Deltares

enabling delta life

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Efficient Model Calibration using Sub-models

New development within iPESTP of iMOD

Peter Vermeulen

Gijs Janssen

Timo Kroon

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Status Quo

What

Investigate an innovative solution to support large-scale parameter estimation for groundwater flow models

Clients

LHM (National Model NL, RWS) and Zeeland Model (Regional Model Prov. Zeeland)

Context

Spatial Calibration of the transient LHM- and Zeeland Model (SeaWAT).

Status

Currently available as prototype in iMOD v5.6

Applicability

Regional models might be able to be calibrated more efficiently

Information

iMOD Manual; PPTX of Modflow-and-More conference; paper (Groundwater) in prep.

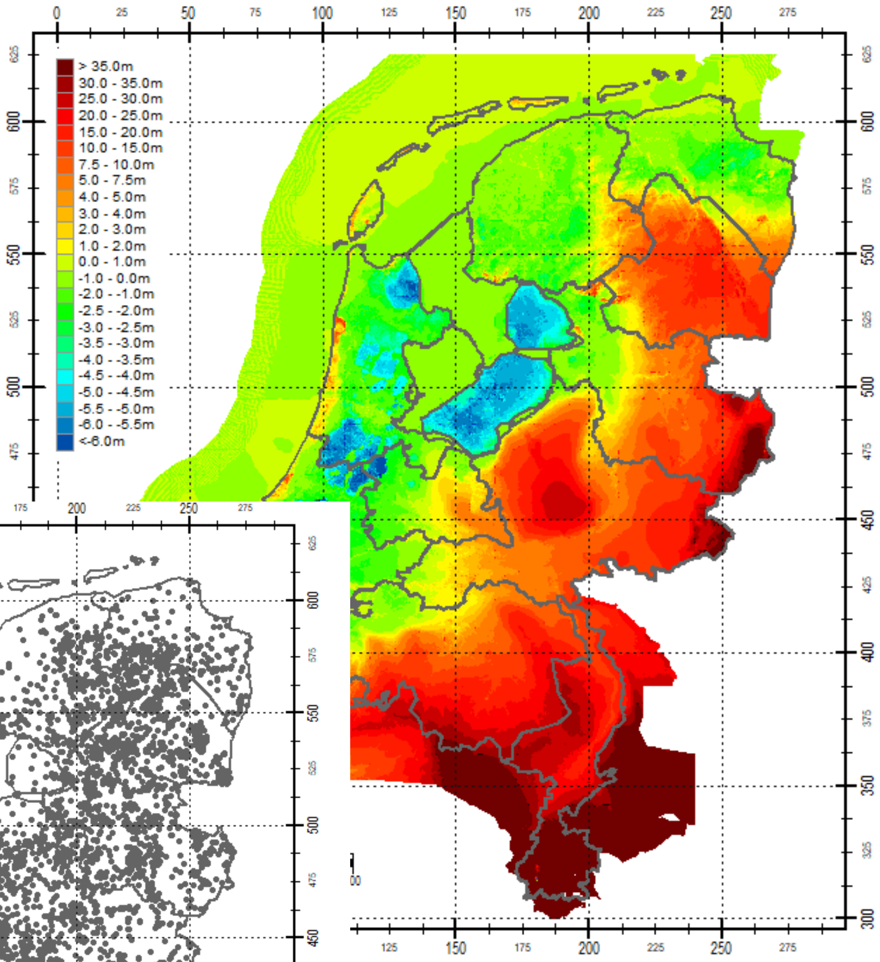
… in highlights some results …

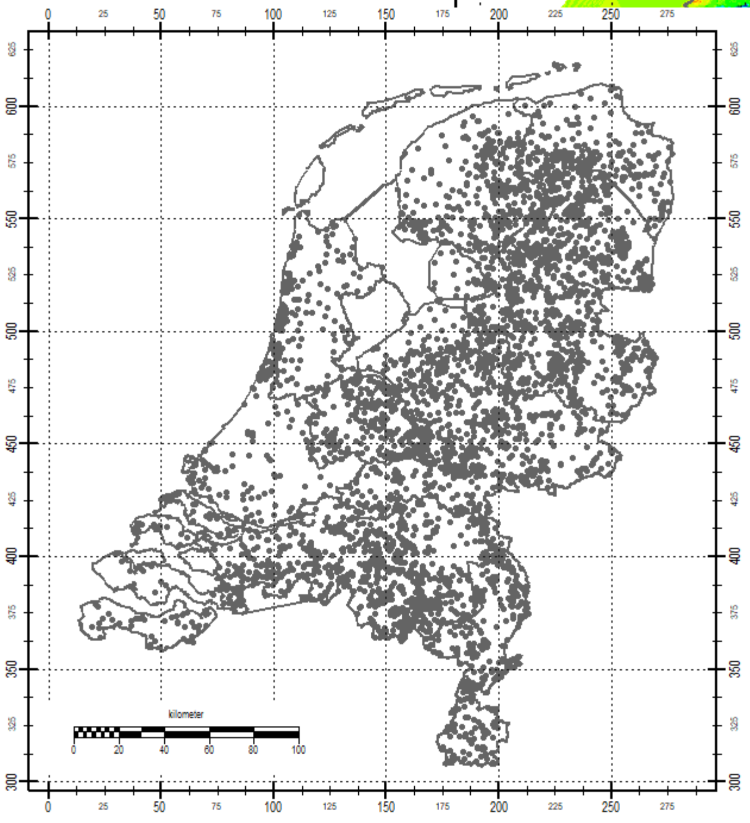
Challenge

Optimize

- 3D Groundwater Flow model
  - Transient Model (171 stresses)
  - 12.5 millions nodes
- Totally 2,050 parameters
  - REGIS units in aquifers and aquitards
  - GeoTOP lithology in “deklaag”
  - Drainage- and river conductance
  - Infiltration factor rivers
  - Storage coefficients
- Observations
  - 0.5 million time-variant observations
  - 60,000 artificial observations GxG

Groundwater Level

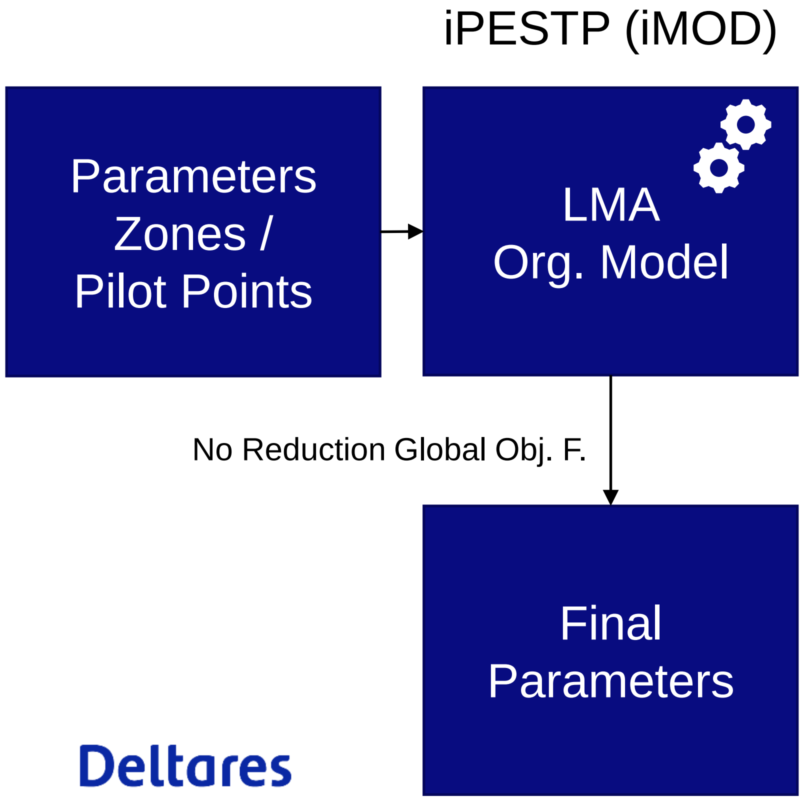




Observations

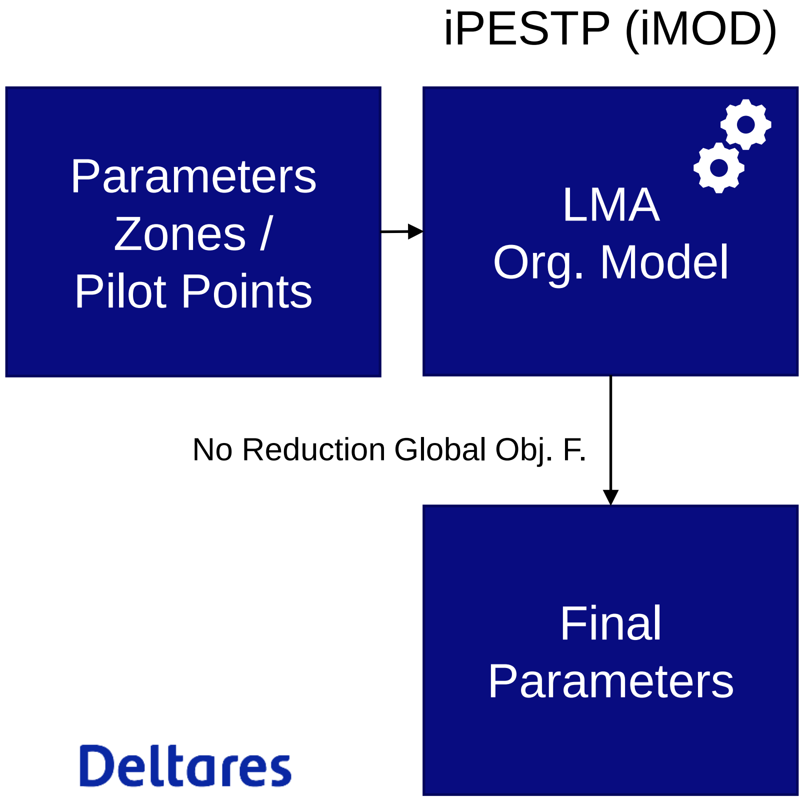
Deltares

LMA Optimization Method

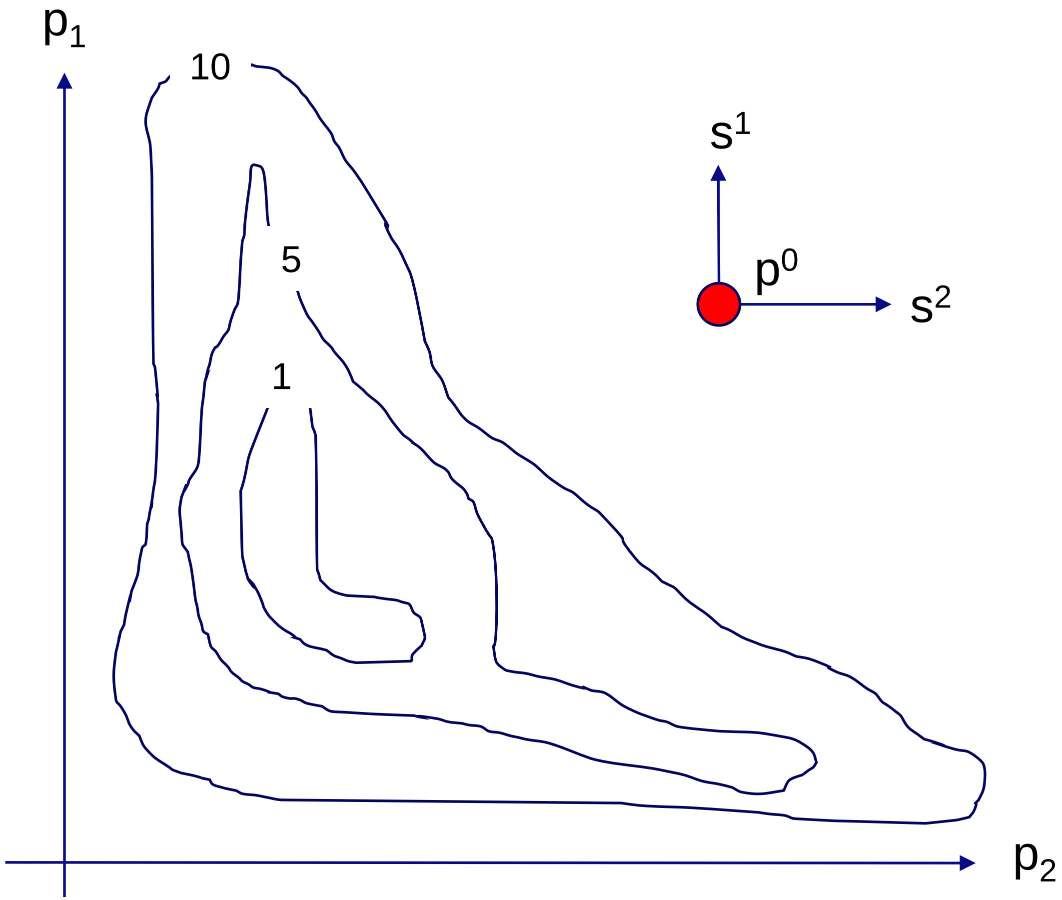


Deltares

LMA Optimization Method

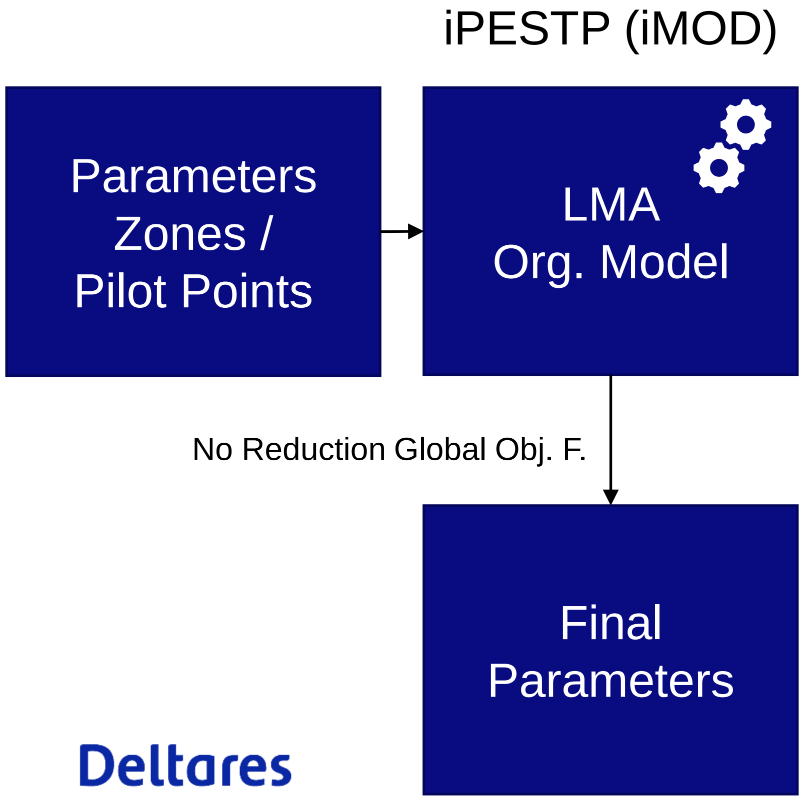


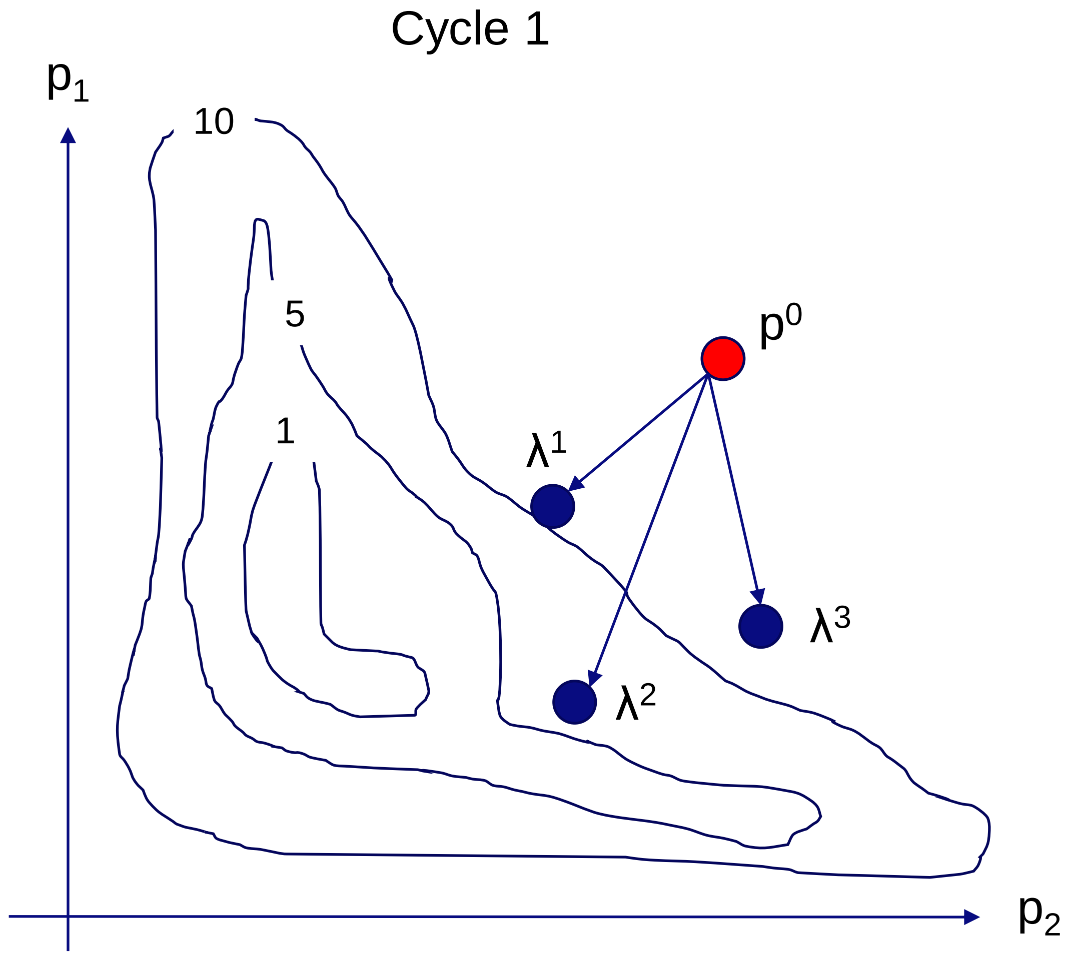
Cycle 1



Sensitivities for each parameter

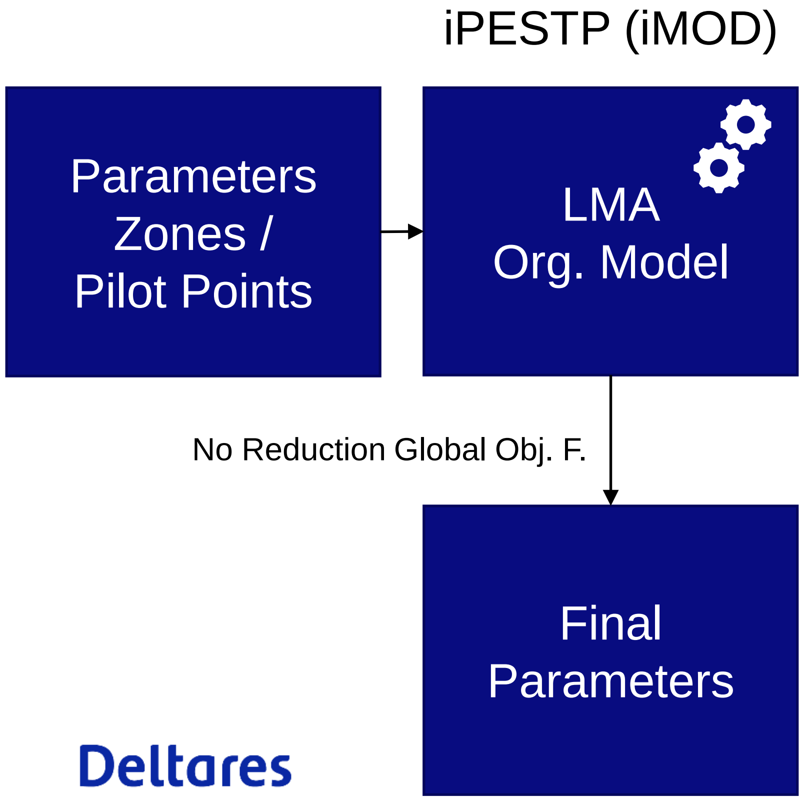
LMA Optimization Method

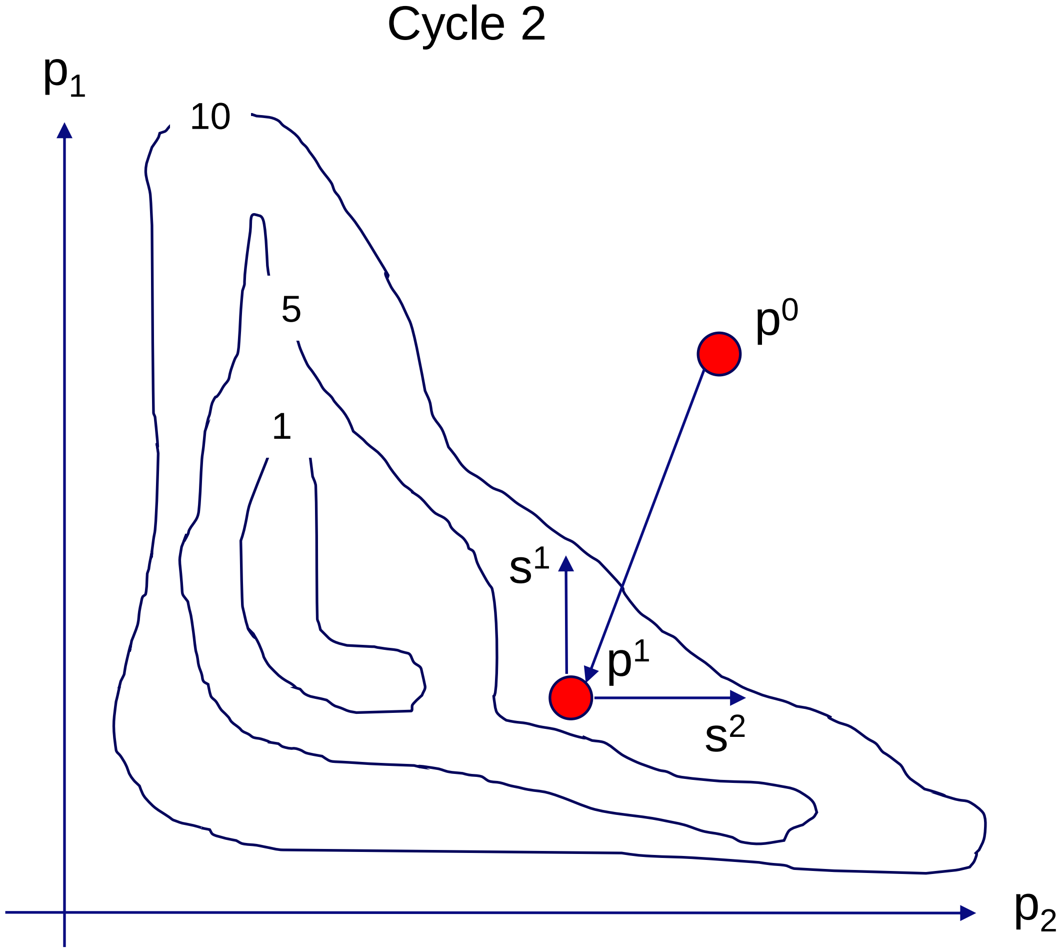




Effectiveness is caused significantly by λ, try multiple λ's

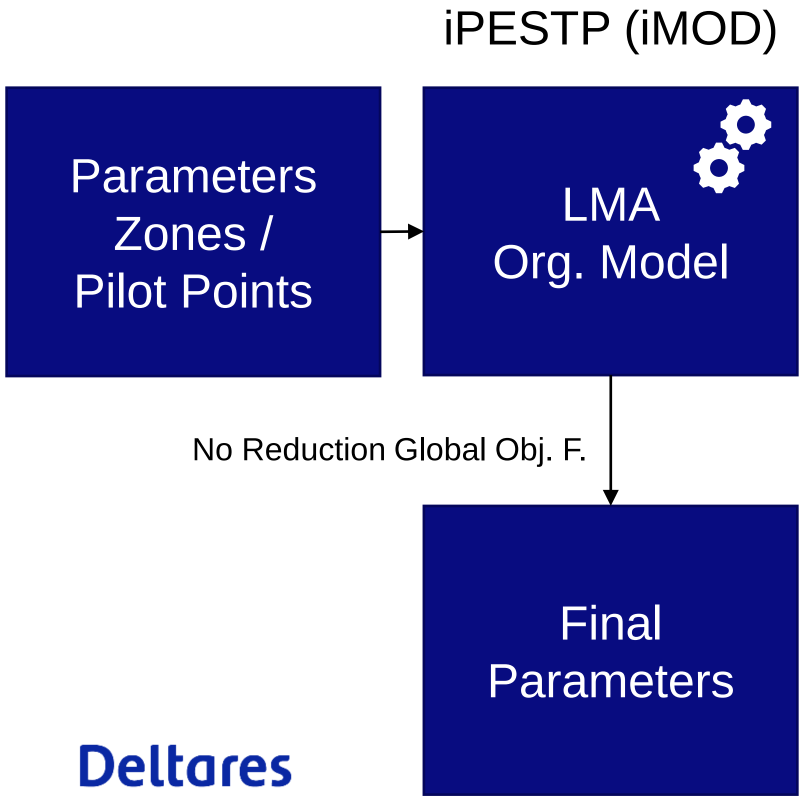
LMA Optimization Method



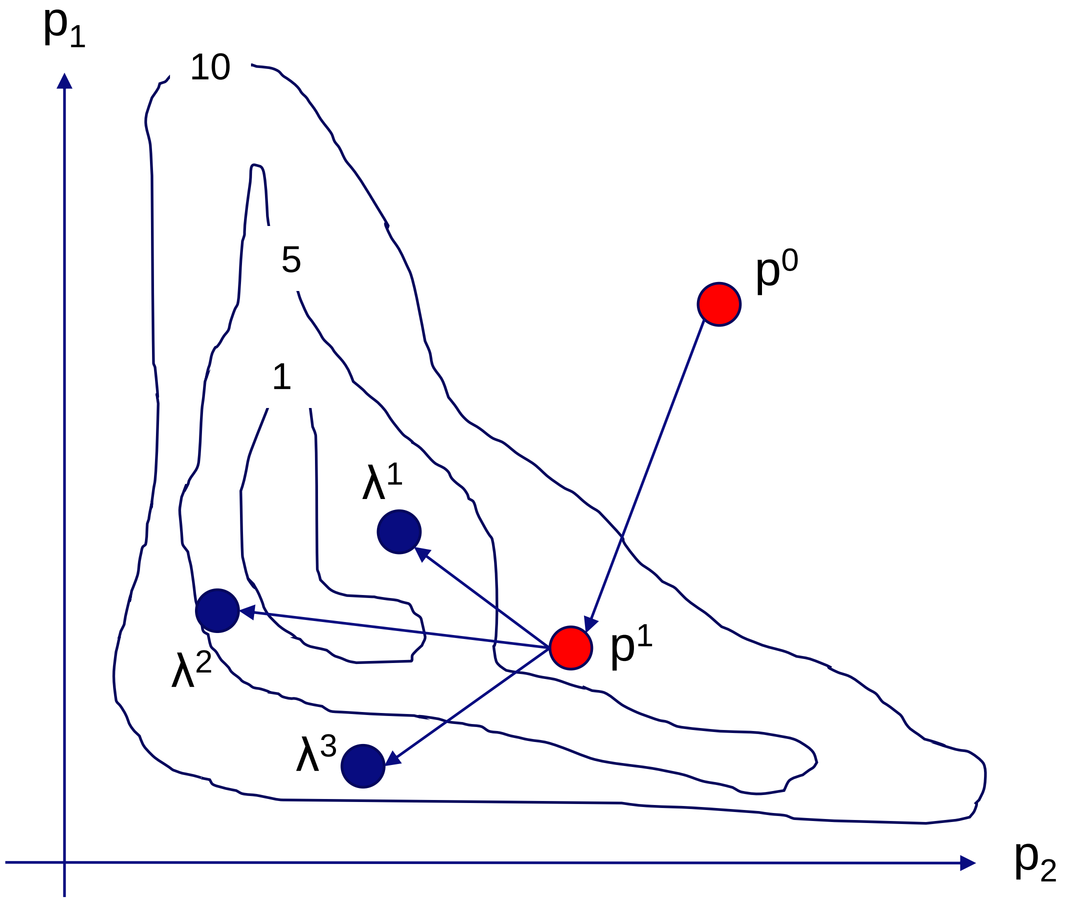


Sensitivities for each parameter

LMA Optimization Method



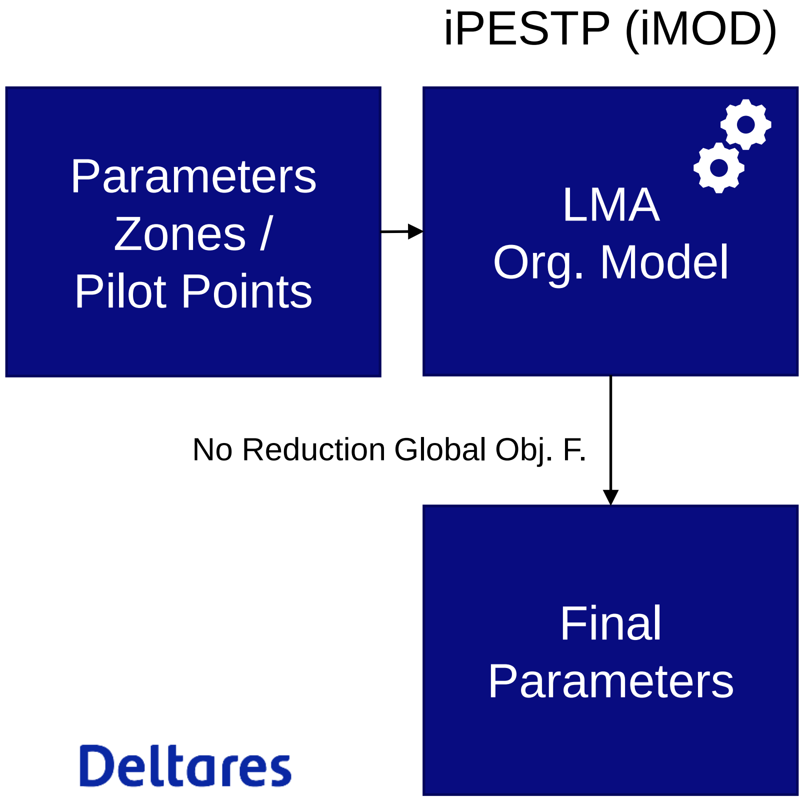
Cycle 2

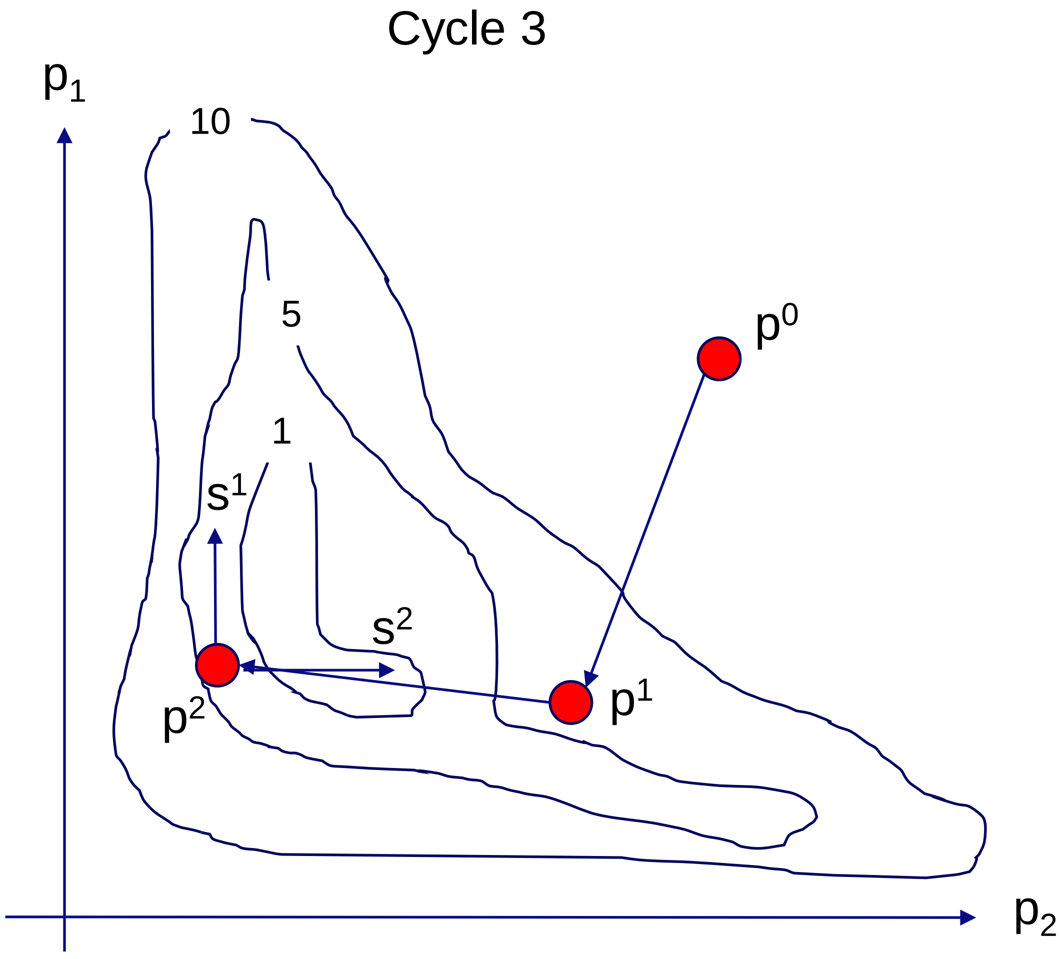


Effectiveness is caused significantly by λ

Deltares

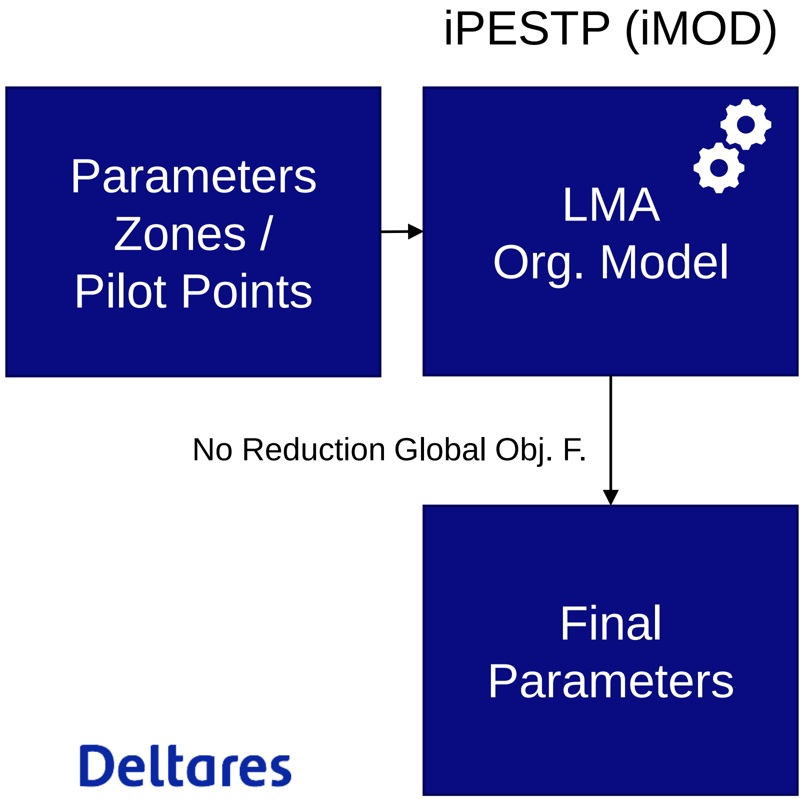
LMA Optimization Method



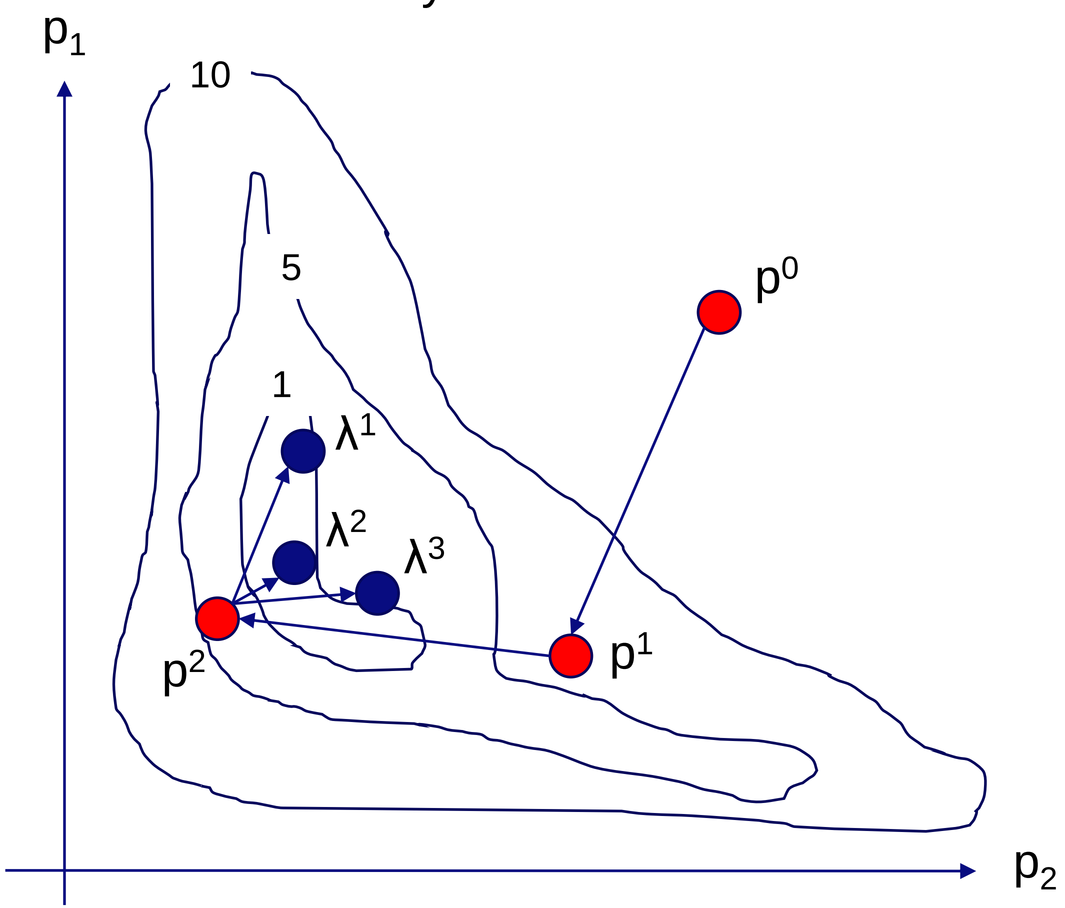


Effectiveness is caused significantly by λ

LMA Optimization Method



Cycle 3



Effectiveness is caused significantly by λ

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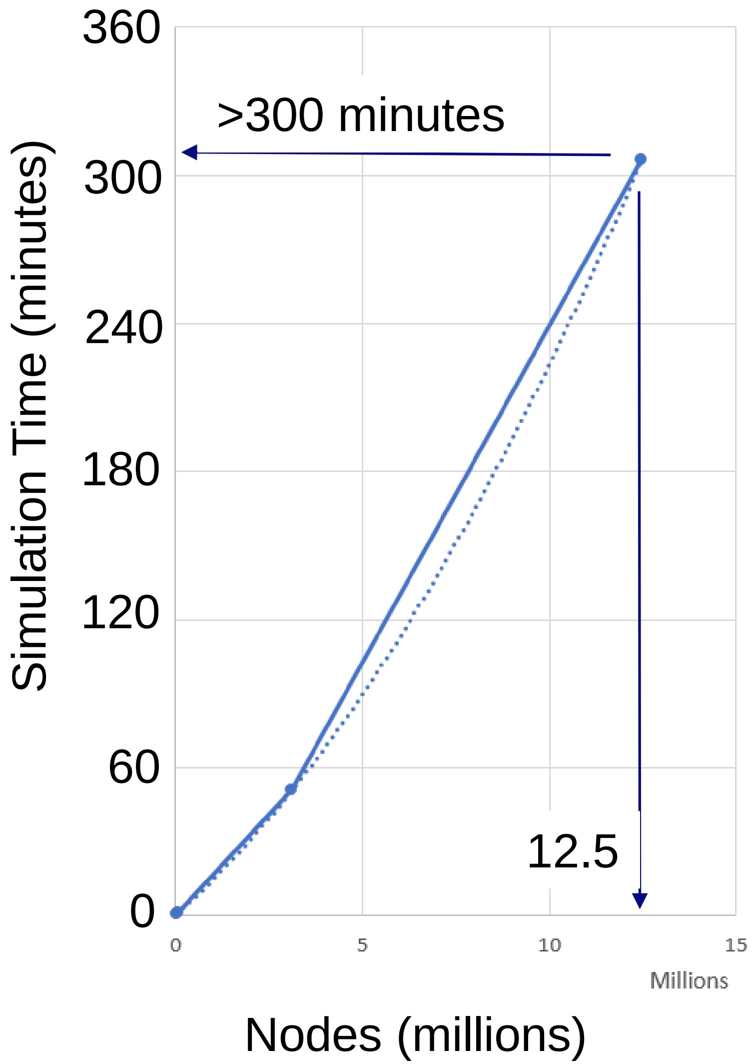
Efficiency of LMA Optimization Method



		Single CPU	20 CPU
Sensitivity	2050	427 days	21 days
Lambda	3	5 hours	5 hours
Totally	10 cycles		~0.5 year

It never goes right the first, second, third time …

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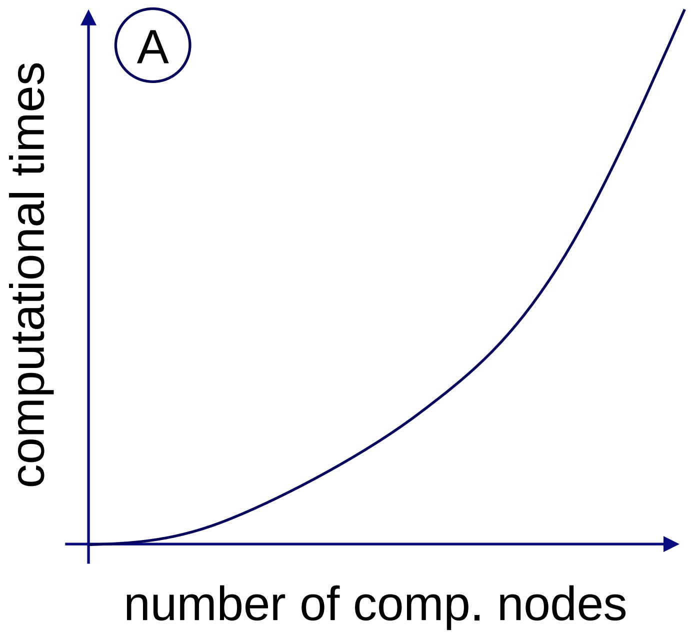
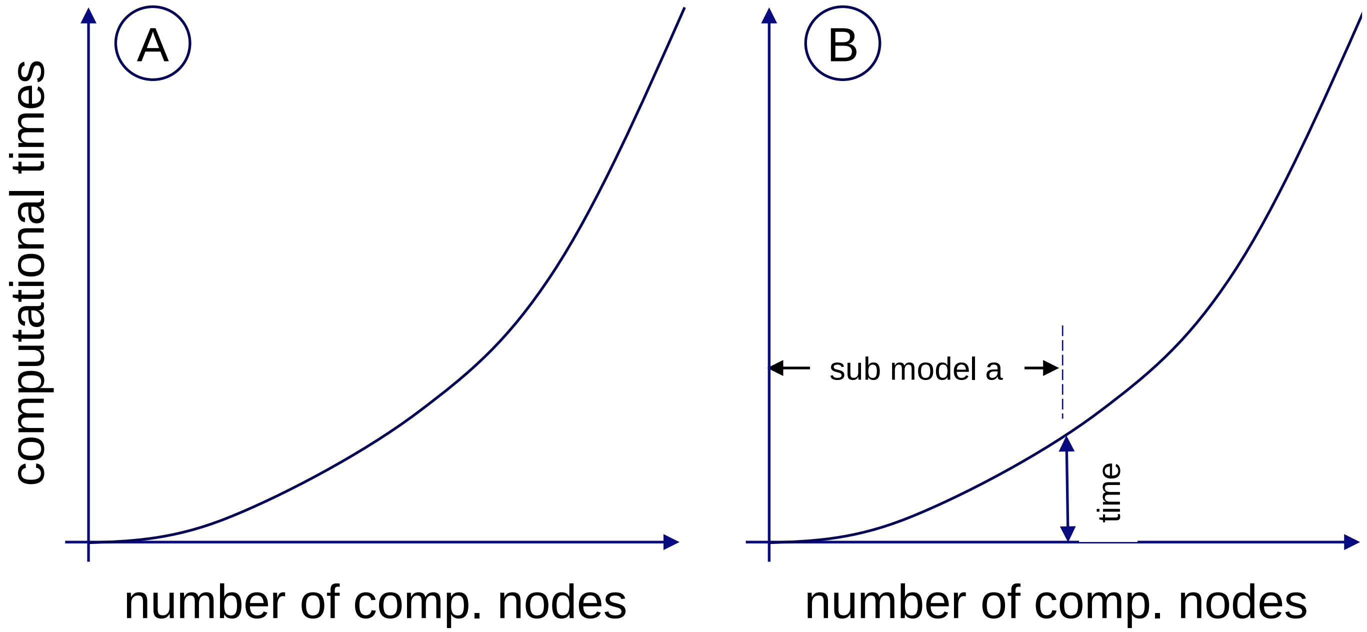
Runtimes of Models



Single CPU

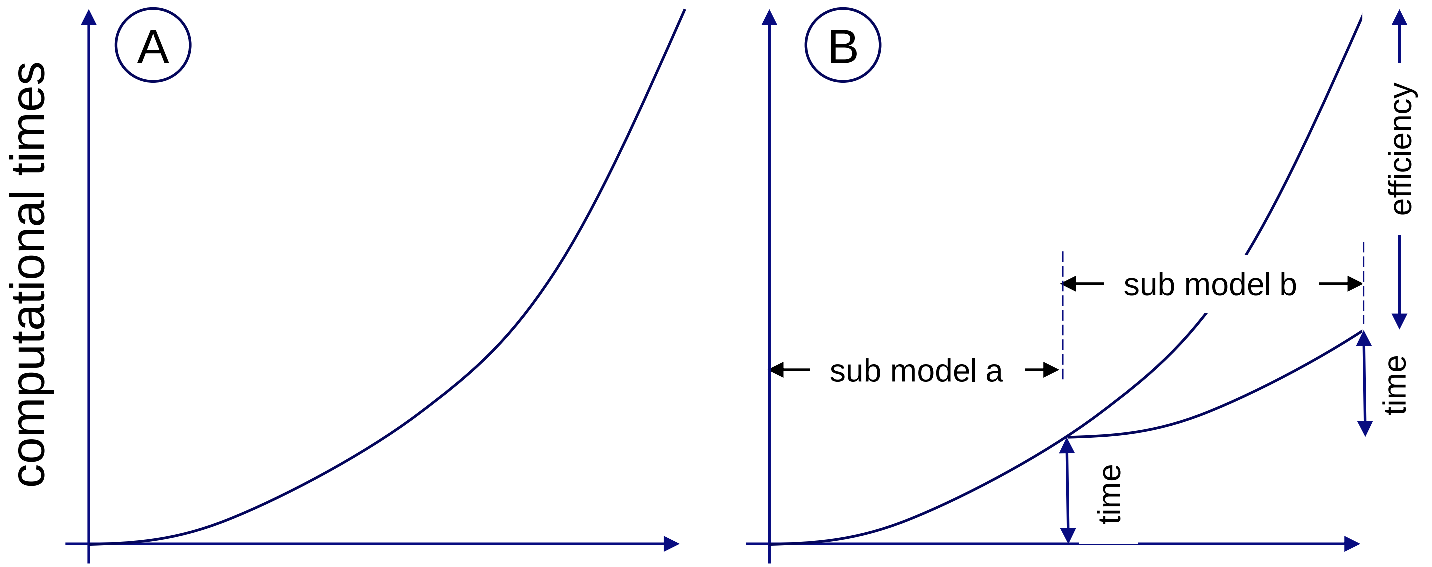
Runtimes of Models



Single CPU

Single CPU/Submodel

Runtimes of Models

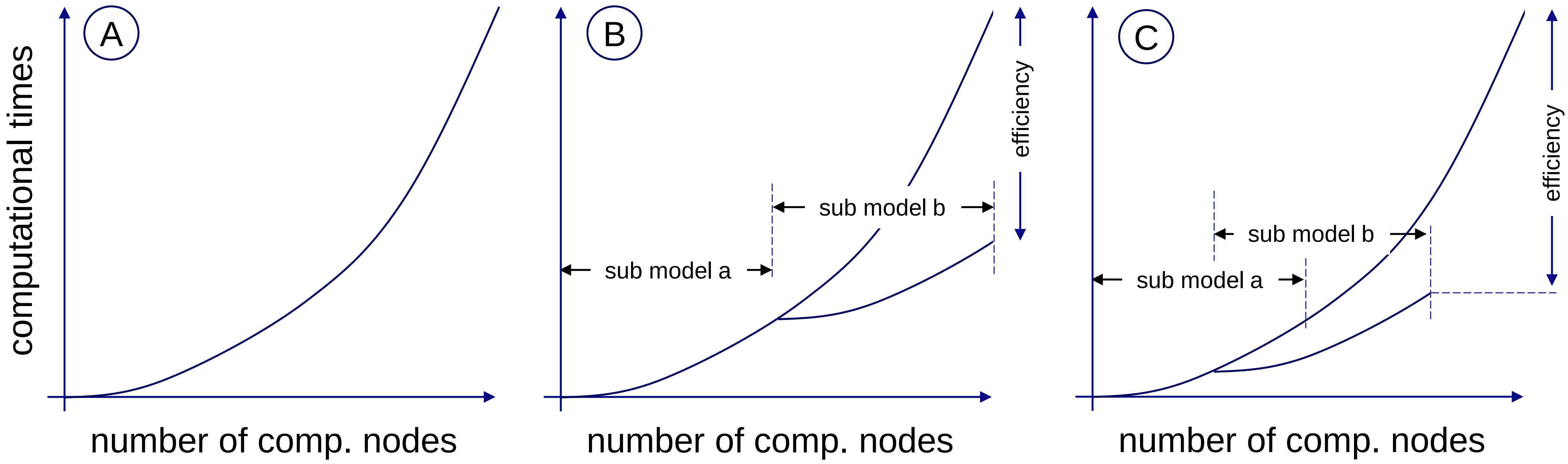


number of comp. nodes
Single CPU

number of comp. nodes
Single CPU/ Two submodels

Deltares

Runtimes of Models

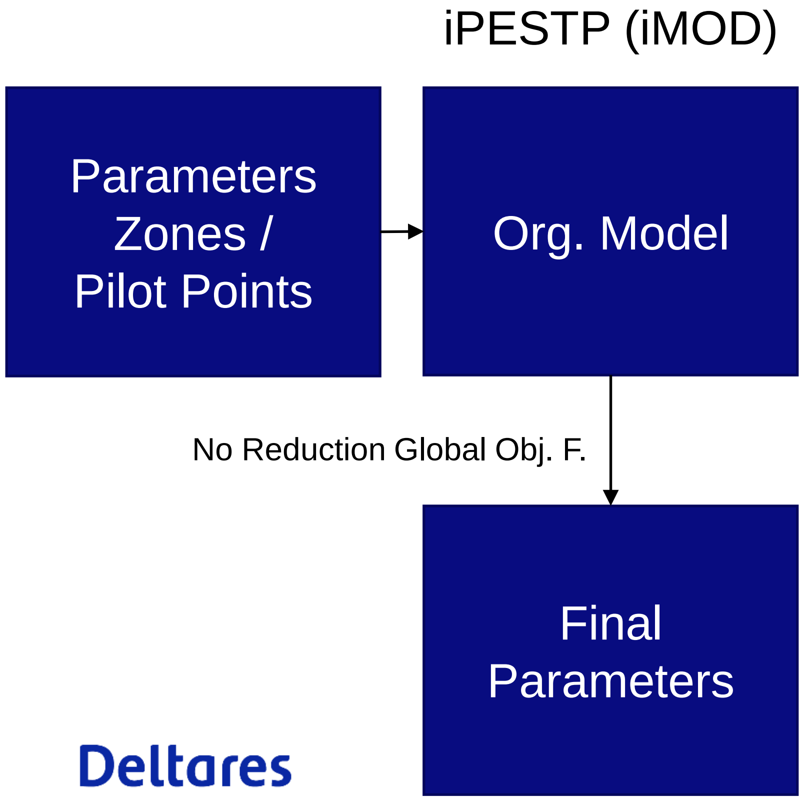


Single CPU

Single CPU/ Two submodels

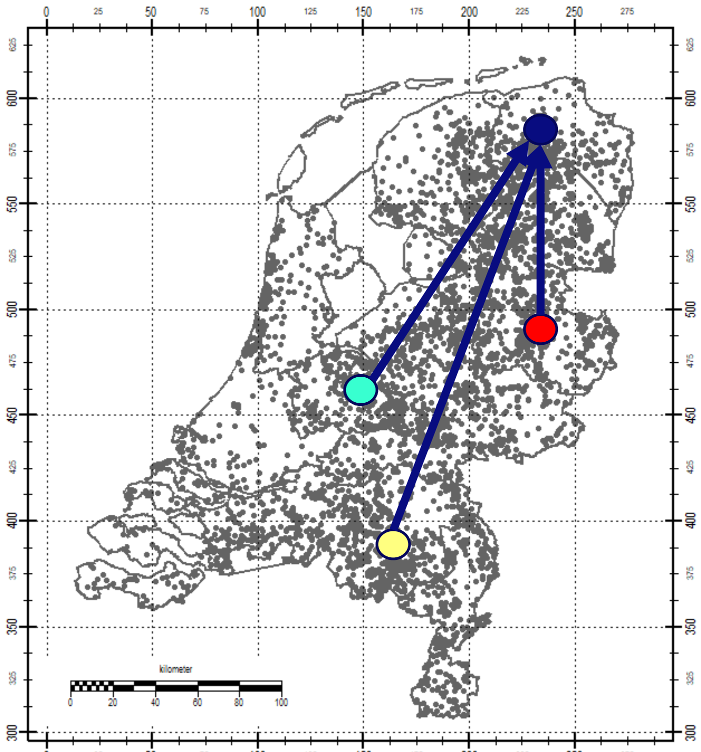
Two CPU/ Two submodels

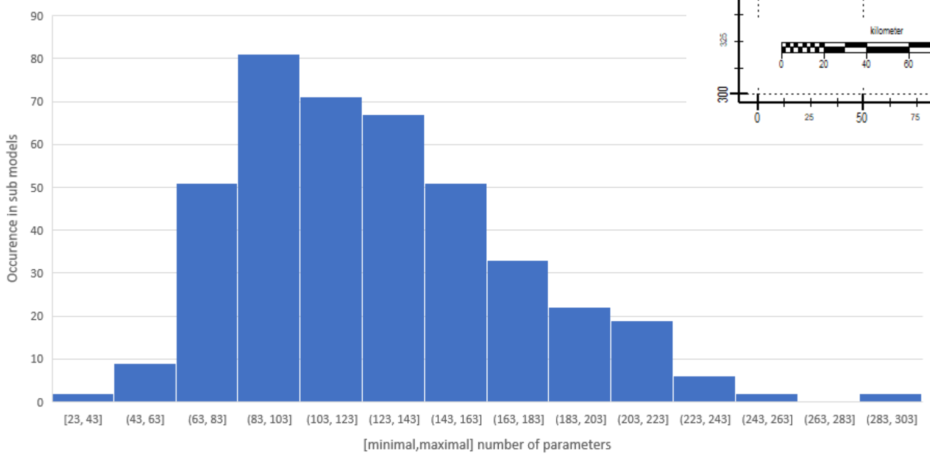
Submodel Model Optimization Method (SMOM)



Questions:

- Effects groundwater in Groningen that of Twente, Utrecht of Brabant?
- Can sensitivities be approximated by smaller models?
- Why compute Groningen for parameters that do not extent in that region?

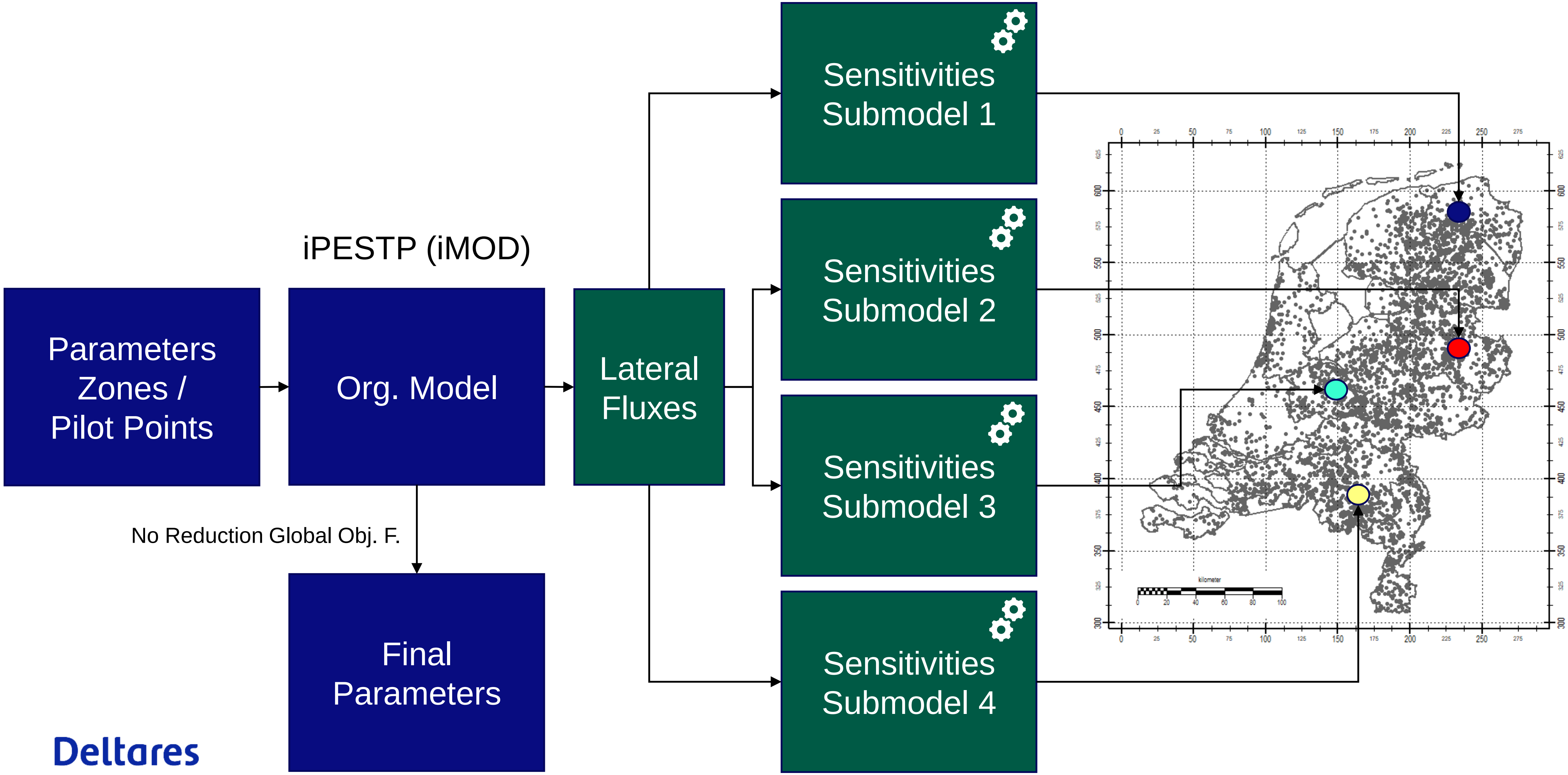




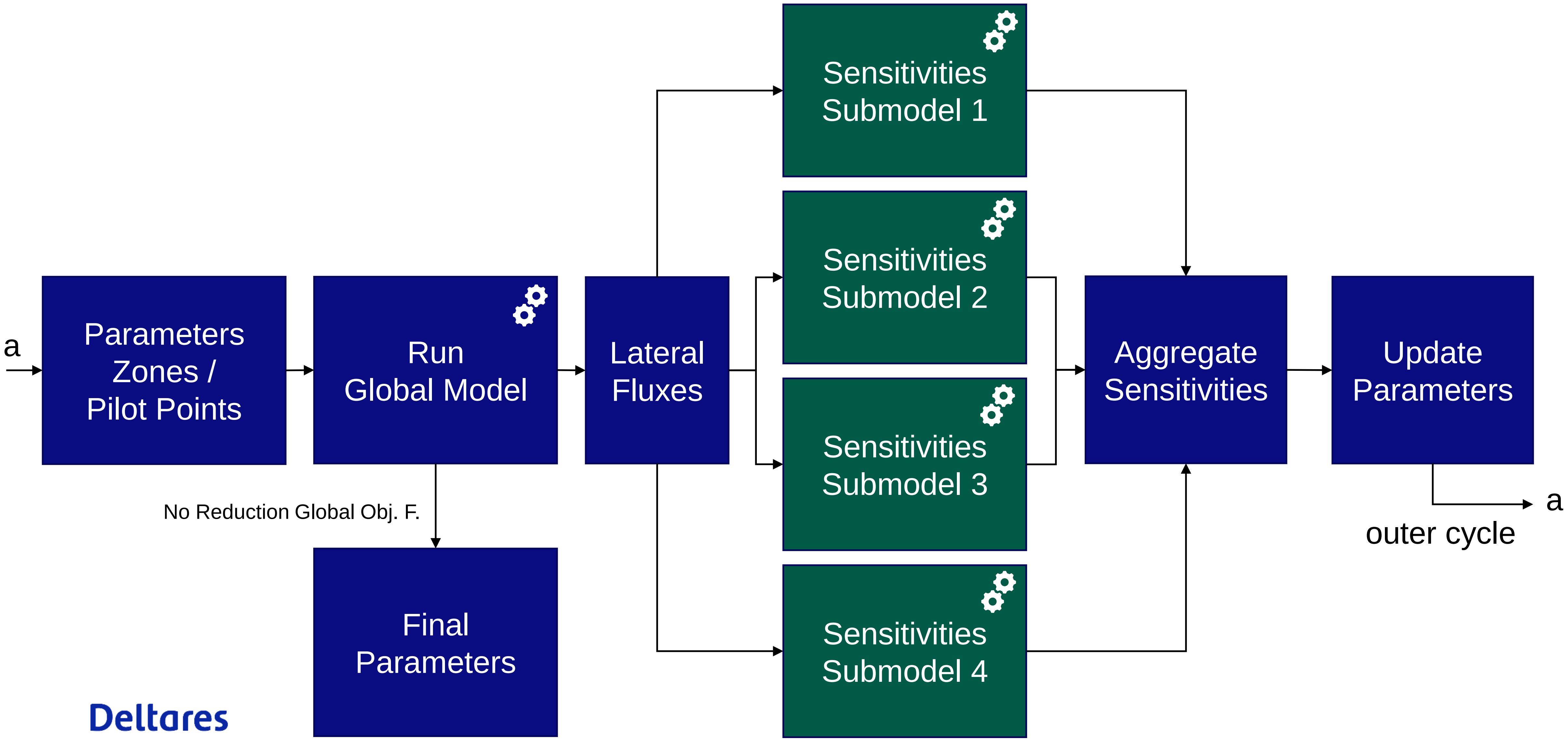
number of parameter per submodel

Deltares

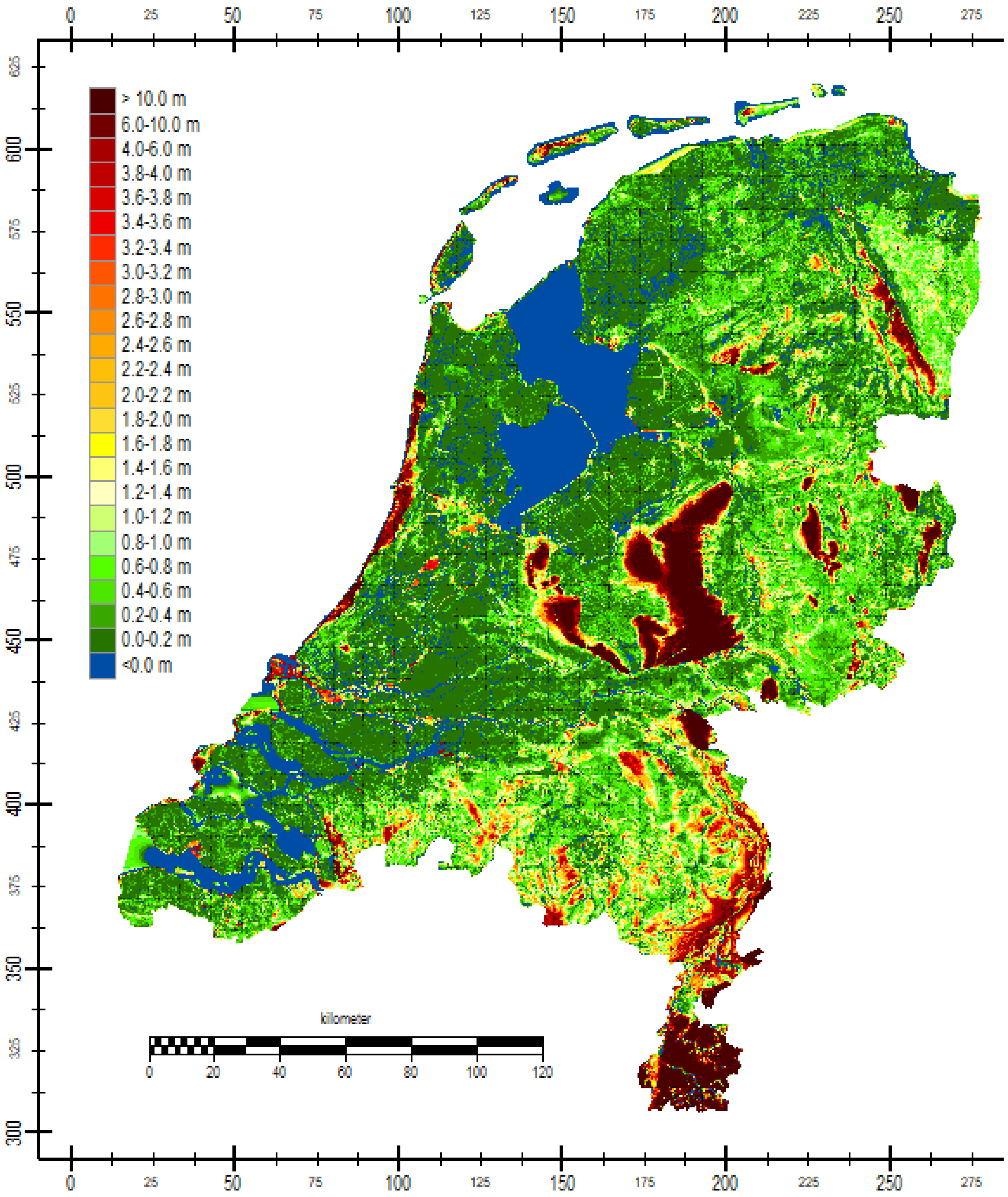
Submodel Model Optimization Method (SMOM)



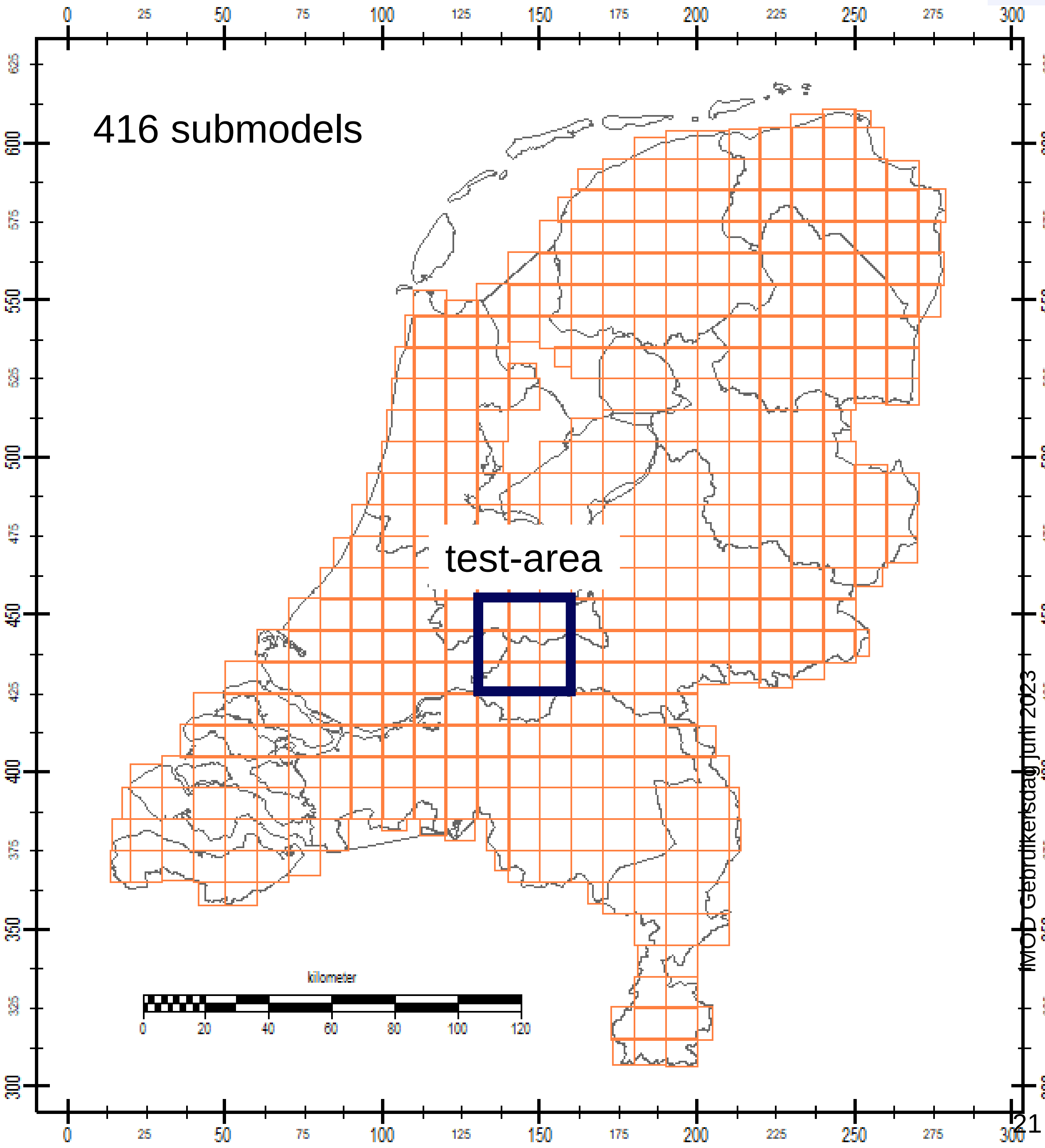
Submodel Model Optimization Method (SMOM)



Deltares



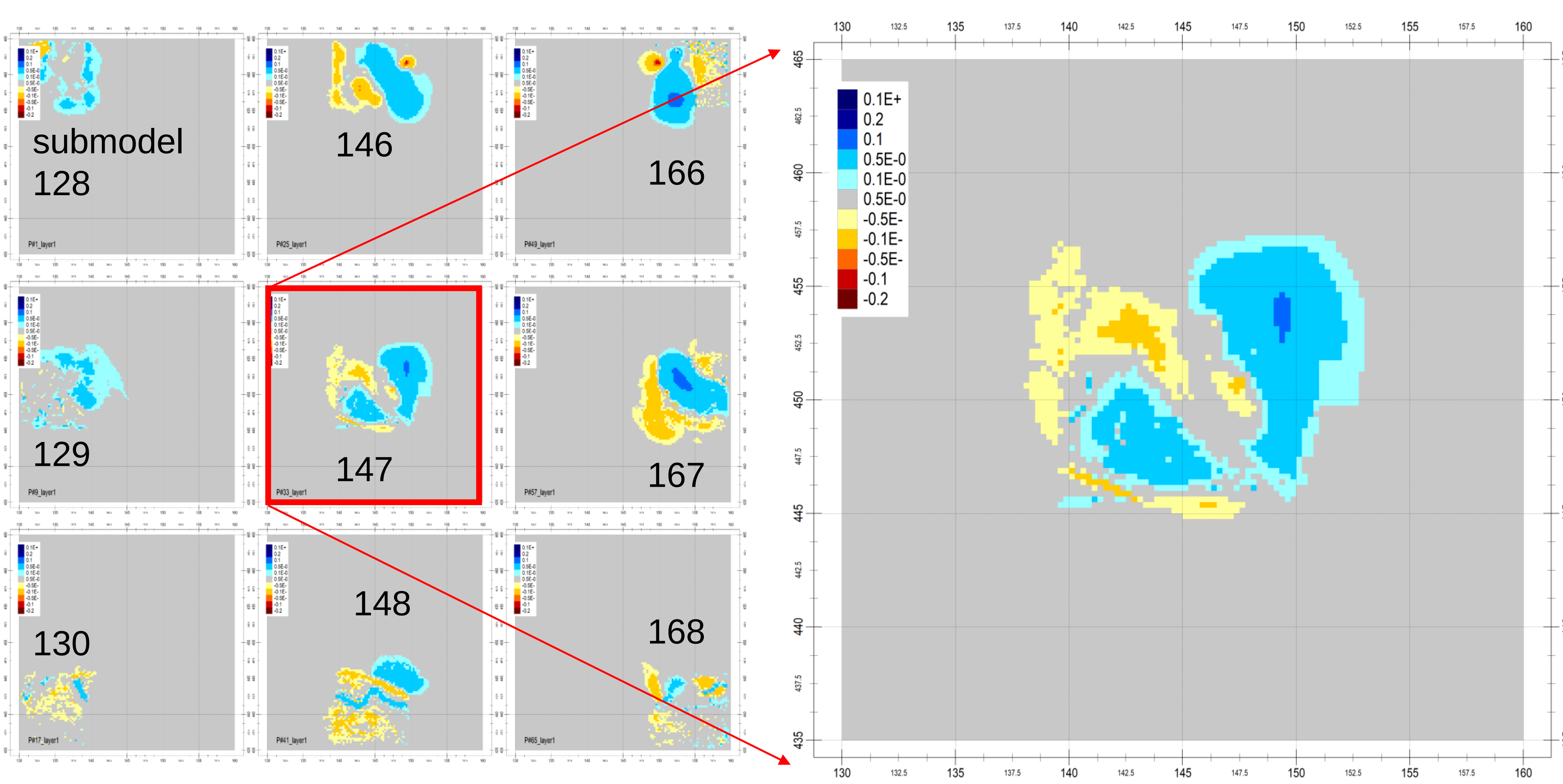
> 10.0 m
6.0-10.0 m
4.0-6.0 m
3.8-4.0 m
3.6-3.8 m
3.4-3.6 m
3.2-3.4 m
3.0-3.2 m
2.8-3.0 m
2.6-2.8 m
2.4-2.6 m
2.2-2.4 m
2.0-2.2 m
1.8-2.0 m
1.6-1.8 m
1.4-1.6 m
1.2-1.4 m
1.0-1.2 m
0.8-1.0 m
0.6-0.8 m
0.4-0.6 m
0.2-0.4 m
0.0-0.2 m
<0.0 m
kilometer



416 submodels
test-area
kilometer

Submodel Model Optimization Method (SMOM)

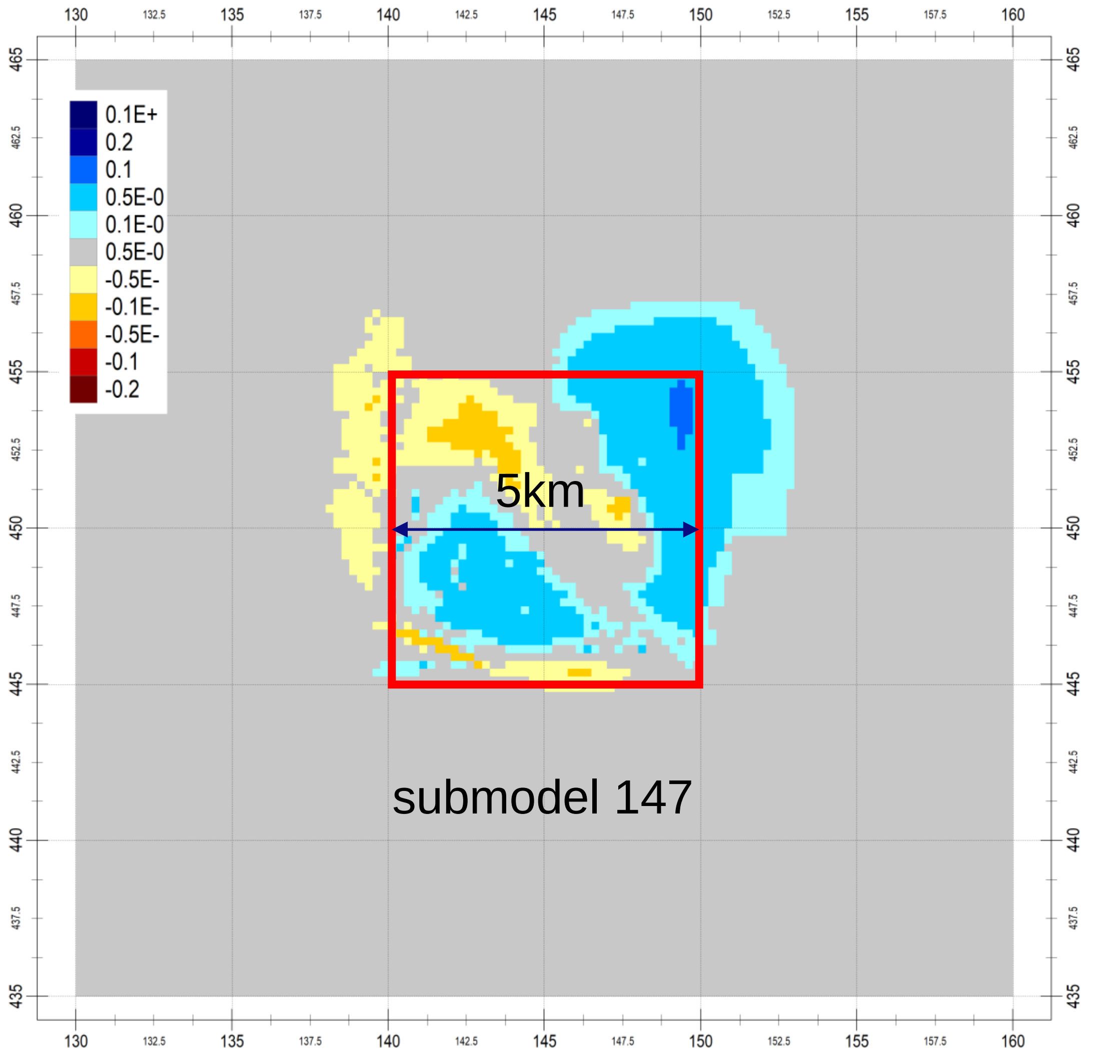
kd$_n$*1.1



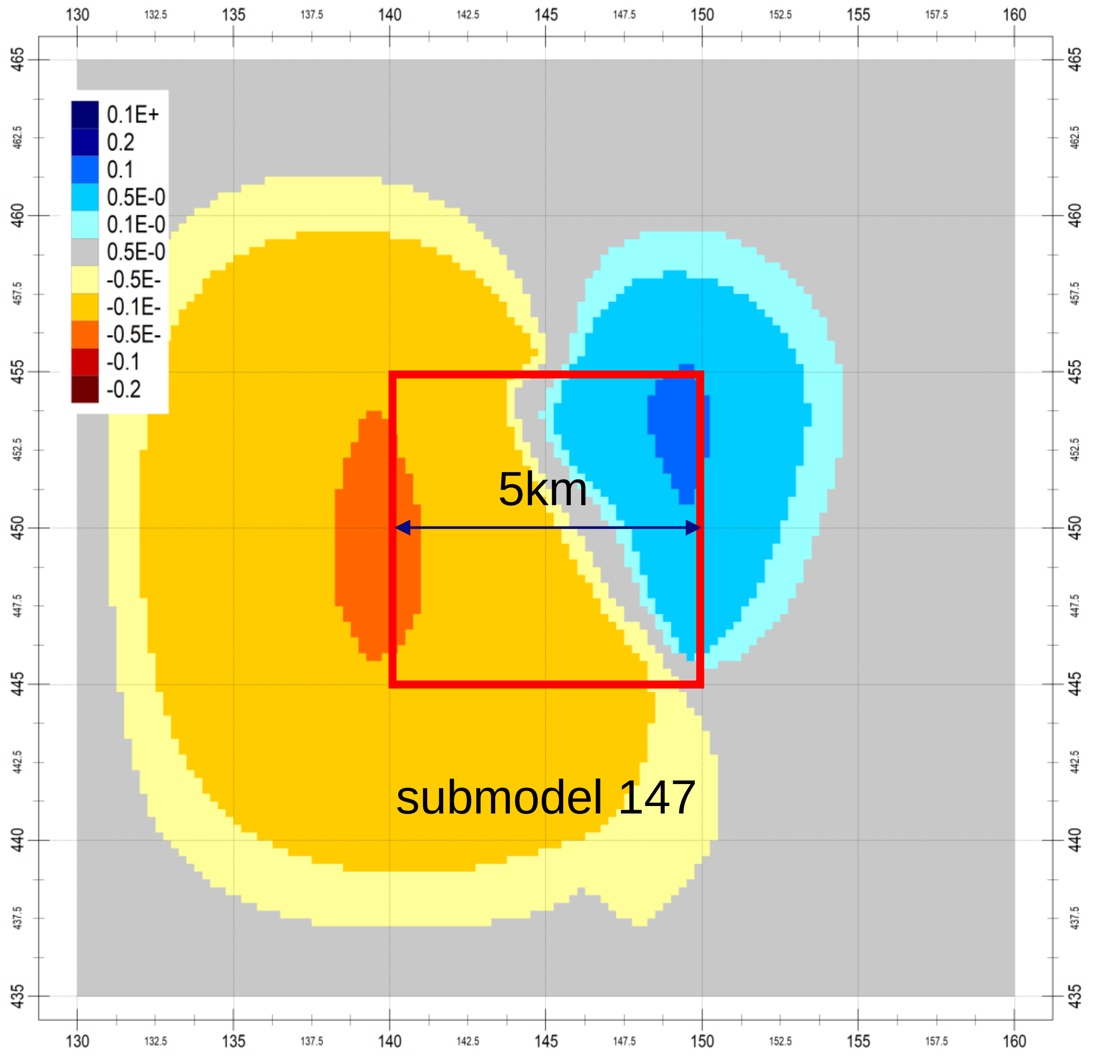
sensitivities in layer 1 per parameter

Deltares

Submodel Model Optimization Method (SMOM)



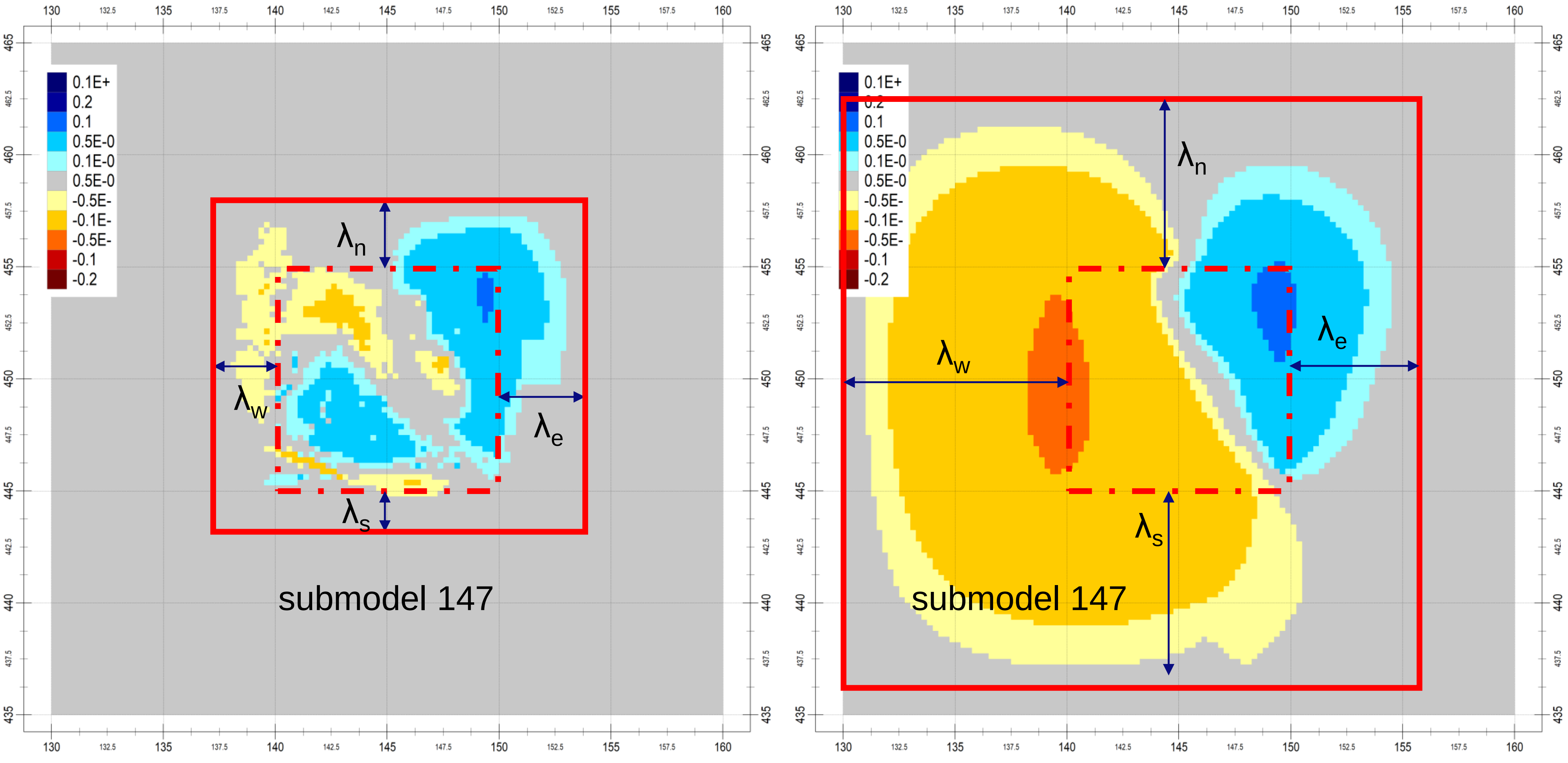
LAYER 1



LAYER 8

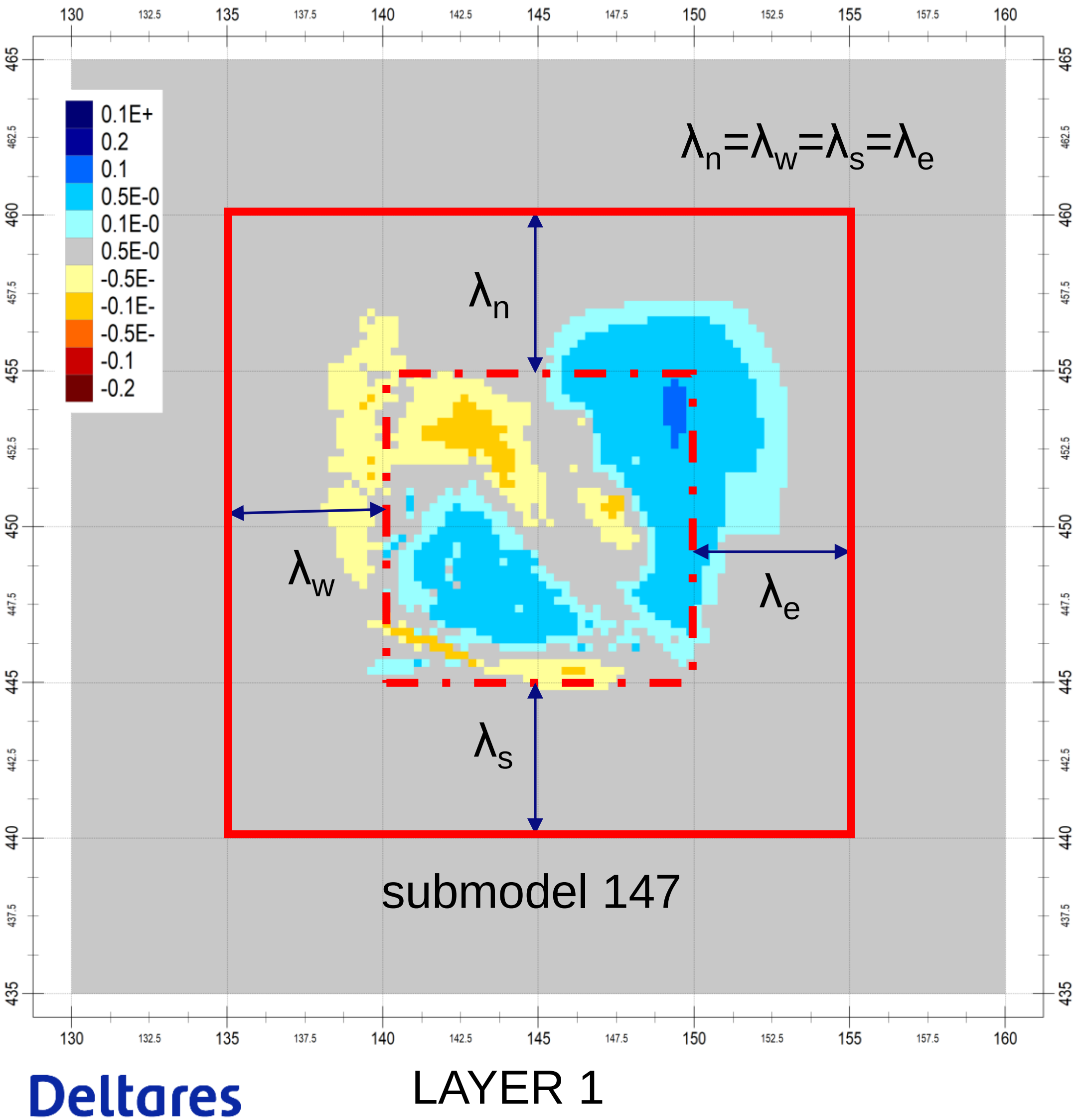
Deltares

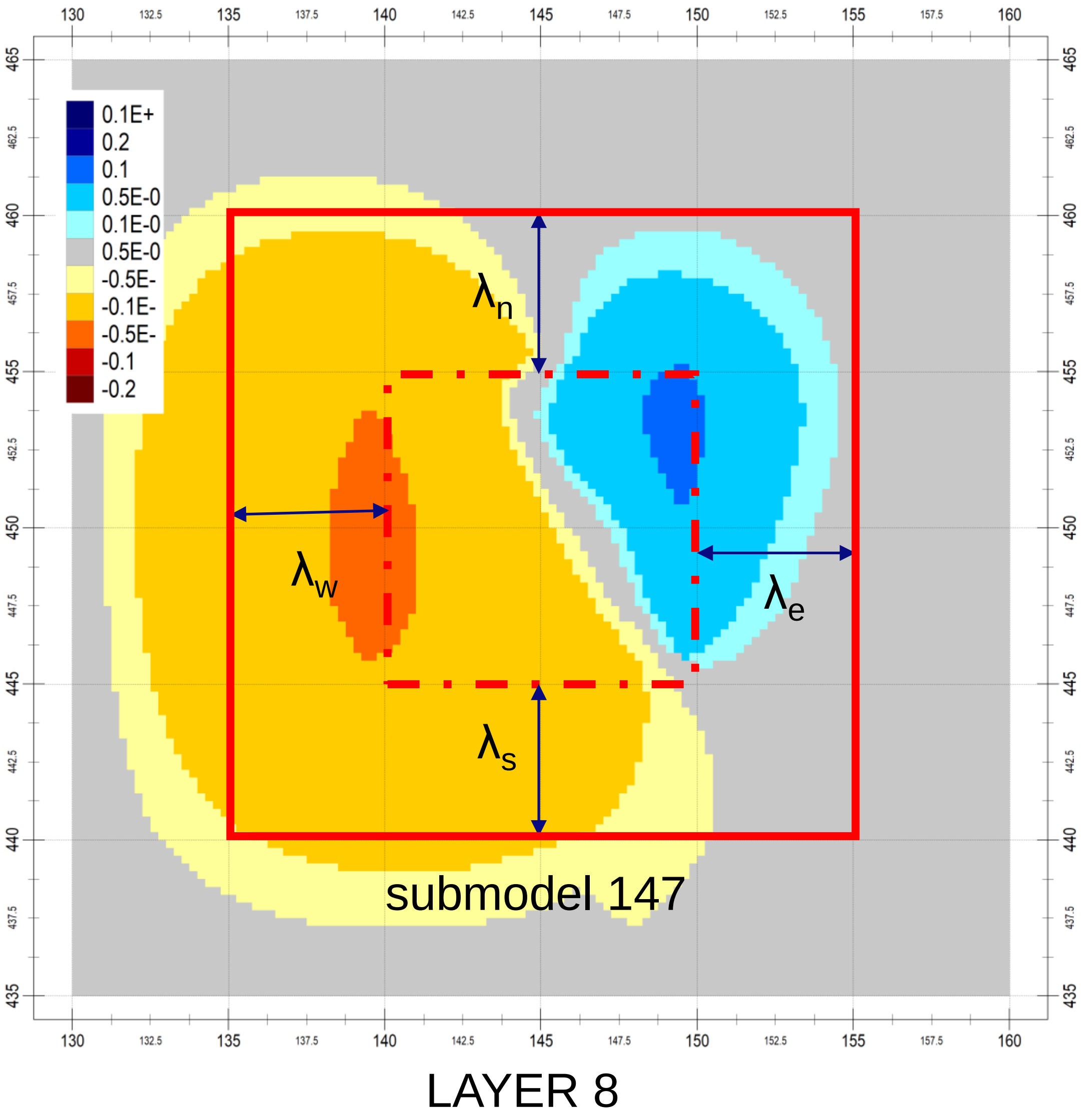
Submodel Model Optimization Method (SMOM)



Deltares

Submodel Model Optimization Method (SMOM)





Deltares

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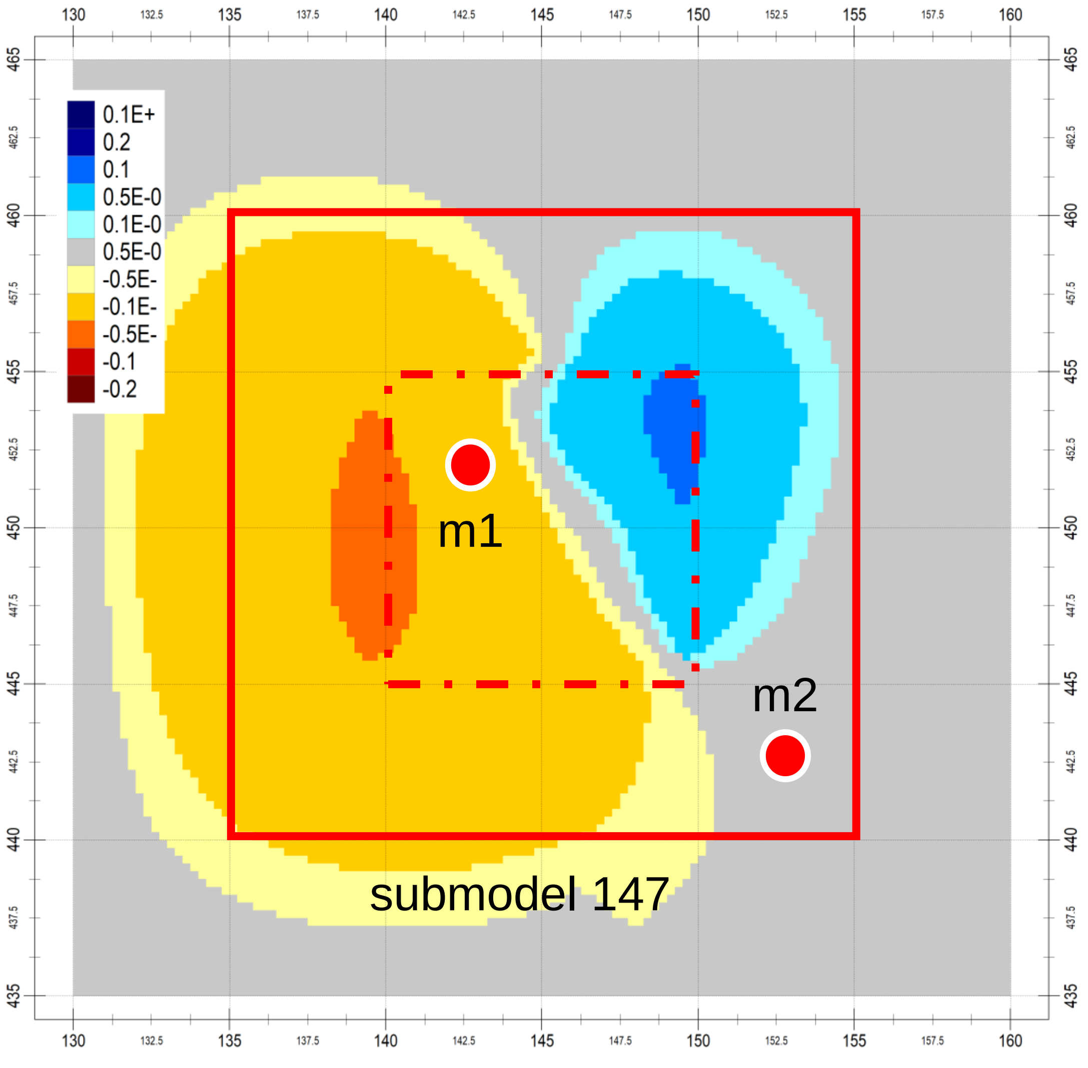

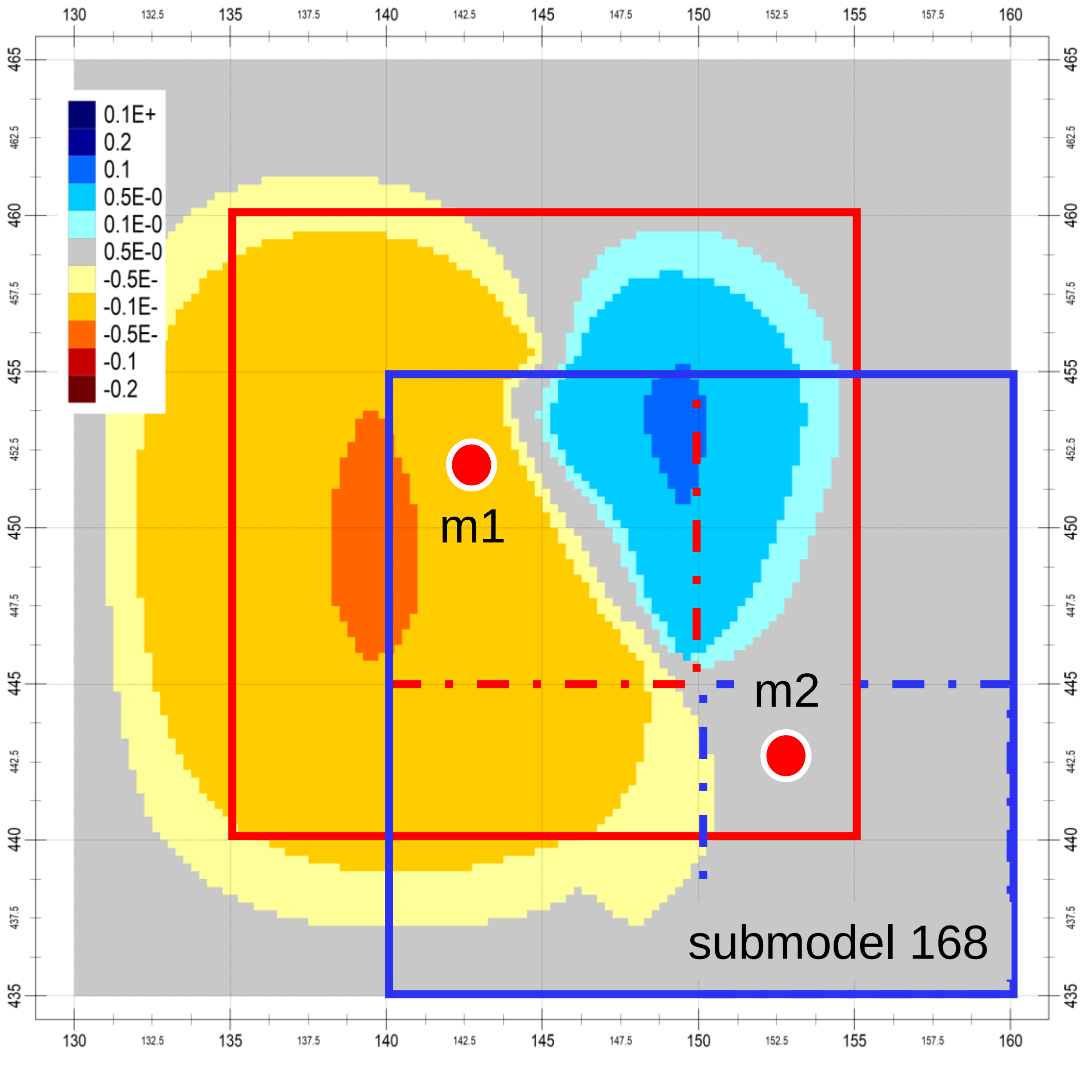

Deltares

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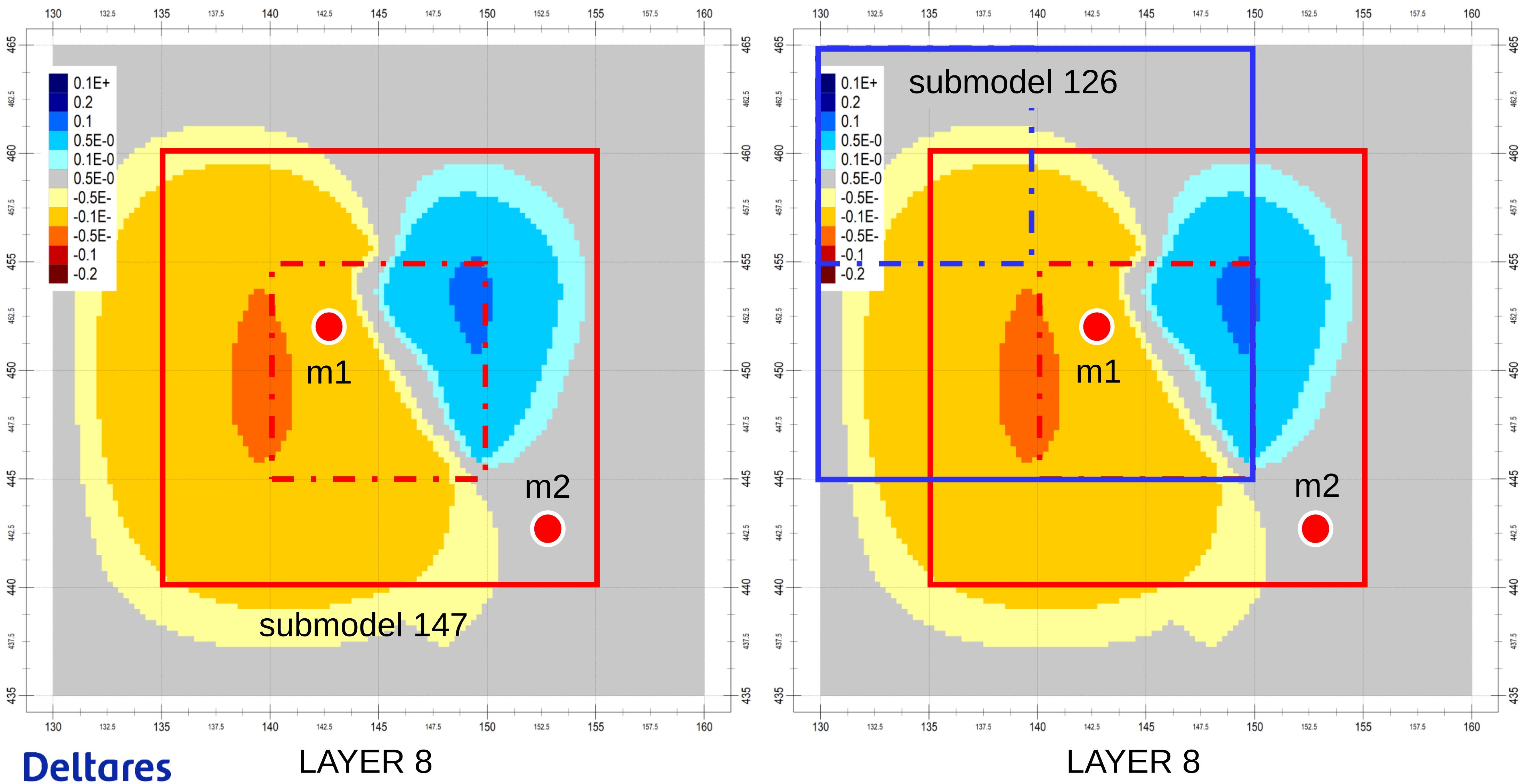
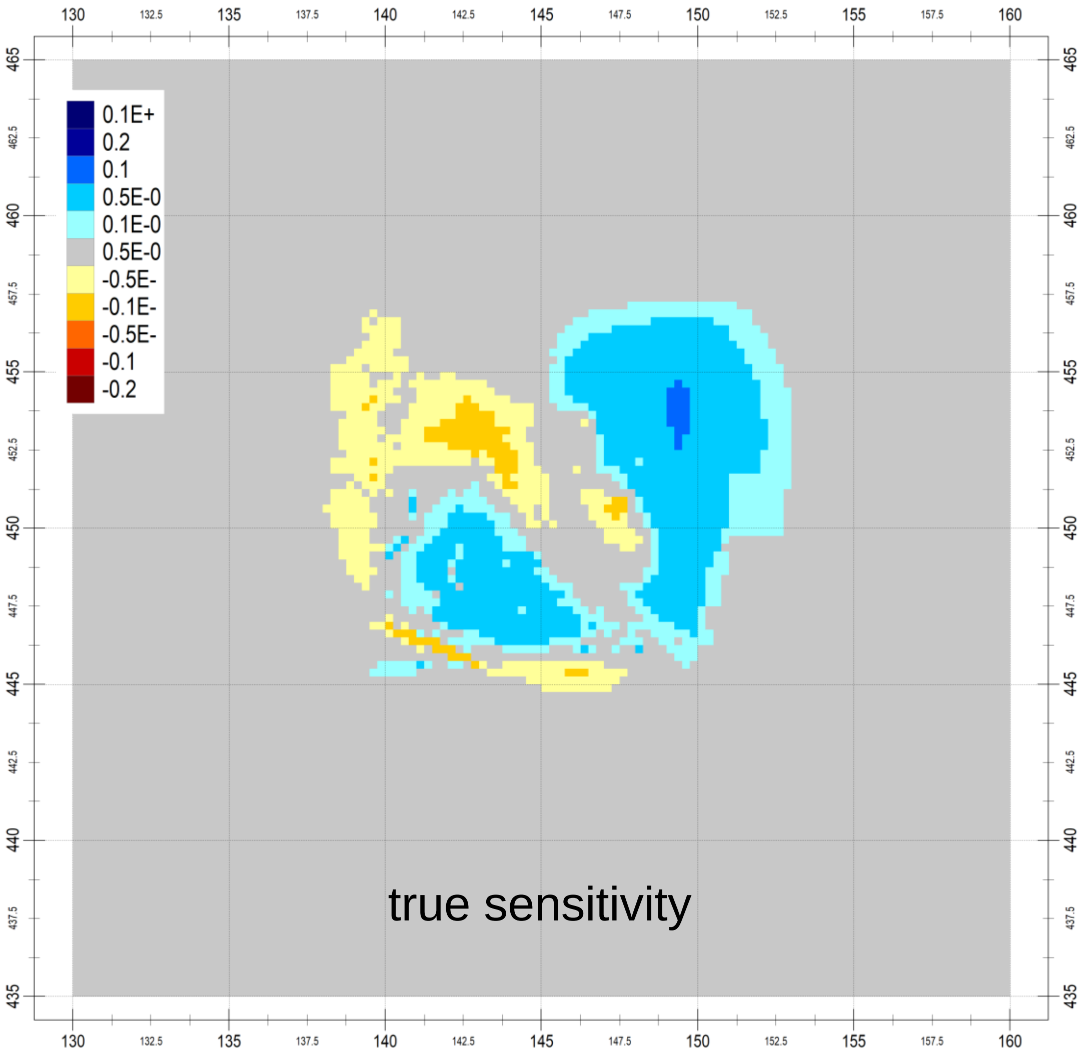


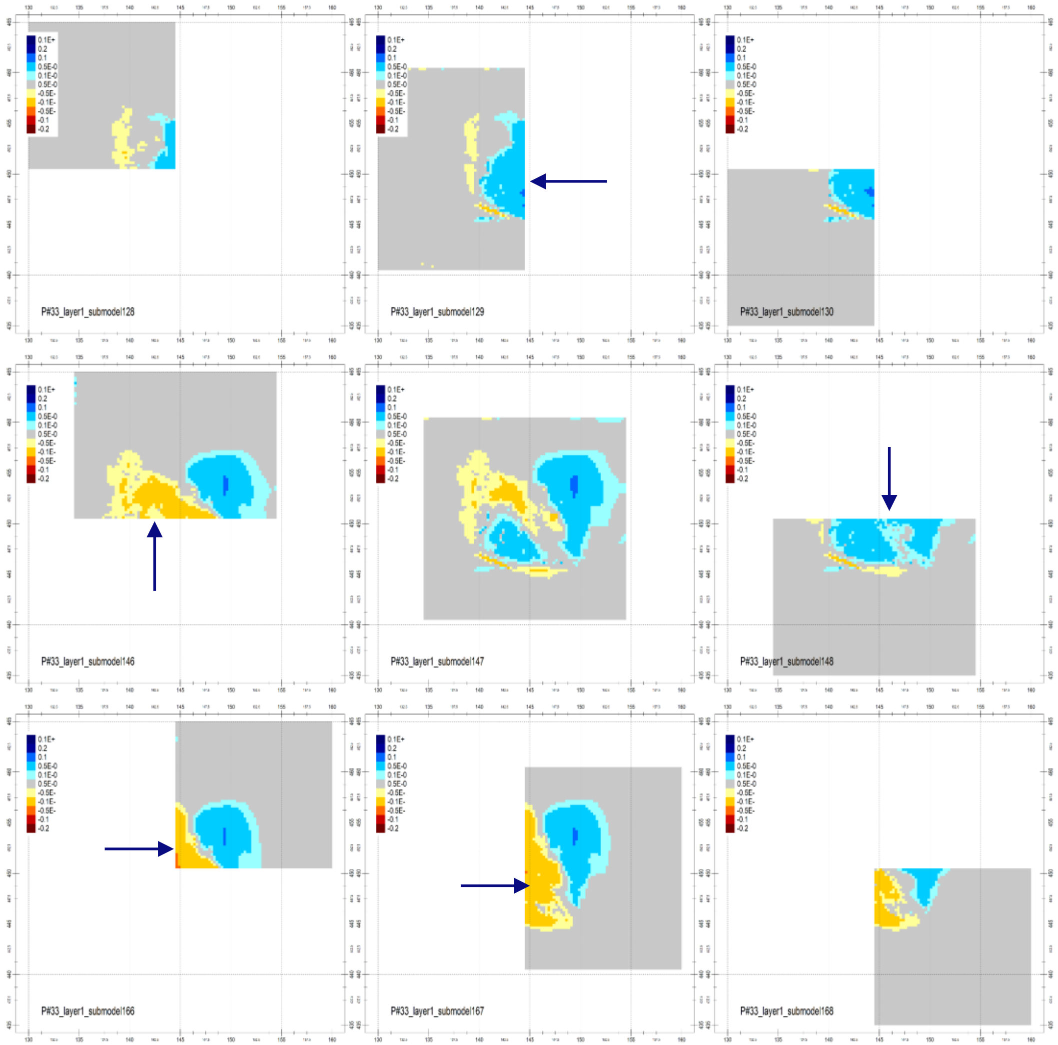
Deltares

SMOM – Q-EDGE



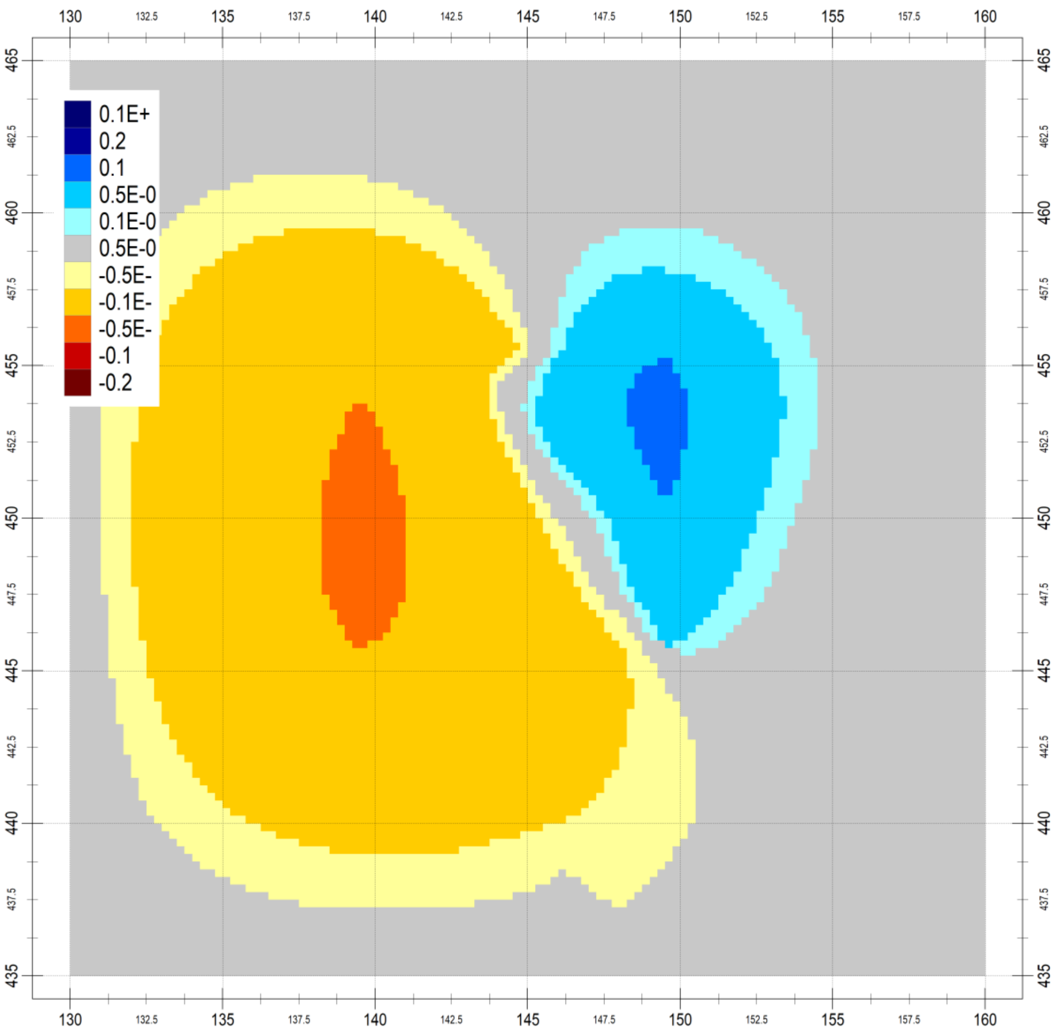
LAYER 1

sensitivities per submodel

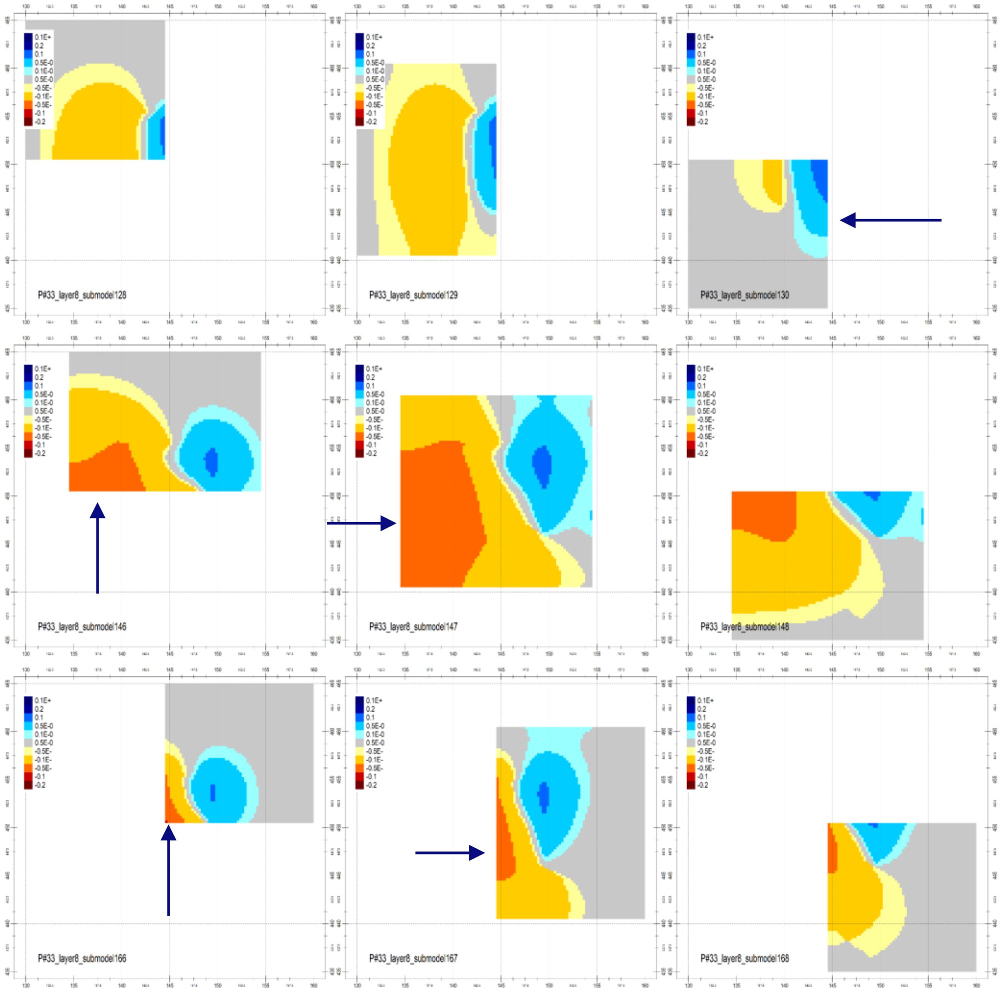


Deltares

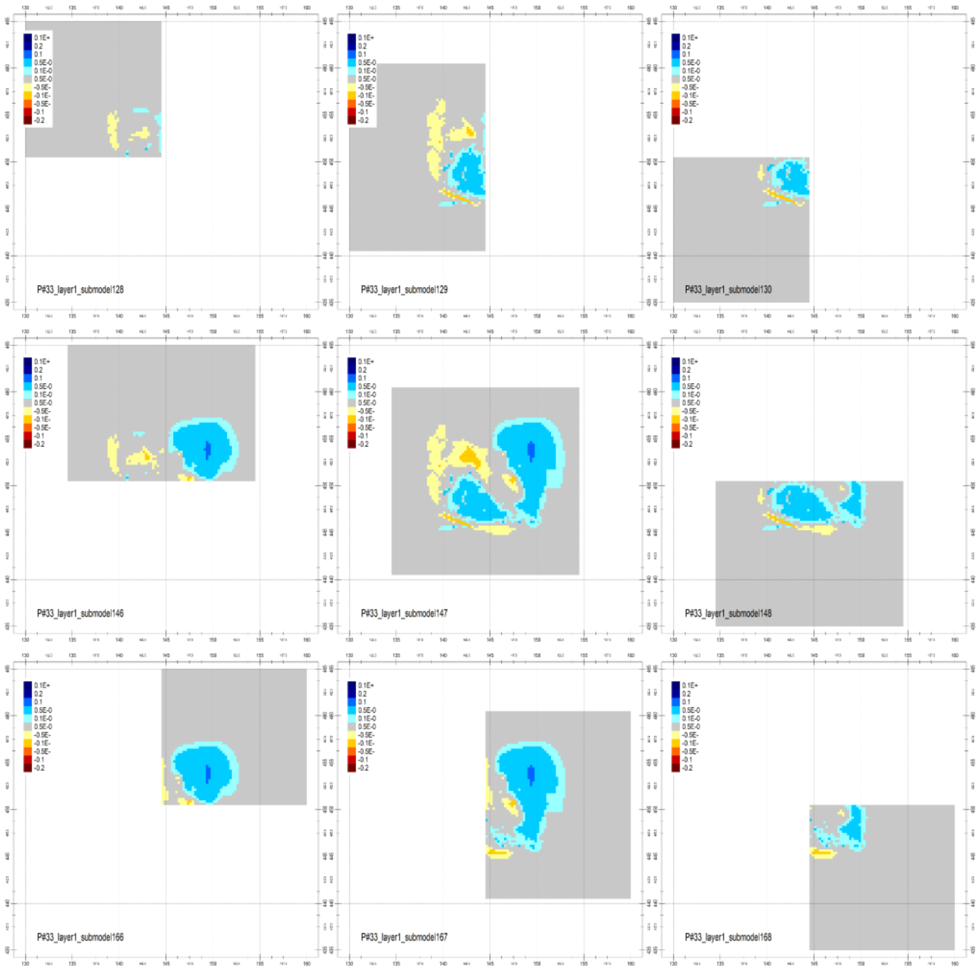
SMOM – Q-EDGE



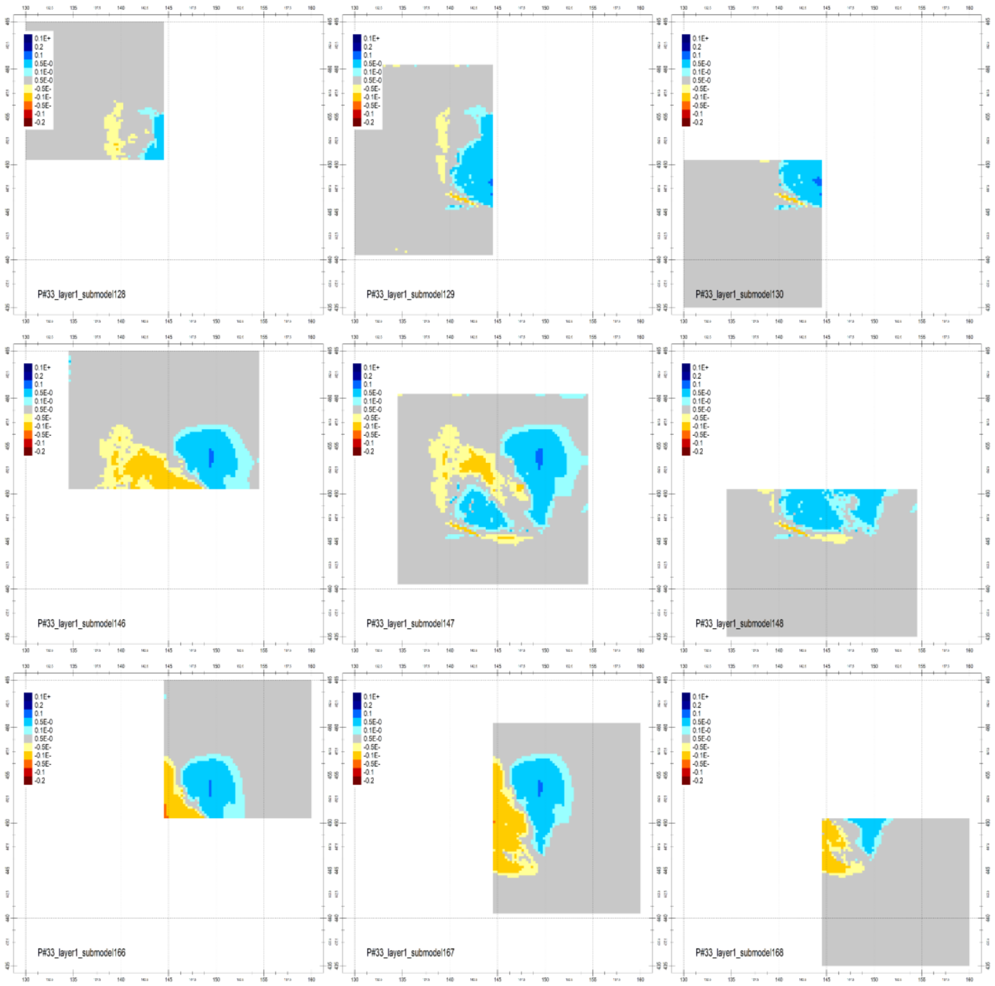
LAYER 8



SMOM – GHB-EDGE cond=q/dh

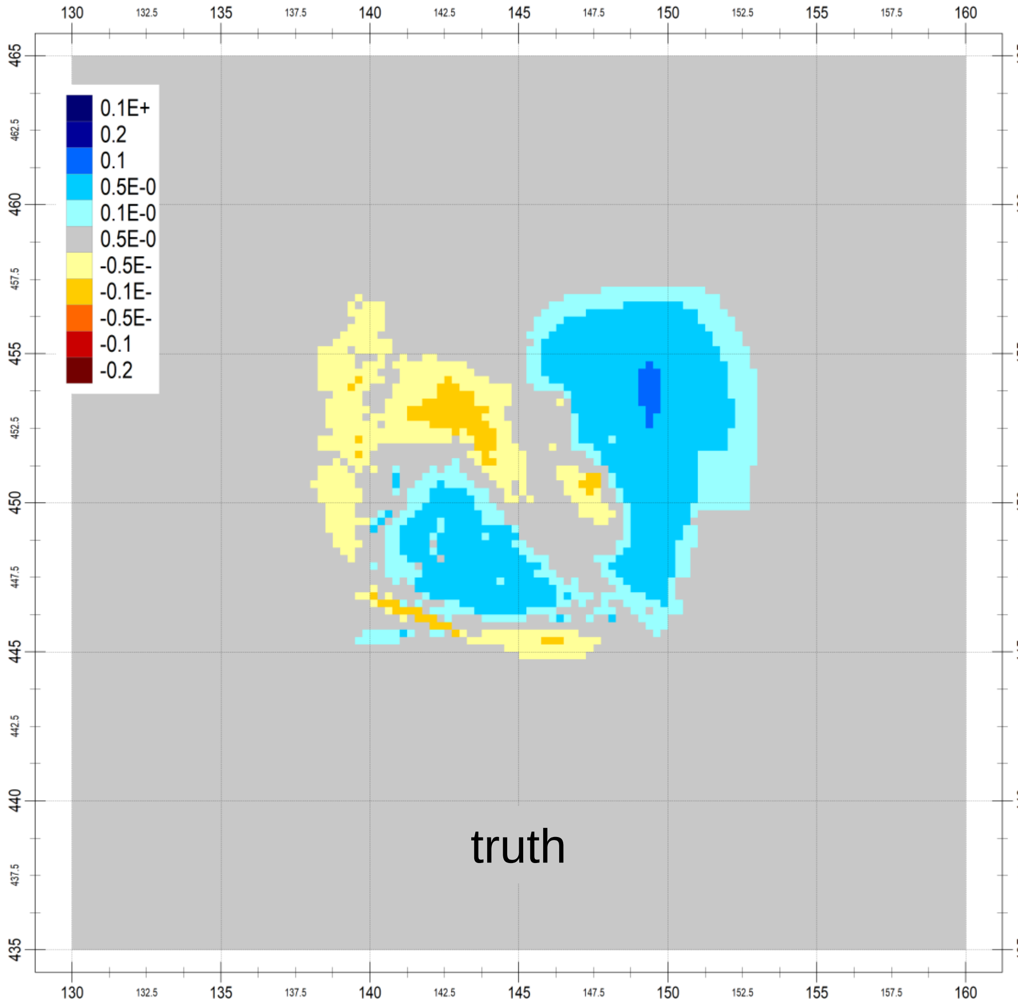


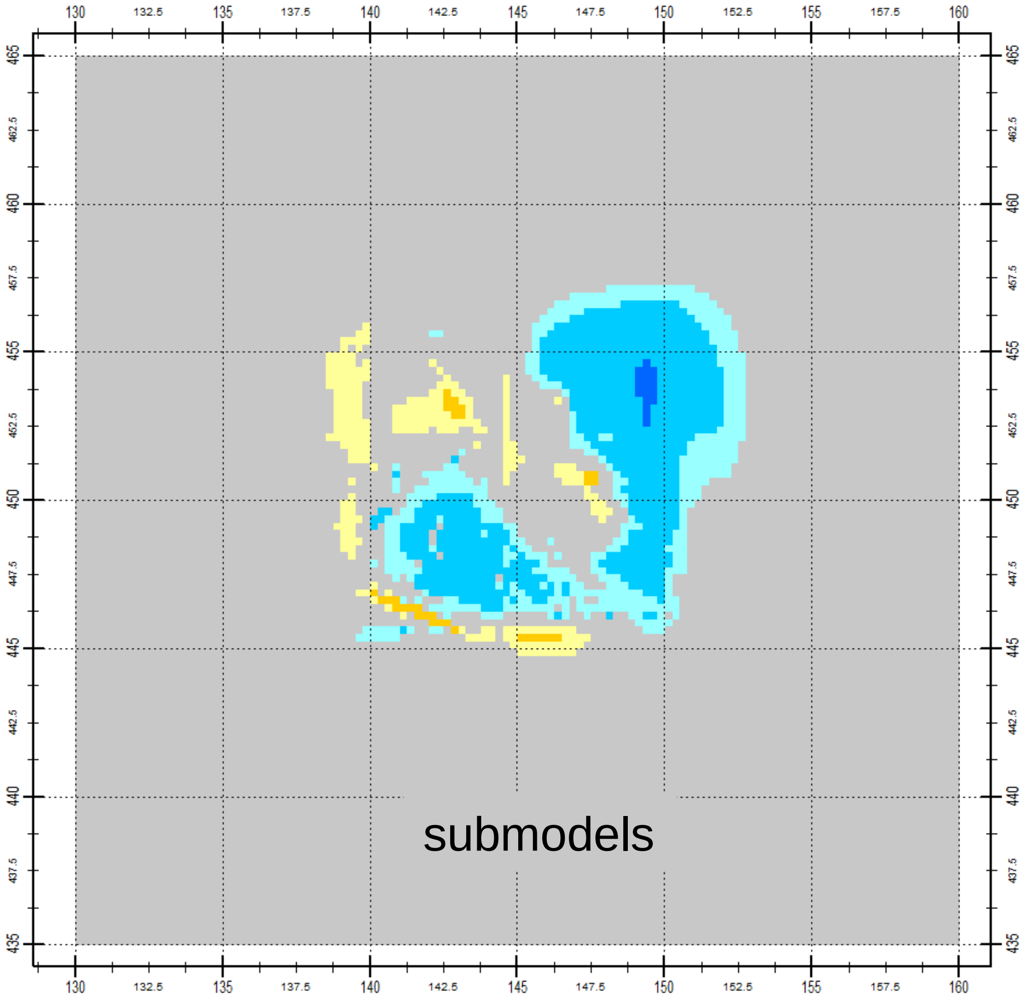
GHB-edge



Q-edge

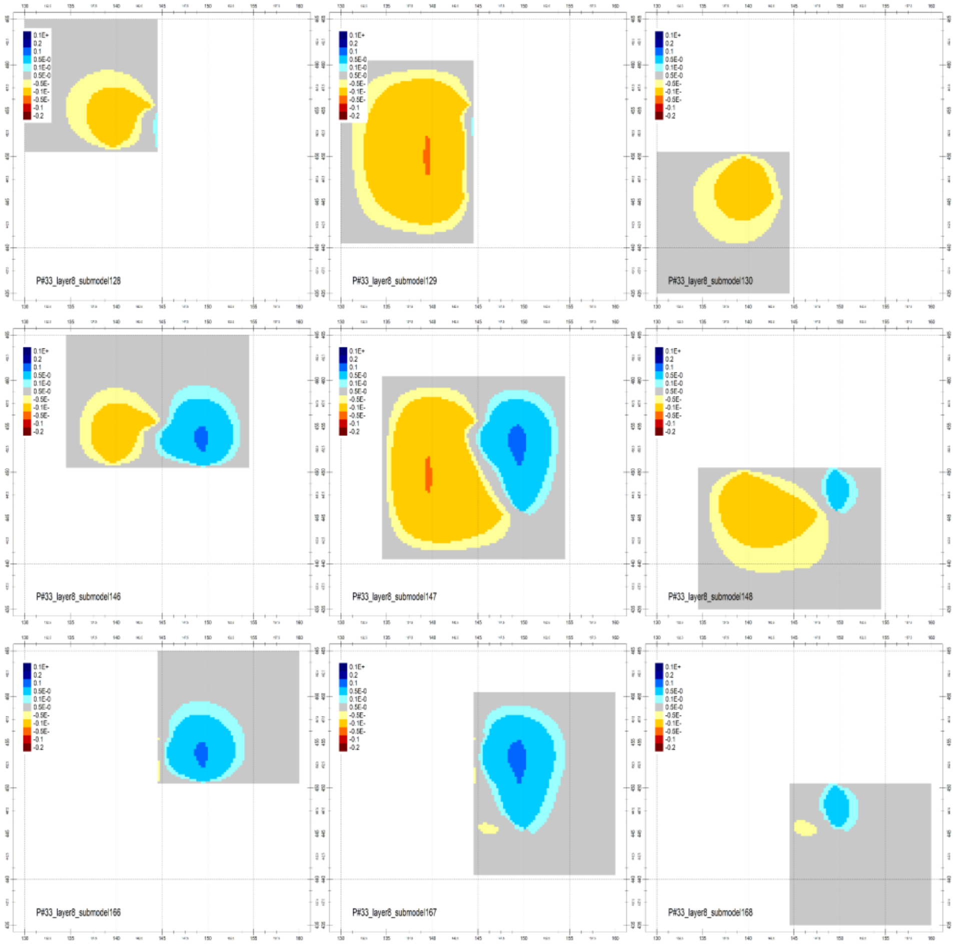
Submodel Model Optimization Method (SMOM)



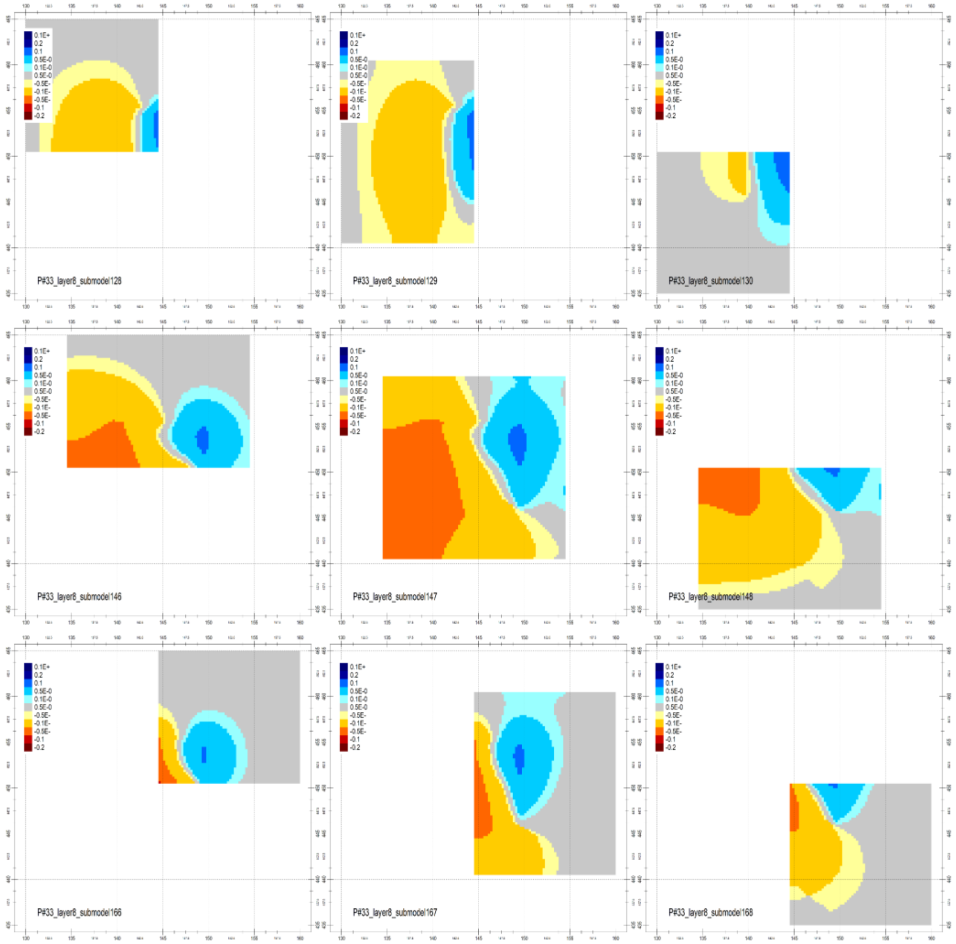


Deltares

SMOM – GHB-EDGE cond=q/dh



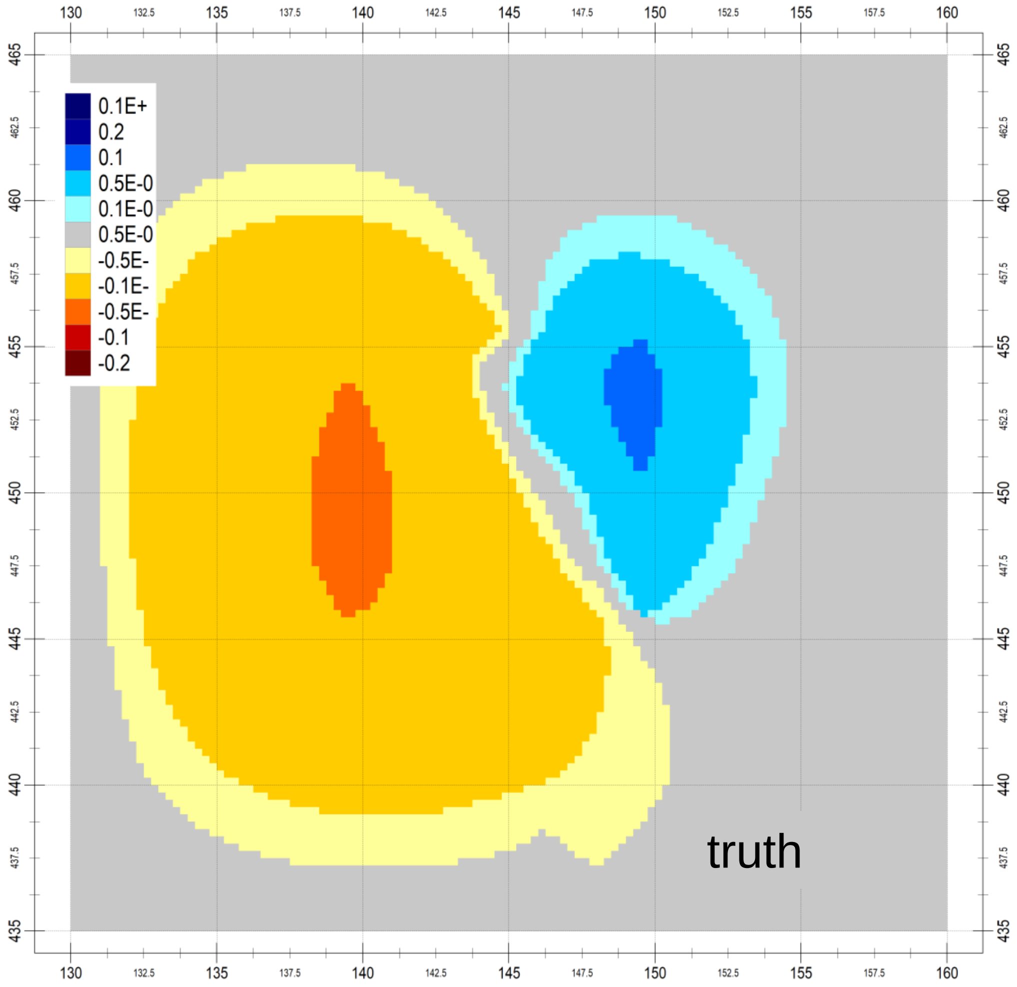
GHB-edge

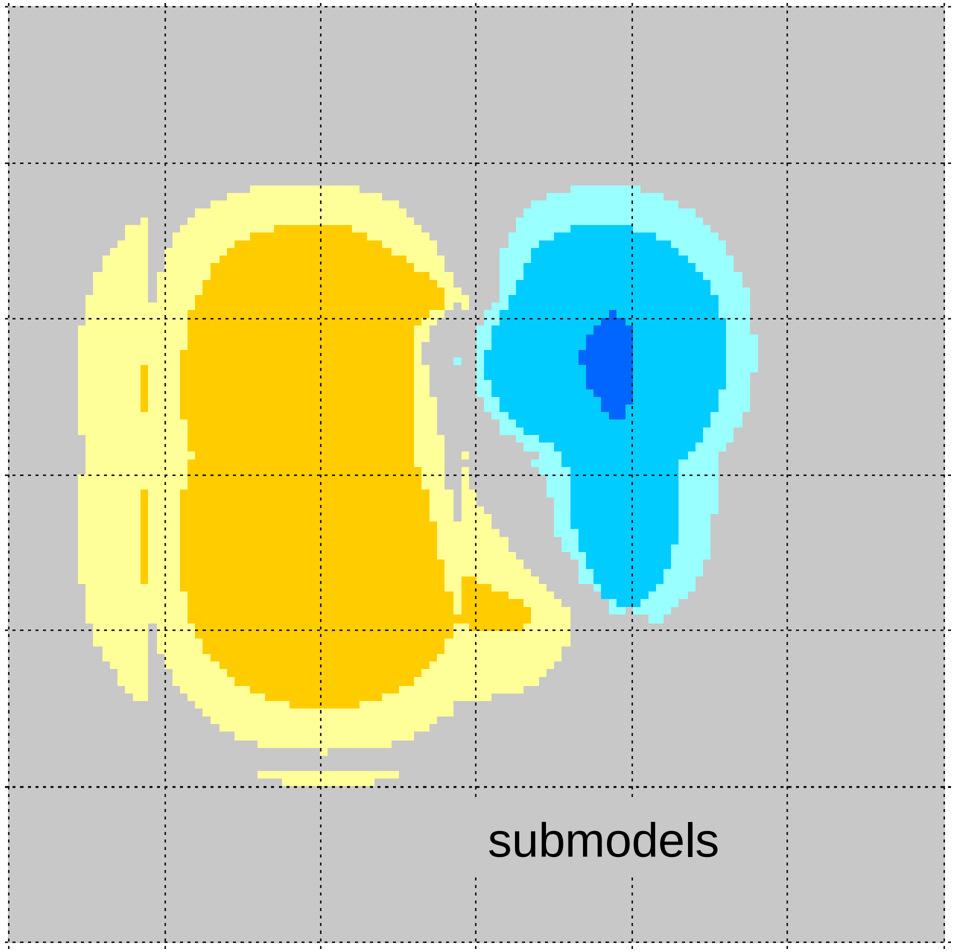


Q-edge

Deltares

SMOM – GHB-EDGE





SMOM – RESULTS

full overlap
half overlap
quarter overlap

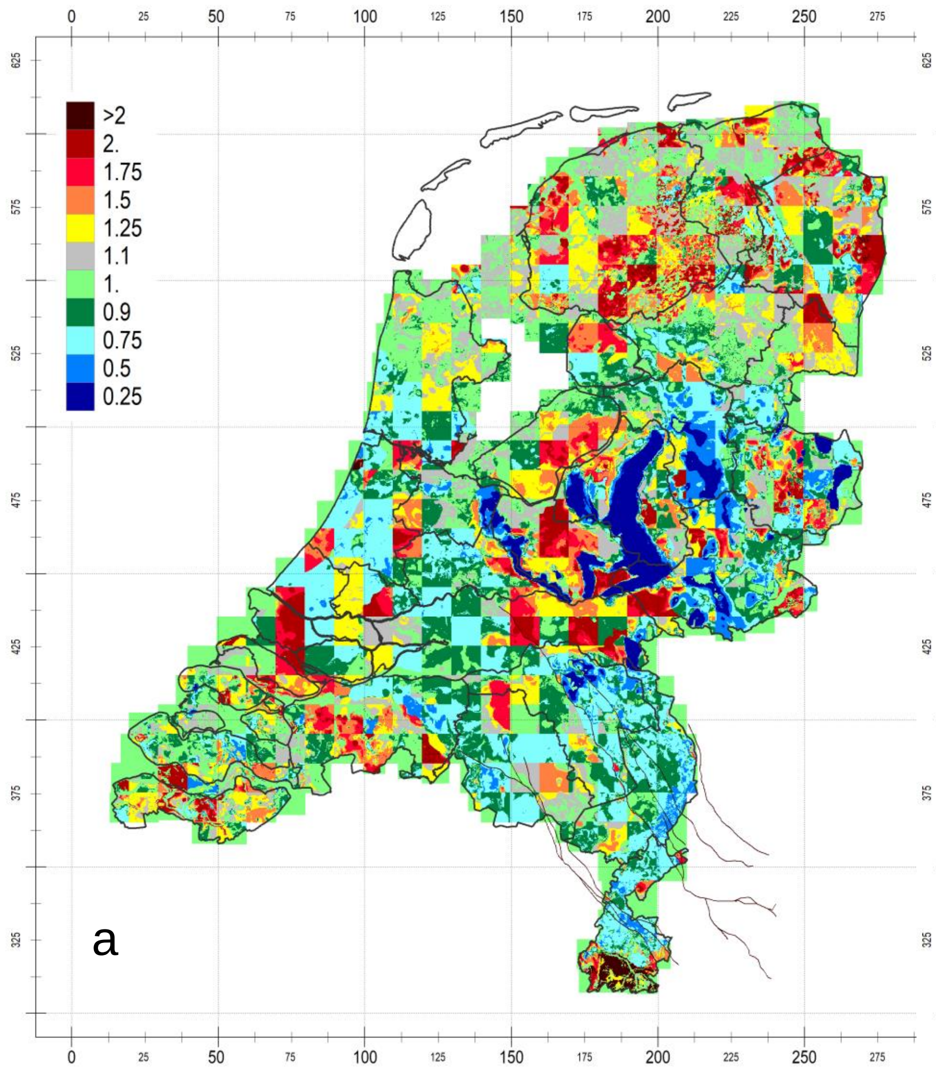
fractional errors

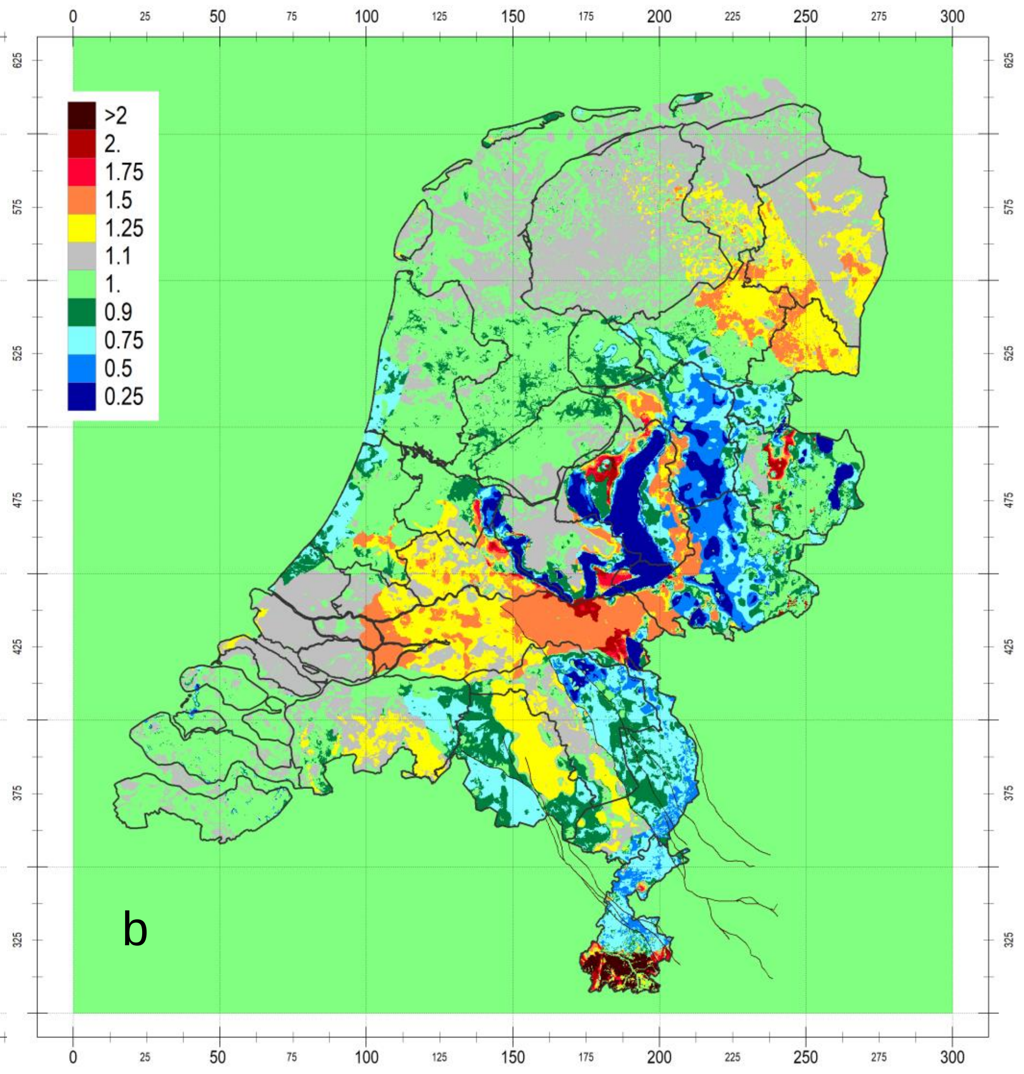
			TRUTH	10000	5000	2500	1000	0		10000	5000	2500	1000	0
	iteraties	0	4	4	4	4	4	4						
	doelf.	199.687	162.829	160.951	162.757	169.232	181.881	228.278		0.98847	0.99956	1.03932	1.11701	1.40195
	kd_z128	1	0.4894	0.538	0.56	0.595	0.759	1.467		1.09929	1.14425	1.21576	1.55086	2.99752
	kd_z129	1	3.65549	3.025	4.289	8.427	10	0.171		0.82752	1.1733	2.3053	2.73561	0.04678
	kd_z130	1	9.7792	10	5.769	9.707	10	1		1.02258	0.58993	0.99262	1.02258	0.10226
GHB-BOUNDARY	kd_z146	1	0.67596	0.678	0.686	0.671	0.68	0.648		1.00302	1.01486	0.99267	1.00598	0.95864
	kd_z147	1	3.46153	3.625	3.688	3.542	2.638	0.591		1.04723	1.06543	1.02325	0.76209	0.17073
	kd_z148	1	4.66887	7.408	6.155	2.238	1.13	0.457		1.58668	1.31831	0.47934	0.24203	0.09788
	kd_z166	1	0.33774	0.343	0.33	0.331	0.338	0.29		1.01557	0.97708	0.98004	1.00077	0.85865
	kd_z167	1	4.75738	5.612	5.17	4.337	6.615	7.479		1.17964	1.08673	0.91164	1.39047	1.57208
	kd_z168	1	0.58062	0.582	0.591	0.398	0.535	0.26		1.00238	1.01788	0.68548	0.92143	0.4478
									sum	1.0871	1.04308	1.06512	1.18131	0.80582
	iteraties	0	4	4	4	4	4	4						
	doelf.	199.687	162.829	164.933	164.939	178.618	175.524	183.853		1.01292	1.01296	1.09697	1.07797	1.12912
	kd_z128	1	0.4894	0.629	0.823	0.61	0.492	0.456		1.28523	1.68163	1.24641	1.0053	0.93174
	kd_z129	1	3.65549	4.524	0.165	2.224	1.585	0.923		1.23759	0.04514	0.6084	0.43359	0.2525
Q-BOUNDARY	kd_z130	1	9.7792	10	10	0.922	2.169	1		1.02258	1.02258	0.09428	0.2218	0.10226
	kd_z146	1	0.67596	0.672	0.683	0.692	0.675	0.646		0.99414	1.01042	1.02373	0.99858	0.95568
	kd_z147	1	3.46153	3.631	3.48	2.122	2.517	1.942		1.04896	1.00534	0.61302	0.72714	0.56102
	kd_z148	1	4.66887	9.067	10	1.038	2.545	1.128		1.94201	2.14184	0.22232	0.5451	0.2416
	kd_z166	1	0.33774	0.413	0.382	0.338	0.325	0.422		1.22283	1.13105	1.00077	0.96228	1.24948
	kd_z167	1	4.75738	7.103	4.686	4.828	5.667	4.131		1.49305	0.985	1.01484	1.1912	0.86833
	kd_z168	1	0.58062	0.177	1.673	0.229	0.182	0.1		0.30485	2.88142	0.39441	0.31346	0.17223
									sum	1.17236	1.32271	0.69091	0.71094	0.59276

RESULTS

kd$_2$ submodel

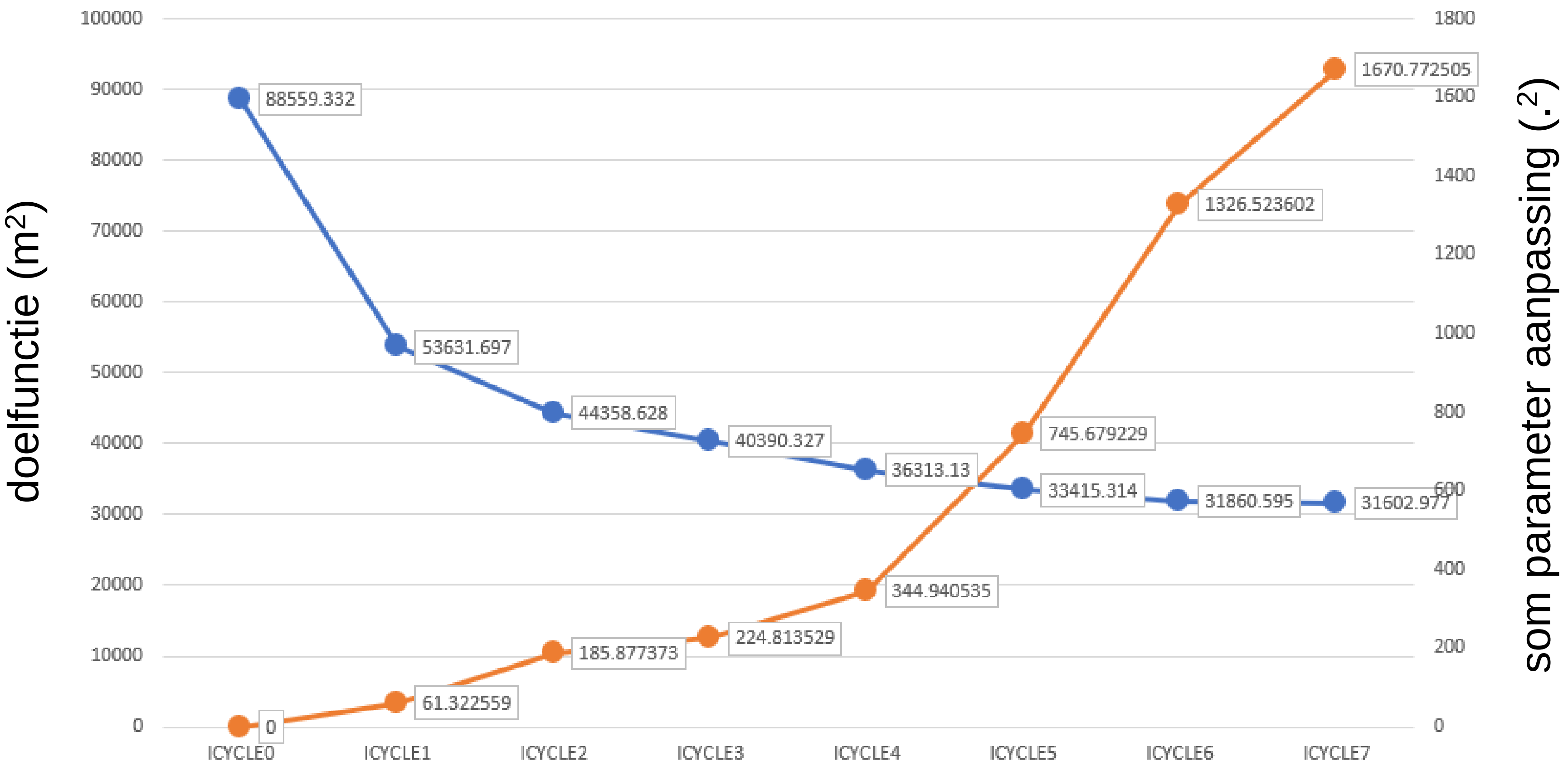
kd$_2$ globalmodel





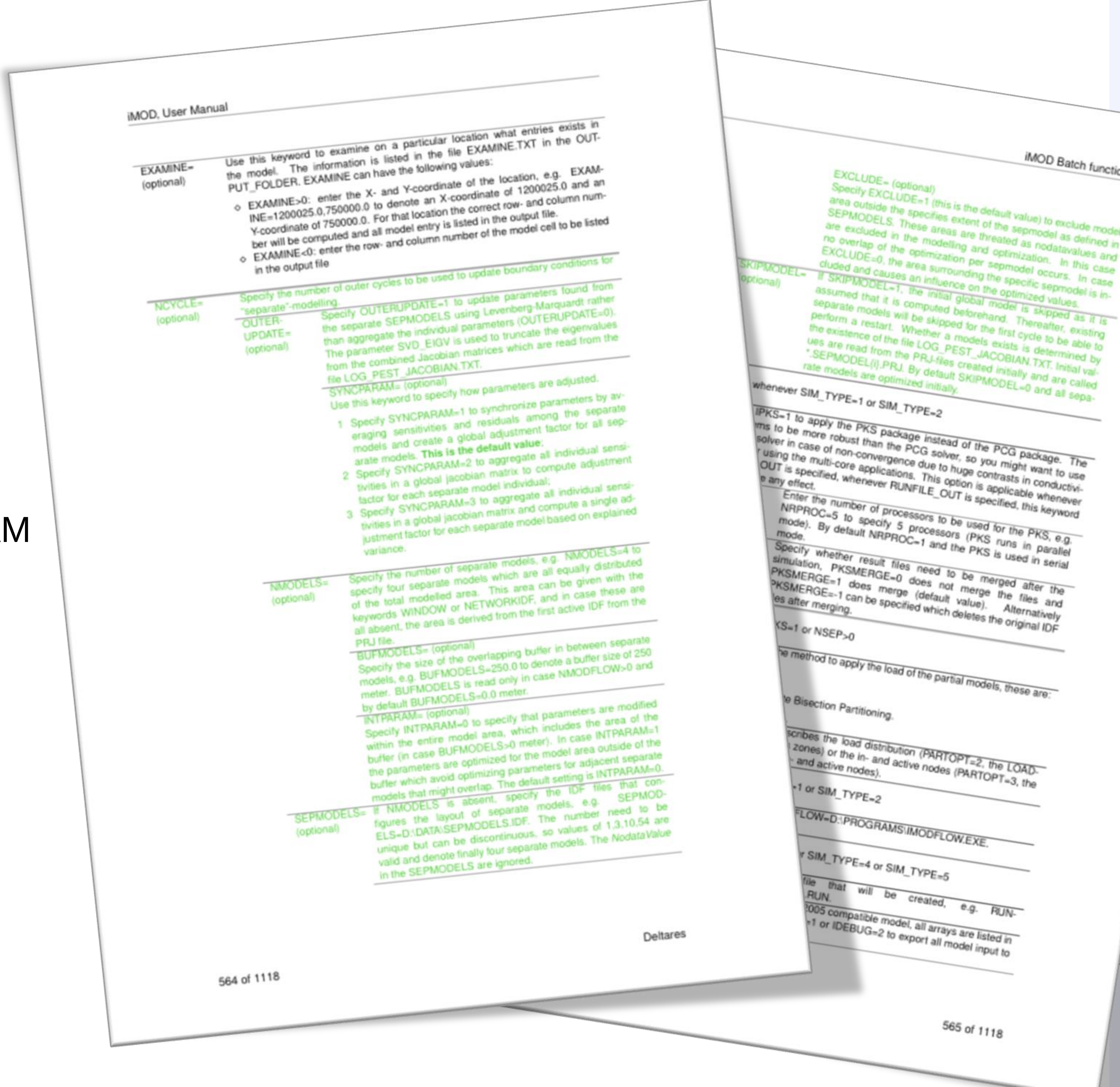
Deltares

RESULTS



doelfunctie (m2)
som parameter aanpassing (.2)
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
1800
1600
1400
1200
1000
800
600
400
200
0
88559.332
53631.697
44358.628
40390.327
36313.13
33415.314
31860.595
31602.977
0
61.322559
185.877373
224.813529
344.940535
745.679229
1326.523602
1670.772505
ICYCLE0
ICYCLE1
ICYCLE2
ICYCLE3
ICYCLE4
ICYCLE5
ICYCLE6
ICYCLE7

Synthetic Example


iMOD, User Manual

EXAMINE= (optional) — Use this keyword to examine on a particular location what entries exists in the model. The information is listed in the file EXAMINE.TXT in the OUTPUT_FOLDER. EXAMINE can have the following values:
- EXAMINE>0: enter the X- and Y-coordinate of the location, e.g. EXAMINE=1200025.0,750000.0 to denote an X-coordinate of 1200025.0 and an Y-coordinate of 750000.0. For that location the correct row- and column number will be computed and all model entry is listed in the output file.
- EXAMINE<0: enter the row- and column number of the model cell to be listed in the output file

NCYCLE= (optional) — Specify the number of outer cycles to be used to update boundary conditions for "separate"-modelling.

OUTERUPDATE= (optional) — Specify OUTERUPDATE=1 to update parameters found from the separate SEPMODELS using Levenberg-Marquardt rather than aggregate the individual parameters (OUTERUPDATE=0). The parameter SVD_EIGV is used to truncate the eigenvalues from the combined Jacobian matrices which are read from the file LOG_PEST_JACOBIAN.TXT.

SYNCPARAM= (optional) — Use this keyword to specify how parameters are adjusted.
1. Specify SYNCPARAM=1 to synchronize parameters by averaging sensitivities and residuals among the separate models and create a global adjustment factor for all separate models. **This is the default value**;
2. Specify SYNCPARAM=2 to aggregate all individual sensitivities in a global jacobian matrix to compute adjustment factor for each separate model individual;
3. Specify SYNCPARAM=3 to aggregate all individual sensitivities in a global jacobian matrix and compute a single adjustment factor for each separate model based on explained variance.

NMODELS= (optional) — Specify the number of separate models, e.g. NMODELS=4 to specify four separate models which are all equally distributed of the total modelled area. This area can be given with the keywords WINDOW or NETWORKIDF, and in case these are all absent, the area is derived from the first active IDF from the PRJ file.

BUFMODELS= (optional) — Specify the size of the overlapping buffer in between separate models, e.g. BUFMODELS=250.0 to denote a buffer size of 250 meter. BUFMODELS is read only in case NMODFLOW>0 and by default BUFMODELS=0.0 meter.

INTPARAM= (optional) — Specify INTPARAM=0 to specify that parameters are modified within the entire model area, which includes the area of the buffer (in case BUFMODELS>0 meter). In case INTPARAM=1 the parameters are optimized for the model area outside of the buffer which avoid optimizing parameters for adjacent separate models that might overlap. The default setting is INTPARAM=0.

SEPMODELS= (optional) — If NMODELS is absent, specify the IDF files that configures the layout of separate models, e.g. SEPMODELS=D:\DATA\SEPMODELS.IDF. The number need to be unique but can be discontinuous, so values of 1,3,10,54 are valid and denote finally four separate models. The NodataValue in the SEPMODELS are ignored.

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FUNCTION=RUNFILE

PRJFILE_IN=D:\MODELS\TEST.PRJ
NAMFILE_OUT=D:\MODELS\TEST.NAM
IPESTP=1
NCPU=6
ISOLVE=1
MODFLOW=D:\IMODFLOW.EXE

NCYCLE=10
SEPMODELS=D:\MODELS\SBM.IDF
BNDSUBMODEL=3

Synthetic Example

BND for Submode
Original Moc

PEST information
after aggregation
Original Modelinput
Submodels

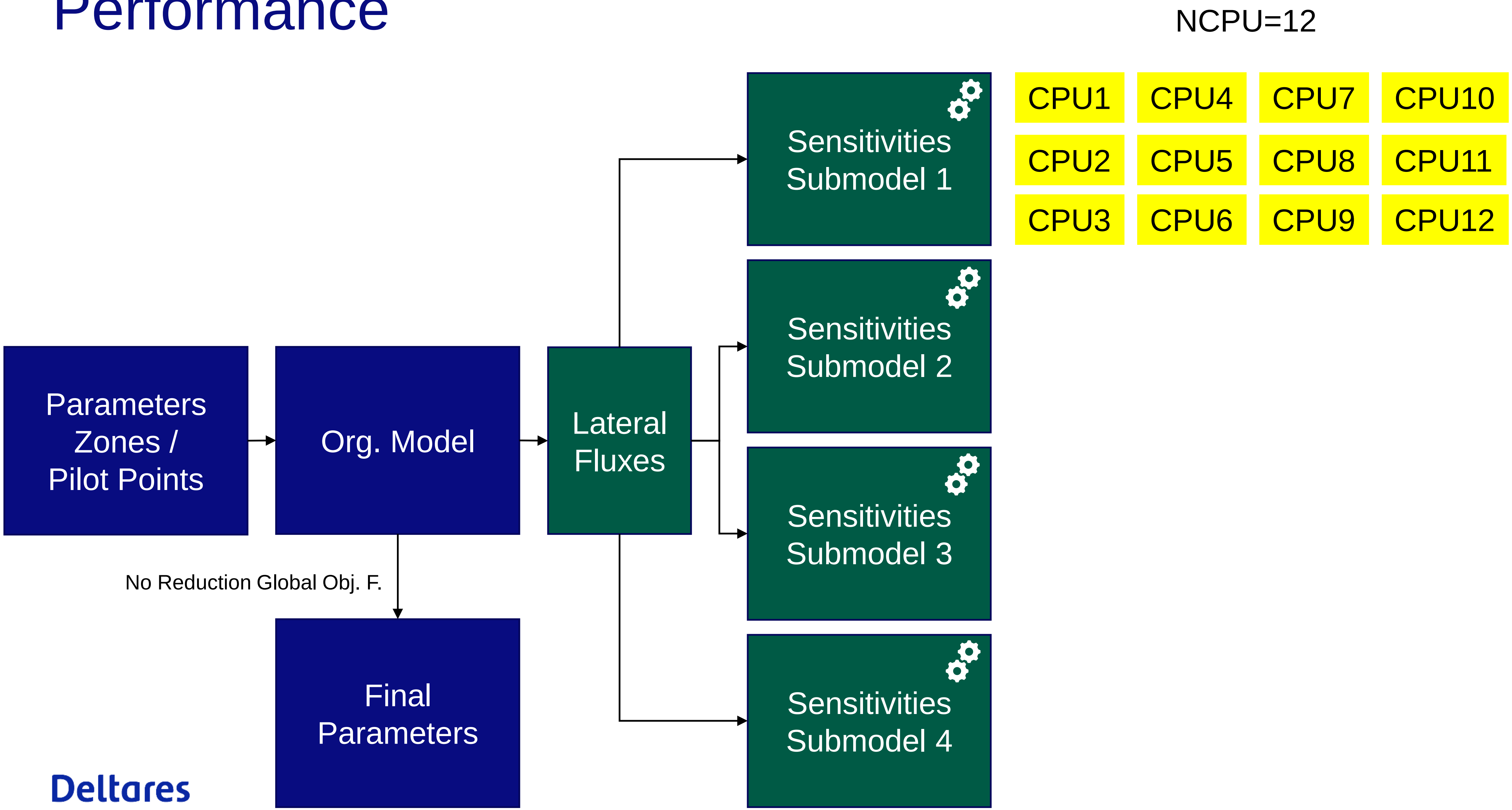
single_zone_sm500mtr_4msr_2param.TXT - Notepad

```
SUMMARY OF SEP-MODELLING
                        cycle1   cycle2   cycle3
      0      0.270       0.015    0.008    0.004
      1                  0.059    0.000    0.000
      2                  0.008    0.000    0.000
      3                  0.100    0.000    0.000

  ICYCLE=         1
 IPRM PT         PARAM    F_FINAL      MEAN      STDEV     F_MDL1     F_MDL2     F_MDL3
    1 KH   AQUIFER1_KH      0.298     0.254      0.114      0.151      0.236      0.376
    2 KH   AQUIFER2_KH      0.979     1.152      0.603      0.599      1.062      1.794

  ICYCLE=         2
 IPRM PT         PARAM    F_FINAL      MEAN      STDEV     F_MDL1     F_MDL2     F_MDL3
    1 KH   AQUIFER1_KH      0.233     0.226      0.049      0.281      0.186      0.211
    2 KH   AQUIFER2_KH      1.228     0.800      0.350      0.396      0.996      1.008

  ICYCLE=         3
 IPRM PT         PARAM    F_FINAL      MEAN      STDEV     F_MDL1     F_MDL2     F_MDL3
    1 KH   AQUIFER1_KH      0.265     0.269      0.048      0.292      0.214      0.302
    2 KH   AQUIFER2_KH      1.384     0.942      0.361      0.538      1.231      1.058
```

Global Objective Function
Local Objective Functions

Sub models

Performance



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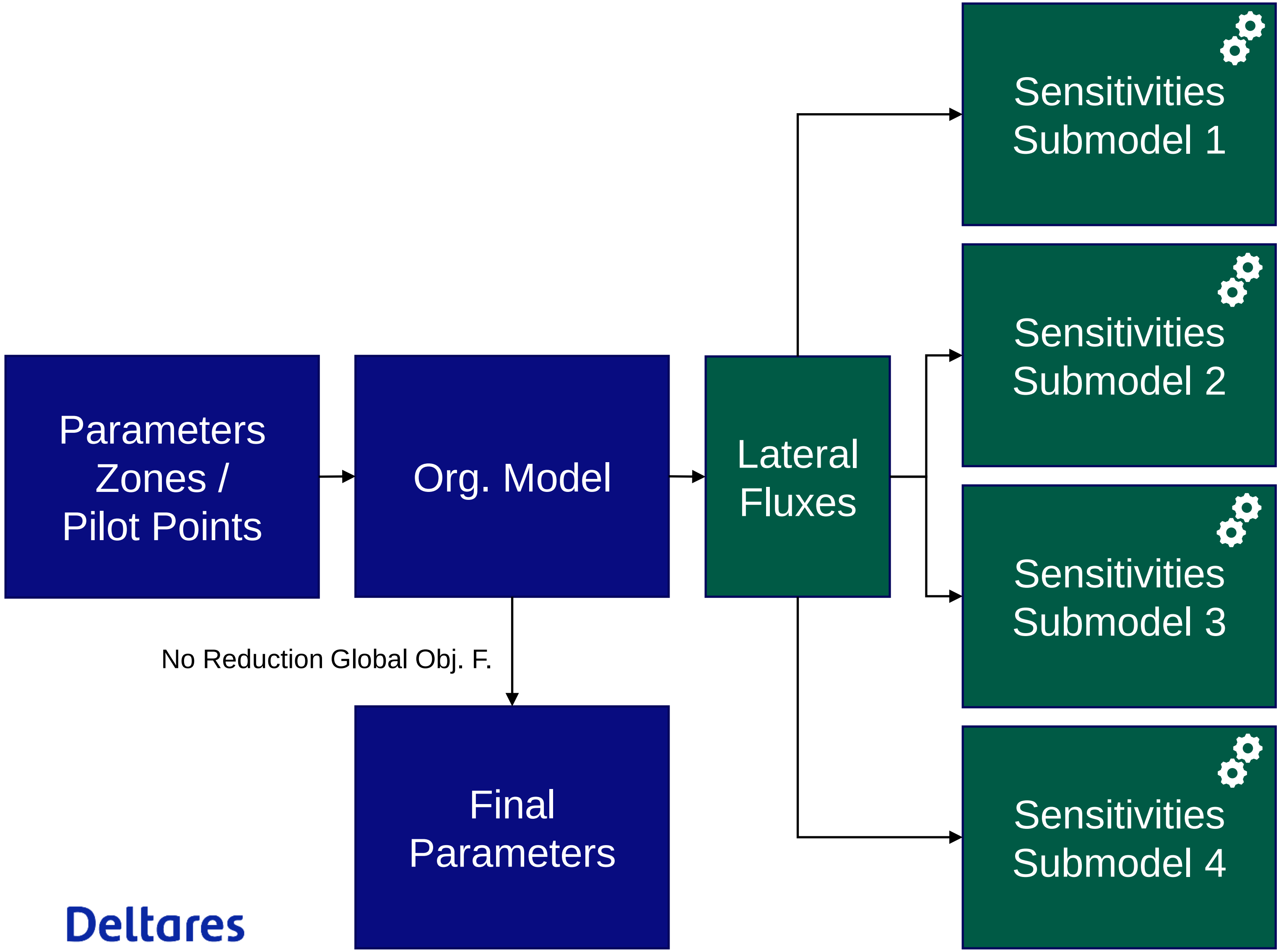
Performance



NCPU=12

CPU1	CPU4	CPU7	CPU10
CPU2	CPU5	CPU8	CPU11
CPU3	CPU6	CPU9	CPU12

$$N_{cpu} = \frac{t_{iter}}{t_{io}}$$

If N_{cpu} is too high performance drops significantly

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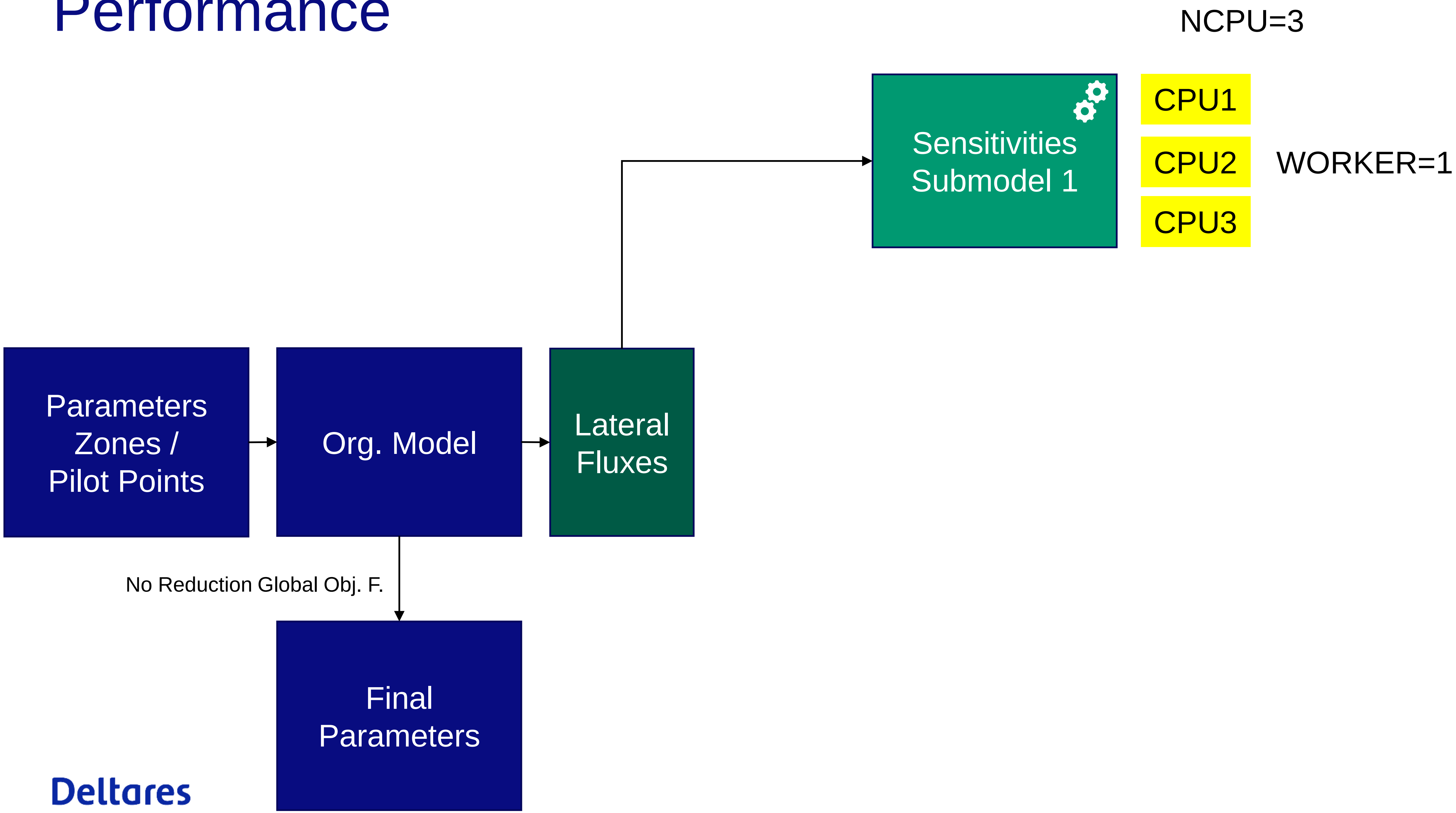
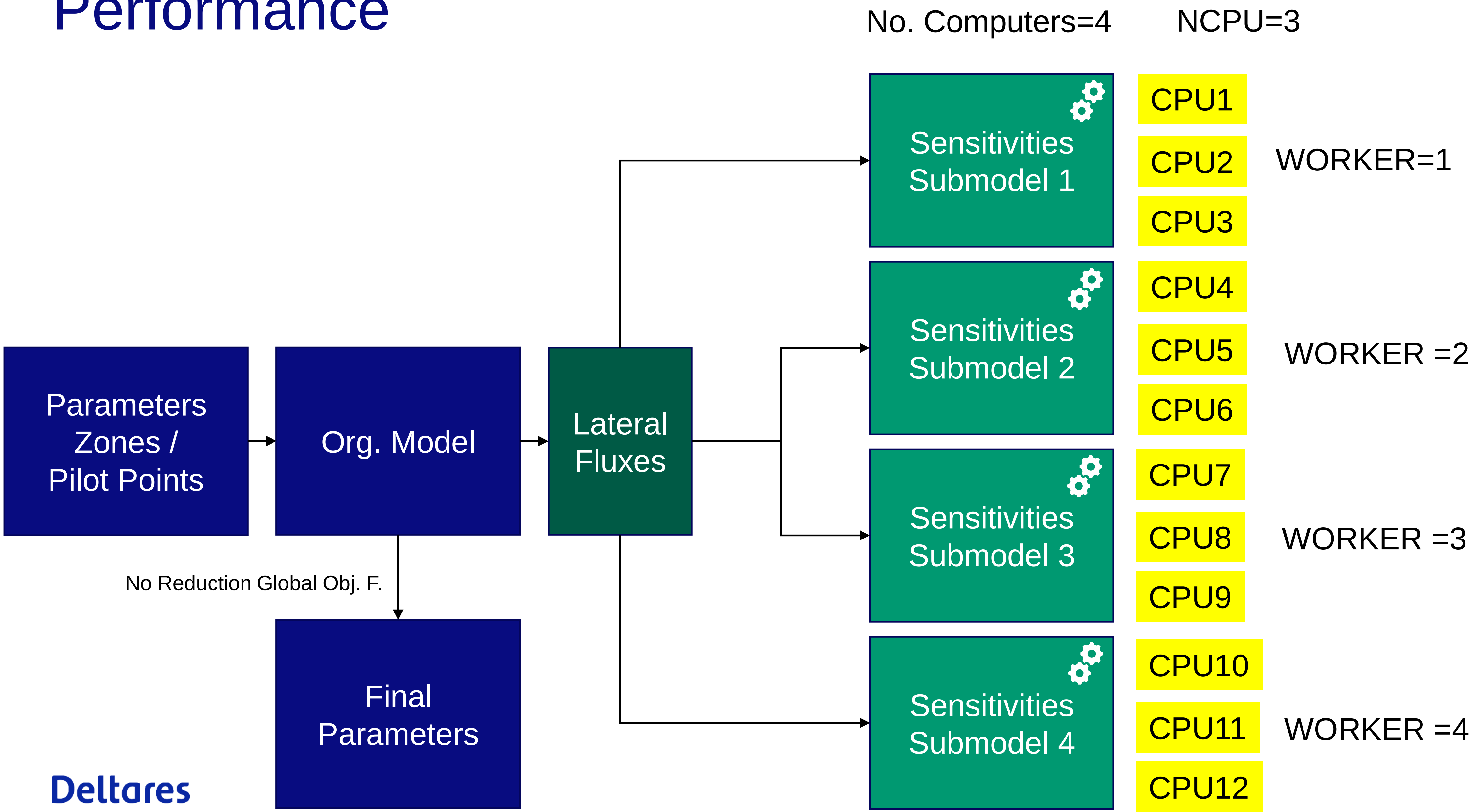
Performance



Performance



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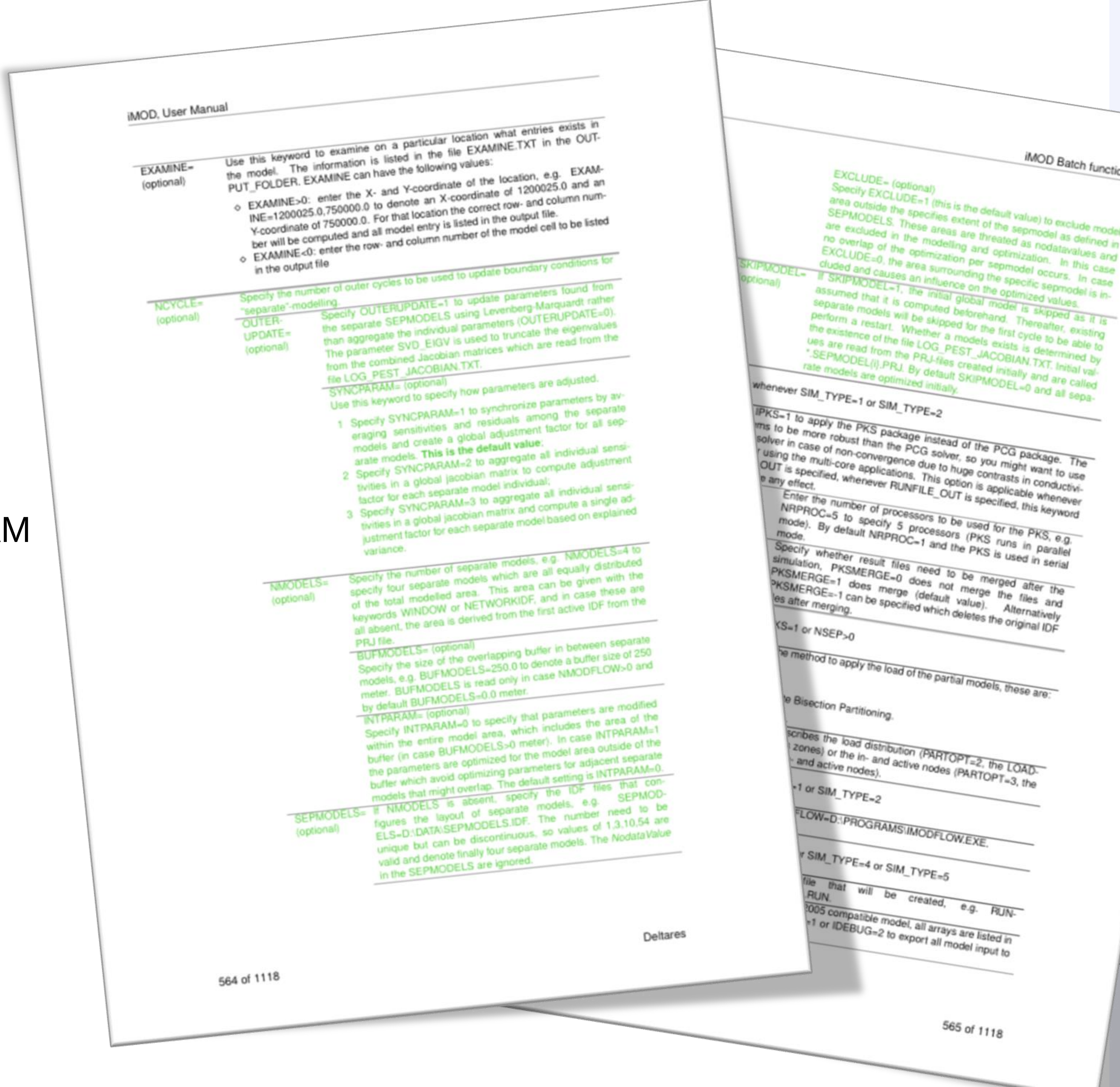
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NCPU=6
ISOLVE=1
MODFLOW=D:\IMODFLOW.EXE

NCYCLE=10
SEPMODELS=D:\MODELS\SBM.IDF
BNDSUBMODEL=3
NWORKERS=3

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Conclusies

- Met half overlappende submodellen wordt voldoende gevoeligheid per parameter verkregen om parameters op globale schaal aan te passen. Het effect wordt dan, gezien vanuit het meetpunt, door het gehele model gebied door gegeven;
- Het noodzakelijkerwijs opschalen van het model voor de kalibratie wordt hiermee voorkomen;
- Het verspreiden van submodellen over verschillende computers vergroot de efficientie;
- Grotere spreidingslengte dwingen grotere buffers af rondom submodellen maar doordat submodellen elkaar allemaal overlappen wordt dit verholpen;
- Met 15 computers en 416 submodellen is het LHM niet-stationair gekalibreerd op basis van de GxG binnen 1-2 weken.

Deltares

Contact

www.deltares.nl

info@deltares.nl

@deltares

@deltares

linkedin.com/company/deltares

facebook.com/deltaresNL