it should prove most useful.



- VARS-TOOL includes an innovative bootstrap-based "factor grouping" strategy that employs a clustering mechanism to handle high-dimensional problems, involving tens to hundreds of factors. It:
  - Estimates Optimal Number of Groups
  - Measures and Maximizes "Robustness"

References:
Sheikholeslami, R., Razavi, S., Gupta, H., Becker, W., Haghnegahdar, A., *Global Sensitivity Analysis of High-Dimensional Problems: How to Objectively Group Factors and Measure Robustness and Convergence of the Results?*, subm. to Environmental Modelling & Software.

VARS-TOOL is a comprehensive, multi-approach, multi-algorithm toolbox equipped with a set of tools to enable GSA for any application.