

Framework for time-varying uncertainty quantification and global sensitivity analysis

Use Case - LARSIM Model

LARSIM-Anwenderworkshop 2022

Ivana Jovanovic Buha

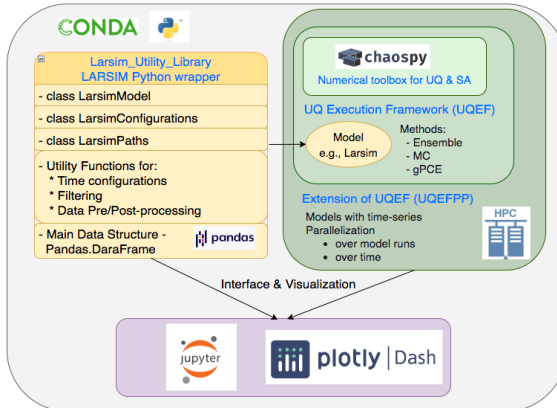
TUM Chair for Scientific Computing in Computer Science & LRZ & LfU Bayern
Hydro-BITS Project



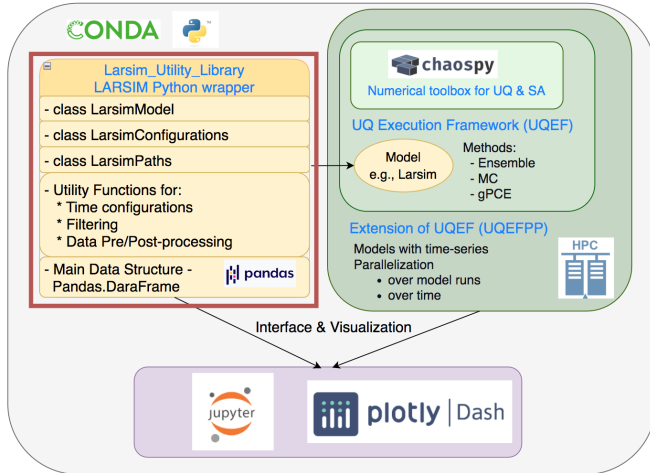
TUM Uhrenturm

Sketch of Python Framework for Data Analysis & UQ & SA

Use Case - LARSIM Model



LARSIM Python Wrapper & Data Analysis



LARSIM Python Wrapper & Data Analysis I

```
precipitation_DF = larsimInputOutputUtilities.any_lila_parser_toPandas(precipitation_file)
precipitation_DF.drop(columns=["Index_run"], inplace=True)
precipitation_DF
```

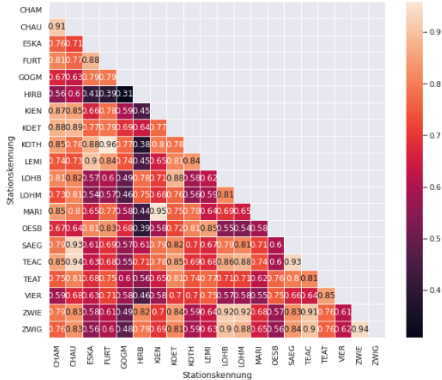
Stationskennung	Type	TimeStamp	Value
0	AHOL	n 2003-11-01 00:00:00	0.0
1	HAGE	n 2003-11-01 00:00:00	0.0
2	ALTE	n 2003-11-01 00:00:00	0.0
3	BERA	n 2003-11-01 00:00:00	0.0
4	BOGE	n 2003-11-01 00:00:00	0.0
...
6832315	POES	n 2018-01-01 23:00:00	0.0
6832316	ALMD	n 2018-01-01 23:00:00	0.0
6832317	EISZ	n 2018-01-01 23:00:00	0.2
6832318	KIRG	n 2018-01-01 23:00:00	0.0
6832319	ESCL	n 2018-01-01 23:00:00	0.0

6832320 rows x 4 columns

```
n_time_vs_stations_reduced.describe().transpose()
```

	count	mean	std	min	25%	50%	75%	max
Stationskennung								
AHOL	123988.0	0.080434	0.509341	0.0	0.0	0.0	0.0	41.37
ALTE	123781.0	0.079997	0.495976	0.0	0.0	0.0	0.0	59.17
BERA	124179.0	0.086166	0.484846	0.0	0.0	0.0	0.0	28.67
BOGE	124162.0	0.090110	0.509354	0.0	0.0	0.0	0.0	36.12
HAGE	124106.0	0.076225	0.476697	0.0	0.0	0.0	0.0	45.75
KELH	116803.0	0.078604	0.473264	0.0	0.0	0.0	0.0	30.83
KIBE	122192.0	0.108258	0.551743	0.0	0.0	0.0	0.0	34.42
KITE	122987.0	0.086367	0.504402	0.0	0.0	0.0	0.0	31.20
KOEF	122686.0	0.074154	0.485481	0.0	0.0	0.0	0.0	36.30
LAML	120349.0	0.125160	0.587278	0.0	0.0	0.0	0.0	33.13
LIND	112672.0	0.144519	0.669033	0.0	0.0	0.0	0.0	40.94
METT	112918.0	0.106285	0.550700	0.0	0.0	0.0	0.0	34.94
MOOS	120498.0	0.094245	0.479406	0.0	0.0	0.0	0.0	30.51
NABB	124032.0	0.075600	0.449435	0.0	0.0	0.0	0.0	25.80
NENB	116823.0	0.088651	0.494034	0.0	0.0	0.0	0.0	36.10
NEUH	120606.0	0.097862	0.520582	0.0	0.0	0.0	0.0	31.34
NITT	123995.0	0.083208	0.496404	0.0	0.0	0.0	0.0	31.80
OBEV	113716.0	0.081888	0.488048	0.0	0.0	0.0	0.0	32.72
OSTH	121262.0	0.090827	0.507465	0.0	0.0	0.0	0.0	53.23
POES	122954.0	0.082003	0.488182	0.0	0.0	0.0	0.0	27.70
REGG	124026.0	0.073788	0.451910	0.0	0.0	0.0	0.0	30.13
RODI	124129.0	0.082270	0.499960	0.0	0.0	0.0	0.0	39.84

LARSIM Python Wrapper & Data Analysis II



AutoCorrelation of Discharge Time-Signal for MARI station

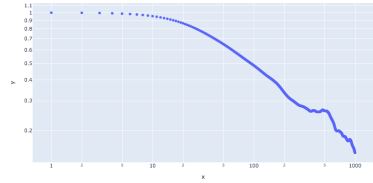
```

In [52]: print("MARI Q Autocorr Lag=1: {}".format(discharge_DF_MARI.Value.autocorr(lag=1)))
         print("MARI Q Autocorr Lag=1000: {}".format(discharge_DF_MARI.Value.autocorr(lag=1000)))

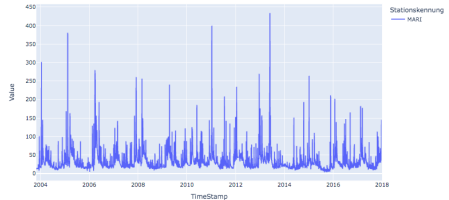
MARI Q Autocorr Lag=1: 0.999267861133339
MARI Q Autocorr Lag=1000: 0.1474019470162516
    
```

```

In [53]: # get how correlated are hourly measures of the discharge at MARI station
         list_of_autocorr = []
         for lag in range(1,1000):
             list_of_autocorr.append(discharge_DF_MARI.Value.autocorr(lag=lag))
         fig = plt.subplots(figsize=(10,10), gridspec_kw={'x_ticks': [1, 1000]})
         fig.update_layout(xaxis_type='log', yaxis_type='log')
         fig.show()
    
```



Measured Q MARI



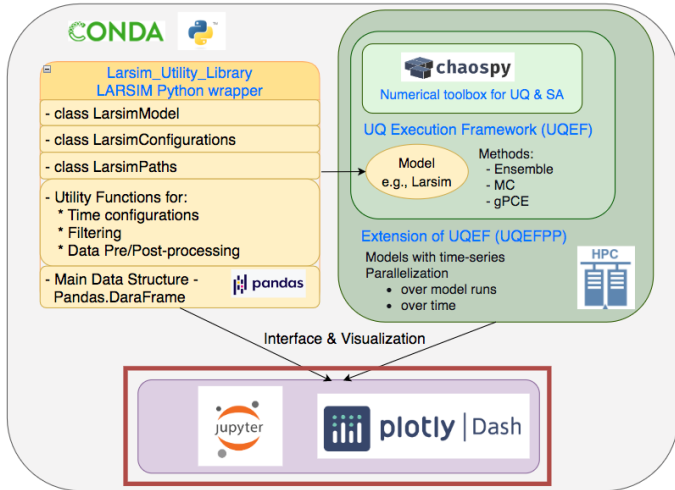
LARSIM Python Wrapper & Data Analysis III

```
result_DF_MARI = larsimDataPostProcessing.filterResultForStationAndTypeOfOutput\
                 (resultsDataFrame=result_array_of_tuples[0]['result_time_series'],\
                  station="MARI",\
                  type_of_output=['Abfluss Messung'])
result_DF_MARI
```

Index_run	Stationskennung	TimeStamp	Type	Value
59146	0	MARI 2013-03-03 05:00:00	Abfluss Messung + Vorhersage	35.766
59148	0	MARI 2013-03-03 06:00:00	Abfluss Messung + Vorhersage	35.935
59150	0	MARI 2013-03-03 07:00:00	Abfluss Messung + Vorhersage	36.113
59152	0	MARI 2013-03-03 08:00:00	Abfluss Messung + Vorhersage	36.275
59154	0	MARI 2013-03-03 09:00:00	Abfluss Messung + Vorhersage	36.395
59156	0	MARI 2013-03-03 10:00:00	Abfluss Messung + Vorhersage	36.470
59158	0	MARI 2013-03-03 11:00:00	Abfluss Messung + Vorhersage	36.518
59160	0	MARI 2013-03-03 12:00:00	Abfluss Messung + Vorhersage	36.556
59162	0	MARI 2013-03-03 13:00:00	Abfluss Messung + Vorhersage	36.594
59164	0	MARI 2013-03-03 14:00:00	Abfluss Messung + Vorhersage	36.631
59166	0	MARI 2013-03-03 15:00:00	Abfluss Messung + Vorhersage	36.660
59168	0	MARI 2013-03-03 16:00:00	Abfluss Messung + Vorhersage	36.679
...
191496	0	MARI 2013-05-31 12:00:00	Abfluss Messung + Vorhersage	80.470
191498	0	MARI 2013-05-31 13:00:00	Abfluss Messung + Vorhersage	81.990
191500	0	MARI 2013-05-31 14:00:00	Abfluss Messung + Vorhersage	83.840
191502	0	MARI 2013-05-31 15:00:00	Abfluss Messung + Vorhersage	86.080
191504	0	MARI 2013-05-31 16:00:00	Abfluss Messung + Vorhersage	88.710
191506	0	MARI 2013-05-31 17:00:00	Abfluss Messung + Vorhersage	91.750
191508	0	MARI 2013-05-31 18:00:00	Abfluss Messung + Vorhersage	95.410
191510	0	MARI 2013-05-31 19:00:00	Abfluss Messung + Vorhersage	100.670
191512	0	MARI 2013-05-31 20:00:00	Abfluss Messung + Vorhersage	107.640
191514	0	MARI 2013-05-31 21:00:00	Abfluss Messung + Vorhersage	114.890
191516	0	MARI 2013-05-31 22:00:00	Abfluss Messung + Vorhersage	122.080
191518	0	MARI 2013-05-31 23:00:00	Abfluss Messung + Vorhersage	128.820

2155 rows x 5 columns

Interface for LARSIM Python Wrapper - Dash Application



Interface for LARSIM Python Wrapper - Dash Application I

Automatic and **adaptable** LARSIM simulation runs

Features: inspecting the forcing and output data, changing parameters, computing GoF functions, etc.



Interface for LARSIM Python Wrapper - Dash Application II

Show Old Simulations Do not show Simulations

Stations

TDR Rain Station Station with Reservoir

WHM [State Data]

Parameters and GoF Tabel

	Index	max	min	std	coefdet	coefadj	coefadj2	coefadj3	coefadj4	coefadj5	coefadj6	coefadj7	coefadj8	coefadj9	coefadj10	coefadj11	coefadj12	coefadj13	coefadj14	coefadj15		
R	9682	24.24932772	1.462289239	0.009292407	0	0.9995	0.9997	0.9998	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	
M	9598	14.3348987389	0.889264616	0.007370444	0	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999

The path to the configuration file you specified

```
g:\project\gms\larsim\python\larsim\configurations\larsim_main.py
```

Set the warm up period

Choose warm up duration:

Warm-up duration: 60h

Set Larsim Parameters

Run simulation without changing any parameters
 Change parameters of the simulation
 Run feasible Sim. & MS

Specify folder to save results

Result folder:

The output of the simulation will be saved in the following folder:

```
g:\project\gms\larsim\python\larsim\configurations\larsim_main.py
```

Select Discharge Station

Select GoF

Model Run (.Log)
 You have just run the simulation with predefined parameters in larsim.py and larsim.py

Interface for LARSIM Python Wrapper - Dash Application III

Set Larsim Parameters

Run simulation without changing any parameters
 Change parameters of the simulation
 Run Ensamble Sim. & UQ

+ ADD NEW SET OF PARAMETERS

ID:1

Tape35 Parameters:

all x

<input type="checkbox"/> EQB:	<input type="checkbox"/> EQI:	<input type="checkbox"/> EQD:
<input type="text" value="40000"/>	<input type="text" value="1000"/>	<input type="text" value="450"/>
<input type="checkbox"/> EQD2:	<input type="checkbox"/> A2:	<input type="checkbox"/> BSF:
<input type="text" value="250"/>	<input type="text" value="1.5"/>	<input type="text" value="0.3"/>
<input type="checkbox"/> beta:	<input type="checkbox"/> Dmin:	<input type="checkbox"/> Dmax:
<input type="text" value="0.012"/>	<input type="text" value="5"/>	<input type="text" value="1"/>
<input type="checkbox"/> KG:	<input type="checkbox"/> EKM:	<input type="checkbox"/> EKL:
<input type="text" value="0.93"/>	<input type="text" value="0.9"/>	<input type="text" value="0.9"/>
<input type="checkbox"/> EKR:		
<input type="text" value="0.9"/>		

LAI Parameters:

<input type="checkbox"/> Acker:	<input type="text" value="Select..."/>	<input type="text" value="5.2"/>
<input type="checkbox"/> locker baumbest.:	<input type="text" value="Select..."/>	<input type="text" value="7.5"/>
<input type="checkbox"/> Mischwald:	<input type="text" value="Select..."/>	<input type="text" value="11"/>
<input type="checkbox"/> Laubwald:	<input type="text" value="Select..."/>	<input type="text" value="11"/>

SUBMIT ENSEMBLE OF THE PARAMETERS

Set Larsim Parameters

Run simulation without changing any parameters
 Change parameters of the simulation
 Run Ensamble Sim. & UQ

+ ADD NEW UNCERTAIN PARAMETER

BSF x

Uniform x

lower	upper
<input type="text" value="0.01"/>	<input type="text" value="0.5"/>
mu	sigma
<input type="text" value="0.3"/>	<input type="text" value="0.1"/>
Depends on v	
Direction of Depen. v	

UQ Setting

UQ Method

Number of MC Evaluations

Sampling Rule

Sample from standard dist?

Quadrature Rule

Quadrature Order

gPCE Poly. Order

gPCE Poly Rule

gPCE Poly Normalized?

Sparse Quadrature?

MPI Solver?

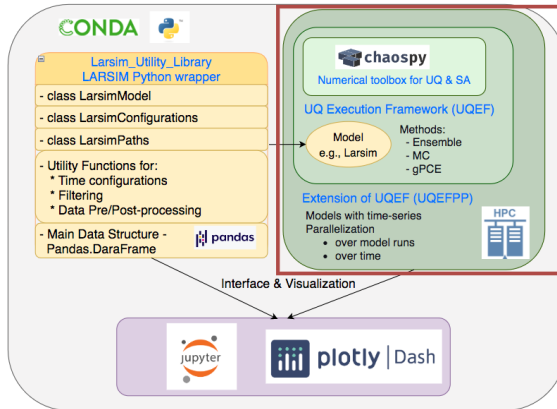
Mpi Method?

Disable Statistics?

SUBMIT ENSEMBLE OF THE PARAMETERS

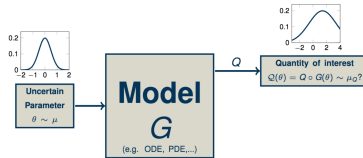
Uncertainty Quantification Execution Framework (UQEF) & UQEFPP

For efficient, comprehensive, time-varying uncertainty quantification and global sensitivity analysis



General Story - UQ & SA & Environmental models

UQ - Quantifying uncertainty in the output of the model; Forward propagation of the input uncertainty to the uncertainty in the model output or some QoI [Smith 2013]



SA - Apportioning output uncertainty to the different input factors; [Razavi et al. 2021]

Reasons for UQ & SA:

- Scientific discovery, explore causalities
- Decision support
- Support and complement model calibration
- Ranking - rank input factors according to the contribution on the output
- Screening - identifying (ir)relevant input factors (i.e., dimensionality reduction)
- Mapping - relating regions of the inputs and outputs

UQEF & UQEFPP Functionalities I

Methods

1. Ensemble runs with predefined values
2. Monte Carlo methods (i.e., sampling strategies - Halton, Sobol, Latin Hypercube)
3. Generalized Polynomial Chaos Expansion (gPCE)
 - Transformation - from dependent variables to independent
 - Point collocation method
 - Pseudo-spectral projection with (sparse) quadrature rule

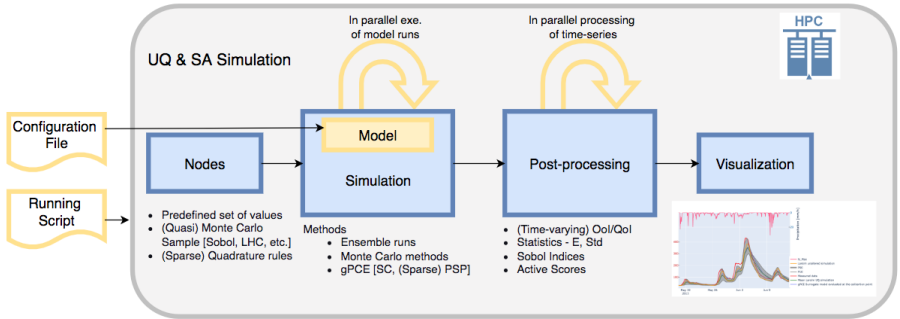
Definition of Ool and Qol

1. (Temporally varying) model output (e.g., discharge)
2. Some objective function / goodness-of-fit (i.e., NSE, RMSE) summing up the whole period, or computed in the sliding window manner

Postprocessing

1. Statistics - mean, std
2. Surrogate gPCE model
3. Sensitivity Analysis
 - Local, gradient-based analysis
 - Global Variance-based - Sobol Indices
 - Global active scores indices
4. Different visualization methods

UQEF & UQEFPP Functionalities II



General Polynomial Chaos Expansion (gPCE) I

$$f(t, \theta) \approx \sum_{n=0}^{N-1} \hat{f}_n(t) \phi_n(\theta) = \sum_{n=0}^{N-1} \langle f(t, \theta), \phi_n(\theta) \rangle_{\rho} \phi_n(\theta) \quad (1)$$

Compute statistical properties of Ool

$$E[f(t, \theta)] \approx \hat{f}_0(t) \quad (2)$$

$$\text{Var}[f(t, \theta)] \approx \sum_{n=1}^{N-1} \hat{f}_n^2(t) \quad (3)$$

The Pseudo-spectral Projection (PSP) Method

- Use quadrature rule to compute coefficients [Constantine, Eldred, and Phipps 2012]

$$\hat{f}_n(t) \approx \sum_{k=0}^{K-1} f(t, x_k) \phi_n(x_k) w_k \quad (4)$$

- nodes, weights $\{x_k, w_k\}_{k=0}^{K-1}$ chosen w.r.t. the input probability distribution $\rho(\theta)$
- evaluate the forward model $f(t, \theta)$ at each x_k !
- From 1-d to d -dimensional space via tensor product formulations
- Sparse grids - minimize the number of deterministic forward simulations

Sensitivity Analysis I

Problem

- How sensitive is $f(t, \theta)$ (or some other QoI) to changes in $\theta \in \mathbf{X}$?
- What is the relative contribution of $\theta_i, i = 1, \dots, d$ to the output uncertainty?

Local sensitivity analysis

- assesses the “sensitivity” around some nominal value, e.g. using gradients of output w.r.t. inputs

Global sensitivity analysis

- based on analyzing a suitable “measure” of uncertainty, e.g. the variance

One-at-Time (OAT) vs. All-at-Time (AAT)

Time-varying vs. Aggregation over-time

Global Variance-based Sensitivity Analysis II

Sobol' Indices (SI) [Bauwens, Nossent, and Elsen 2011; Saltelli et al. 2010]

First order SI

fraction of the model output variance that would disappear on average if θ_i is fixed

$$S_i(t) = \frac{\text{Var}[E[f|\theta_i]]}{\text{Var}[f(\theta)]} = \frac{\text{Var}[f] - E[\text{Var}[f|\theta_i]]}{\text{Var}[f]} = \frac{V_i(t)}{\text{Var}[f]} \quad (5)$$

Total order SI evaluate the total effect of an input parameter

$$S_i^T(t) = \frac{E[\text{Var}[f|\theta_{-i}]]}{\text{Var}[f]} = \frac{\sum_{n \in A_i} V_n}{\text{Var}[f]} = 1 - \frac{V_{-i}(t)}{\text{Var}[f]} \quad (6)$$

- Computing by MC samples $\Rightarrow \#model_runs = N(d + 2)$

SI and gPCE [Sudret 2008]

$$S_i^T(t) \approx \frac{\sum_{n \in A_i} \hat{f}_n^2(t)}{\sum_{n=1}^{N-1} \hat{f}_n^2(t)} \quad (7)$$

UQ & SA in Hydrology

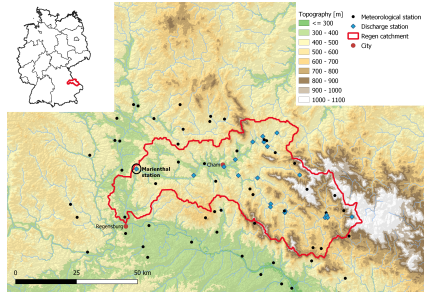
- Variogram Analysis of Response Surfaces (VARS Tool) [Bajracharya et al. 2020; Gupta and Razavi 2018; Razavi 2016]
- Distribution-based sensitivity analysis - PAWN & Sensitivity Analysis For Everybody - A Matlab toolbox for Global Sensitivity Analysis - SAFE [Pianosi, Sarrazin, and Wagener 2015; Pianosi and Wagener 2018]
- Fourier based sensitivity analysis - FAST [Collins and Avissar 1994; Koo et al. 2020; McRae, Tilden, and Seinfeld 1982]
- gPCE and stochastic collocation or PSP approach [Fan et al. n.d.; Miller et al. n.d.]

Important aspects of our framework:

- Different choice of the Ool/Qol
- Sparse Grid based PSP - optimizing the number of model runs [Buha et al. 2022; Obersteiner 2020]
- Parallel execution of independent model runs [Künzner 2021]
- Parallel processing over time

Study Case - Regen Catchment I

Catchment size: 2613,40km²
 Gauge zero point: 336,95mNHN
 River chainage: 29.54km
 Data from 2003-2018
 1h temporal and 1km² spatial resolution
 Data source - LfU Bayern



Study Case - Regen Catchment II

UQ & SA Scenario:

- Examining the impact of 5 model parameters on model output (i.e., discharge) under high-flow conditions
- Hindcasting past data (i.e., measured forcing data)
- Simultaneously changing the parameter values over the whole catchment

Goal:

- Estimation of predictive model uncertainty due to assumed uncertainty in 5 model parameters
- Get a better insight into the model parameters -> model output relation
- Get the posterior distribution of the parameters conditioned on some objective function (e.g., goodness-of-fit)

```

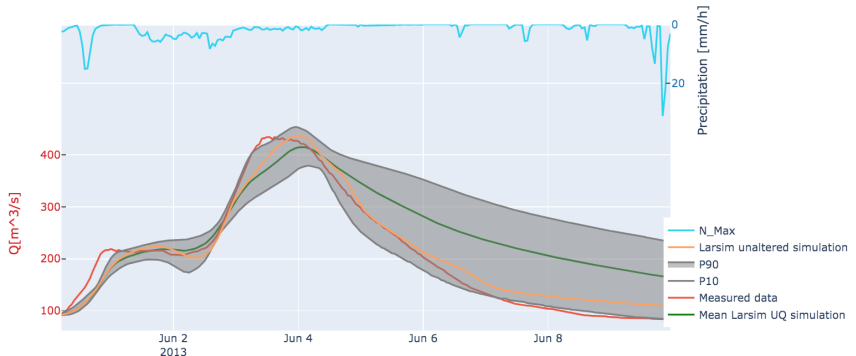
"parameters": [
  {
    "name": "EQD",
    "type": "tape35",
    "distribution": "Uniform",
    "lower": 0,
    "upper": 1,
    "lower_limit": 50,
    "upper_limit": 5000,
    "depends_on": "EQI",
    "direction": "decreasing",
    "default": 450.0
  },
  {
    "name": "EQD2",
    "type": "tape35",
    "distribution": "Uniform",
    "lower": 0,
    "upper": 1,
    "lower_limit": 10,
    "upper_limit": 1000,
    "depends_on": "EQD",
    "direction": "decreasing",
    "default": 250.0
  },
  {
    "name": "A2",
    "type": "tape35",
    "distribution": "Uniform",
    "mu": 1.5,
    "sigma": 0.75,
    "lower": 0.5,
    "upper": 4.0,
    "lower_limit": 0.5,
    "upper_limit": 4.0,
    "default": 1.5
  },
  {
    "name": "BSF",
    "type": "tape35",
    "distribution": "Uniform",
    "mu": 0.3,
    "sigma": 0.1,
    "lower": 0.01,
    "upper": 0.5,
    "lower_limit": 0.01,
    "upper_limit": 0.5,
    "default": 0.3
  },
  {
    "name": "Dmax",
    "type": "tape35",
    "distribution": "Uniform",
    "lower": 0.06,
    "upper": 10,
    "lower_limit": 0.06,
    "upper_limit": 10,
    "default": 1.0
  }
]

```

Visualization of the results I

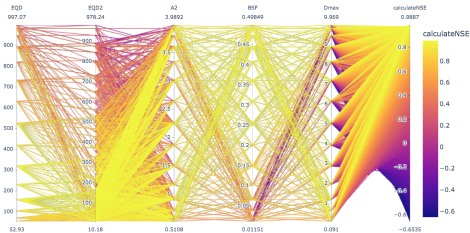
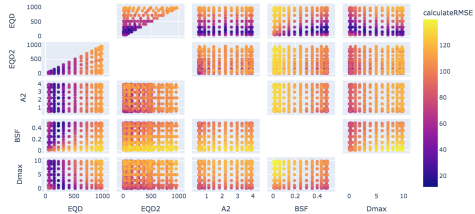
Time-varying influence of 5 parameters on model predictions under the high-flow conditions

- **QoI:** Hourly discharge values
- **Method:** gPCE (Kronrod-Patterson sparse quadrature) $q = 11$; $p = 6$
- **#model evaluations:** 17103
- **Computation time:** ~ 2 hours on 4 compute nodes (28CPU+55GB RAM per node)



Visualization of the results II

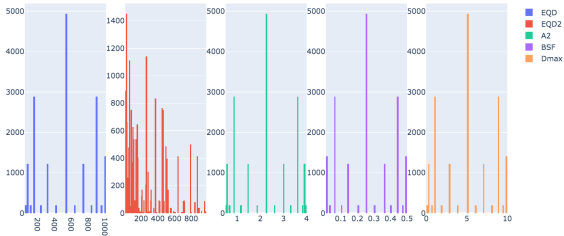
Parameters vs. GoF



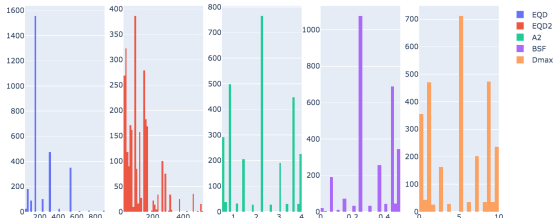
Visualization of the results IV

Parameters prior and “posterior” distribution

Prior Distribution of the Parameters

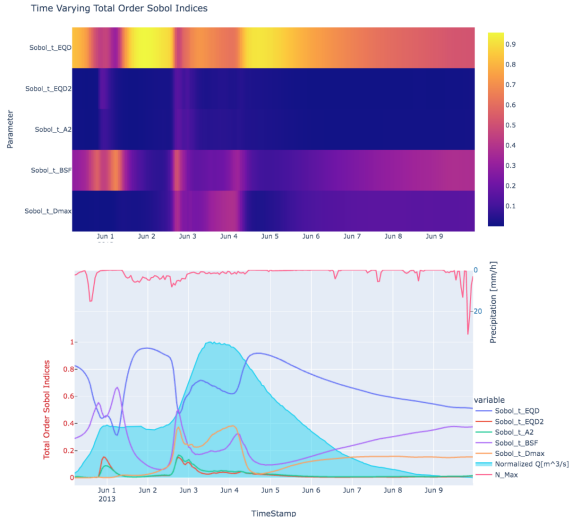


Posterior Distribution of the Parameters - conditioned on 'good' LogNSE



Visualization of the results V

Sobol Total SI over time



Conclusion and Future Works

- Proof of concept - we can run many LARSIM runs in a reasonable time
- Useful prior calibration tool (i.e., getting a better insight into the model parameters -> model output relation)
- Produce surrogate models in the parameter space, e.g., gPCE or Active Subspaces

Next steps...





- Account for distributed model parameters
- Account for other sources of the uncertainty, e.g., (spatial) input data
- Test learned surrogate models and uncertain bands on a future forecasting events and measure their predictive skills Leandro et al. 2019

Note: Frameworks UQEF & UQEFPP Will be soon open-source on GitHub/GitLab





Thank you!

Please feel free to contact me if you have further questions
ivana.jovanovic@tum.de





References I

-  Bajracharya, Ajay et al. (2020). "Time variant sensitivity analysis of hydrological model parameters in a cold region using flow signatures". In: [Water \(Switzerland\)](#) 12.4. ISSN: 20734441. DOI: 10.3390/W12040961.
-  Bauwens, Willy, Jiri Nossent, and Pieter Elsen (2011). "Sobol' sensitivity analysis of a complex environmental model". In: DOI: 10.1016/j.envsoft.2011.08.010. URL: www.elsevier.com/locate/envsoft.
-  Buha, Ivana Jovanovic et al. (Apr. 2022). "Efficient Uncertainty Quantification and Global Time-Varying Sensitivity Analysis Using the Spatially Adaptive Combination Technique". en. In: [SIAM Conference on Uncertainty Quantification \(UQ22\)](#). SIAM. Atlanta, Georgia: SIAM.
-  Collins, Dan and Roni Avissar (June 1994). "An Evaluation with the Fourier Amplitude Sensitivity Test (FAST) of Which Land-Surface Parameters Are of Greatest Importance in Atmospheric Modeling". In: [Journal of Climate](#) 7. DOI: 10.1175/1520-0442(1994)007<0681:AEWTFA>2.0.CO;2.





References II

-  Constantine, Paul G, Michael S Eldred, and Eric T Phipps (2012). “Sparse pseudospectral approximation method”. In: [Computer Methods in Applied Mechanics and Engineering](#) 229, pp. 1–12.
-  Fan, Y R et al. (n.d.). “Parameter uncertainty and temporal dynamics of sensitivity for hydrologic models: A hybrid sequential data assimilation and probabilistic collocation method”. In: (). DOI: [10.1016/j.envsoft.2016.09.012](https://doi.org/10.1016/j.envsoft.2016.09.012). URL: <http://dx.doi.org/10.1016/j.envsoft.2016.09.012>.
-  Gupta, Hoshin V. and Saman Razavi (2018). “Revisiting the Basis of Sensitivity Analysis for Dynamical Earth System Models”. In: [Water Resources Research](#) 54.11, pp. 8692–8717. ISSN: 19447973. DOI: [10.1029/2018WR022668](https://doi.org/10.1029/2018WR022668). URL: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2018WR022668>.
-  Koo, Hyeongmo et al. (May 2020). “A global sensitivity analysis approach for identifying critical sources of uncertainty in non-identifiable, spatially distributed environmental models: A holistic analysis applied to SWAT for input datasets and model parameters”. In: [Environmental Modelling and Software](#) 127. ISSN: 13648152. DOI: [10.1016/j.envsoft.2020.104676](https://doi.org/10.1016/j.envsoft.2020.104676).

References III

-  Künzner, Florian (2021). “Efficient non-intrusive uncertainty quantification for large-scale simulation scenarios”. *Dissertation*. München: Technische Universität München.
-  Leandro, J. et al. (2019). “Forecasting upper and lower uncertainty bands of river flood discharges with high predictive skill”. In: *Journal of Hydrology* 576. February, pp. 749–763. ISSN: 00221694. DOI: 10.1016/j.jhydro1.2019.06.052. URL: <https://doi.org/10.1016/j.jhydro1.2019.06.052>.
-  McRae, Gregory J., James W. Tilden, and John H. Seinfeld (1982). “Global sensitivity analysis—a computational implementation of the Fourier Amplitude Sensitivity Test (FAST)”. In: *Computers Chemical Engineering* 6.1, pp. 15–25. ISSN: 0098-1354. DOI: [https://doi.org/10.1016/0098-1354\(82\)80003-3](https://doi.org/10.1016/0098-1354(82)80003-3). URL: <https://www.sciencedirect.com/science/article/pii/0098135482800033>.
-  Miller, K L et al. (n.d.). Efficient Uncertainty Quantification in Fully-Integrated Surface and Subsurface Hydrology. Tech. rep.


References IV

-  Obersteiner, Michael (2020). SparseSpACE - The Sparse Grid Spatially Adaptive Combination Environment. <https://github.com/obersteiner/sparseSpACE>.
-  Pianosi, Francesca, Fanny Sarrazin, and Thorsten Wagener (Aug. 2015). “A Matlab toolbox for Global Sensitivity Analysis”. In: [Environmental Modelling and Software](#) 70, pp. 80–85. ISSN: 13648152. DOI: 10.1016/j.envsoft.2015.04.009.
-  Pianosi, Francesca and Thorsten Wagener (Oct. 2018). “Distribution-based sensitivity analysis from a generic input-output sample”. In: [Environmental Modelling and Software](#) 108, pp. 197–207. ISSN: 13648152. DOI: 10.1016/j.envsoft.2018.07.019.
-  Razavi, Saman (2016). “A new framework for comprehensive, robust, and efficient global sensitivity analysis: 1. Theory IMPC: Integrated Modelling Program for Canada View project Changing Cold Regions Network (CCRN) View project”. In: DOI: 10.1002/2015WR017558. URL: <https://www.researchgate.net/publication/287149711>.

References V

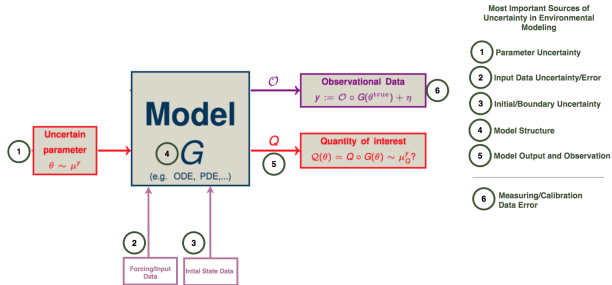
-  Razavi, Saman et al. (Mar. 2021). “The Future of Sensitivity Analysis: An essential discipline for systems modeling and policy support”. In: Environmental Modelling and Software 137, p. 104954. ISSN: 13648152. DOI: [10.1016/j.envsoft.2020.104954](https://doi.org/10.1016/j.envsoft.2020.104954).
-  Saltelli, Andrea et al. (2010). “Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index”. In: Computer Physics Communications 181.2, pp. 259–270. ISSN: 0010-4655. DOI: <https://doi.org/10.1016/j.cpc.2009.09.018>. URL: <https://www.sciencedirect.com/science/article/pii/S0010465509003087>.
-  Smith, Ralph C (2013). Uncertainty quantification: theory, implementation, and applications. Vol. 12. Siam.
-  Sudret, Bruno (2008). “Global sensitivity analysis using polynomial chaos expansions”. In: Reliability Engineering and System Safety 93, pp. 964–979. ISSN: 09518320. DOI: [10.1016/j.ress.2007.04.002](https://doi.org/10.1016/j.ress.2007.04.002).

References VI

-  Xiu, D and G E Karniadakis (2002). “The Wiener-Askey Polynomial Chaos for Stochastic Differential Equations”. In: [SIAM Journal of Scientific Computing](#) 24, pp. 619–644.

Extra Slides

General Story - UQ & SA & Environmental models I



Terms of Interest:

- Uncertain Inputs, e.g., parameters, forcing data, initial state, etc.
- Output of Interest (Ool), e.g., any (spatio-temporal) model response
- Quantity of interest (Qol), e.g., objective function, goodness-of-fit, etc.

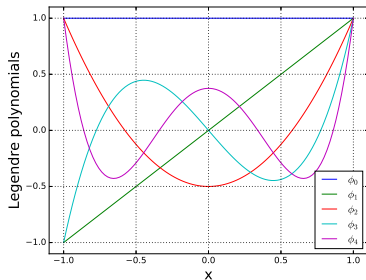
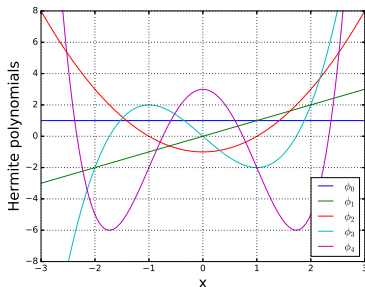
General Polynomial Chaos Expansion (gPCE) I

- Approximate a random variable $f(t, \theta)$ by truncated expansion of orthogonal polynomials (analogy with Fourier series) [Xiu and Karniadakis 2002]

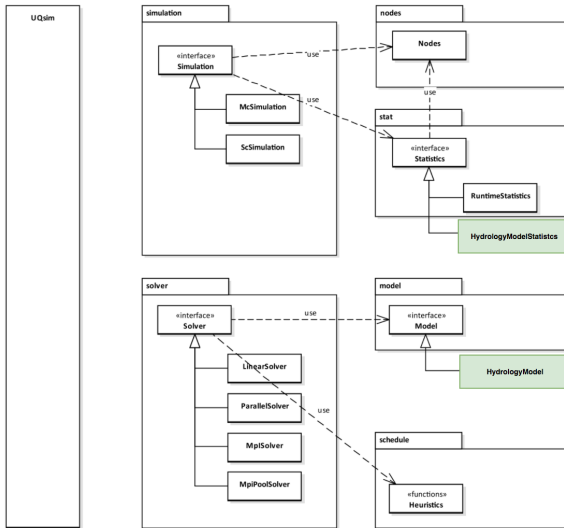
$$f(t, \theta) = \sum_{n=0}^{\infty} \hat{f}_n(t) \phi_n(\theta) \approx \sum_{n=0}^{N-1} \hat{f}_n(t) \phi_n(\theta) \quad (8)$$

- type of polynomials chosen w.r.t. parameter distribution $\rho(\theta)$**
- exploit orthonormality of the underlying basis

$$\hat{f}_n(t) = \langle f(t, \theta), \phi_n(\theta) \rangle_{\rho} = \int_{\Omega} f(t, \theta) \phi_n(\theta) \rho(\theta) d\theta \quad (9)$$

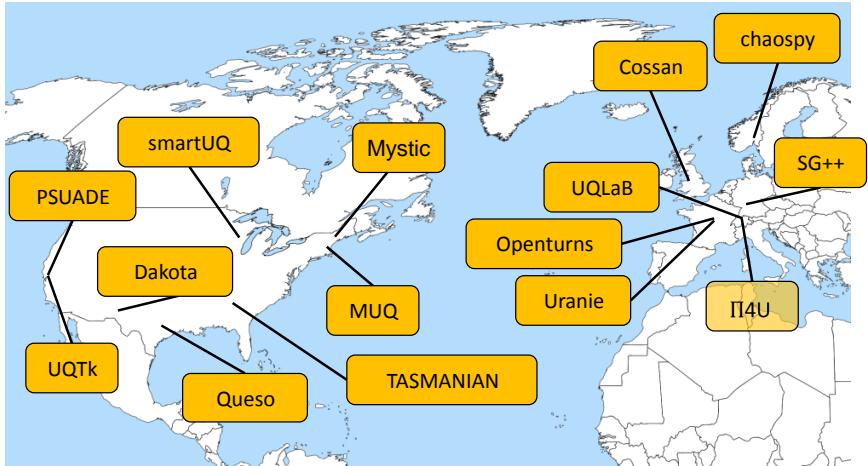


Sketch of our In-house software solution



Our software relies on Chaospy library, UQEF library Künzner 2021, and other Python libraries (e.g., mpi4py, Pandas, Plotly)

World of UQ Software - No need to code from scratch



source of world map: <http://en.wikipedia.org>

SIAM conference UQ 18, minisymposia 88, 102, 115, and 128: Software for UQ, Tobias Neckel & Dirk Pflüger
 see also https://www5.in.tum.de/wiki/index.php/SIAMUQ18_-_Slides_Minisymph_Software4UQ

Study Case - Regen Catchment

UQ & SA Scenario:

- Examining the impact of 5 model parameters on model output (i.e., discharge) under high-flow conditions

Parameters:

- EQD - Retaining constant of the slow runoff storage
- EQD2 - Retaining constant of the fast runoff storage
- Dmax - maximum drainage of the soil storage at filling level
- A2 - Threshold value of the fast and slow direct runoff
- BSF - Exponent of the soil moisture saturation area function