Tobias K Andersen, Xiangzhen Kong

Parallel sensitivity and auto-calibration tool (parsac) tutorial

Parsac
Parallel sensitivity and auto-calibration Tool

parsac is a Python package for sensitivity analysis and auto-calibration in parallel. It is designed for analysis of models that take significant time to run. It works with models that are run by calling one binary, that use text-based configuration files based on yaml or Fortran namelists, and that write their output to netcdf.

Developed by Jorn Bruggeman and Karsten Bolding.

Source code: https://github.com/BoldingBruggeman/parsac

Installation: pip install parsac --user (in your Python console window)

Auto-calibration

Brief intro to auto-cal with parsac

Auto-cal iteration

1) **define/update** parameter space and observations

2) **run** auto-calibration via parsac

3) **analyze** calibration results

Brief intro to auto-cal with parsac

Auto-cal iteration

1) **define/update** parameter space and observations

U:\20-PostDoc\0-Ravn\model_setup\dennis_2020_version\parsac\wet_cal.xml - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

wet_cal.xml

```xml
<config xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespaceSchemaLocation="../client/config.xsd">
  <transports>
    <transport type="sqlite" path="LakeRavn.db"/>
  </transports>
  <executable path="E:/Model_setups/GOTM-WET/Ravn/gotm.exe"/>
  <setup path="../"/>
  <parameters>
  <!-- all steps include plus/minus 40% of the default value, be cautious of sediment initialization values -->
  <!-- STEP 1A: Calibration of physical dynamics - TEMPERATURE -->
  <!-- xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx -->
  <!-- Physical parameters             -->
  <!-- xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx -->
  <!-- scale factor for heat fluxes  -->
  <!--<parameter file="gotm.yaml"   variable="surface/fluxes/heat/scale_factor" minimum="0.93" maximum="1.0"/> -->
  <!-- scale factor for short-wave radiation -->
  <parameter file="gotm.yaml"   variable="surface/meteo/swr/scale_factor" minimum="0.9" maximum="1.0"/>
  <!-- wind speed in West-East direction @ 10 m -->
  <parameter file="gotm.yaml"   variable="surface/meteo/u10/scale_factor" minimum="1.1" maximum="1.22"/>
  <!-- wind speed in North-South direction @ 10 m -->
  <parameter file="gotm.yaml"   variable="surface/meteo/v10/scale_factor" minimum="0.75" maximum="0.9"/>
  <!-- minimum turbulent kinetic energy [m^2/s^2; min=0.0; default=1.00000000E-10] -->
  <parameter file="gotm.yaml"   variable="turbulence/turb_param/k_min" minimum="0.00000001" maximum="0.0000010" logscale="True"/>
  <!-- non-visible fraction of shortwave radiation [fraction; min=0.0; max=1.0; default=0.7] -->
  <parameter file="gotm.yaml"   variable="light_extinction/A/constant_value" minimum="0.50" maximum="0.56"/>
  <!-- e-folding depth of non-visible shortwave radiation [m; min=0.0; default=0.4] -->
  <parameter file="gotm.yaml"   variable="light_extinction/g1/constant_value" minimum="0.1" maximum="0.8"/>
  <!-- e-folding depth of visible shortwave radiation [m; min=0.0; default=8.0] -->
  <parameter file="gotm.yaml"   variable="light_extinction/g2/constant_value" minimum="6.0" maximum="11.0"/>

```

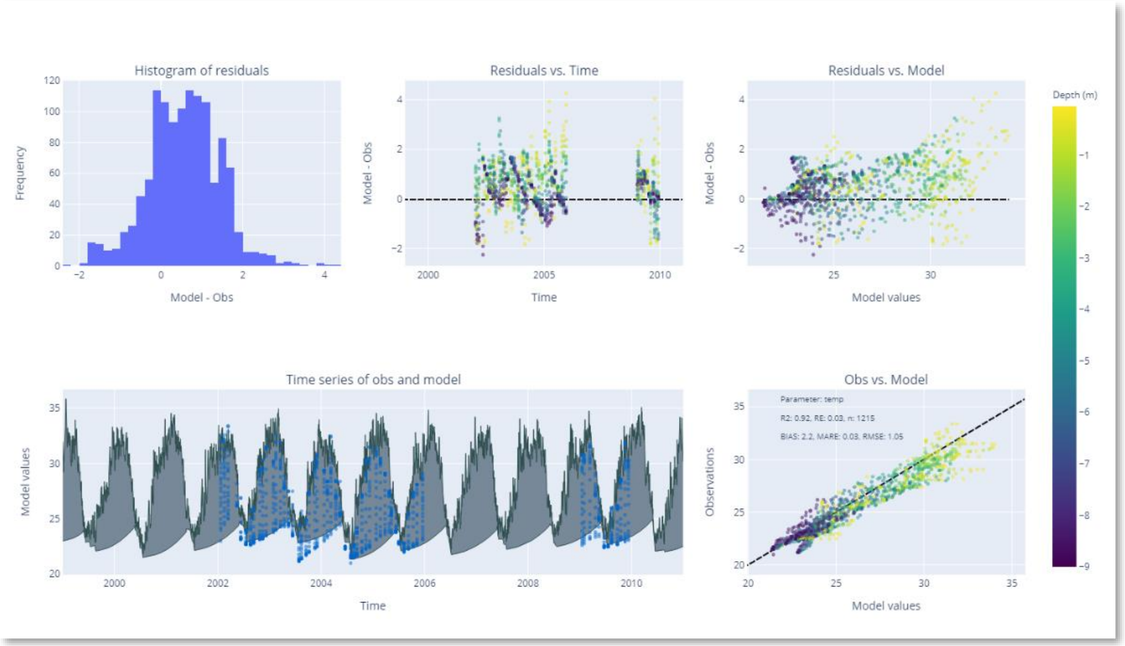
Brief intro to auto-cal with parsa

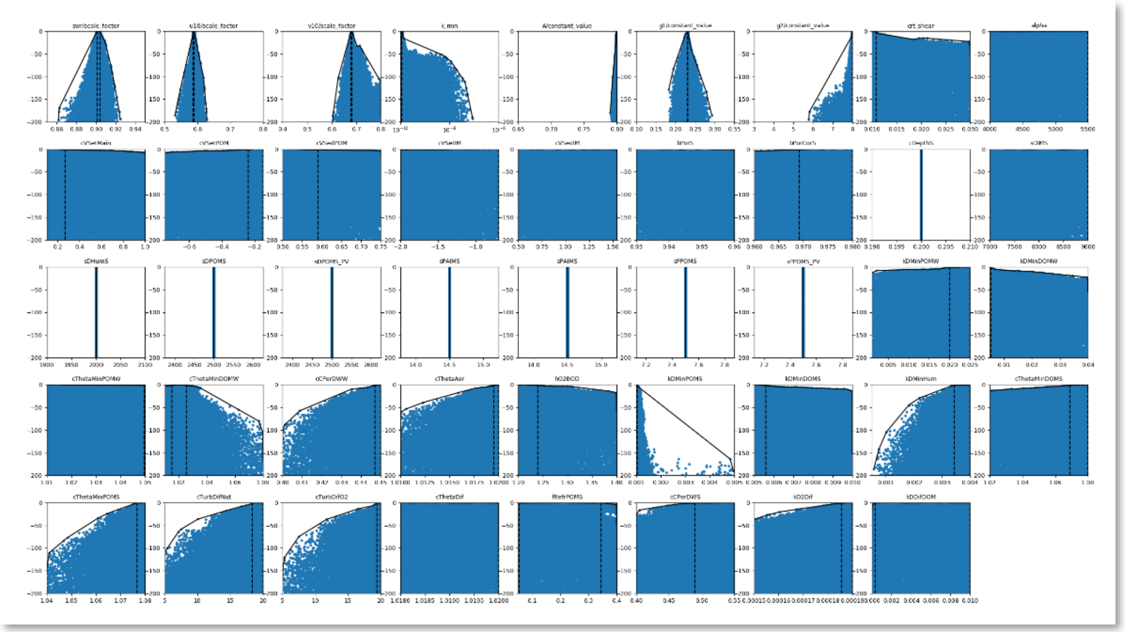
Auto-cal iteration

1) **define/update** parameter space and observations

2) **run** auto-calibration via parsac

3) **analyze** calibration results





Brief intro to auto-cal with parsac

Auto-cal iteration

1) **define/update** parameter space and observations

2) **run** auto-calibration via parsac

3) **analyze** calibration results

C:\Users\tkan\OneDrive - Danmarks Tekniske Universitet\WET_teaching material\Nanjing_workshop-2024\files\wet_dashahe-step1.xml - Notepad++

wet_dashahe-step1.xml

```xml
<config xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespaceSchemaLocation="../client/config.xsd">
  <transports>
    <transport type="sqlite" path="LakeDashahe_step5.db"/>
  </transports>
  <executable path="../gotm_release.exe"/>
  <setup path="../"/>
  <parameters>
  <!-- all steps include plus/minus 40% of the default value or based on user experience -->
  <!-- be cautious of sediment initialization values -->
  <!-- STEP 1A: Calibration of physical dynamics - TEMPERATURE -->
  <!-- BIOSHADE IN GOTM.YAML = FALSE -->
  <!-- xxxxxxxxxxxxxxxxxxxxxxxxxxxxxx -->
  <!-- Physical parameters            -->
  <!-- xxxxxxxxxxxxxxxxxxxxxxxxxxxxxx -->
  <!-- wind speed in West-East direction @ 10 m -->
  <parameter file="gotm.yaml"   variable="surface/meteo/u10/scale_factor" minimum="0.6" maximum="1.4"/>
  <!-- wind speed in North-South direction @ 10 m -->
  <parameter file="gotm.yaml"   variable="surface/meteo/v10/scale_factor" minimum="0.6" maximum="1.4"/>
  <!-- shortwave radiation -->
  <parameter file="gotm.yaml"   variable="surface/meteo/swr/scale_factor" minimum="0.6" maximum="1.4"/>
  <!-- cloud cover, can be calibrated -->
  <!-- <parameter file="gotm.yaml"   variable="surface/meteo/cloud/scale_factor" minimum="1.0" maximum="1.0"/> -->
  <!-- minimum turbulent kinetic energy [m^2/s^2; min=0.0; default=1.00000000E-10] -->
  <parameter file="gotm.yaml"   variable="turbulence/turb_param/k_min" minimum="1e-9" maximum="5e-7" logscale="True"/>
  <!-- non-visible fraction of shortwave radiation [fraction; min=0.0; max=1.0; default=0.7] -->
  <parameter file="gotm.yaml"   variable="light_extinction/A/constant_value" minimum="0.65" maximum="0.75"/>
  <!-- e-folding depth of non-visible shortwave radiation [m; min=0.0; default=0.4] -->
  <parameter file="gotm.yaml"   variable="light_extinction/g1/constant_value" minimum="0.30" maximum="0.5"/>
  <!-- e-folding depth of visible shortwave radiation [m; min=0.0; default=8.0] -->
  <parameter file="gotm.yaml"   variable="light_extinction/g2/constant_value" minimum="6.0" maximum="10.0"/>

  </parameters>
  <observations>
    <variable source="tempv.obs" modelpath="output.nc" modelvariable="temp" spinupyears = "5"/>
    <!-- <variable source="do.obs" modelpath="output.nc" modelvariable="abiotic_water_sO2W" spinupyears = "5"/> -->
    <!-- <variable source="no3.obs" modelpath="output.nc" modelvariable="abiotic_water_sNO3W" spinupyears = "5"/> -->
    <!-- <variable source="nh4.obs" modelpath="output.nc" modelvariable="abiotic_water_sNH4W" spinupyears = "5" /> -->
    <!-- <variable source="po4.obs" modelpath="output.nc" modelvariable="abiotic_water_sPO4W" spinupyears = "5"/> -->
    <!-- <variable source="tp.obs" modelpath="output.nc" modelvariable="wet_totP_calculator_result" spinupyears = "5" /> -->
    <!-- <variable source="tn.obs" modelpath="output.nc" modelvariable="wet_totN_calculator_result" spinupyears = "5" /> -->
    <!-- <variable source="chla.obs" modelpath="output.nc" modelvariable="wet_chla_calculator_result" spinupyears = "5" /> -->
    <!-- <variable source="cyano_chla.obs" modelpath="output.nc" modelvariable="cyanobacteria_oChla" spinupyears = "5" /> -->
    <!-- <variable source="diat_chla.obs" modelpath="output.nc" modelvariable="diatoms_oChla" spinupyears = "5" /> -->
  </observations>
  <extra_outputs>
    <statistic name="correlation" expression="corrcoef(x,y)[0,1]"/>
    <statistic name="rmse" expression="sqrt(mean((y-x)**2))"/>
    <statistic name="R2" expression="corrcoef(x,y)[0,1]**2"/>
    <statistic name="pbias" expression="sum((y-x)*100)/sum(x)"/>
  </extra_outputs>
</config>
```

Specify database file name

Specify GOTM-WET executable

Specify GOTM-WET parameters and their ranges

parsac only includes .obs files under <observation>

Optional: include calculated performance metrics for each obs in database file

eXtensible Markup Language file | length : 3,619 | lines : 52 | Ln : 52 | Col : 1 | Pos : 3,620 | Unix (LF) | UTF-8 | INS

```
D:\Models\lake_dashahe_qwet\parsac>C:\Users\Administrator\anaconda3\Scripts\parsac calibration plotbest D:/Models/lake_d
ashahe_qwet/parsac/wet_dashahe-step5.xml
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\tempv.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\do.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\no3.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\nh4.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\po4.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\tp.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\tn.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\chla.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\cyano_chla.obs...
Loading cached copy of D:\Models\lake_dashahe_qwet\parsac\diat_chla.obs...
Retrieving results...
Found 1029843 results, of which 0 were invalid.
1th best parameter set:
  gotm.yaml/surface/meteo/u10/scale_factor = 1.2217
  gotm.yaml/surface/meteo/v10/scale_factor = 1.0077
  gotm.yaml/surface/meteo/swr/scale_factor = 0.941884
  gotm.yaml/turbulence/turb_param/k_min = 3.28413e-06
  gotm.yaml/light_extinction/A/constant_value = 0.738787
  gotm.yaml/light_extinction/g1/constant_value = 0.398411
  gotm.yaml/light_extinction/g2/constant_value = 7.40694
  fabm.yaml/instances/abiotic_water/parameters/kDMinPOMW = 0.0629678
  fabm.yaml/instances/abiotic_water/parameters/kDMinDOMW = 0.0416152
  fabm.yaml/instances/abiotic_water/parameters/cThetaMinPOMW = 1.03687
  fabm.yaml/instances/abiotic_water/parameters/cThetaMinDOMW = 1.06267
  fabm.yaml/instances/abiotic_sediment/parameters/kDMinPOMS = 0.00998945
  fabm.yaml/instances/abiotic_sediment/parameters/kDMinDOMS = 0.00990978
  fabm.yaml/instances/abiotic_sediment/parameters/cThetaMinDOMS = 1.05223
  fabm.yaml/instances/abiotic_sediment/parameters/cThetaMinPOMS = 1.04707
  fabm.yaml/instances/abiotic_sediment/parameters/kO2Dif = 0.000159337
  fabm.yaml/instances/abiotic_sediment/parameters/cTurbDifO2 = 2.89222
  fabm.yaml/instances/abiotic_water/parameters/kNMinPOMW = 0.0034557
  fabm.yaml/instances/abiotic_water/parameters/kNMinDOMW = 0.0150304
  fabm.yaml/instances/abiotic_water/parameters/kNitrW = 0.149681
  fabm.yaml/instances/abiotic_water/parameters/hNO3DenitW = 1.51189
  fabm.yaml/instances/abiotic_water/parameters/hO2BOD = 0.777001
  fabm.yaml/instances/abiotic_water/parameters/hO2Nitr = 1.57426
  fabm.yaml/instances/abiotic_water/parameters/NO3PerCW = 0.917556
```

How many model simulations in the calibration did not complete

Parameter value for plotbest model execution (you can also find these in fabm.yaml in plotbest model folder)

```
C:\windows\system32\cmd.ex
  fabm.yaml/instances/cladocerans/parameters/cClearPrey2 = 1.54922
  fabm.yaml/instances/cladocerans/parameters/cClearPrey3 = 2.03721
  fabm.yaml/instances/cladocerans/parameters/cClearPrey4 = 2.48719
  fabm.yaml/instances/cladocerans/parameters/fGutOccPrey2 = 1.50008
  fabm.yaml/instances/cladocerans/parameters/fGutOccPrey4 = 4.8261
  fabm.yaml/instances/cladocerans/parameters/kDConsMaxZoo = 0.949981
  fabm.yaml/instances/cladocerans/parameters/cTmOptZoo = 28.7824
  fabm.yaml/instances/cladocerans/parameters/cSigTmZoo = 12.3742
  fabm.yaml/instances/cladocerans/parameters/fDAssZoo = 0.301235
  fabm.yaml/instances/cladocerans/parameters/fZooDOMW = 0.0515662
  fabm.yaml/instances/cladocerans/parameters/kMortZoo = 0.001
  fabm.yaml/instances/cladocerans/parameters/kDRespZoo = 0.132183
Original ln likelihood = 110.49561
Copying files for model setup to C:\Users\ADMINI~1\AppData\Local\Temp\gotmopt99csz5oo...
   skipping parsac because it is a directory
   skipping restart.nc because it is a NetCDF file
Evaluating fitness with parameter set [1.2217,1.0077,0.941884,3.28413e-06,0.738787,0.398411,7.40694,0.0629678,0.0416152,
1.03687,1.06267,0.00998945,0.00990978,1.05223,1.04707,0.000159337,2.89222,0.0034557,0.0150304,0.149681,1.51189,0.777001,
1.57426,0.917556,2.08223,1.079,0.000597438,0.000861677,0.670612,1.08654,0.972069,1.05063,1.11325,27.9326,0.00235275,0.00
26888,0.0222718,0.809709,1.95042,0.0184772,1.44527,1.03694,0.039098,1.51618,0.0199577,0.00947401,0.0282785,0.643669,0.64
0192,0.0297333,-0.5,0.0155308,0.0460541,0.0301086,2.1968,25.8694,10.7991,1,7.41933,14.1283,-0.5,0.5,0.247615,1.3709,5.17
096,30.4412,2,35.1659,0.773731,0.483398,23.2962,14.7578,1,11.4078,46.9837,1.56476,1.54922,2.03721,2.48719,1.50008,4.8261
,0.949981,28.7824,12.3742,0.301235,0.0515662,0.001,0.132183].
Starting model run...
 ------------------------------------------------------------------------
 GOTM started on 2024/10/04 at 03:50:28
 ------------------------------------------------------------------------
    init_gotm
 ------------------------------------------------------------------------
        Reading yaml configuration from: gotm.yaml
        configuring modules ....
    init_airsea_yaml
        done
    init_stim_yaml
        done.
    init_observations_yaml
    configure_streams_yaml
        done
    init_turbulence_yaml
        done.
```

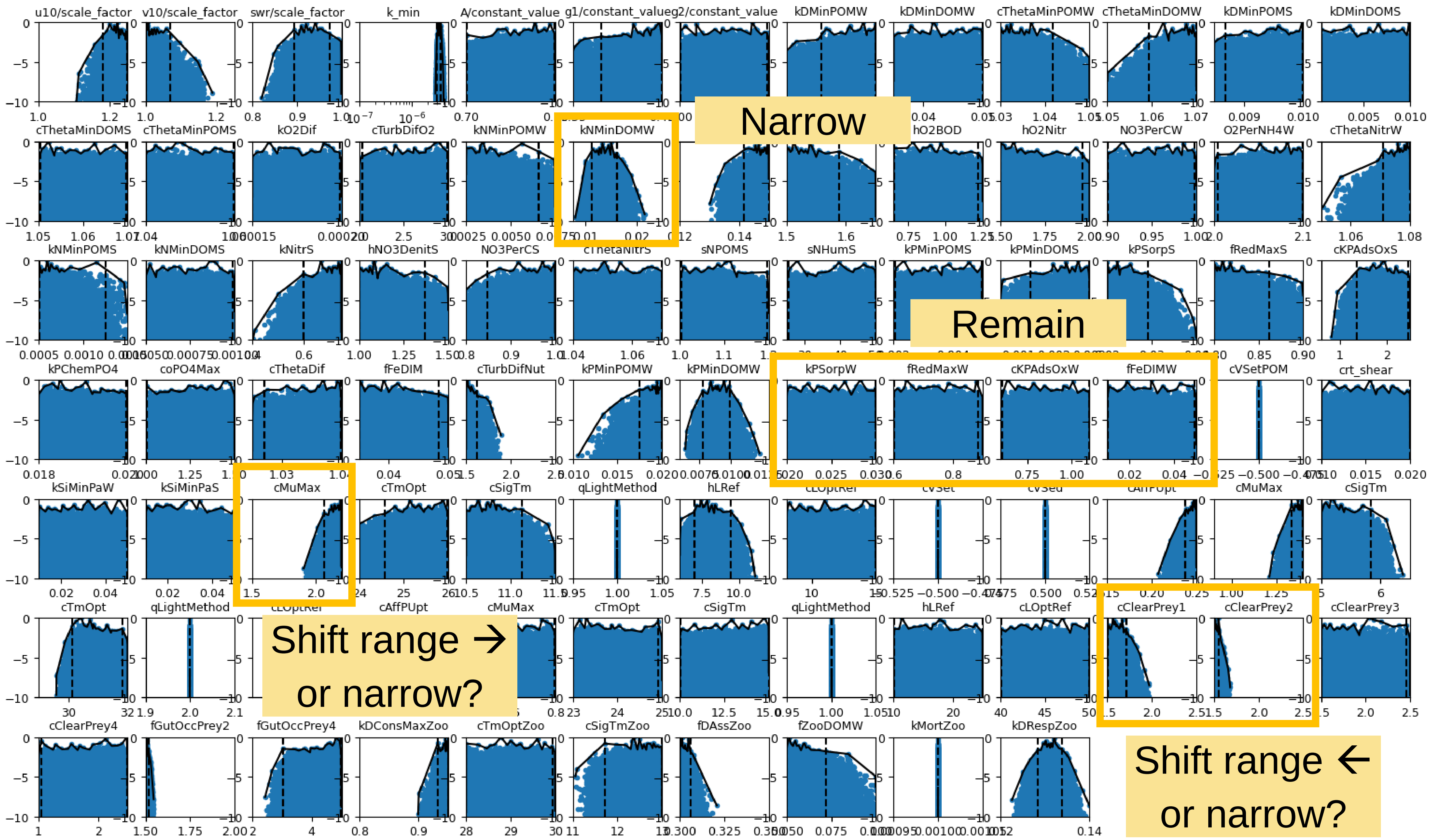
parsac created the plotbest folder and executed the model from this folder

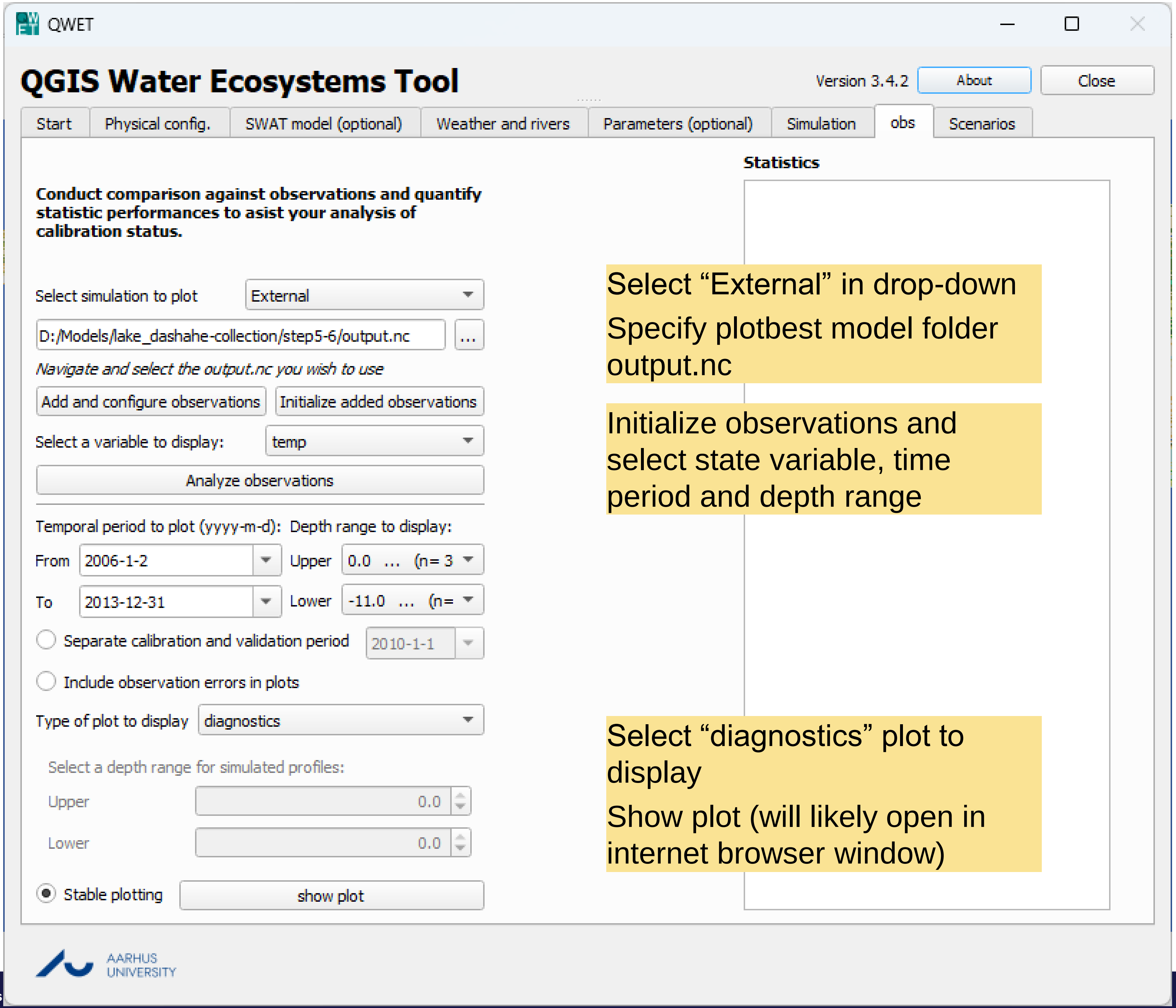
DTU

```
Calculating weights for linear interpolation to "wet_totP_calculator_result" observations...done.
Calculating weights for linear interpolation to "wet_totN_calculator_result" observations...done.
Calculating weights for linear interpolation to "wet_chla_calculator_result" observations...done.
Calculating weights for linear interpolation to "cyanobacteria_oChla" observations...done.
Calculating weights for linear interpolation to "diatoms_oChla" observations...done.
Using optimal s.d. for temp = 2.12557.
Using optimal s.d. for abiotic_water_sO2W = 1.27727.
Using optimal s.d. for abiotic_water_sNO3W = 0.206254.
Using optimal s.d. for abiotic_water_sNH4W = 0.0408296.
Using optimal s.d. for wet_totP_calculator_result = 0.0109255.
Using optimal s.d. for wet_totN_calculator_result = 0.161355.
ln Likelihood = 110.496.
Newly calculated ln likelihood = 110.49561. Original value was 110.49561.
temp:
- bias: 0.4878
- mean absolute error = 1.48
- rmse = 2.111
- cor = 0.9743
- s.d. mod = 8.656
- s.d. obs = 7.793
abiotic_water_sO2W:
- bias: 0.7978
- mean absolute error = 1.012
- rmse = 1.268
- cor = 0.9659
- s.d. mod = 3.748
- s.d. obs = 3.448
abiotic_water_sNO3W:
- bias: 0.05684
- mean absolute error = 0.1763
- rmse = 0.2034
- cor = 0.8241
- s.d. mod = 0.3133
- s.d. obs = 0.3397
abiotic_water_sNH4W:
- bias: 0.009641
- mean absolute error = 0.02944
- rmse = 0.04026
- cor = 0.229
- s.d. mod = 0.0199
```

parsac estimated sd to use for weights in optimization

State variable performance calculated by parsac, worth saving for each calibration iteration


Narrow
Remain
Shift range → or narrow?
Shift range ← or narrow?



Select “External” in drop-down

Specify plotbest model folder output.nc

Initialize observations and select state variable, time period and depth range

Select “diagnostics” plot to display

Show plot (will likely open in internet browser window)

Sensitivity analysis

tkan@aqua.dtu.dk

or you can write to me
on wechat ☺

Currently, WET website at Aarhus University is not maintained. WET team is working on a new solution.

We let you know via wechat when new website with updated material is ready.

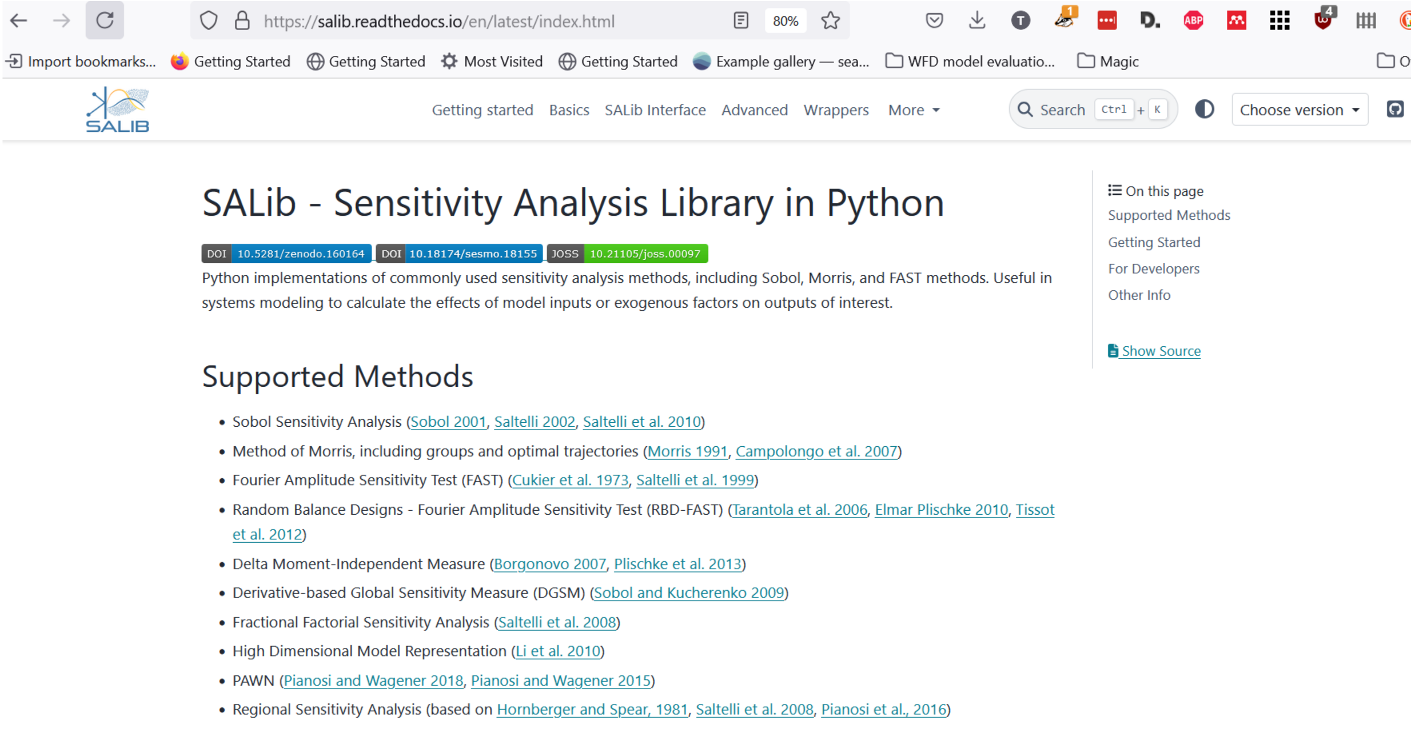
wet.au.dk

The modelling process

1. Definition of idea / problem and system
2. Conceptual diagram
3. Mathemati-cal formulation
4. Verification
5. Sensitivity analysis
6. Calibration and validation
7. Application (scenarios, hypothesis)

parsac and SALib

For sensitivity analysis, parsac relies on the Python package Sensitivity Analysis Library in Python (SALib) published by Herman & Usher (2017) and Iwanaga, Usher and Herman (2022).



SALib: Match sampling with SA method

Table 1. parsac supported SALib methods and their corresponding sampling schemes with their parsac names.

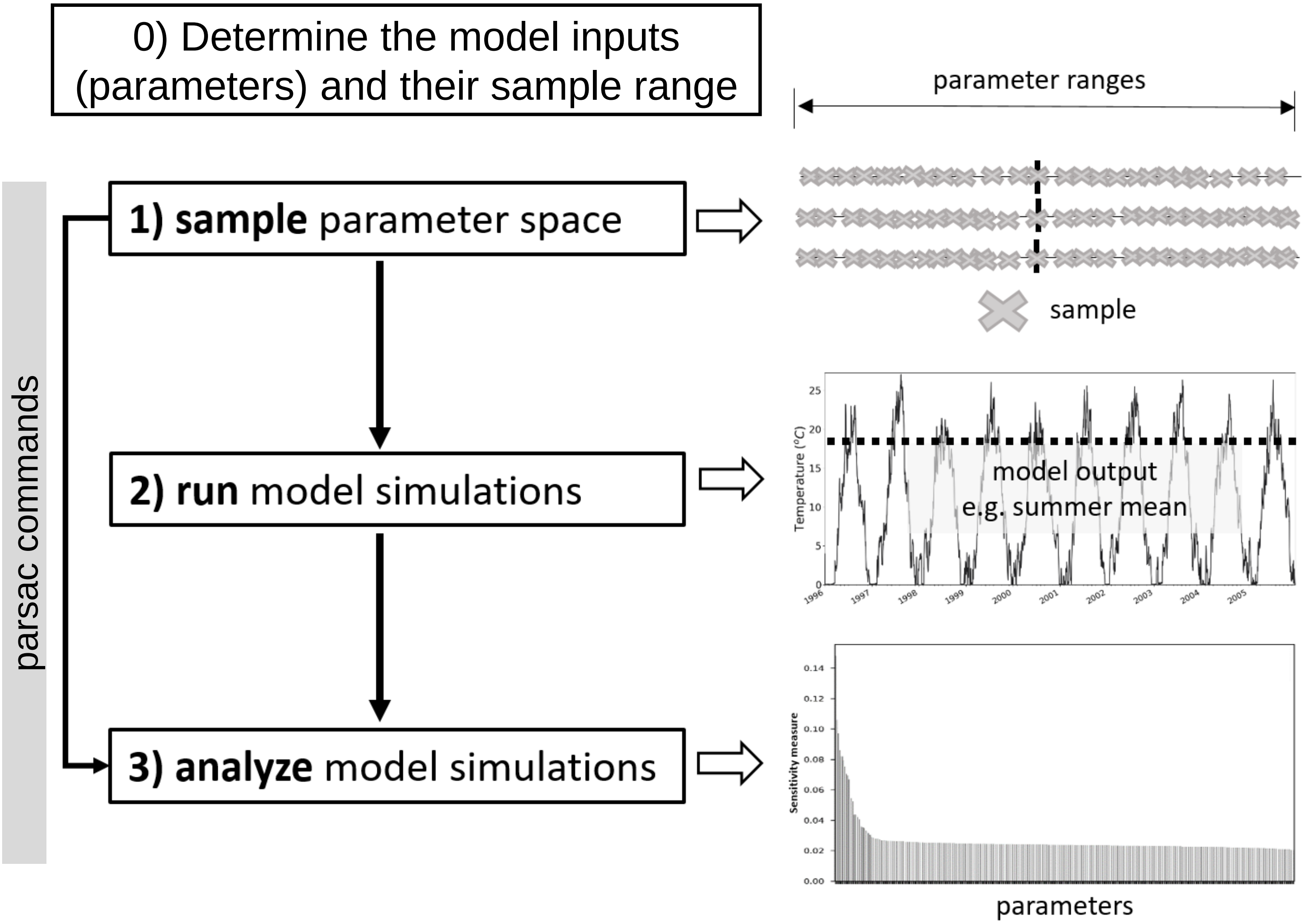
Sensitivity method	parsac name	**Sampling**	parsac name
Fourier Amplitude Sensitivity Test (FAST)	fast		fast
Random Balance Designs - Fourier Amplitude Sensitivity Test	rbd_fast	Latin hypercube sampling	latin
Method of Morris	morris		morris
Sobol Sensitivity Analysis	sobol	Saltelli's sampling	saltelli
Delta Moment-Independent Measure	delta	Latin hypercube sampling	latin
Derivative-based Global Sensitivity Measure	dgsm		
Fractional Factorial Sensitivity Analysis	ff		ff

Brief intro to sensitivity analysis with parsac

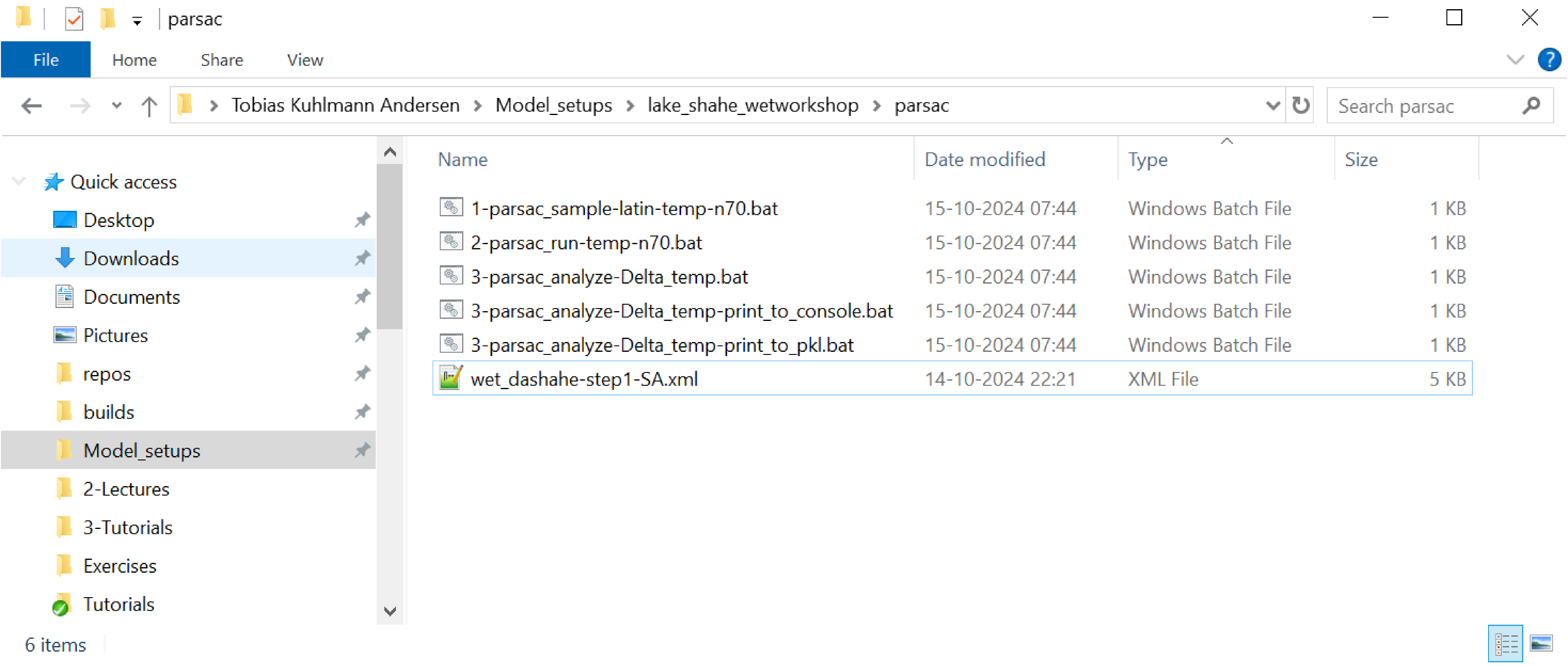
parsac relies on the Python package Sensitivity Analysis Library for Python (SALib) for SA methods.

Full SA procedure documented in Andersen et al. (2021)

General parsac sensitivity analysis



Working parsac folder for SA



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File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

bryrup_sa_epi_summer_tp_25.xml

```xml
<config xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespaceSchemaLocation="../client/confi
  <transports>
    <transport type="sqlite" path="Arreskov_SA_all.db"/>
  </transports>
  <executable path="../gotm.exe"/>
  <setup path="../"/>
  <parameters>
  <parameter dummy="True" maximum="1" minimum="0"/>
  <parameter file="gotm.yaml"   variable="surface/fluxes/heat/scale_factor" minimum="0.75" maximum="1.25"/>
  <parameter file="gotm.yaml"   variable="surface/meteo/swr/scale_factor" minimum="0.75" maximum="1.25"/>
  <parameter file="gotm.yaml"   variable="surface/meteo/u10/scale_factor" minimum="0.75" maximum="1.25"/>
  <parameter file="gotm.yaml"   variable="surface/meteo/v10/scale_factor" minimum="0.75" maximum="1.25"/>
  <parameter file="gotm.yaml"   variable="turbulence/turb_param/k_min" minimum="1E-10" maximum="1-E6" logscale="True"/>
  <parameter file="gotm.yaml"   variable="light_extinction/A/constant_value" minimum="0.45" maximum="0.75"/>
  <parameter file="gotm.yaml"   variable="light_extinction/g1/constant_value" minimum="0.3" maximum="0.5"/>
  <parameter file="gotm.yaml"   variable="light_extinction/g2/constant_value" minimum="6.0" maximum="10.0"/>
  <parameter file="fabm.yaml" maximum="2.0" minimum="1.2" variable="instances/abiotic_sediment/parameters/cKPAdsOx"/>
  <parameter file="fabm.yaml" maximum="18.47" minimum="11.082" variable="instances/abiotic_sediment/parameters/cTurbDifNut"/>
  <parameter file="fabm.yaml" maximum="0.125" minimum="0.075" variable="instances/abiotic_sediment/parameters/cDepthS"/>
  <parameter file="fabm.yaml" maximum="0.92125" minimum="0.55275" variable="instances/abiotic_sediment/parameters/bPorCorS"/>
  <parameter file="fabm.yaml" maximum="0.95" minimum="0.64425" variable="instances/abiotic_sediment/parameters/fRedMax"/>
  <parameter file="fabm.yaml" maximum="0.625" minimum="0.375" variable="instances/abiotic_sediment/parameters/fDepthDifS"/>
  <parameter file="fabm.yaml" maximum="0.0125" minimum="0.0075" variable="instances/abiotic_sediment/parameters/fAlDIM"/>
  <parameter file="fabm.yaml" maximum="0.20125" minimum="0.12075" variable="instances/abiotic_sediment/parameters/cRelPAdsAl"/>
  <parameter file="fabm.yaml" maximum="0.00375" minimum="0.00225" variable="instances/abiotic_sediment/parameters/kDMinPOMS"/>
  </parameters>
  <observations>
    <!-- linkage between observation files and model output for objective function in calibration   -->
    <!-- Step 1 -->
    <!-- <variable source="./DO.obs" modelpath="output.nc" modelvariable="abiotic_water_sO2W" spinupyears="3"/>  -->
    <!-- <variable source="./CHLA.obs" modelpath="output.nc" modelvariable="pclake_chla_calculator_result" spinupyears="3"/>  -->
  </observations>
  <targets>
    <!-- MEAN  -->
    <target expression="filter_by_time(wet_totP_calculator_result[:,:],months=(1,2,3,4,5,6,7,8,9,10,11,12)).mean()" path="output.nc"/>
    <target expression="filter_by_time(wet_totP_calculator_result[:,:],months=(1,2,12)).mean()" path="output.nc"/>
    <target expression="filter_by_time(wet_totP_calculator_result[:,:],months=(3,4,5)).mean()" path="output.nc"/>
    <target expression="filter_by_time(wet_totP_calculator_result[:,:],months=(6,7,8)).mean()" path="output.nc"/>
    <target expression="filter_by_time(wet_totP_calculator_result[:,:],months=(9,10,11)).mean()" path="output.nc"/>
  </targets>
</config>
```

Specify database file name (not used)

Specify GOTM-WET executable

Specify GOTM-WET parameters and their ranges

parsac sensitivity does not use observations

Specify GOTM-WET output, netcdf, time period and descriptive metric (mean, etc)

eXtensible Markup Language file   length : 3,374   lines : 42   Ln : 42   Col : 1   Pos : 3,375   Unix (LF)   UTF-8   INS

How to determine parameter ranges

What is the aim of the sensitivity analysis?

Some ideas to determine parameter ranges:

- % ranges from default values
- % ranges from calibrated values
- Min and max based on literature

parsac SA commands

The corresponding parsac command lines, arguments and options are:

1. **“parsac sensitivity sample xmlfile info {fast,latin,morris,saltelli,ff} samplesize”**

xmlfile	XML formatted configuration file (xml file)
info	Path to output of the "sample" step (pickle file, .pkl)
samplesize	Number of samples generated by sampling scheme

2. **“parsac sensitivity run info”**

info	Path to output of the "sample" step (pickle file, .pkl)

3. **“parsac sensitivity analyze [-h] [--print_to_console]
 [--select SELECT SELECT] [--pickle PICKLE] info
 {fast,rbd_fast,morris,sobol,delta,dgsm,ff}
 --num_resamples RESAMPLES”**

info	Path to output of the "sample" step (pickle file, .pkl)
--print_to_console	Print results directly to console
--select SELECT SELECT	This requires two values: N OUTPUTXML. Selects the N most sensitive parameters for a calibation run and save it to OUTPUTXML
--pickle PICKLE	Path of pickle file to write with analysis results
--num_resamples	The number of resamples when computing confidence intervals

Sample size

Andersen et al (2020) used

Screening (all some GOTM + all WET parameters: approx. 360)

100 samples per parameter

In-depth SA (most sensitive parameters, 20-50)

250 samples per parameter

Most important, check confidence intervals in SA results.

Parsac SA command for delta analysis

1. **parsac sensitivity sample xmlfile info latin samplesize**

xmlfile = wet_dashahe-step1-SA.xml

info = “C:\folder_to_\parsac\delta_temp_n30.pkl

samplesize = 30

2. **parsac sensitivity run info**

3. parsac sensitivity analyze --print_to_console info delta

3. parsac sensitivity analyze --pickle pickle info delta

pickle = delta_temp_SA_results.pkl

Example of SA results

Anaconda Prompt - parsac sensitivity run C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_n50.pkl

```
Original error was: cannot import name 'Sequence' from 'collections' (C:\Users\tkan\AppData\Local\anaconda3\Lib\collecti
ons\__init__.py)

A fatal error has occured during the function execution
Traceback (most recent call last):
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\pp-1.6.4.4-py3.11.egg\ppworker.py", line 103, in run
    __args = pickle.loads(ppc.b_(__sargs))
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\dill\__init__.py", line 33, in <module>
    from .session import (
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\dill\session.py", line 32, in <module>
    import pathlib
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\pathlib.py", line 10, in <module>
    from collections import Sequence
ImportError: cannot import name 'Sequence' from 'collections' (C:\Users\tkan\AppData\Local\anaconda3\Lib\collections\__i
nit__.py)
Traceback (most recent call last):
  File "<frozen runpy>", line 198, in _run_module_as_main
  File "<frozen runpy>", line 88, in _run_code
  File "C:\Users\tkan\AppData\Local\anaconda3\Scripts\parsac.exe\__main__.py", line 7, in <module>
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\parsac\parsac_run.py", line 12, in main
    parsac.main()
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\parsac\__init__.py", line 48, in main
    args.func(args)
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\parsac\sensitivity.py", line 225, in main
    Y = current_job.evaluate_ensemble([undoLogTransform(X[i, :], logscale) for i in range(X.shape[0])], stop_on_bad_resu
lt=True)
        ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
^^^^^^^^
  File "C:\Users\tkan\AppData\Local\anaconda3\Lib\site-packages\parsac\job\shared.py", line 276, in evaluate_ensemble
```

Anaconda Prompt

```
                                                    Evaluating fitness with parameter set [1.17867,0.938987,0.691318,0.31
6997,7.77171].
Starting model run...
Model run took 257.1 s.




                                                     Evaluating fitness with parameter set [1.05591,1.16061,0.747843,0.40
3331,6.99702].
Starting model run...
Model run took 253.5 s.
 Updating sensitivity info in C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_n50.pkl with model result
s...
ERROR: The process "18760" not found.
ERROR: The process "23008" not found.
ERROR: The process "25460" not found.
ERROR: The process with PID 21520 could not be terminated.
Reason: There is no running instance of the task.

(base) C:\Users\tkan>ERROR: The process "20604" not found.
ERROR: The process "4172" not found.
```

Anaconda Prompt

```
(base) C:\Users\tkan>parsac sensitivity analyze --pickle C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_te
mp_SA_results.pkl C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_n50.pkl delta --num_resamples 100
Reading sensitity samples from C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_n50.pkl...
Reading configuration from C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\wet_dashahe-step1.xml...
Target 0 (output.nc/filter_by_time(temp[:,:],months=(1,2,3,4,5,6,7,8,9,10,11,12)).mean())
  - gotm.yaml/surface/meteo/v10/scale_factor (0.41209798355387056)
  - gotm.yaml/light_extinction/g2/constant_value (0.34144913782427877)
  - gotm.yaml/surface/meteo/u10/scale_factor (0.14255830286030505)
  - gotm.yaml/light_extinction/g1/constant_value (0.09012025527739215)
  - gotm.yaml/light_extinction/A/constant_value (0.08663801836324822)
Writing analysis result to pickle C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_SA_results.pkl.

(base) C:\Users\tkan>
```

Anaconda Prompt

```
(base) C:\Users\tkan>parsac sensitivity analyze --print_to_console C:\Users\tkan\Model_setups\lake_shahe_workshop\parsa
c\delta_temp_n50.pkl delta --num_resamples 100
Reading sensitivity samples from C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\delta_temp_n50.pkl...
Reading configuration from C:\Users\tkan\Model_setups\lake_shahe_workshop\parsac\wet_dashahe-step1.xml...
                                                   delta  delta_conf        S1   S1_conf
gotm.yaml/surface/meteo/u10/scale_factor        0.194747    0.065448  0.189696  0.215314
gotm.yaml/surface/meteo/v10/scale_factor        0.407474    0.087800  0.520617  0.119472
gotm.yaml/light_extinction/A/constant_value     0.141332    0.079204  0.070337  0.151453
gotm.yaml/light_extinction/g1/constant_value    0.232874    0.076295  0.172186  0.148453
gotm.yaml/light_extinction/g2/constant_value    0.089950    0.074734  0.163239  0.178264
Target 0 (output.nc/filter_by_time(temp[:,:],months=(1,2,3,4,5,6,7,8,9,10,11,12)).mean())
  - gotm.yaml/surface/meteo/v10/scale_factor (0.40747447691683986)
  - gotm.yaml/light_extinction/g1/constant_value (0.23287378411118495)
  - gotm.yaml/surface/meteo/u10/scale_factor (0.19474707038533715)
  - gotm.yaml/light_extinction/A/constant_value (0.14133170293054328)
  - gotm.yaml/light_extinction/g2/constant_value (0.08994990623596802)

(base) C:\Users\tkan>
```

Example of SA results