# Towards more general sensitivity estimates

## Applications considering model structural uncertainties, grouping of parameters, and large-scale analyses

Juliane Mai

SAMO 2022 - Florida State University
March 14-16, 2022

UNIVERSITY OF WATERLOO

# Motivation

## – Challenges in Sensitivity Analyses –

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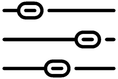
Model parameters only



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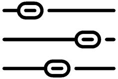

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**Challenge #1:**

Limits process understanding

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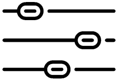

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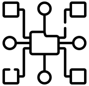
Dependence on model structure



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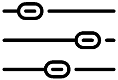

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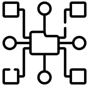

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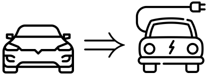
Transferability to other models



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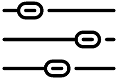

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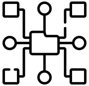

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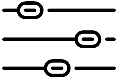

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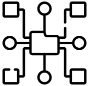

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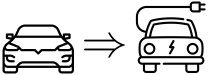

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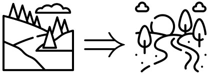
**Challenge #3:**

Sensitivities at new location



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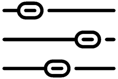

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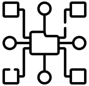

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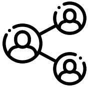
Data sharing & re-usability



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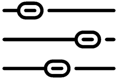

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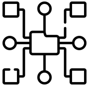

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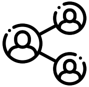

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**Challenge #4:**

Extracting data from previous studies

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- Challenges and **methods presented are general** but presented for applications in hydrologic modeling

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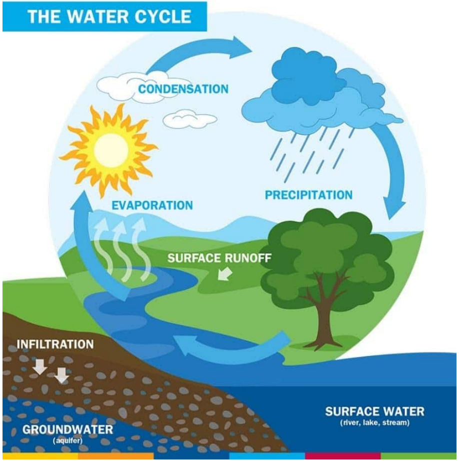


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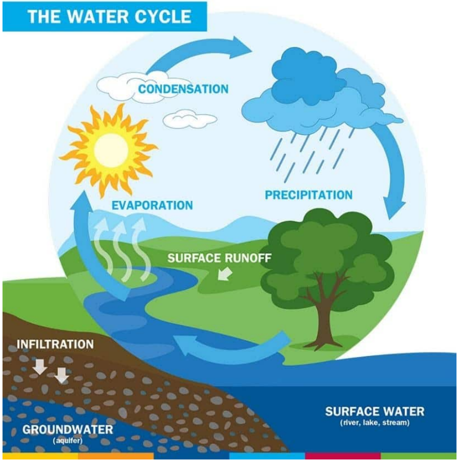


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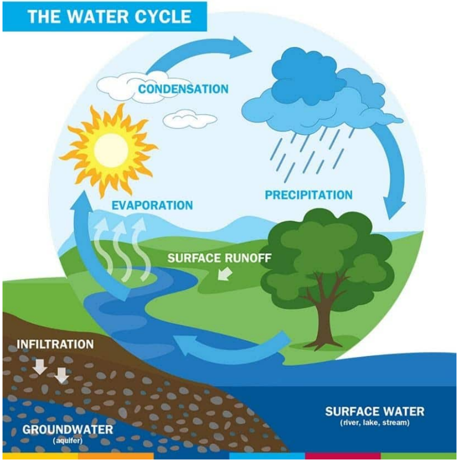
- Output: streamflow
- Inputs:
  - dynamic: radiation, precipitation, temperature, ...
  - static: elevation, slope, latitude, longitude, ...

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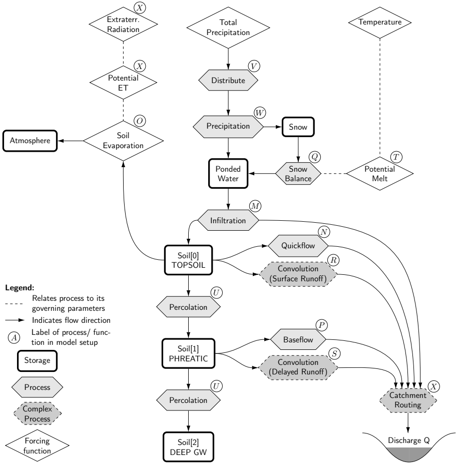
- Output: streamflow
- Inputs:
  - dynamic: radiation, precipitation, temperature, ...
  - static: elevation, slope, latitude, longitude, ...
  - **parameters** describing evaporation, infiltration, etc.

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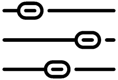
Model parameters only



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Limits process understanding

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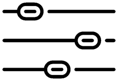

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Define **SA for processes** (groups of parameters) rather than parameters only

# Challenge 1: Define SA for processes

## – Sobol' method for parameters –

**Main effect:**

$$S_i = \frac{\text{Variance of model, if } \textbf{one} \text{ parameter is variable}}{\text{Variance of model, if } \textbf{all} \text{ parameters are variable}}$$

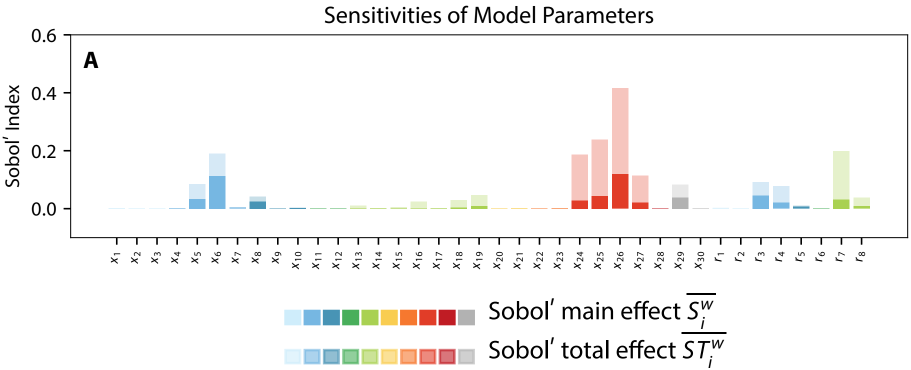
**Total effect:**

$$S_{T_i} = \frac{\text{Variance of model, if } \textbf{all incl. one} \text{ parameters are variable}}{\text{Variance of model, if } \textbf{all} \text{ parameters are variable}}$$

[1] Sobol' (1993). *Sensitivity Estimates for Nonlinear Mathematical Models. Math. Model. Comput. Exp., Engl. Transl., 1(4), 407–414.*

# Challenge 1: Define SA for processes

## – Sobol’ method for parameters –





[2] Mai, J., Craig, J. R., & Tolson, B. A. (2020). *Simultaneously determining global sensitivities of model parameters and model structure.* Hydrology and Earth System Sciences, 24(12), 5835–5858. http://doi.org/10.5194/hess-24-5835-2020

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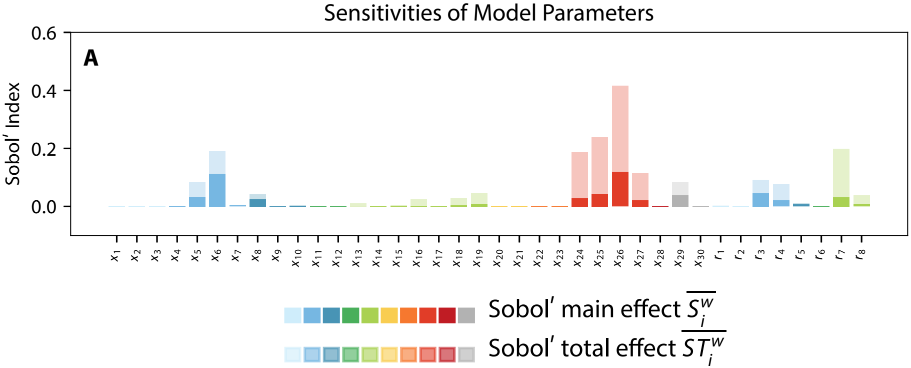


Estimates sensitivity of model regarding choice of model parameters.
(40,000 model runs)

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# Challenge 1: Define SA for processes

## – Sobol' method for grouped parameters –

**Main effect:**

$$S_G = \frac{\text{Variance of model, if } \textbf{only parameters in group G} \text{ are variable}}{\text{Variance of model, if } \textbf{all} \text{ parameters are variable}}$$

**Total effect:**

$$S_{T_G} = \frac{\text{Variance of model, if } \textbf{all parameters that incl. group G} \text{ are variable}}{\text{Variance of model, if } \textbf{all} \text{ parameters are variable}}$$

[3] Sobol, I. M., & Kucherenko, S. S. (2005). *Global Sensitivity Indices for Nonlinear Mathematical Models.* Review. WILMOTT Magazine, 2–7.

# Challenge 1: Define SA for processes

## – Sobol' method for grouped parameters –

| ID | Process | Parameters active |
|---|---|---|
| 1 | Infiltration | $\{x_1, x_2, x_3, x_{29}\}$ |
| 2 | Quickflow | $\{x_4, x_5, x_6, x_7, x_{29}\}$ |
| 3 | Soil evaporation | $\{x_8, x_9, x_{10}, x_{29}\}$ |
| 4 | Baseflow | $\{x_{11}, x_{12}\}$ |
| 5 | Snow balance | $\{x_{13}, x_{14}, x_{15}, x_{16}, x_{17}, x_{18}, x_{19}\}$ |
| ... | ... | ... |

[2] Mai, J., Craig, J. R., & Tolson, B. A. (2020). *Simultaneously determining global sensitivities of model parameters and model structure.* Hydrology and Earth System Sciences, 24(12), 5835–5858. http://doi.org/10.5194/hess-24-5835-2020

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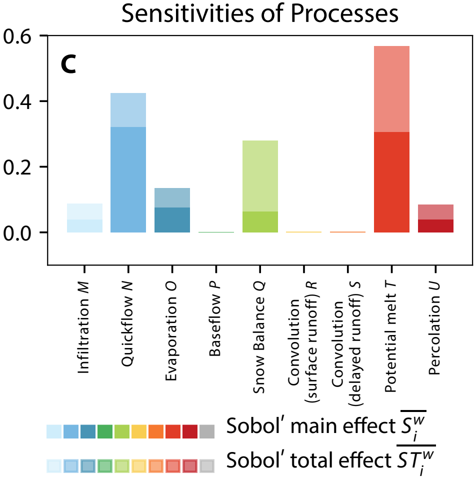
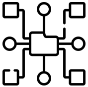



Estimates sensitivity of model regarding choice of model parameters.

↷ 11,000 model runs for 9 processes
instead of
40,000 model runs for 38 parameters

[2] Mai, J., Craig, J. R., & Tolson, B. A. (2020). *Simultaneously determining global sensitivities of model parameters and model structure.* Hydrology and Earth System Sciences, 24(12), 5835–5858. http://doi.org/10.5194/hess-24-5835-2020

Dependence on model structure



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# Challenge #2:

Transferability to other models

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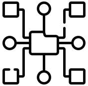

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Define model **blending multiple model structures** into one hyper-model

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# Challenge 2: Define blended models

## – Sensitivity Analysis regarding Model Structure –

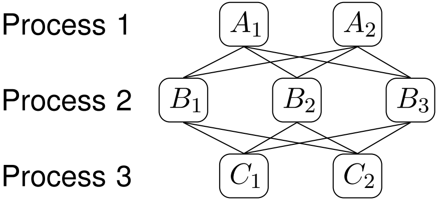
Process 1 $\boxed{A_1}$ $\boxed{A_2}$

Process 2 $\boxed{B_1}$ $\boxed{B_2}$ $\boxed{B_3}$

Process 3 $\boxed{C_1}$ $\boxed{C_2}$

# Challenge 2: Define blended models

## – Sensitivity Analysis regarding Model Structure –




Model: $f(\vec{x}) = A_i \cdot B_j + C_k$ with $i \in \{1,2\}$, $j \in \{1,2,3\}$, $k \in \{1,2\}$

$2 \times 3 \times 2 = 12$ models with varying "active" parameters
$\Rightarrow$ 12 sensitivity analyses

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# Challenge 2: Define blended models

## – Sensitivity Analysis regarding Model Structure –

| n | Model | | | $S^n_{x_1}$ | $S^n_{x_2}$ | $S^n_{x_3}$ | $S^n_{x_4}$ | $S^n_{x_5}$ | $S^n_{x_6}$ | $S^n_{x_7}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $A_1$ | $B_1$ | $C_1$ | 0.383 | 0.000 | – | – | – | 0.001 | – |
| 2 | $A_1$ | $B_1$ | $C_2$ | 0.171 | 0.000 | 0.007 | – | – | – | 0.548 |
| 3 | $A_1$ | $B_2$ | $C_1$ | 0.656 | – | 0.000 | – | – | 0.036 | – |
| 4 | $A_1$ | $B_2$ | $C_2$ | 0.013 | – | 0.012 | – | – | – | 0.968 |
| 5 | $A_1$ | $B_3$ | $C_1$ | 0.000 | – | – | 0.000 | 0.000 | 0.132 | – |
| 6 | $A_1$ | $B_3$ | $C_2$ | 0.000 | – | 0.013 | 0.000 | 0.000 | – | 0.983 |
| 7 | $A_2$ | $B_1$ | $C_1$ | 0.024 | 0.937 | – | – | – | 0.000 | – |
| 8 | $A_2$ | $B_1$ | $C_2$ | 0.024 | 0.926 | 0.000 | – | – | – | 0.012 |
| 9 | $A_2$ | $B_2$ | $C_1$ | 0.145 | 0.382 | 0.224 | – | – | 0.001 | – |
| 10 | $A_2$ | $B_2$ | $C_2$ | 0.052 | 0.138 | 0.138 | – | – | – | 0.583 |
| 11 | $A_2$ | $B_3$ | $C_1$ | 0.000 | 0.000 | – | 0.237 | 0.237 | 0.003 | – |
| 12 | $A_2$ | $B_3$ | $C_2$ | 0.000 | 0.000 | 0.010 | 0.043 | 0.043 | – | 0.810 |

**What is the overall most sensitive parameter?**

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# Challenge 2: Define blended models

## – Sensitivity Analysis regarding Model Structure –

$f^n(\vec{x}) = A_i \cdot B_j + C_k$ with $i \in \{1,2\}$, $j \in \{1,2,3\}$, $k \in \{1,2\}$

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$$\Downarrow$$

$$g(\vec{x}) = (w_1 A_1 + w_2 A_2) \cdot (w_3 B_1 + w_4 B_2 + w_5 B_3) + (w_6 C_1 + w_7 C_2)$$

with

$$\begin{aligned} w_1 + w_2 &= 1 \\ w_3 + w_4 + w_5 &= 1 \\ w_6 + w_7 &= 1 \end{aligned}$$

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Sampling of weights is another story... See [4].

[4] Mai, J., Craig, J. R., & Tolson, B. A. (2022). *The pie sharing problem: Unbiased sampling of N+1 summative weights.* Environmental Modelling & Software, 148, 105282. http://doi.org/10.1016/j.envsoft.2021.105282

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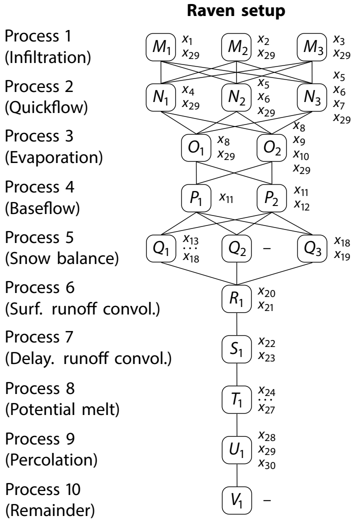


108 models with 30 model parameters and 8 additional parameters to generate weights

[2] Mai, J., Craig, J. R., & Tolson, B. A. (2020). *Simultaneously determining global sensitivities of model parameters and model structure.* Hydrology and Earth System Sciences, 24(12), 5835–5858. http://doi.org/10.5194/hess-24-5835-2020

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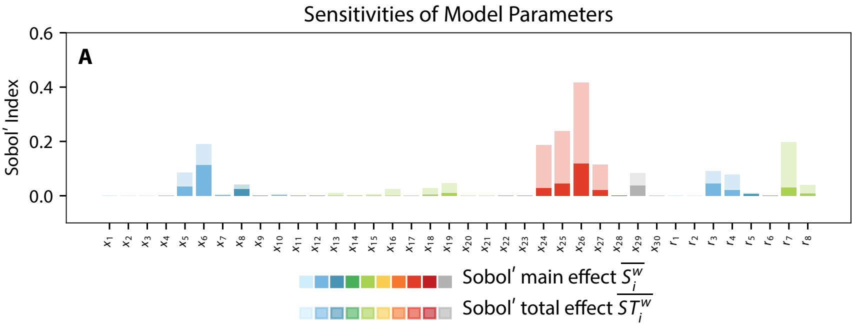


↷ 40,000 model runs for blended model with 38 parameters
instead of
2,718,000 model runs to analyze 108 models individually each with 18 to 29 parameters

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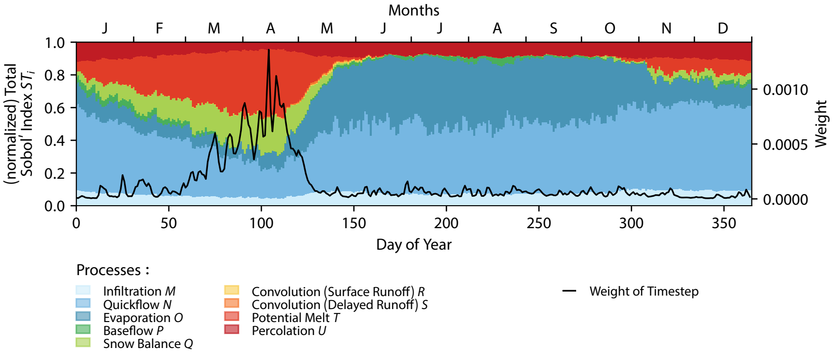


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## Challenge #3:

Dependence on location

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Sensitivities at new location

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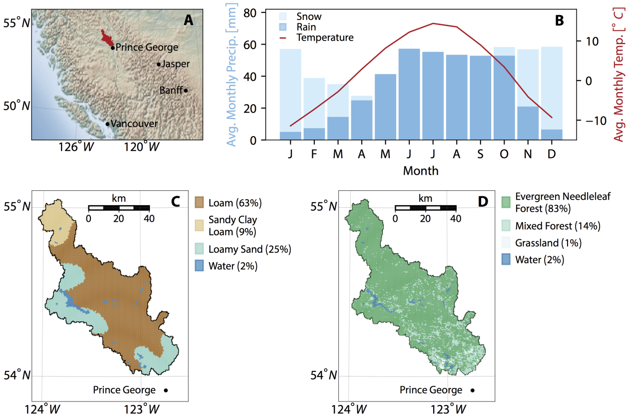
**Large-sample experiment** to obtain functional relationships to approx. sensitivities

# Challenge 3: Large-sample experiments

## – Inferring functional relationships for sensitivities –

Example model setup for Salmon River catchment ($4230 km^2$)




[2] Mai, J., Craig, J. R., & Tolson, B. A. (2020). *Simultaneously determining global sensitivities of model parameters and model structure.* Hydrology and Earth System Sciences, 24(12), 5835–5858. http://doi.org/10.5194/hess-24-5835-2020

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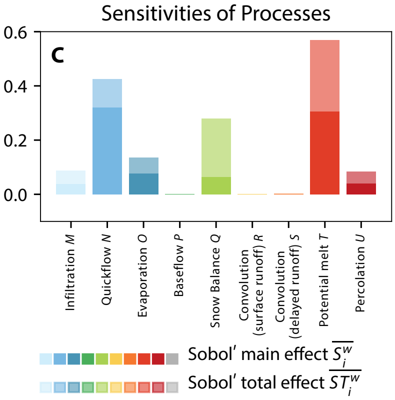



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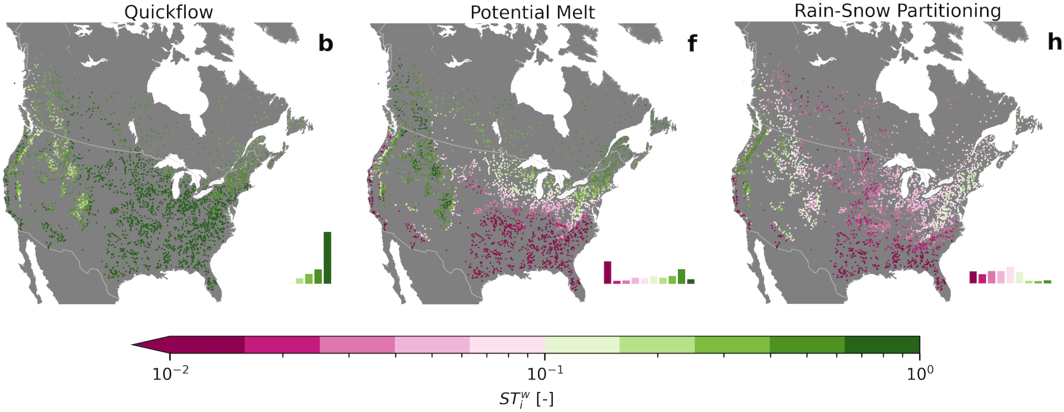
# Challenge 3: Large-sample experiments

## – Inferring functional relationships for sensitivities –

Model setups for 3316 catchments in North America

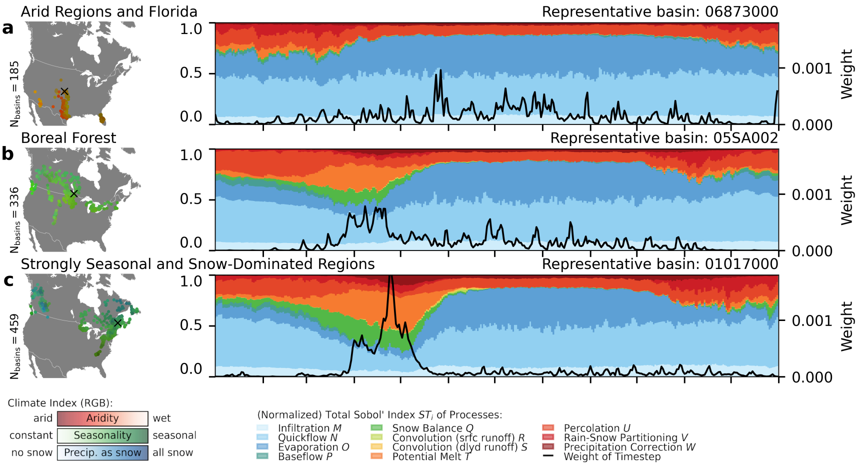




[5] Mai, J., Craig, J. R., Tolson, B. A., & Arsenault, R. (2022). *The sensitivity of simulated streamflow to individual hydrologic processes across North America.* Nature Communications, 13(1), 455. http://doi.org/10.1038/s41467-022-28010-7

# Challenge 3: Large-sample experiments

## – Inferring functional relationships for sensitivities –

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# Challenge 3: Large-sample experiments

## – Inferring functional relationships for sensitivities –

multi-variate regression using location characteristics to approximate sensitivities

**Table 1 Deduced functional relationships using basin attributes to estimate process sensitivities.**

| Process | Pred. x | Pred. y | Estimated functional relationship $\widetilde{ST}_i^w = f(x,y)$ | Adj. Coeff. of Determ. $R^2_{adj}(\widetilde{ST}_i^w, ST_i^w)$ |
|---|---|---|---|---|
| Infiltration | $f_S$ | - | $0.2985 - 0.8113x + 1.0443x^2 - 0.5203x^3$ | 0.905 |
| Quickflow | $f_S$ | $\Sigma P$ | $0.9044 - 3.4122x^2 + 2.6596x^3 - 4.771 \times 10^{-5}y - 0.001153xy + 0.001870x^2y$ | 0.953 |
| Evaporation | $f_S$ | - | $0.3835 - 0.7713x + 0.1945x^2 + 0.3964x^3$ | 0.915 |
| Snow Balance | $f_S$ | - | $-0.009051 + 0.4161x + 1.3796x^2 - 2.0661x^3$ | 0.926 |
| Convolution (srfc runoff) | $\overline{T}$ | $f_{cold}$ | $0.06531 - 0.00639x + 1.645 \times 10^{-4}x^2 - 0.0008165y + 4.104 \times 10^{-5}xy + 2.6508 \times 10^{-6}y^2$ | 0.657 |
| Potential Melt | $f_S$ | - | $-0.01494 + 0.8236x + 2.4265x^2 - 3.1523x^3$ | 0.950 |
| Percolation | $f_S$ | - | $0.2829 - 0.7275x + 0.8276x^2 - 0.3582x^3$ | 0.909 |
| Rain-Snow Partitioning | $f_S$ | $f_{cold}$ | $-0.001715 + 3.7710x - 0.002150y - 0.03638xy + 1.302 \times 10^{-5}y^2 + 8.753 \times 10^{-5}xy^2$ | 0.815 |
| Precipitation Correction | $f_S$ | $I_{m,r}$ | $0.07343 + 0.5829x^2 - 1.0106x^3 + 0.01122y^3 - 0.1677xy^2 + 0.5264x^2y$ | 0.809 |

Note. Results of the regression analysis identifying the functional relationships between predictors and the variance-weighted total Sobol' sensitivities $ST_i^w$ based on the results of the 3316 basins analyzed by xSSA. The regression is performed using polynomials with one predictor (up to degree three with at most six coefficients) and polynomials with two predictors (up to degree three with at most five coefficients). The one-predictor polynomial is used unless the use of a pair of predictors led to an improvement of the adjusted coefficients of determination $R^2_{adj}$ by at least 0.05. The basin characteristics used as predictors are derived from geophysical attributes and the meteorology available for each basin (1950 to 2010). The adjusted coefficients of determination $R^2_{adj}$ between the xSSA-derived sensitivities $ST_i^w$ and the predicted sensitivities $\widetilde{ST}_i^w$ are given in the last column. Description of predictors: $f_S$ is the fraction of precipitation that is snow [mm/mm], $\Sigma P$ is the annual sum of precipitation [mm], $\overline{T}$ is the annual average temperature in [°C], $f_{cold}$ is the average annual number of days below 0 °C, $I_{m,r}$ is the measure of seasonality ranging between [0,2].

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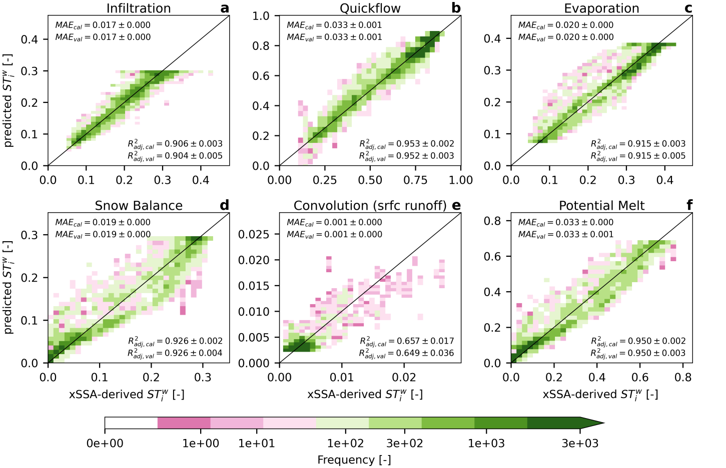


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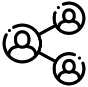
Data sharing &
re-usability



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## Challenge #4:

Extracting data from
previous studies

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juliane.mai@uwaterloo.ca | JulieeeMai

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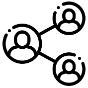
Data sharing & re-usability



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Extracting data from previous studies

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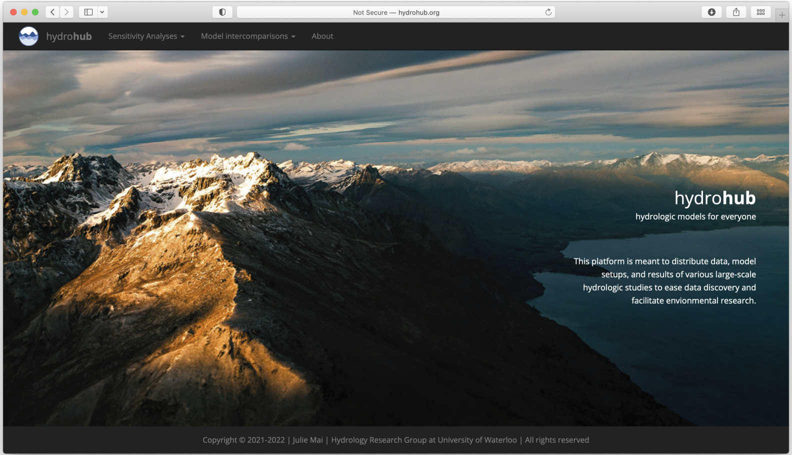
Web-based **interactive presentation** of inputs, setups, and results

# Challenge 4: Sharing of large datasets

## – Interactive websites –




Portal for interactive websites of large-scale projects: **hydrohub.org**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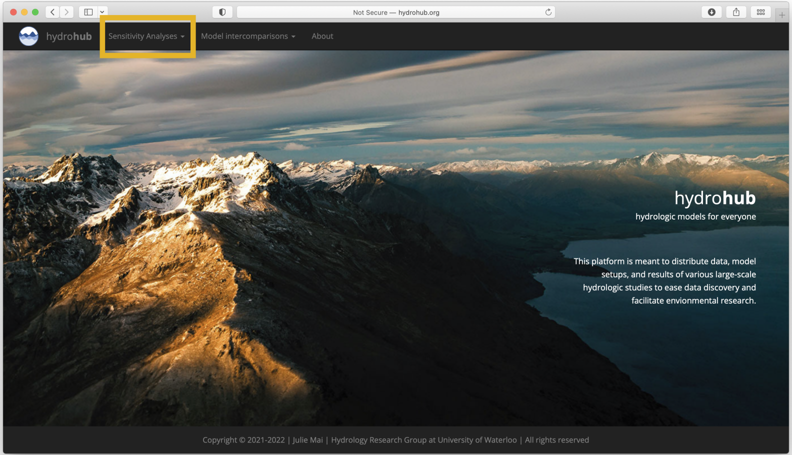


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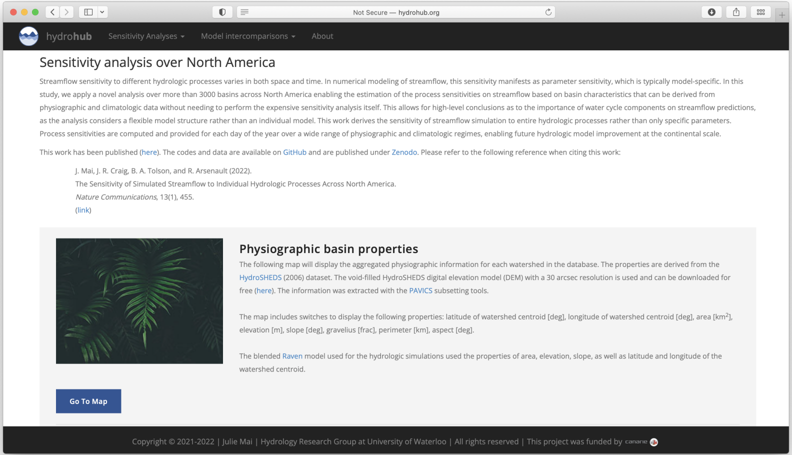


Details about SA over North America

&

List of available **interactive maps**


[5] Mai, J., Craig, J. R., Tolson, B. A., & Arsenault, R. (2022). *The sensitivity of simulated streamflow to individual hydrologic processes across North America.* Nature Communications, 13(1), 455. http://doi.org/10.1038/s41467-022-28010-7

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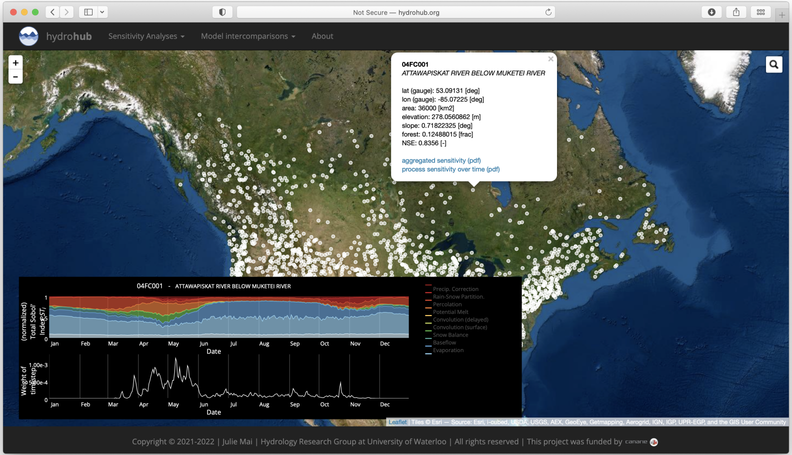


For example, time-dependent **sensitivity of processes** (incl. plots for download)


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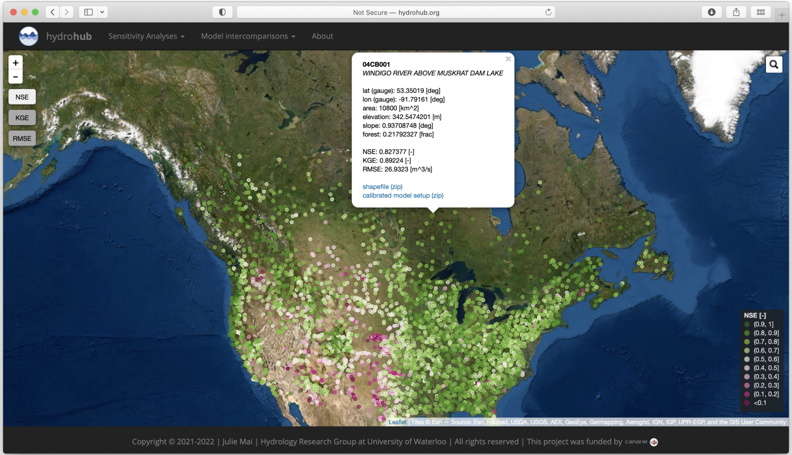


For example, calibration results (incl. **model setups** for download)

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# Summary

## – Challenges and new approaches in Sensitivity Analyses –

Define **SA for processes** (groups of parameters) rather than parameters only

### Challenge #1:

Limits process understanding

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Define model **blending multiple model structures** into one hyper-model

### Challenge #2:

Transferability to other models

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**Large-sample experiment** to obtain functional relationships to approx. sensitivities

### Challenge #3:

Sensitivities at new location

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Web-based **interactive presentation** of inputs, setups, and results

### Challenge #4:

Extracting data from previous studies

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Thanks for your attention!

Looking forward to your questions.

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