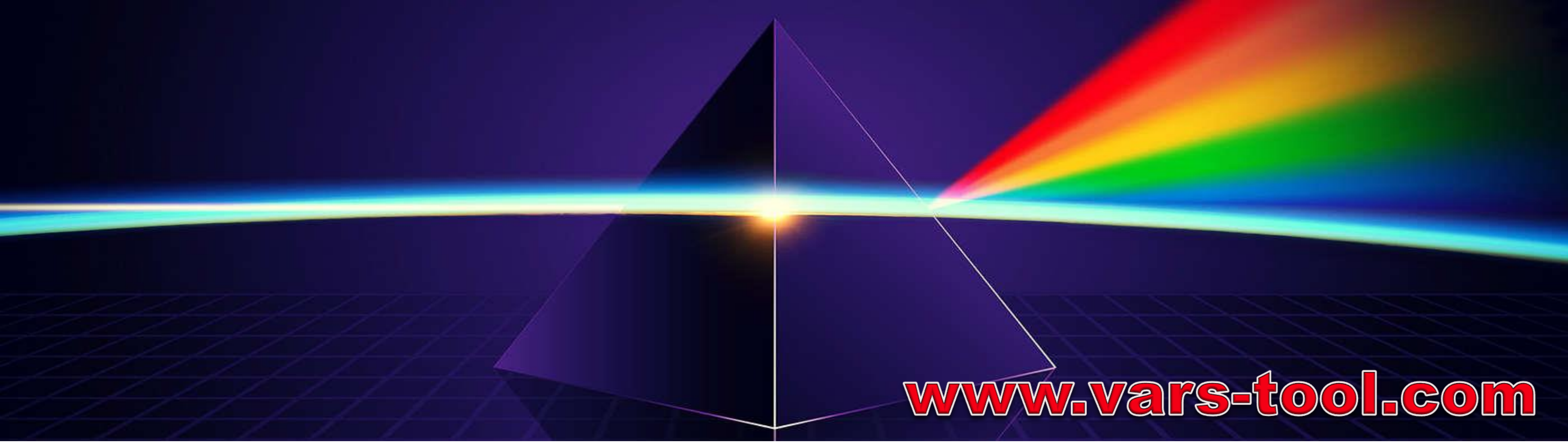


A Toolbox for Comprehensive, Efficient, and Robust Sensitivity and Uncertainty Analysis

Saman Razavi, First Annual General Meeting
Saman Razavi, July 18-19, 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

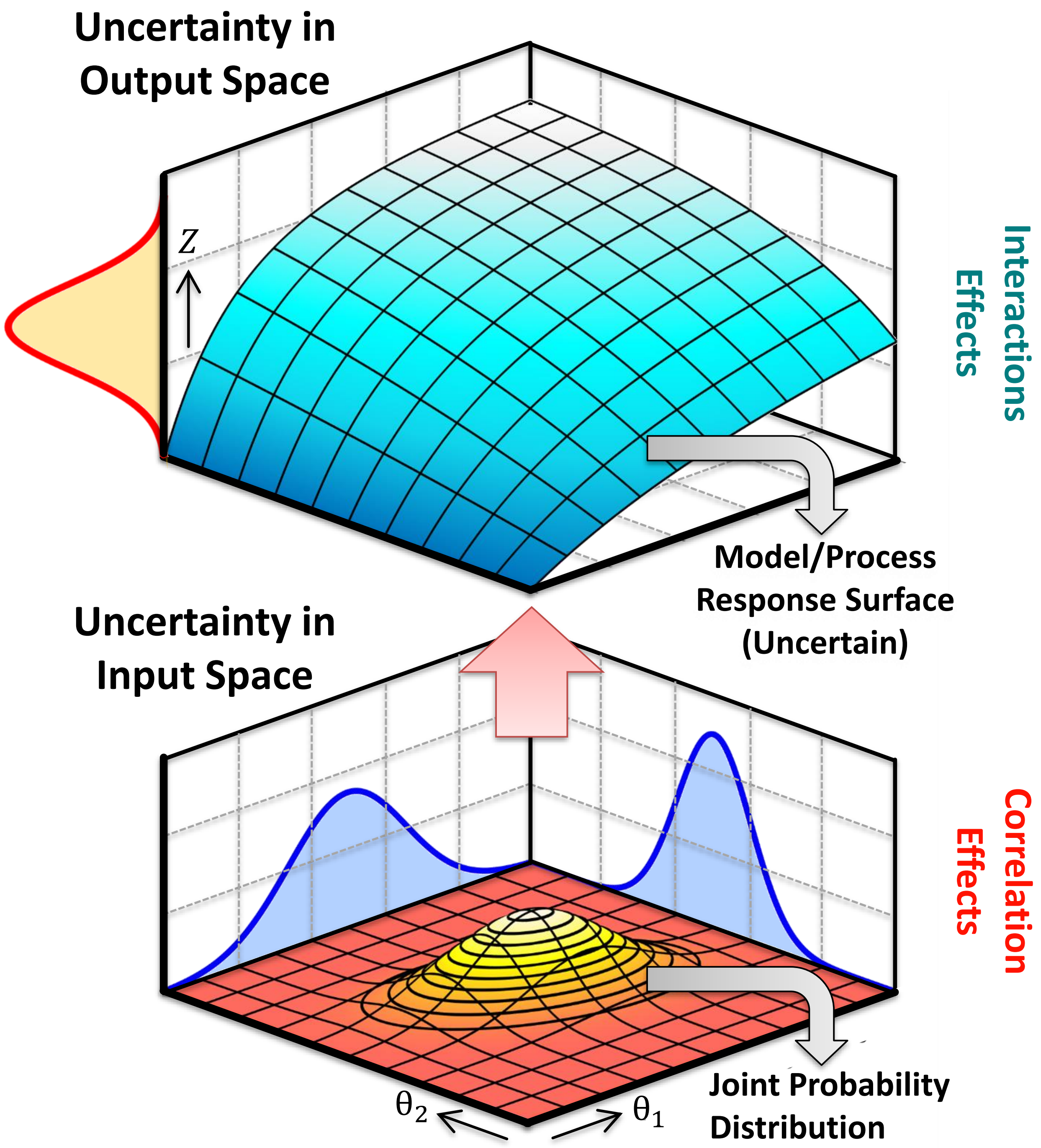
Approaches to Uncertainty Analysis

(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

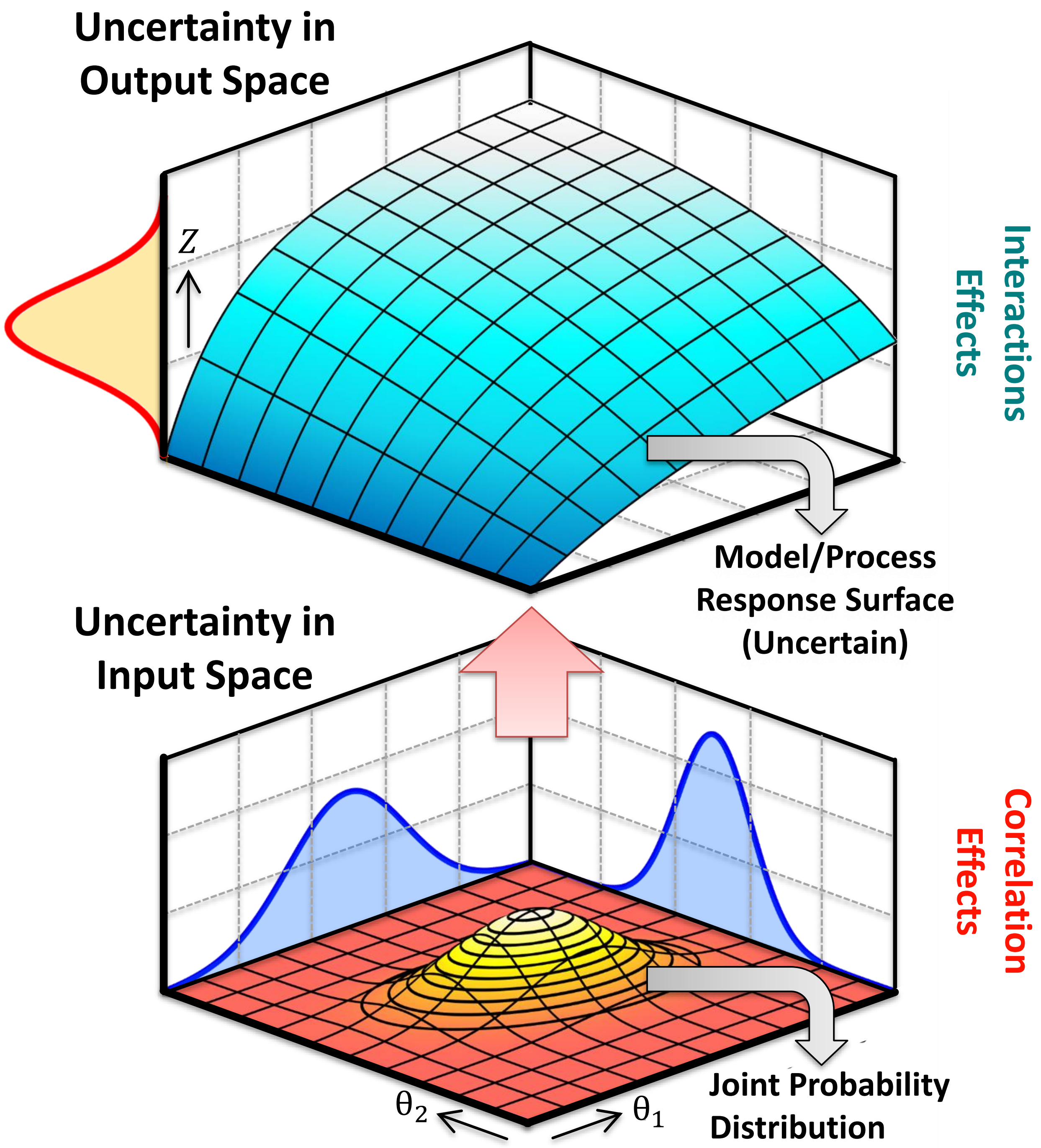
(3) Sensitivity Analysis Approach

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

<u>when does uncertainty matter?</u>

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.



http://vars-tool.com/

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

Saman Razavi[1,2,3], Razi Sheikholeslami[1,2], Hoshin Gupta[4], Amin Haghnegahdar[1,2]

[1]Global Institute for Water Security, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

[2]School of Environment and Sustainability, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

[3]Dept. of Civil, Geological, and Environmental Engineering, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

[4]Department of Hydrology & Atmospheric Sciences, The University of Arizona, Tucson, Arizona, USA

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

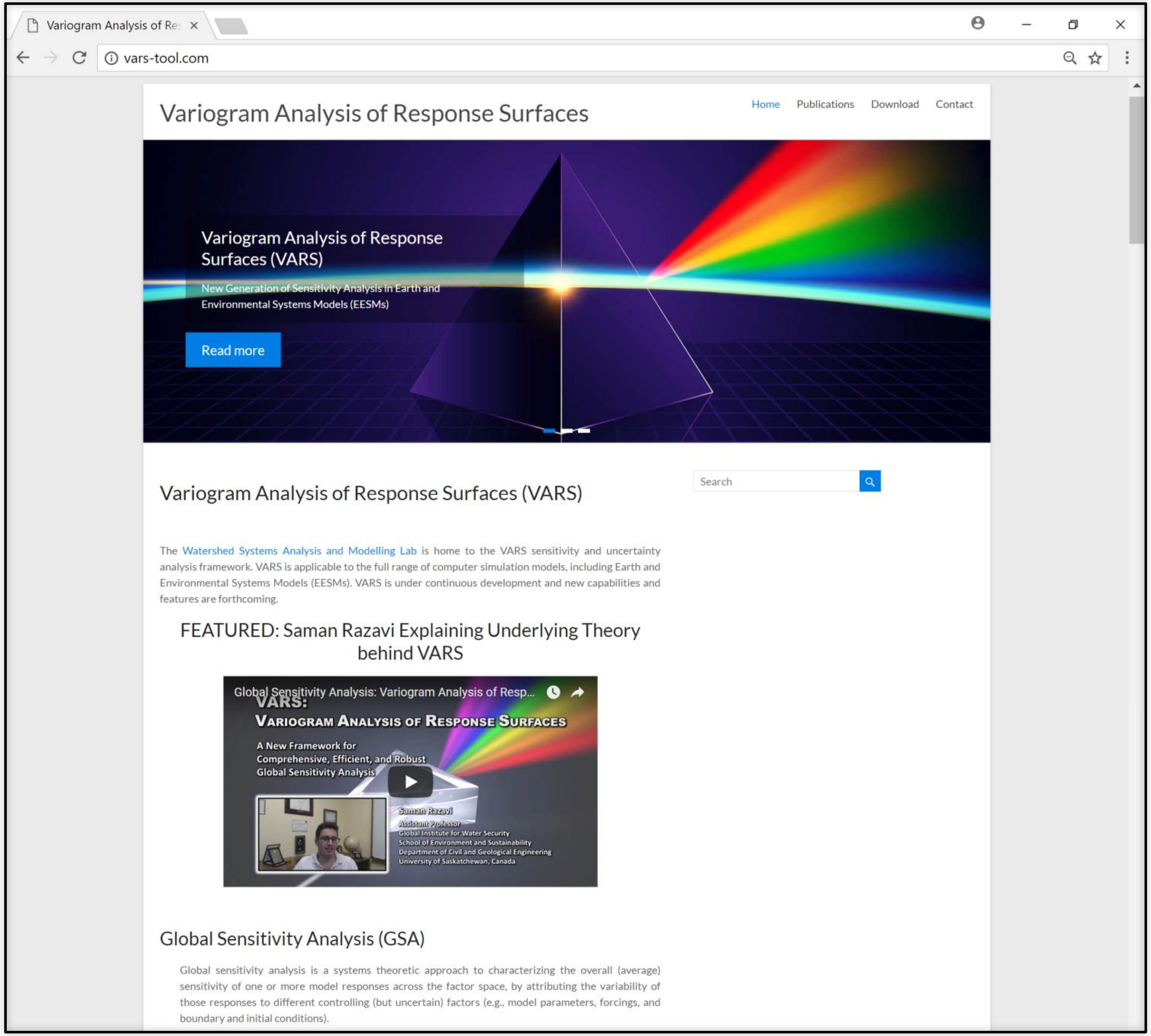
Abstract (150 Words MAX LIMIT):

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



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.

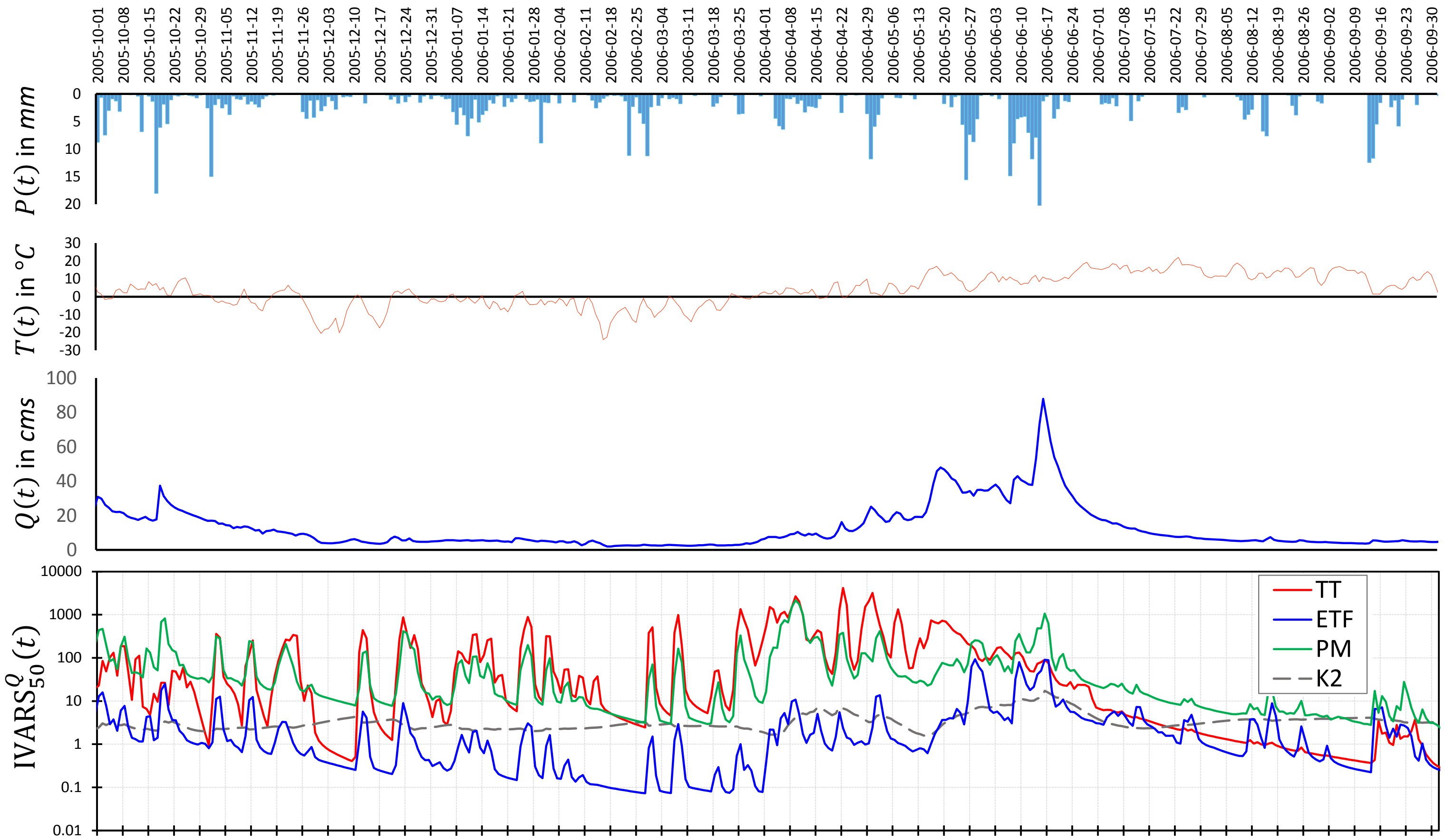
Important Features:

- 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)

Revisiting the Fundamental Basis of Global Sensitivity Analysis for Dynamical Environmental 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:



  - **<u>"Time-varying" sensitivity indices:</u>** time series that reveals time-dependent sensitivities of model responses to factors.
  - **<u>"Time-aggregate" sensitivity indices:</u>** 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.

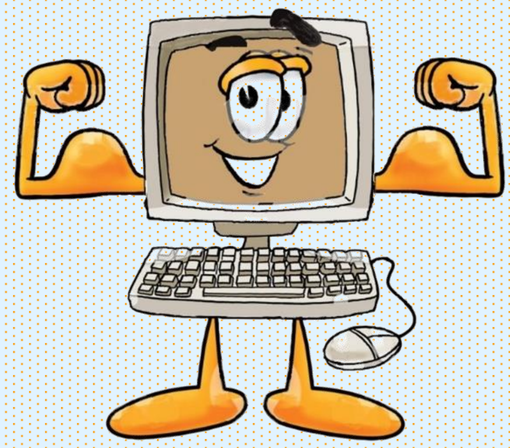
A Dynamical, Input-State-Output Model

Time Step: $t = 1 \text{ to } T$

Sequences of Inputs: $U_t = \{U_t^1, \dots, U_t^{D_u}\}$

Initial State: $X_0 = \{X_0^1, \dots, X_0^{D_x}\}$

D_u, N_Θ, D_x and D_y are the dimensions of the input, parameter, state, and flux vectors, respectively.



Parameter Set: $\Theta = \{\theta_1, \dots, \theta_{N_\Theta}\}$

Sequences of States: $X_t(\Theta) = \{X_t^1(\Theta), \dots, X_t^{D_x}(\Theta)\}$

Sequences of Fluxes:

$Y_t(\Theta) = \{Y_t^1(\Theta), \dots, Y_t^{D_y}(\Theta)\}$

Simulated Time Series

$$Y^k(\Theta^j) = \{Y_1^k(\Theta^j), \dots, Y_T^k(\Theta^j)\}$$

flux k for point j in parameter space

$$Z = \{Z_1, \dots, Z_T\}$$

Observed Time Series

Performance Metric:

$$F^j = F(Y|Z, \Theta^j) = \frac{1}{T}\sum_{t=1}^{T}\left(fZ_t - fY_t(\Theta^j)\right)^2$$

Transformation Function

The ‘Filtering Role’ of Performance Metrics

$$F^j = \frac{1}{T}\sum_{t=1}^{T}\left(fZ_t - fY_t(\Theta^j)\right)^2$$

Gradient Vector Representing Magnitude and Sign of ‘Local Sensitivity’

$$\nabla F^j = \left\{dF^j/d\theta_1, \dots, dF^j/d\theta_{N_\theta}\right\}$$

$$dF^j/d\theta_i = \frac{-2}{T}\sum_{t=1}^{T}\left(fZ_t - fY_t(\Theta^j)\right)\cdot \left.\frac{df}{dY_t}\right|_{\Theta^j}\cdot \left.\frac{dY_t}{d\theta_i}\right|_{\Theta^j}$$

$$dF^j/d\theta_i = \frac{-2}{T}\sum_{t=1}^{T}\overbrace{r_t(\Theta^j)}^{\text{Residual (Error)}}\cdot \underbrace{\beta_t(\Theta^j)}_{\text{Transformation Effect}}\cdot \overbrace{\left.\frac{dY_t}{d\theta_i}\right|_{\Theta^j}}^{\text{Sensitivity Coefficient}}$$

- The critical issue is that the result is obscured by mix effects of the residual term (“goodness of model fit” at that time step), the nature of transformation function, and sensitivity coefficient.
- Unjustified insensitivity of the time steps and parameter locations at which the model fits data well (i.e., where $\mathbf{r}_t(\Theta^j) \sim$ zero). Counter-intuitively, the result is biased to represent time steps and parameter locations where the model performance is not good (where $\mathbf{r}_t(\Theta^j)$ is far from zero).
- Such approaches depend on availability of system state/output observational data, and therefore, the analysis they provide is necessarily incomplete.

The Issues to be Discussed:

(1) 'Sensitivity' Analysis versus 'Identifiability' Analysis: The Need for a Clear Distinction

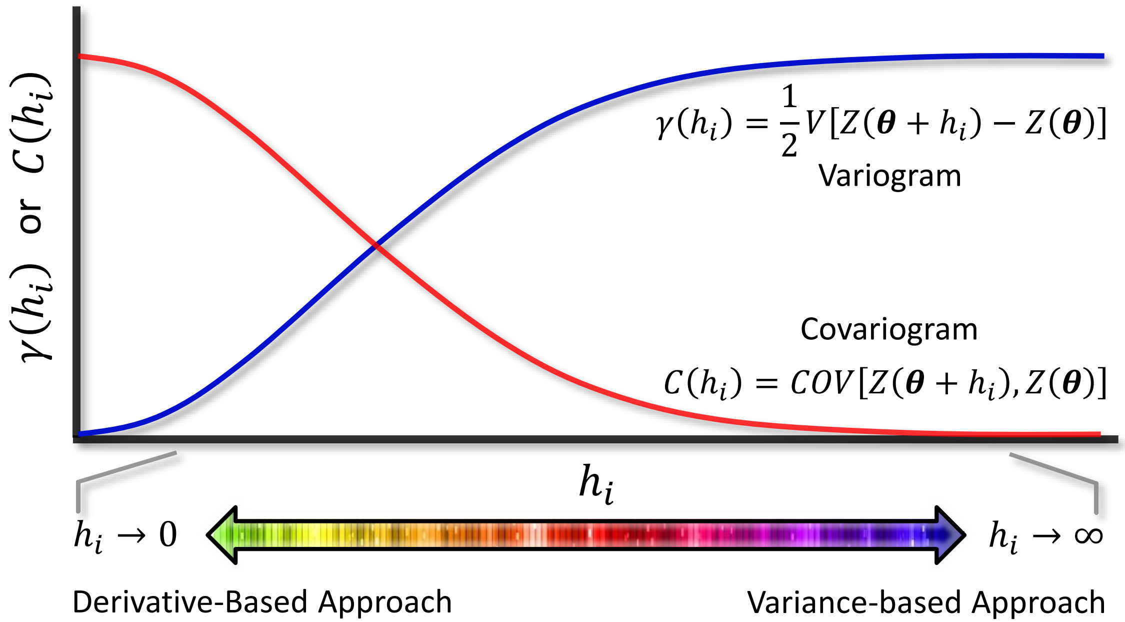
- The former is a specific attribute of the '*forward'* problem to establish which parameters exert stronger (or weaker) controls on the models' dynamical input-state-output behavior.
- The latter is an attribute of the '*inverse'* problem to establish which parameters are more readily identifiable when observational data regarding the system behavior is available.

(2) Methodological Focus on Single-Response Problems: Weakly Informative on Dynamics

- Most sensitivity analysis approaches are primarily designed for applications where the sensitivity of *only* a single model output to factor perturbations is of interest.
- Sensitivity analysis of models with time series outputs is mainly handled by computing some '*performance metric*' that measures the goodness-of-fit to observed data.
- The performance metric-based approach is typically extended (e.g., by a moving window approach) to account for the time-evolving nature dynamical models.

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.

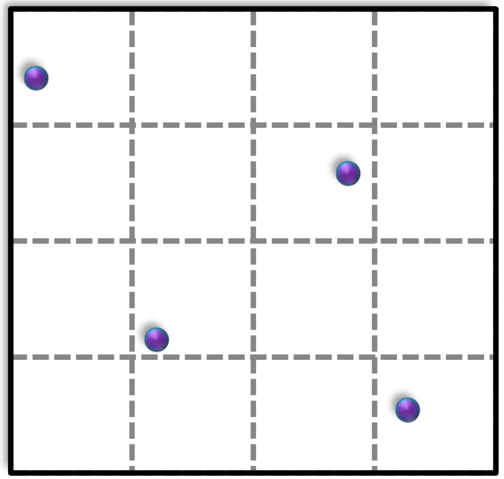
Razavi, S., and Gupta, H. V., (2016), *A new framework for comprehensive, robust, and efficient global sensitivity analysis: 2. Application*, Water Resources Research.

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

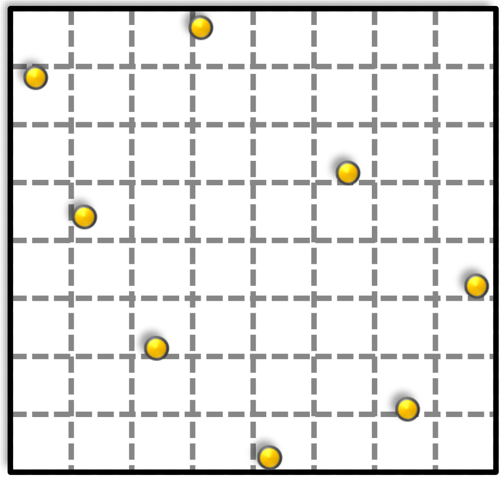
Sampling Strategies

- 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.

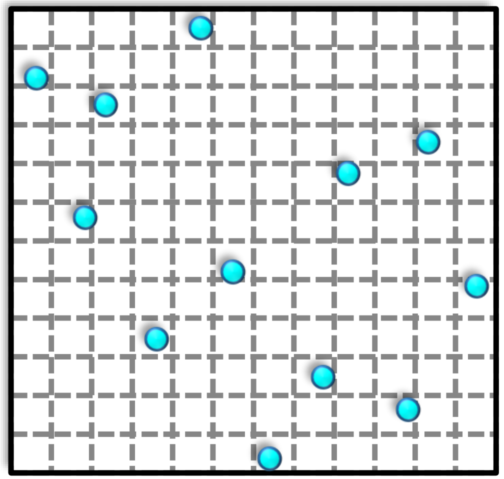
Progressive Sample Size = 4, 8, 12, …



#1



#1 + #2



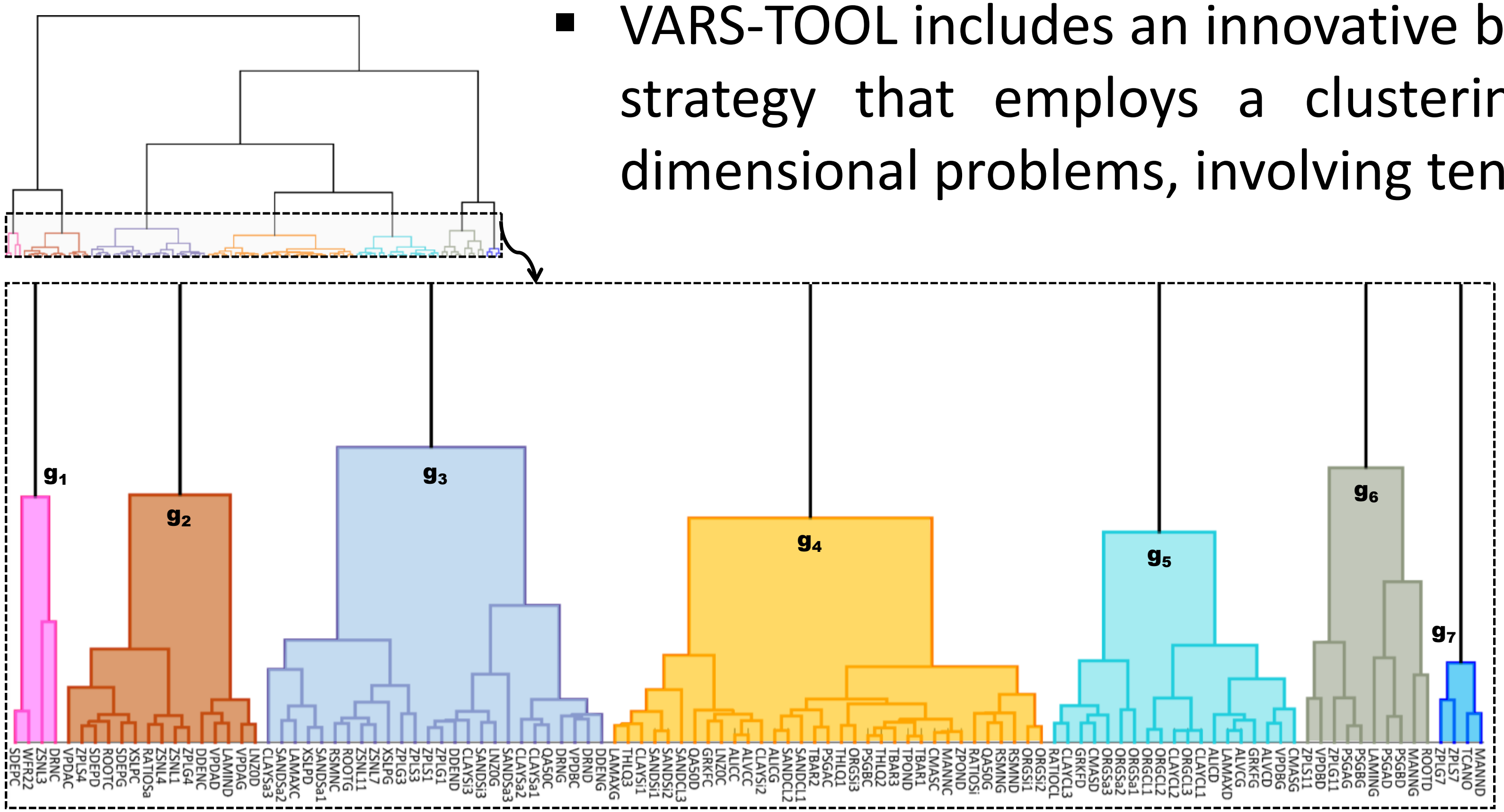
#1 + #2 + #3

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.

VARS_inp.txt - Notepad

File Edit Format View Help

```
% <><><><>          Variogram Analysis of Response Surfaces (VARS) Main Input File          <><><><>
% <><><>           © Saman Razavi 2018; V1 written in 2013-15; V2 written in 2017-18          <><><><>
% <><>          Do not change row numbers and orders. Any text after % is deemed comments          <><><><>
% <>             VARS-TOOL will scale factors in range zero to one before analysis              <><><><>
HBV_out                  % 5. Output folder: name of the folder where VARS results are to be stored
100                      % 6. Number of stars: the total number of stars for a STAR-VARS run
0.1                      % 7. Sampling resolution, Delta h: The minimum h in the VARS analysis
0.1  0.3  0.5            % 8. IVARS scale ranges of interest, H: e.g., 0.1 and 0.3 correspond [0-0.1] and [0-0.3], respectively
eval_HBV_SASK            % 9. Model filename: MATLAB m-file without .m extension
C:\VARS-Tool-v2\HBV-SASK % 10. Folder address: that includes model file, factor space, and star centers (if applicable)
                         % 11. Star-centers file: if blank, VARS generates star centers via the sampling strategy specified in line 12
PLHS                     % 12. Sampling strategy: RND, LHS, PLHS, SobolSeq, or Halton for generation of star centers; if blank, default is LHS
123456789                % 13. Seed number: for randomization of sampling strategy specified in line 12; leave blank for automatic randomization
1                        % 14. Bootstrap-and-grouping flag: enter "1" to bootstrap and group, or "0" not to
1000                     % 15. Bootstrap size: number of sampling iterations with replacement; if bootstrap flag = 0, this line will be ignored
0.9                      % 16. Confidence level: for bootstrap-based confidence intervals on results; if line 14 = 0, this line will be ignored
                         % 17. User-specified number of groups: if blank, VARS-TOOL will find the optimal number; if line 14 = 0, this line will be ignored
0                        % 18. Online/offline flag: enter "0" for online VARS, or "1" for offline VARS
1                        % 19. Offline-stage flag: enter "1" to run STAR & write samples, or "2" to read model output & run VARS; active when line 18 = 1
10                       % 20. Reporting frequency, R: reports after completion of every set of R stars; if line 12 = PLHS, R will also be the slice size
1                        % 21. Plotting flag: enter "1" to generate plots on the results, or "0" not to generate
1                        % 22. Time series length: needed for the GGSM analysis of dynamical systems models; enter "1" for conventional GSA
1                        % 23. Text-report flag: enter "1" to write txt report files, or "0" not to write
```