

Deltares

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Efficient Model Calibration using Sub-models

New development within iPESTP of iMOD

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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 v5.5

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 ...

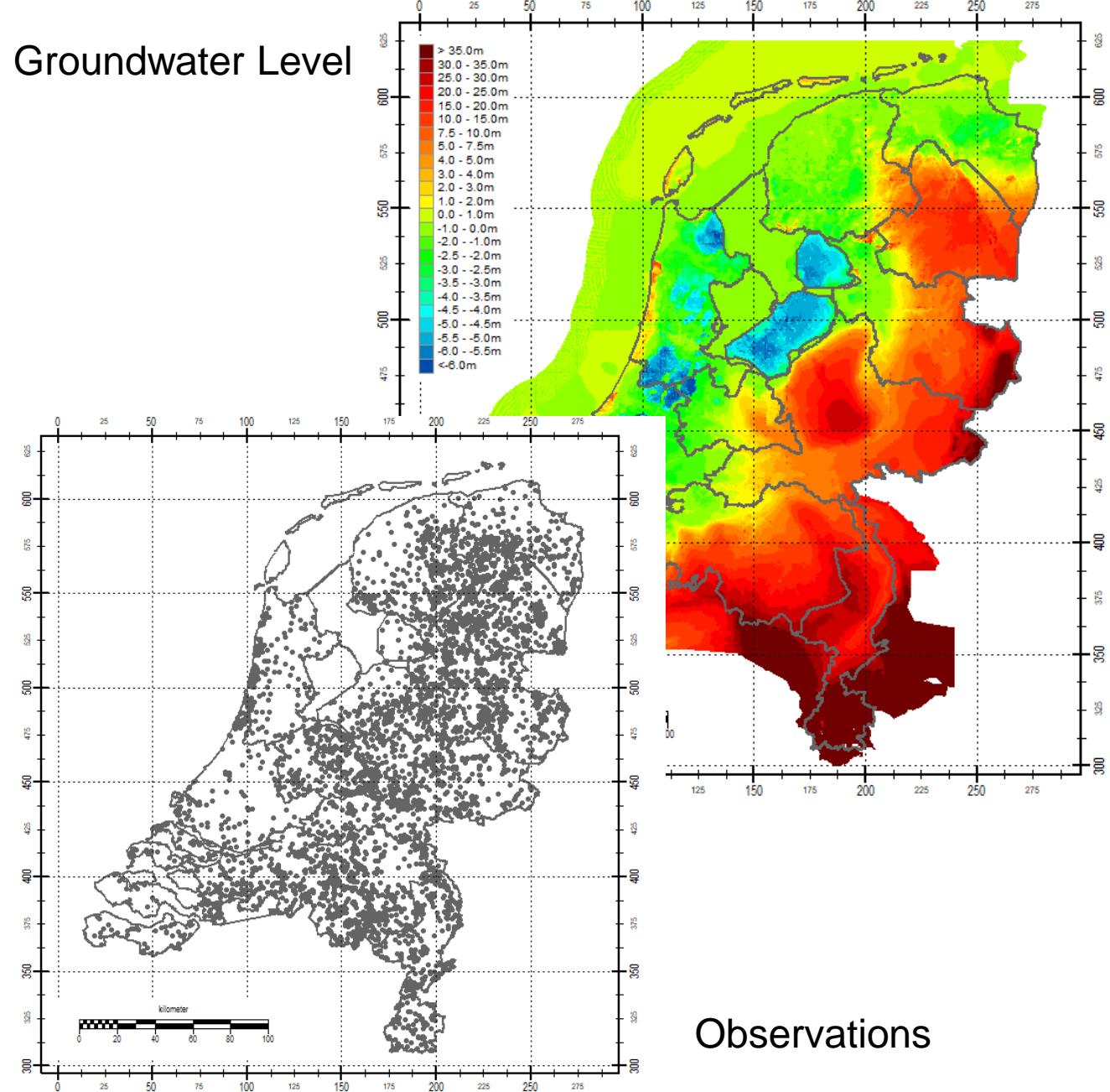
Deltas

Challenge

Optimize

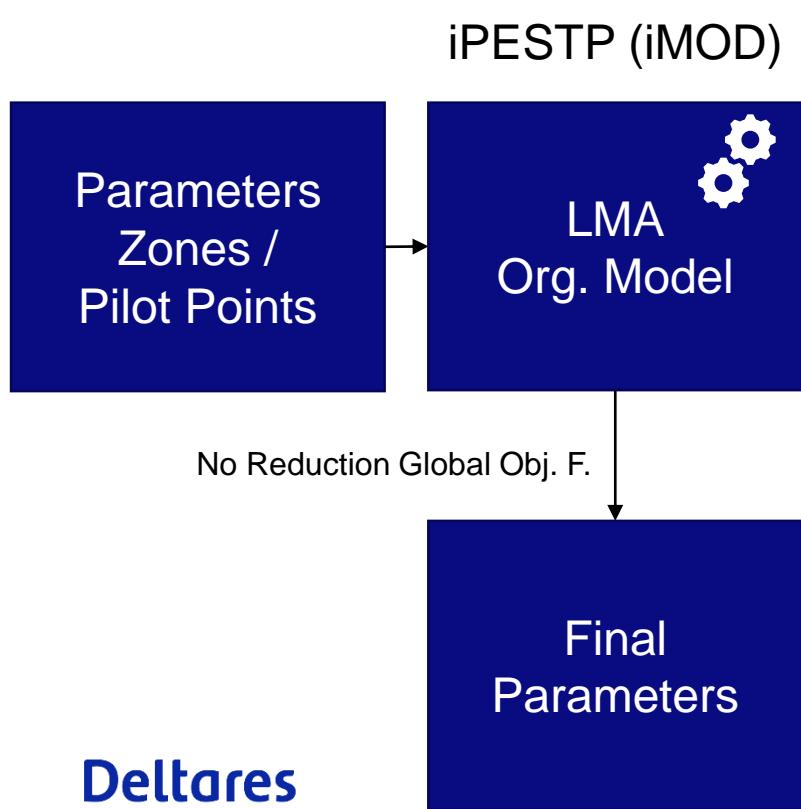
- 3D Groundwater Flow model
 - Transient Model (171 stresses)
 - 12.5 millions nodes
- Totally 2,050 parameters
 - REGIS units in aquifers and aquitards
 - GeoTOP lithology in “deklag”
 - Drainage- and river conductance
 - Infiltration factor rivers
 - Storage coefficients
- Observations
 - 0.5 million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

Groundwater Level

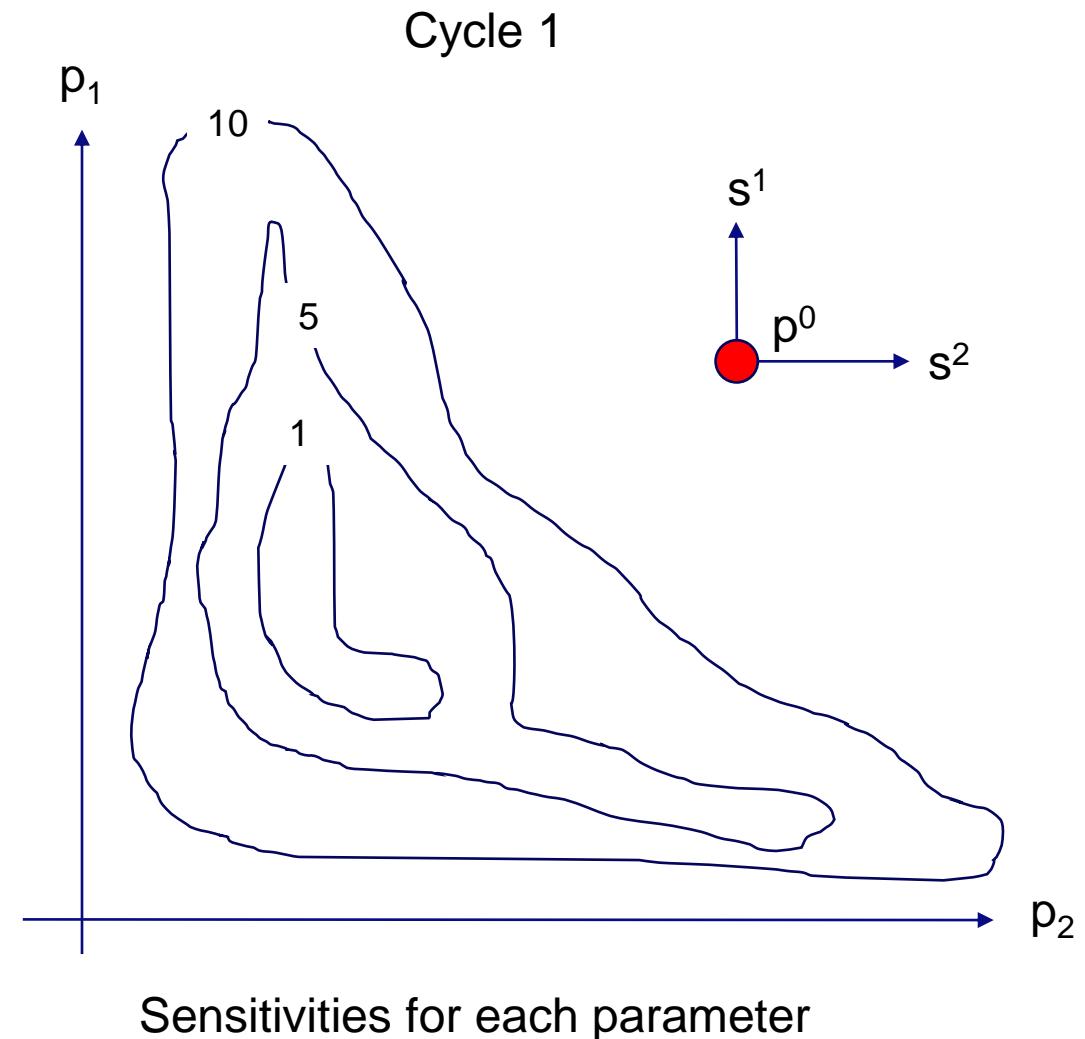
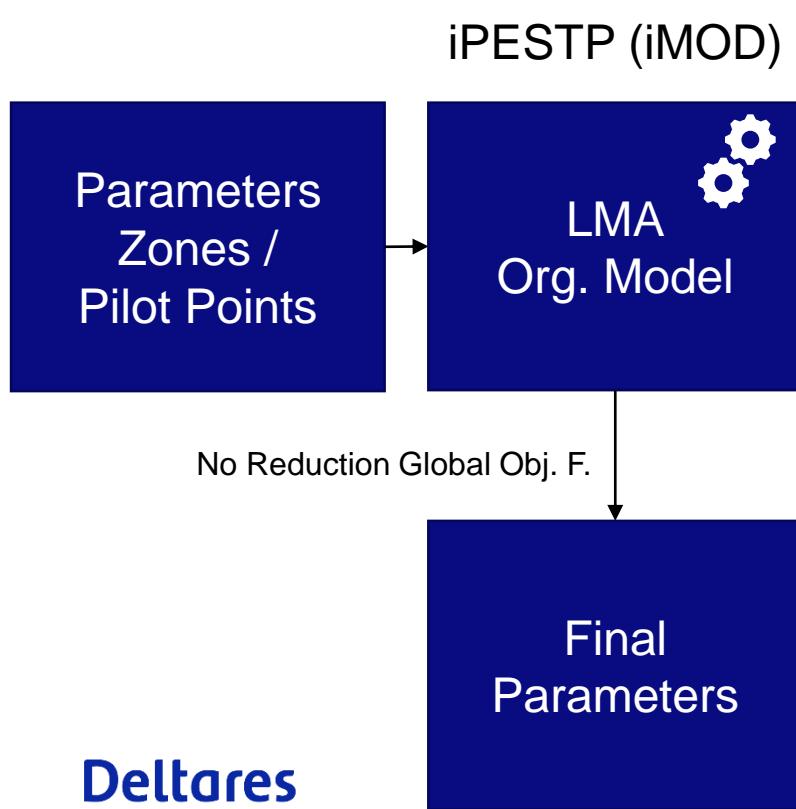


Observations

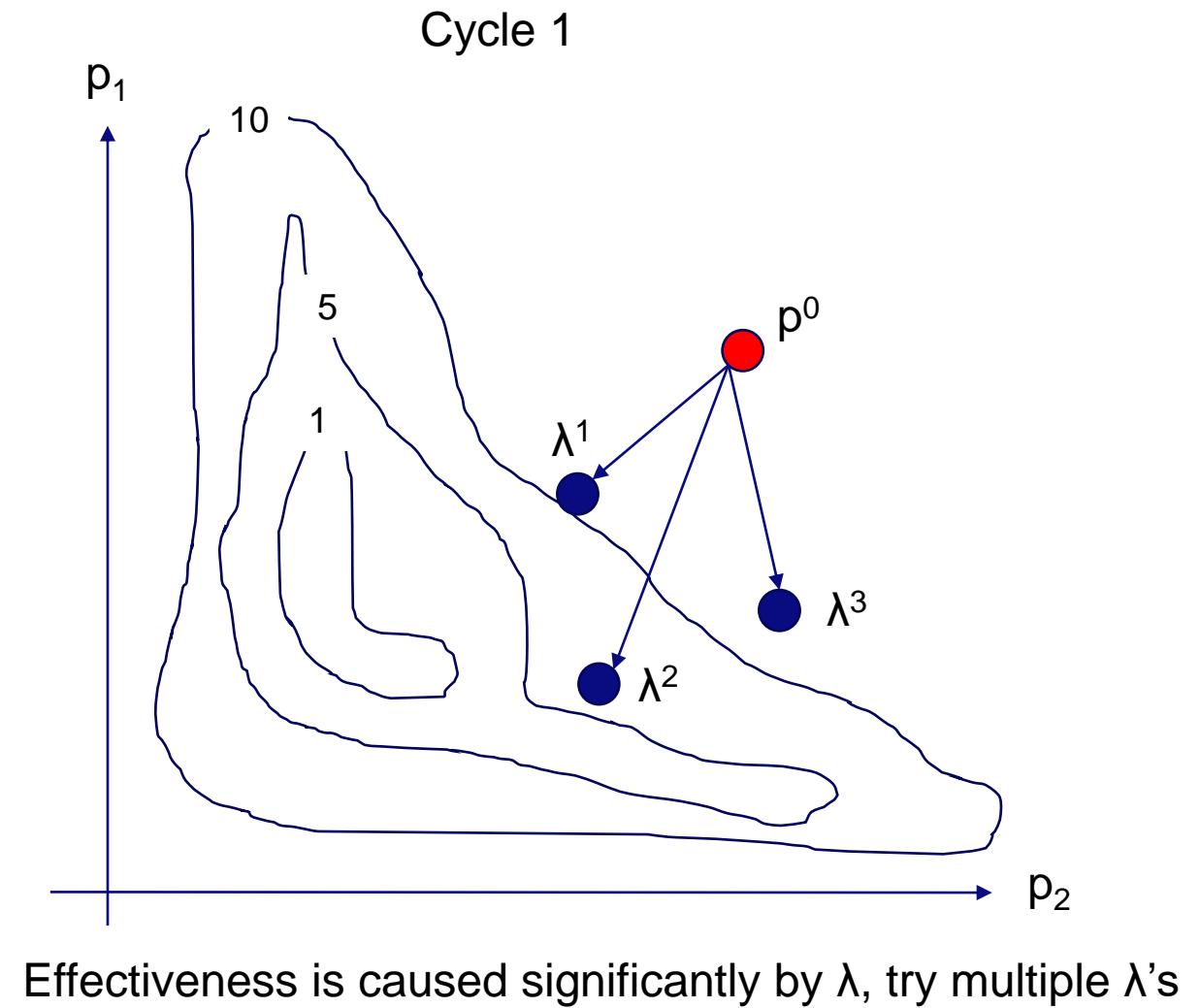
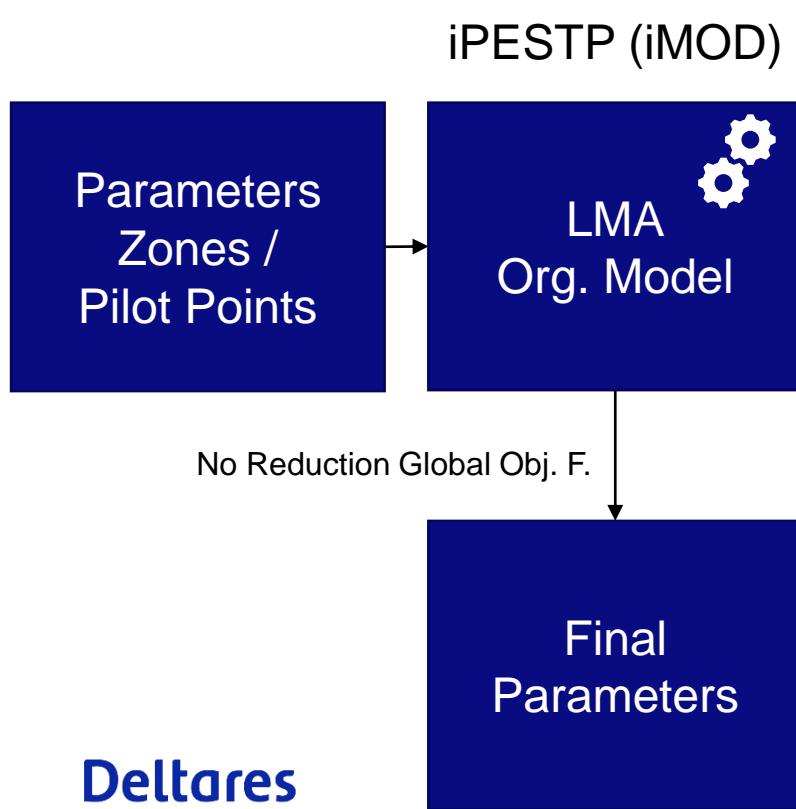
LMA Optimization Method



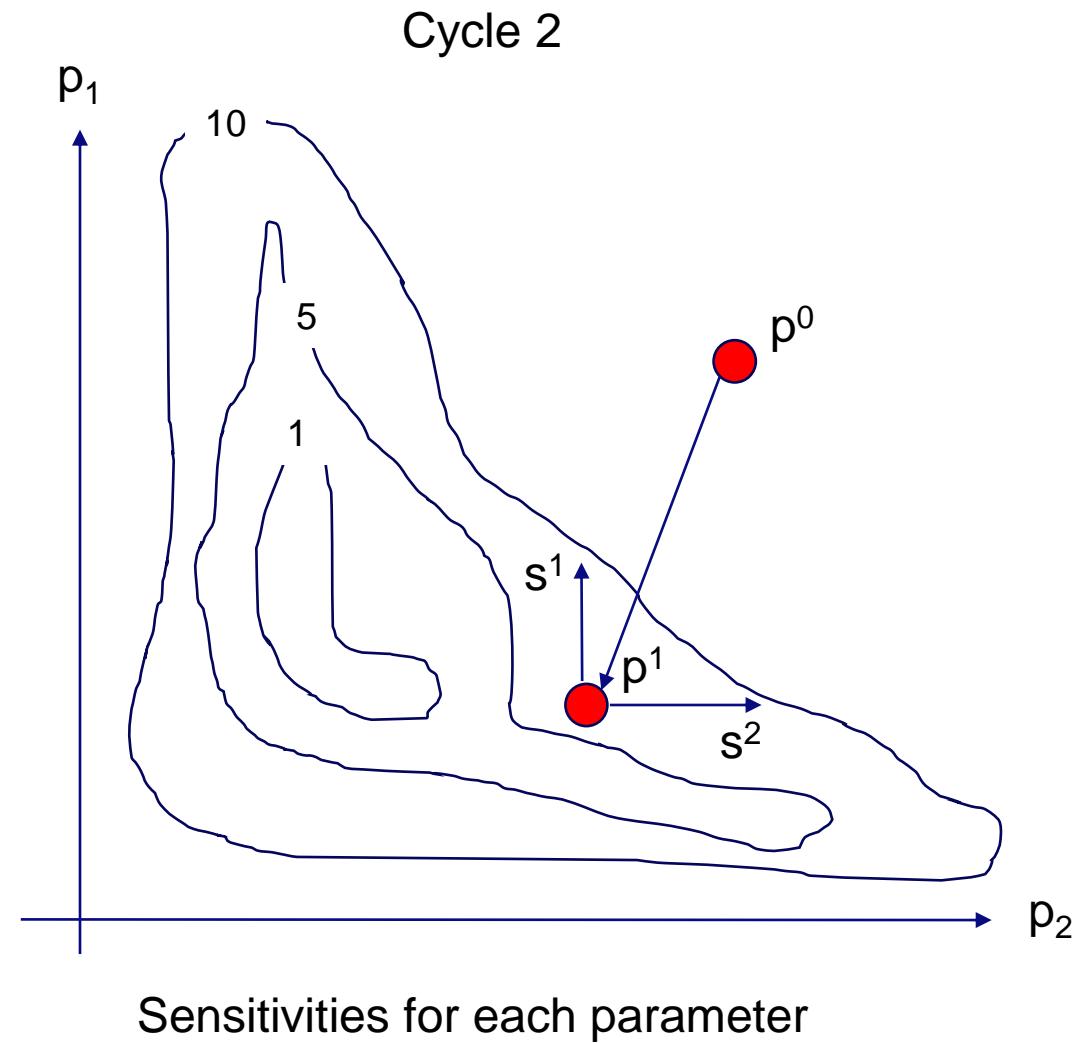
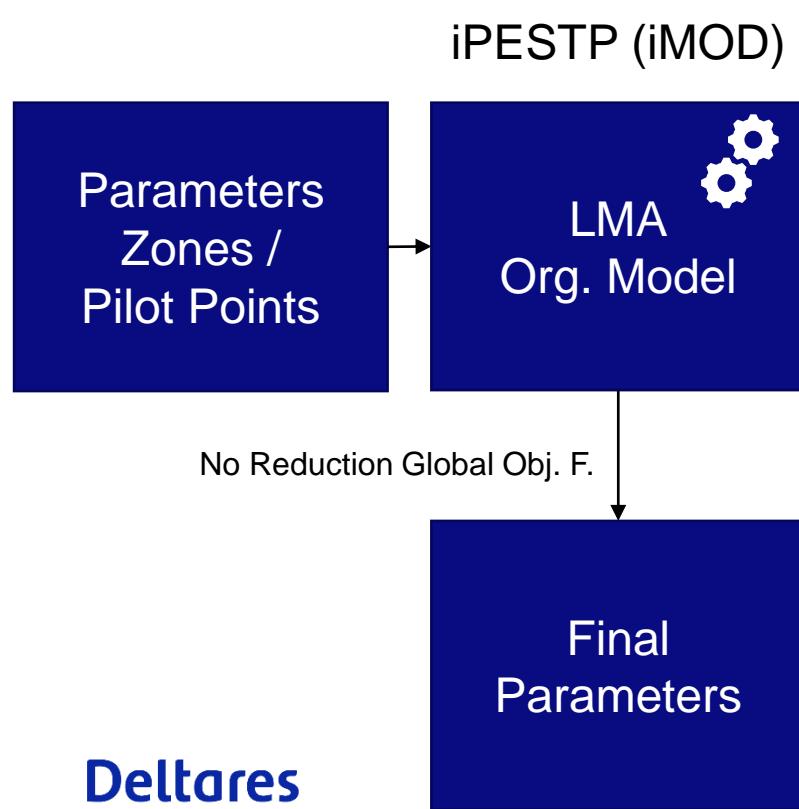
LMA Optimization Method



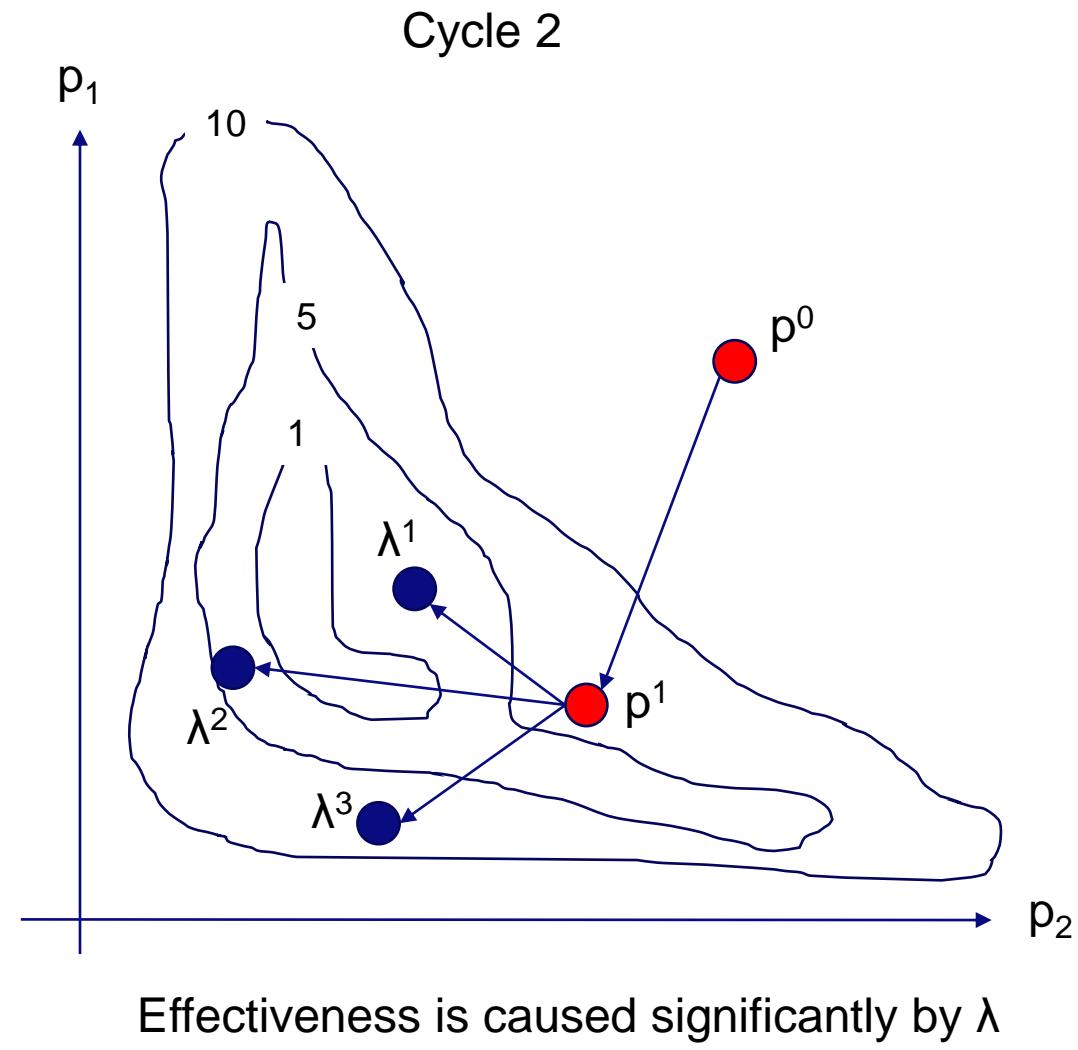
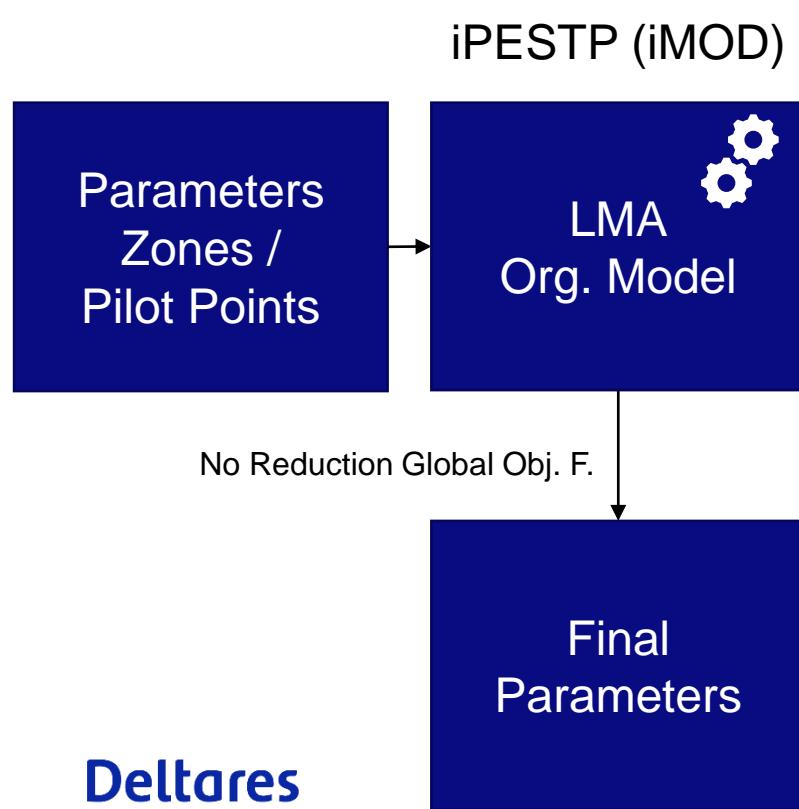
LMA Optimization Method



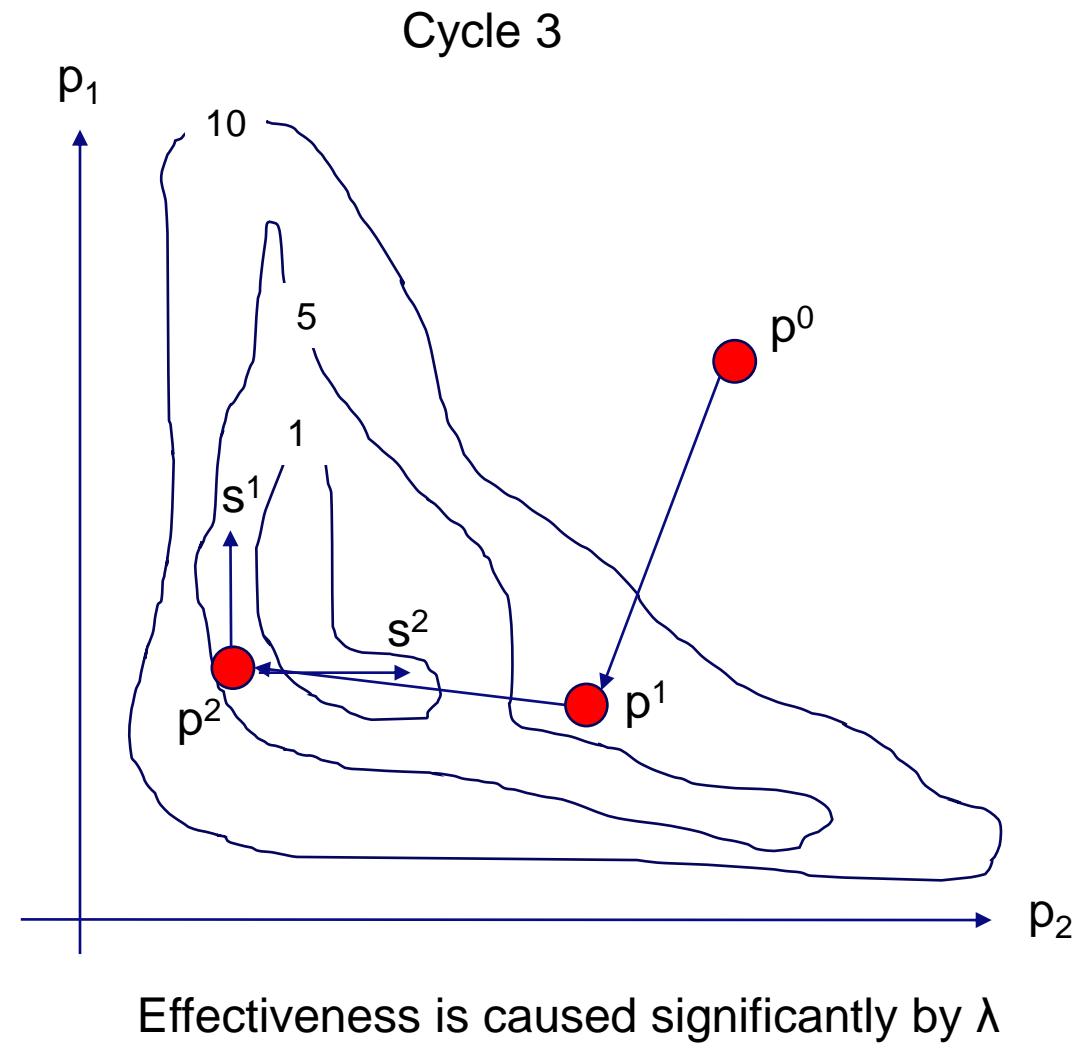
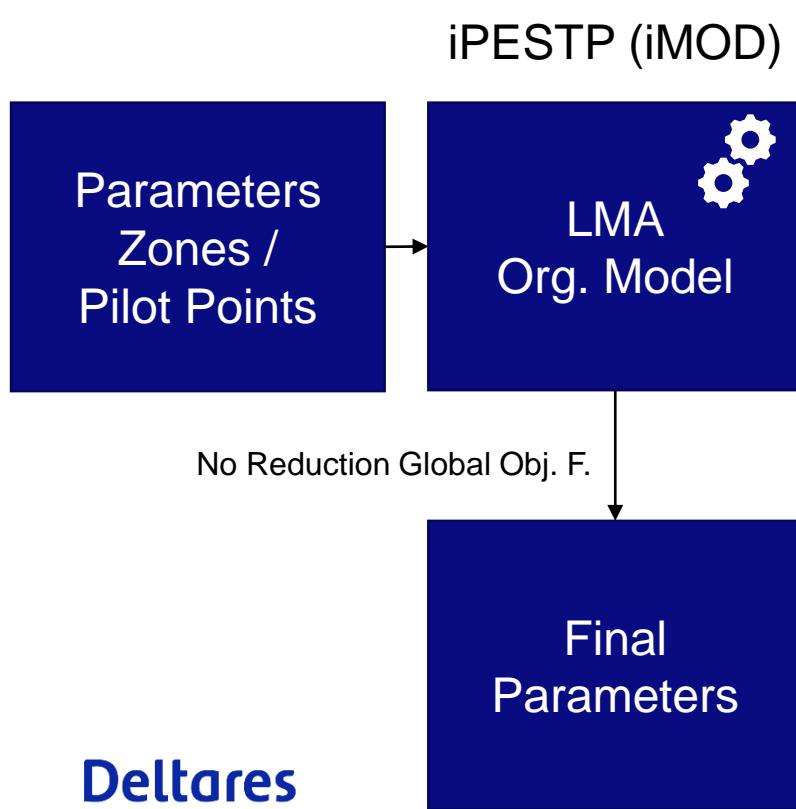
LMA Optimization Method



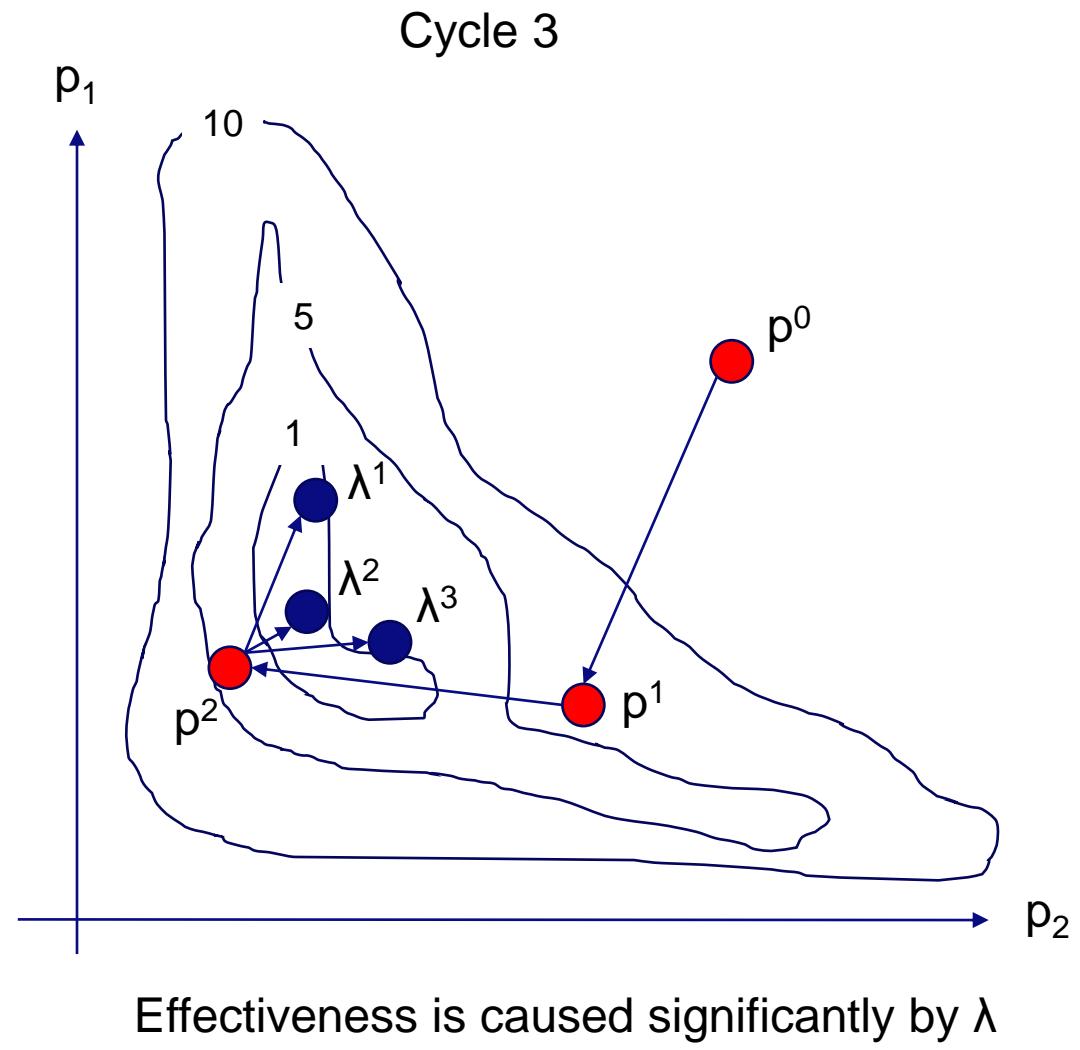
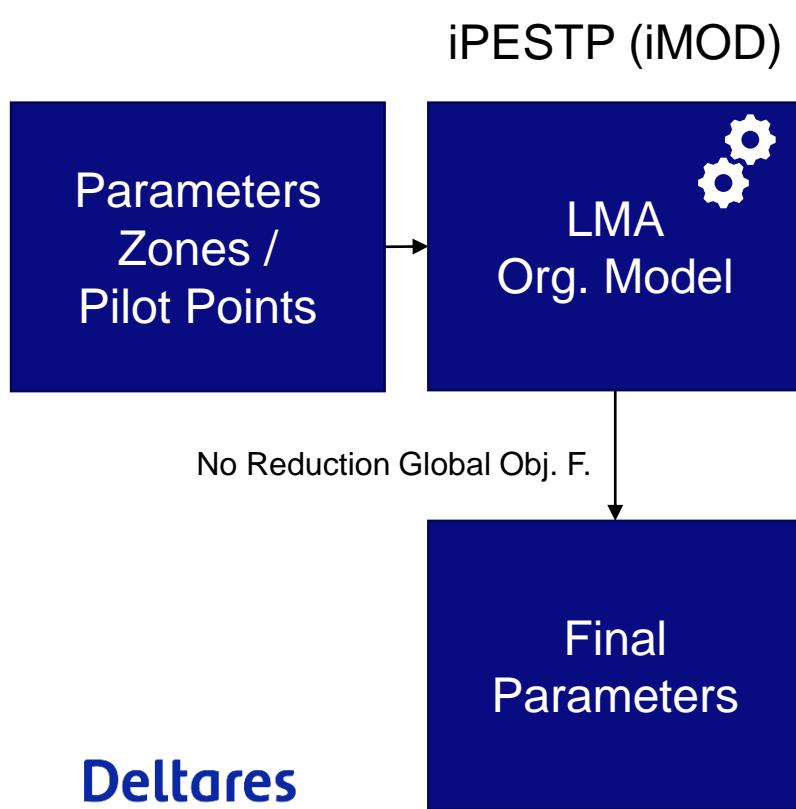
LMA Optimization Method



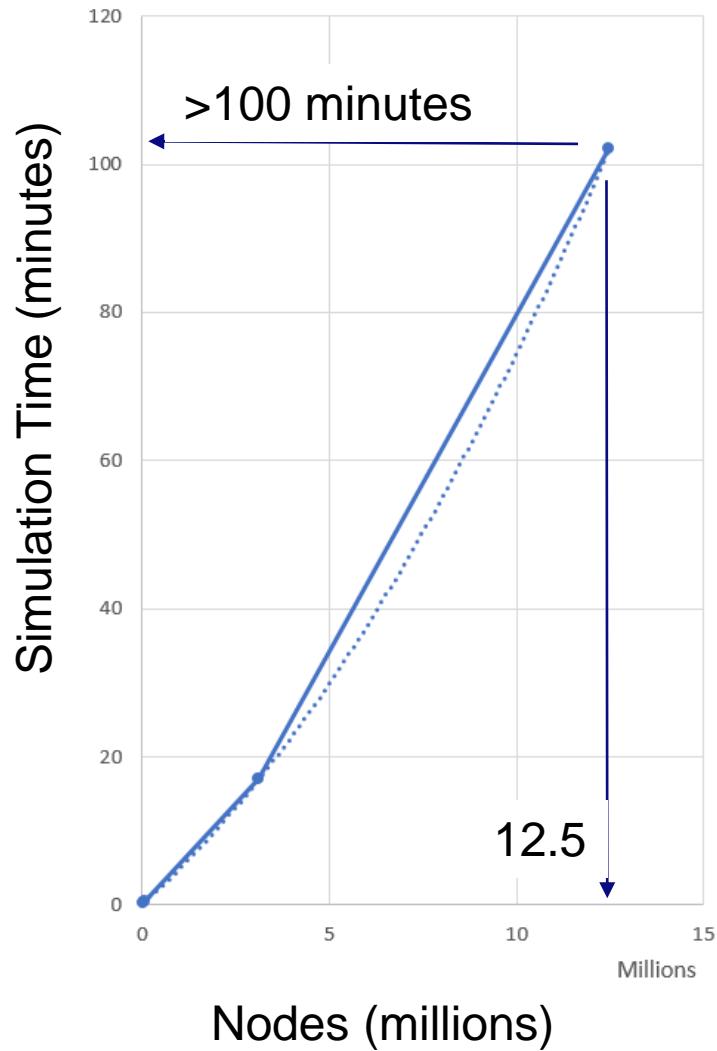
LMA Optimization Method



LMA Optimization Method



Runtimes of Models

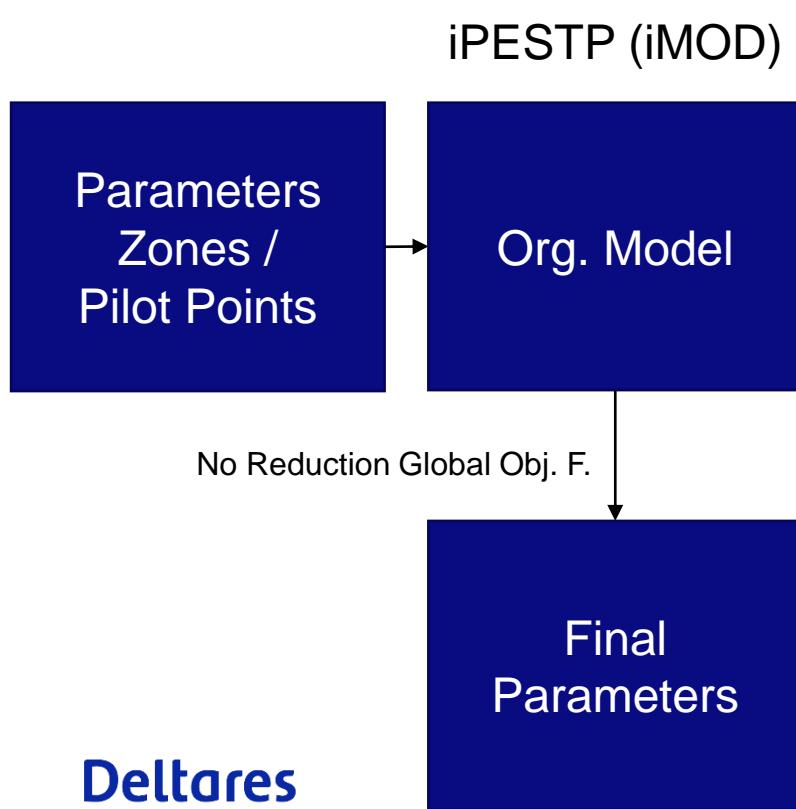


		Days	20 CPU
Sensitivity	2050	141	8 days
Lambda	3	0.25	2 minutes
Totally	3 cycles		24 days

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

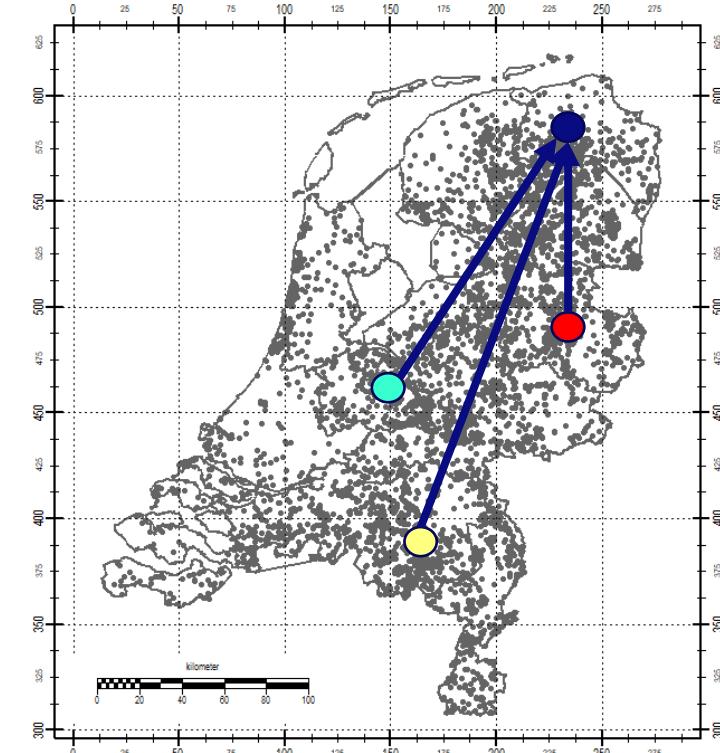
so finally multiple set of 24 days to complete

Submodel Model Optimization Method (SMOM)

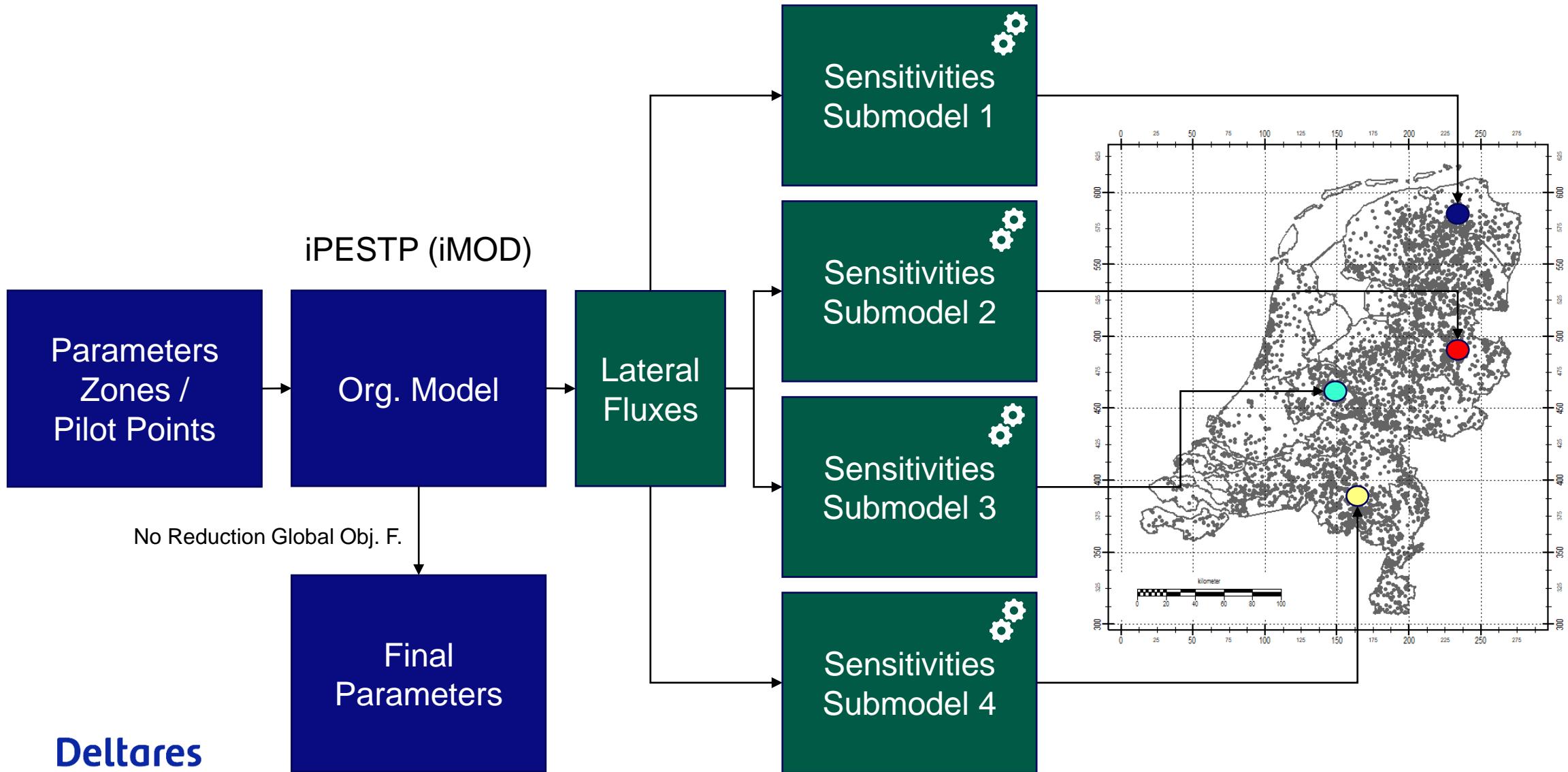


Questions:

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



Submodel Model Optimization Method (SMOM)



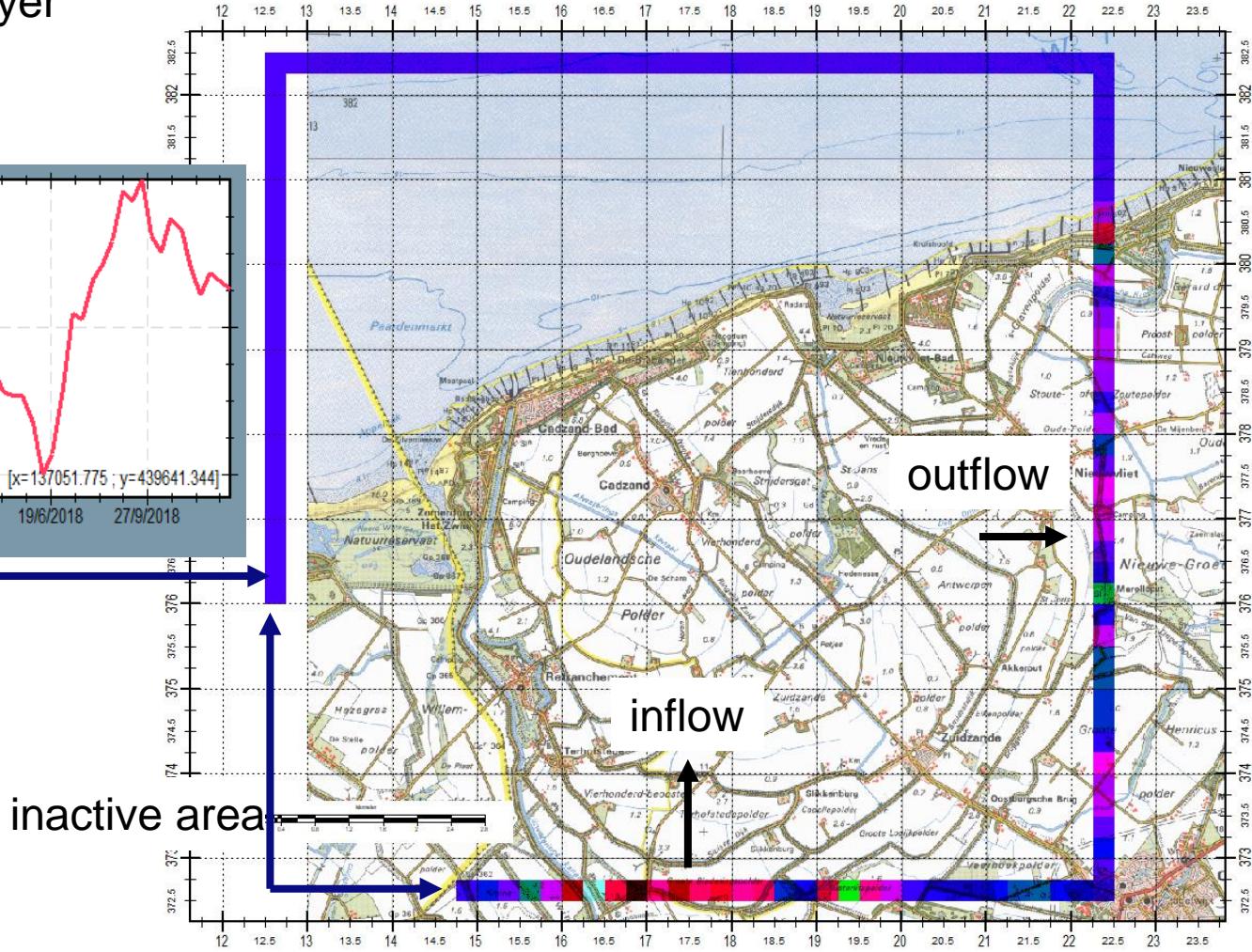
Submodel Model Optimization Method (SMOM)

FHB boundary condition per modellayer
with fluxes from original model

horizontal flux (m^3/d)

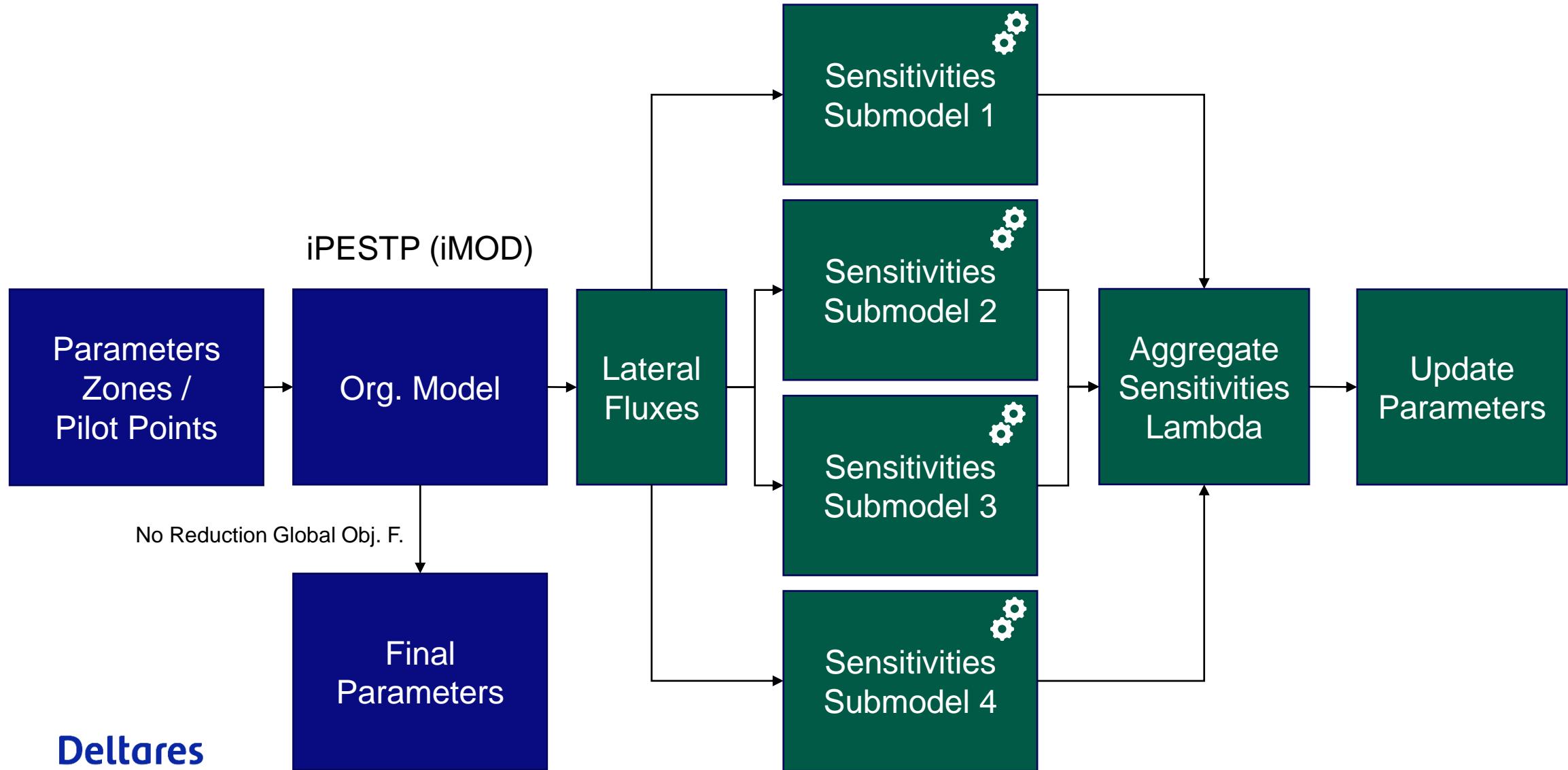


time



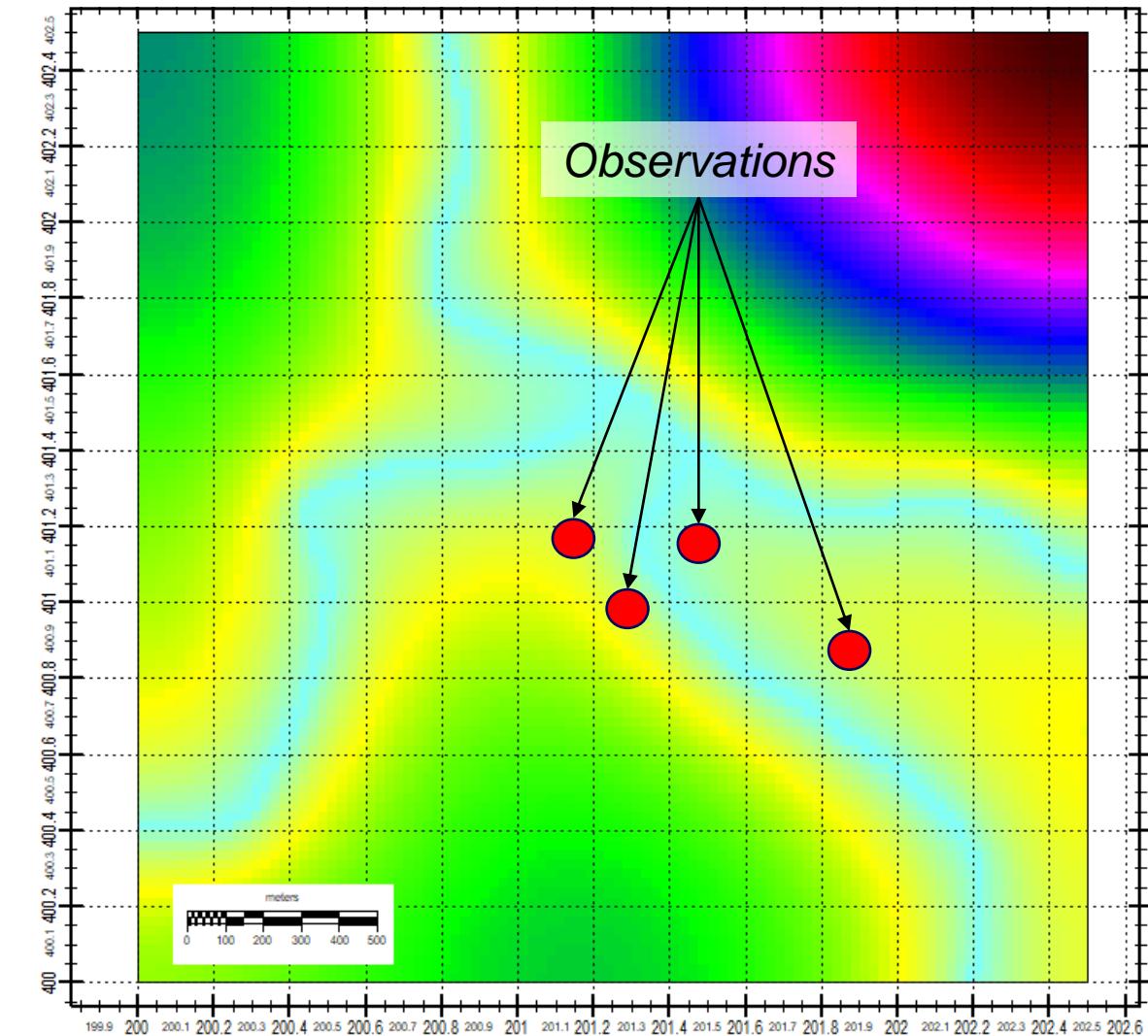
Deltas

Submodel Model Optimization Method (SMOM)



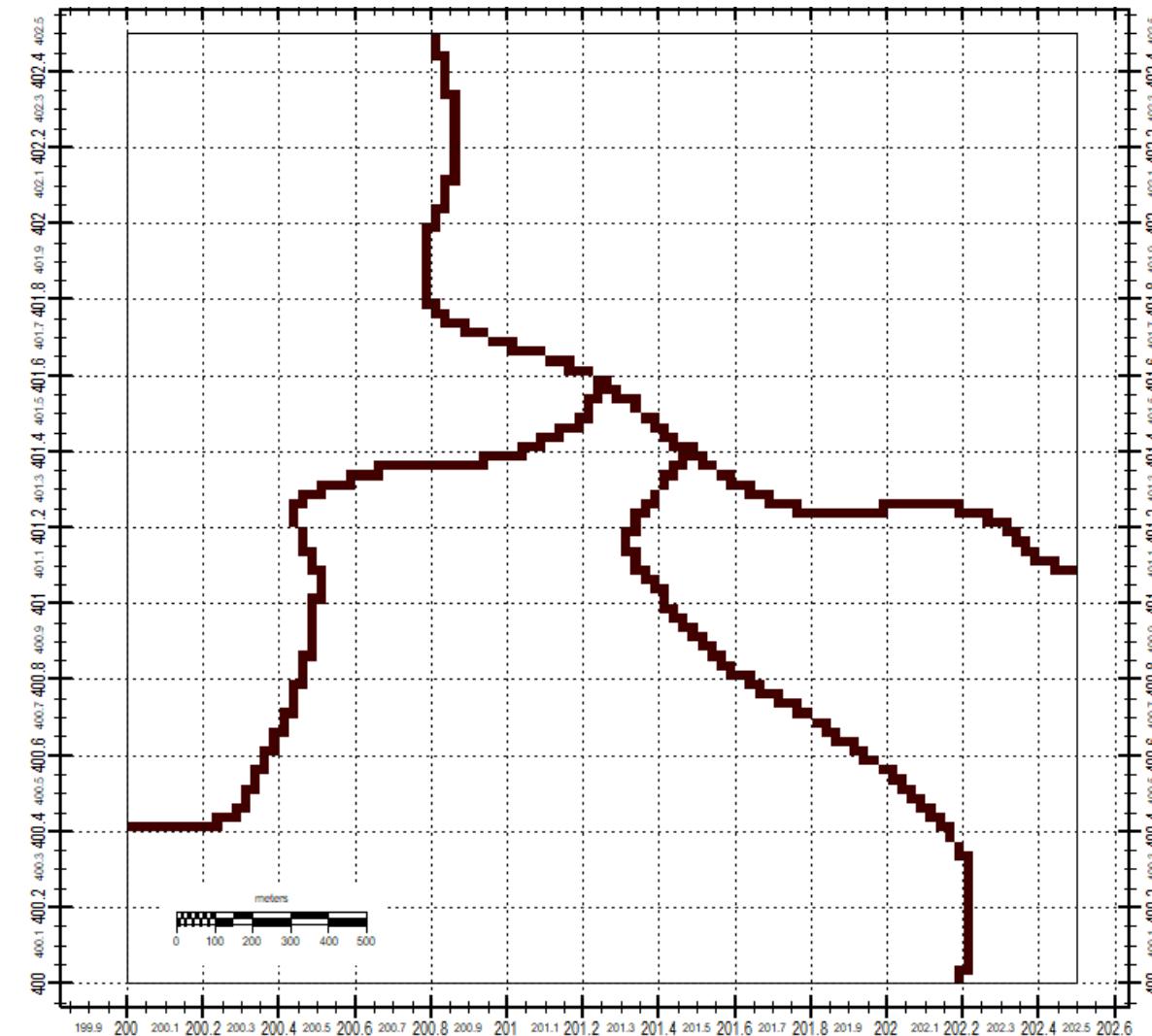
Deltas

Synthetic Example



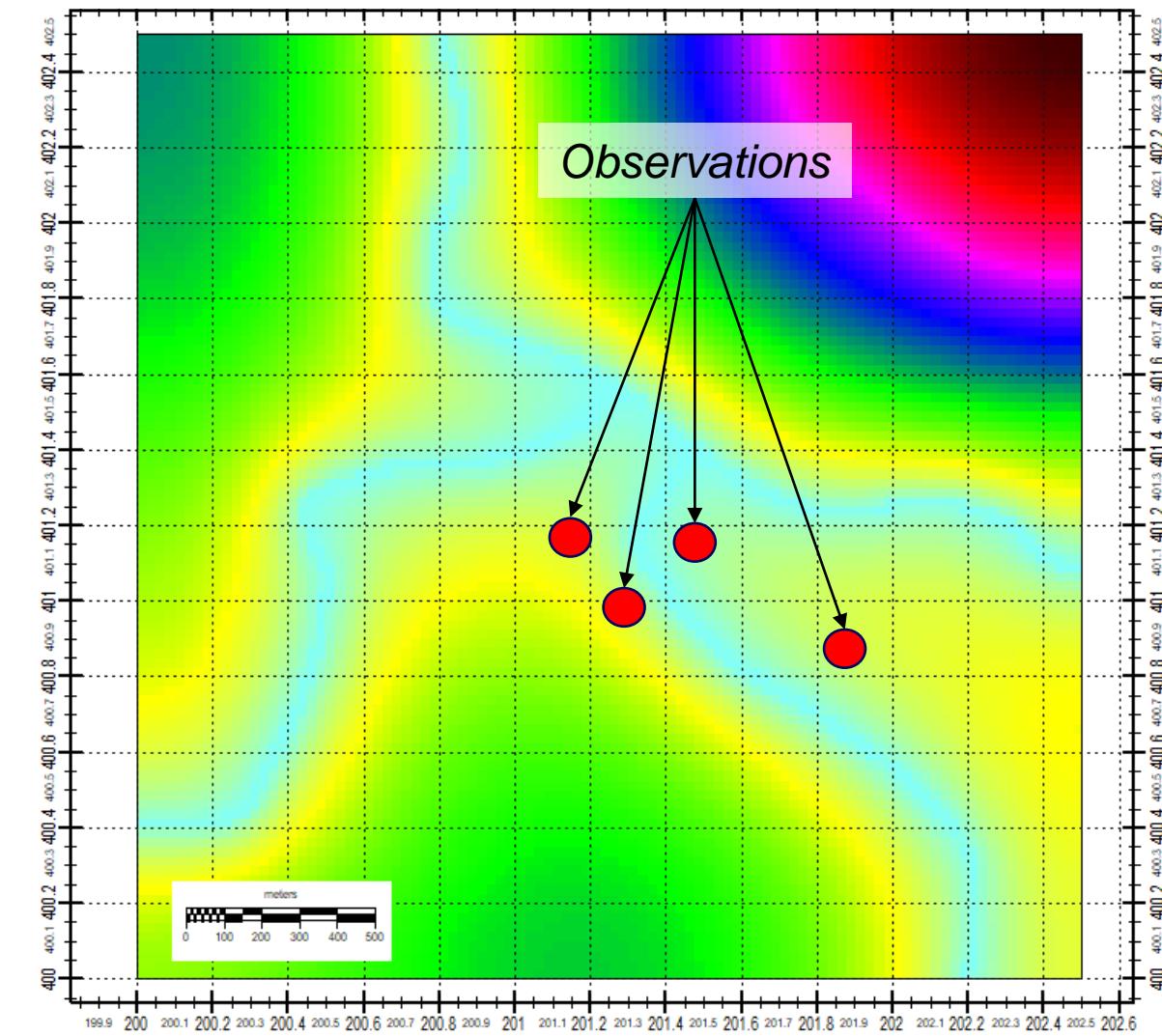
Deltas

Computed Head / Observations

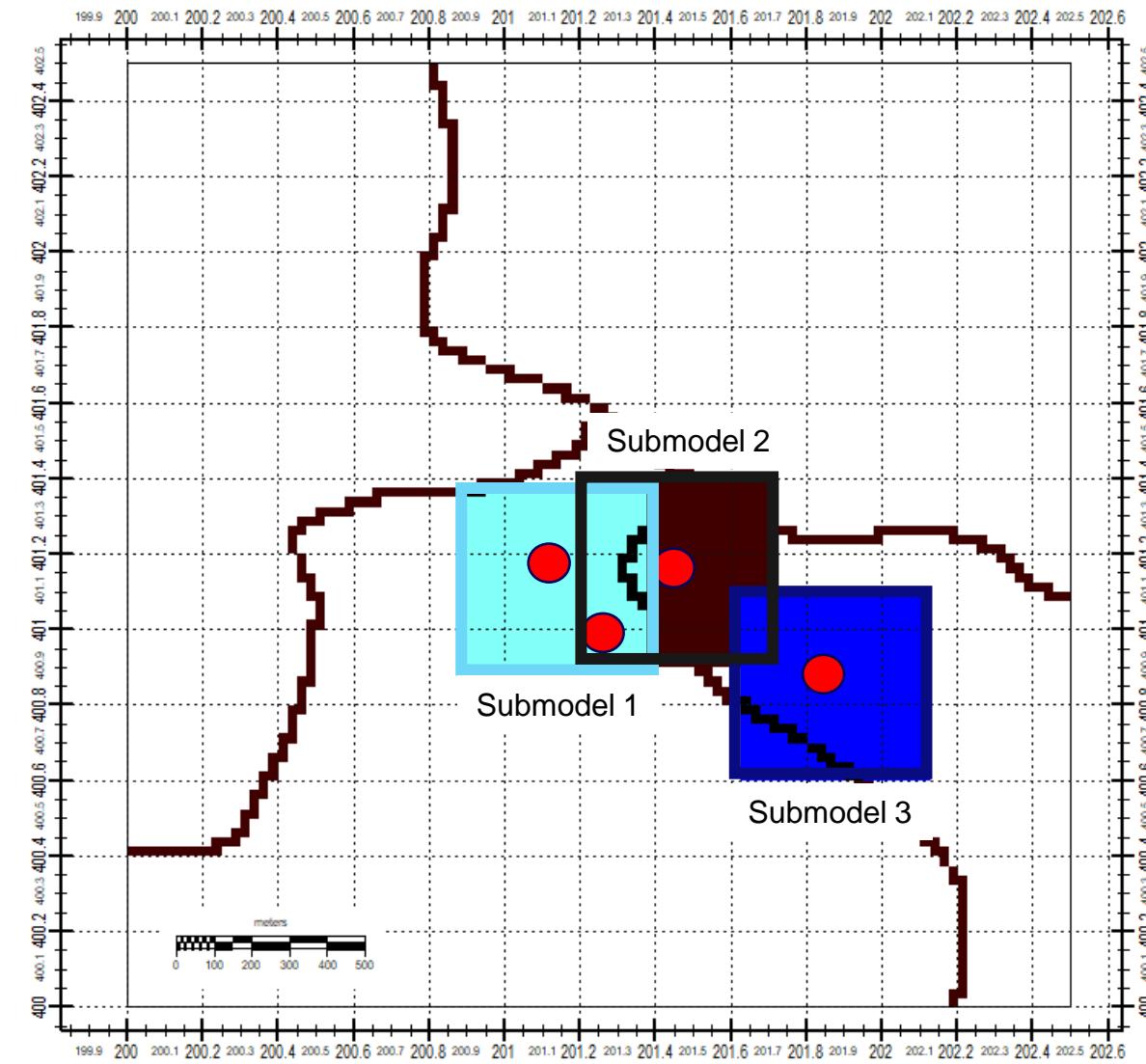


River

Synthetic Example



Deltas



Synthetic Example

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=3
SEPMODELS=D:\MODELS\SBM.IDF
OUTERUPDATE=1
SKIPMODEL=0
```

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 OUT-PUT_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.

OUTER-UPDATE= (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 modeled area. This area can be given with the keywords WINDOW or NETWORKID, 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.

SKIPMODEL= (optional) If SKIPMODEL=1, the initial global model is skipped as it is assumed that it is computed beforehand. Thereafter, existing separate models will be updated for the first cycle to be able to perform the optimization per sepmode. The initial values are taken from the input file. By default SKIPMODEL=0 and all separate models are optimized initially.

SKIPMODEL **IPKS=1** to apply the PKS package instead of the PCG package. The solver is more robust than the PCG solver, so you might want to use IPKS=1 in case of non-convergence due to huge contrasts in conductivity using the multi-core applications. This option is applicable whenever OUT is specified, whenever RUNFILE_OUT is specified, this keyword has any effect.

NRPROC=5 to specify 5 processors (PKS runs in parallel mode). By default NRPROC=1 and the PKS is used in serial mode.

PKSMERGE=0 specifies whether result files need to be merged after the simulation. PKSMERGE=0 does not merge (default value). Alternatively PKSMERGE=1 can be specified which deletes the original IDF file after merging.

XS=1 or **NSEP>0** the method to apply the load of the partial models, these are:
• Bisection Partitioning.

LOADZONES= describes the load distribution (PARTOPT=2, the LOAD-zones) or the in- and active nodes (PARTOPT=3, the active nodes).

PARTOPT=1 or **SIM_TYPE=2** **MODFLOW=D:\PROGRAMS\IMODFLOW.EXE**

PARTOPT=3 or **SIM_TYPE=4** or **SIM_TYPE=5** **RUNFILE=D:\PROGRAMS\IMODFLOW.RUN** file that will be created, e.g. RUNFILE=1005 compatible model, all arrays are listed in RUNFILE=1 or IDEBUG=2 to export all model input to

iMOD Batch functions

EXCLUDE= (optional) Specify EXCLUDE=1 (this is the default value) to exclude model area outside the specifies extent of the sepmode as defined in SEPMODELS. These areas are treated as nodatavalues and are excluded in the modeling and optimization. In this case no overlap of the optimization per sepmode occurs. In case EXCLUDE=0, the area surrounding the specific sepmode is included and causes an influence on the optimized values.

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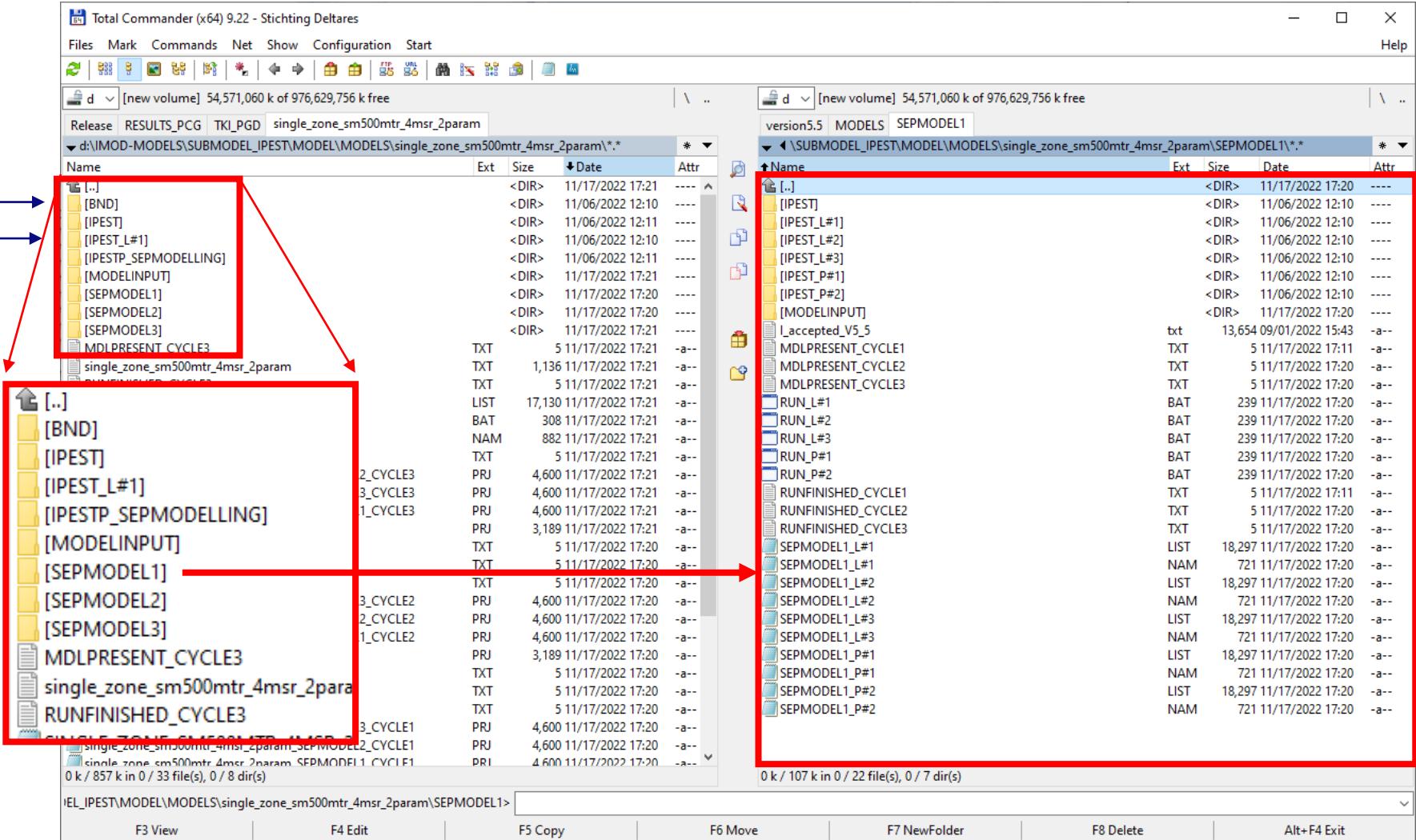
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iMOD International User Day 2022

Synthetic Example

BND for Submodels
Original Model

PEST information
after aggregation
Original Modelinput
Submodels



Synthetic Example

BND for Submodels
Original Model

PEST information
after aggregation
Original Model input
Submodels

Total Commander (x64) 9.22 - Stichting Deltares

single_zone_sm500mtr_4msr_2param.TXT - Notepad

File Edit Format View Help

SUMMARY OF SEP-MODELLING

		cycle1	cycle2	cycle3
0		0.270	0.015	0.008
1			0.059	0.000
2			0.008	0.000
3			0.100	0.000
				0.004

Global Objective Function

Local Objective Functions

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

Sub models

m\SEPMODEL1*.*

Size	Date	Attr
<DIR>	11/17/2022 17:20	---
<DIR>	11/06/2022 12:10	---
<DIR>	11/17/2022 17:20	---
13,654	09/01/2022 15:43	-a--
5	11/17/2022 17:11	-a--
5	11/17/2022 17:20	-a--
5	11/17/2022 17:20	-a--
239	11/17/2022 17:20	-a--
5	11/17/2022 17:11	-a--
5	11/17/2022 17:20	-a--
5	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--
18,297	11/17/2022 17:20	-a--
721	11/17/2022 17:20	-a--

Alt+ F4 Exit

Synthetic Example

single_zone_sm500mtr_4msr_2param.TXT - Notepad

File Edit Format View Help

SUMMARY OF SEP-MODELLING

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
1 KH	AQUIFER1_KH			0.298	0.254	0.114
2 KH	AQUIFER2_KH			0.979	1.152	0.603

ICYCLE=	2	IPRM PT	PARAM	F_FINAL	MEAN	STDEV
1 KH	AQUIFER1_KH			0.233	0.226	0.049
2 KH	AQUIFER2_KH			1.228	0.800	0.350

ICYCLE=	3	IPRM PT	PARAM	F_FINAL	MEAN	STDEV	F_MDL1
1 KH	AQUIFER1_KH			0.265	0.269	0.048	0.292
2 KH	AQUIFER2_KH			1.384	0.942	0.361	0.538

Sub models

LOG_PEST.TXT - Notepad

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*** Lambda Cycle ***

Optimization History:

Statistics	ITER003	ITER002	ITER001	ITER000
Total Obj. Val.	0.004	0.004	0.069	0.270
Meas. Obj. Val.	0.004	0.004	0.069	0.270
Param Obj. Val.	0.000	0.000	0.000	0.000
Number of Obs.	4	4	4	4
Goodness of Fit	-0.554	-0.574	-0.759	-0.882
Nash Sutcliffe	-5.364	-5.445	-100.264	-394.538

Parameter	ITER003	ITER002	ITER001	ITER000
AQUIFER1_KH	0.2617264	0.2578616	0.4228614	1.0000000
AQUIFER2_KH	1.4215247	1.3003882	1.2083414	1.0000000
Adjustment	0.1211982	0.1889380	0.6135919	

*** Next Optimization

LOG_PEST.TXT - Notepad

File Edit Format View Help

AQUIFER1_KH	0.5995011E-01	0.4266653
AQUIFER2_KH	0.4266653	3.376036

Parameter Correlation Matrix (-)

	AQUIFER1_KH	AQUIFER2_KH
AQUIFER1_KH	1.0000000	0.9483939
AQUIFER2_KH	0.9483939	1.0000000

Parameter Variance - Standard Parameter Error (Confidence Limits ~96%)

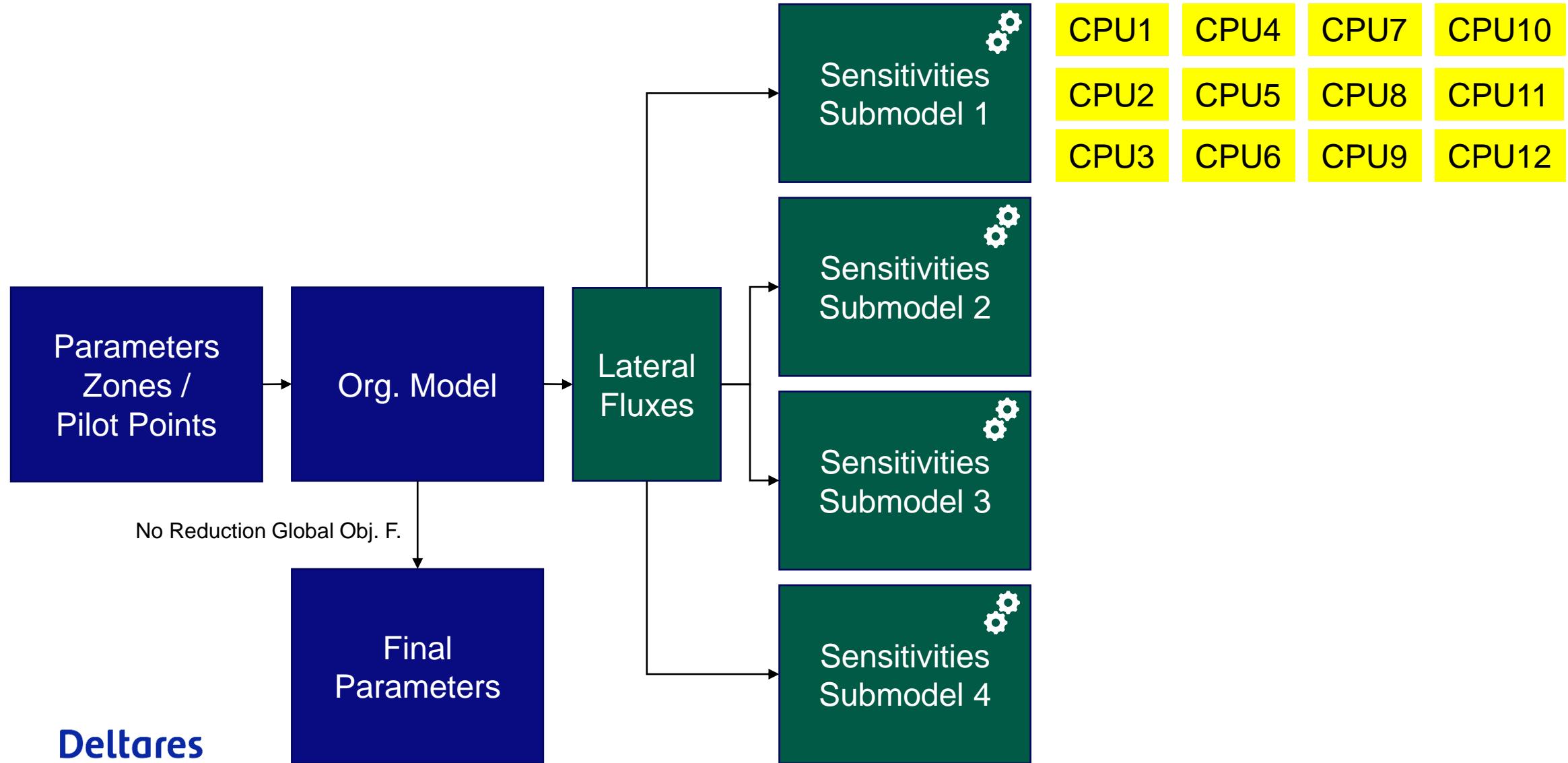
	Lower_Limit	Average	Upper Limit
AQUIFER1_KH	0.1619681	0.2617264	0.4229271
AQUIFER2_KH	0.3879079E-01	1.421525	52.09310

Start Lambda Testing

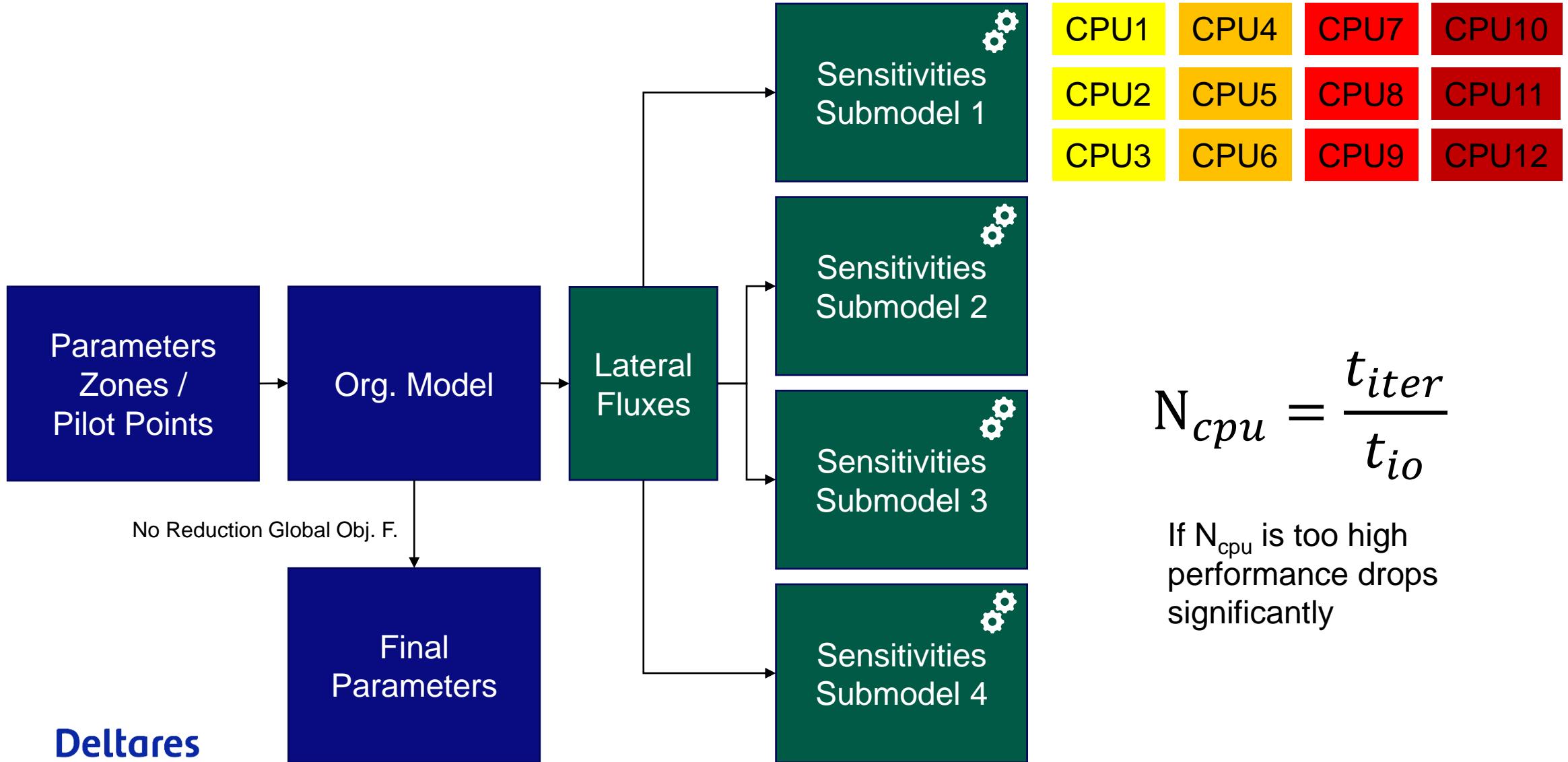
Lambda_0 (lambda number 1) prior to the update vector 0.388E-02

Performance

NCPU=12

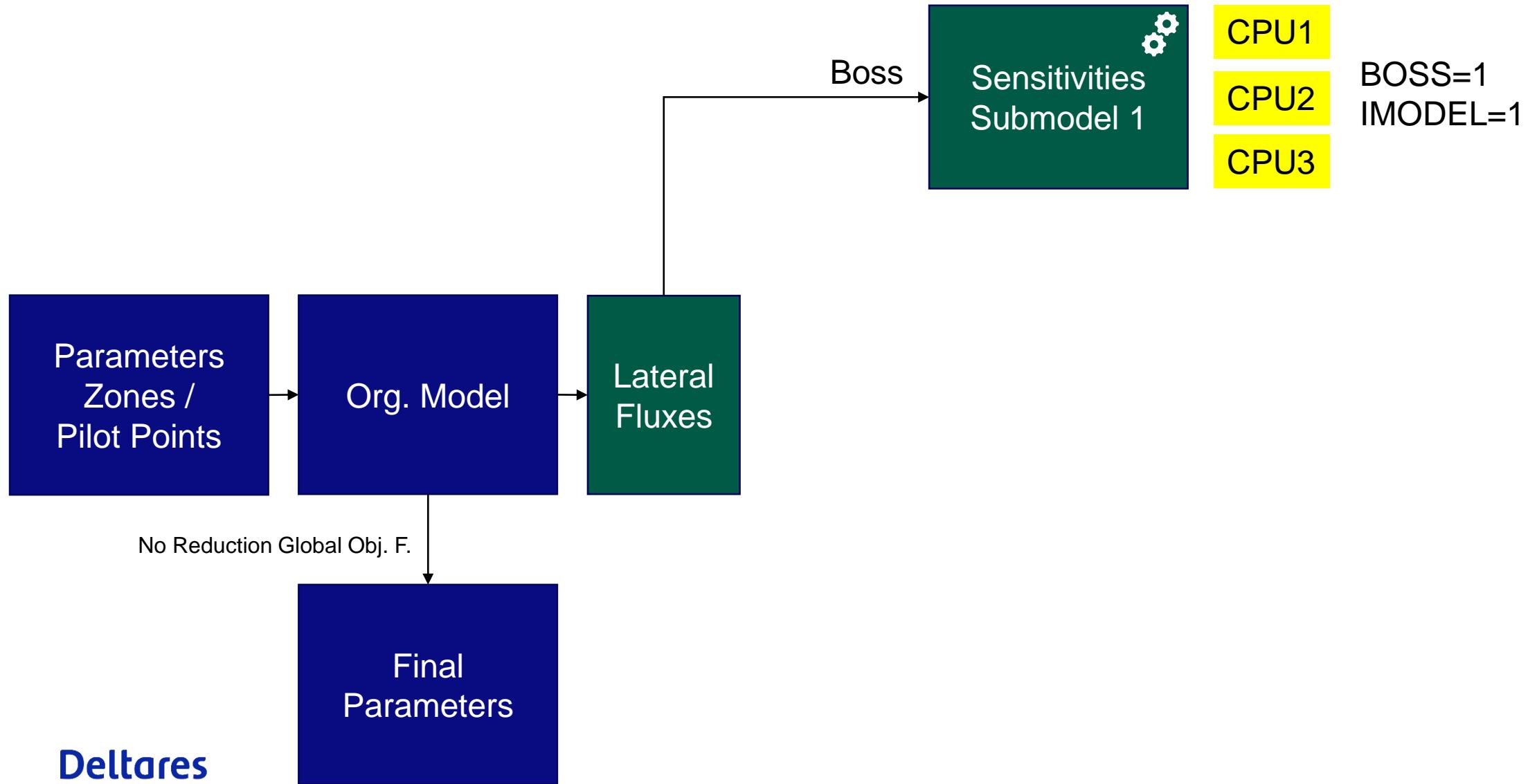


Performance



Performance

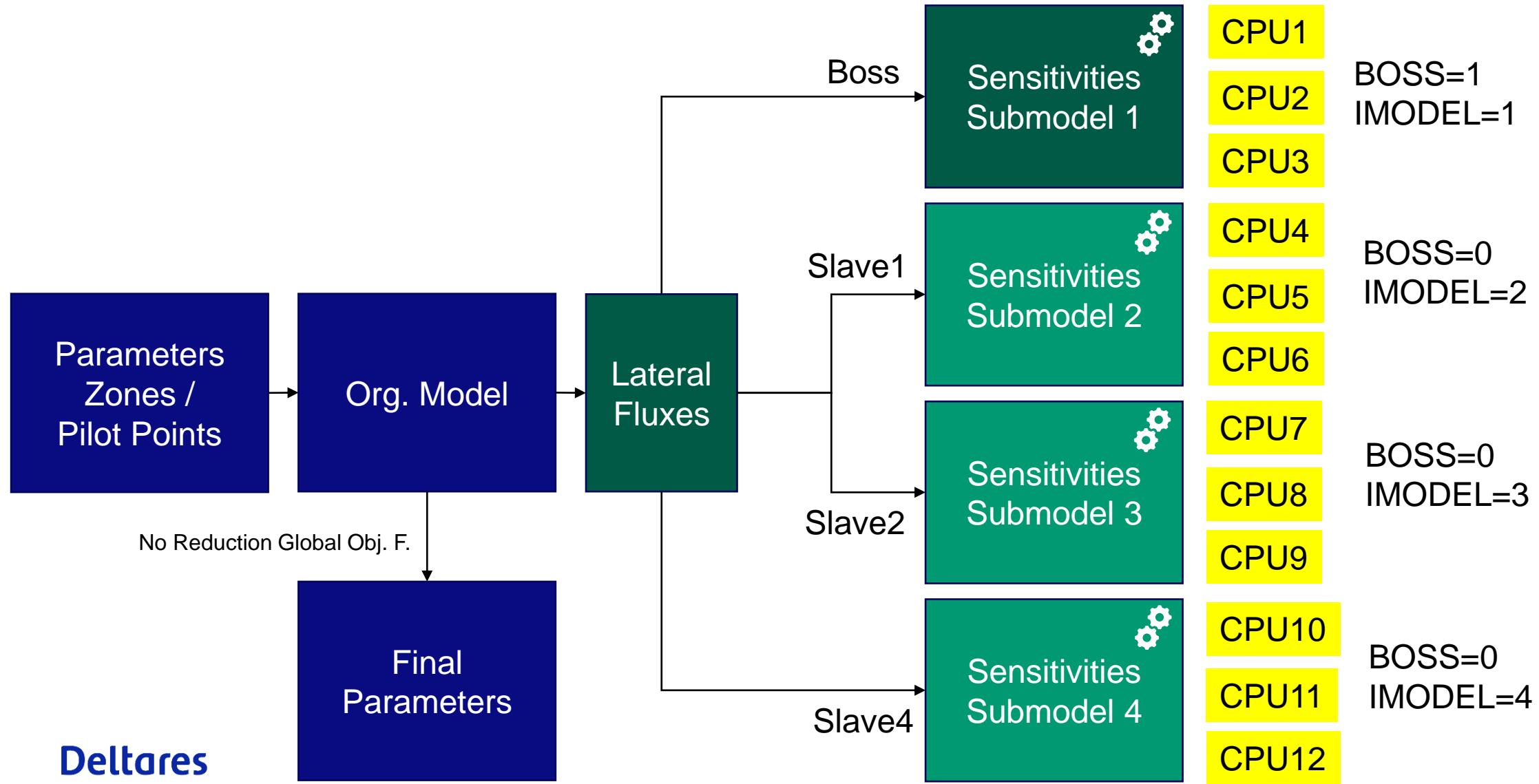
NCPU=3



Performance

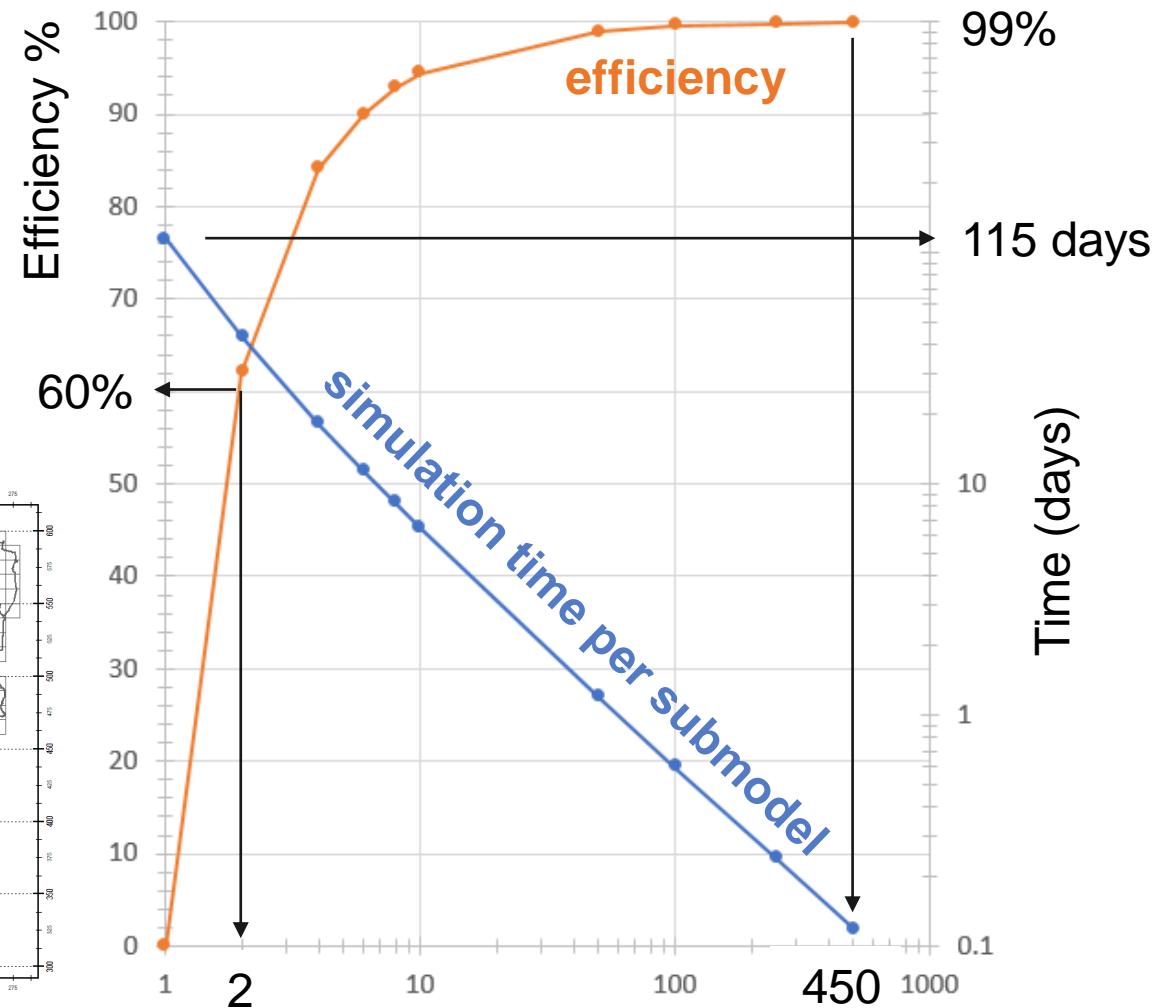
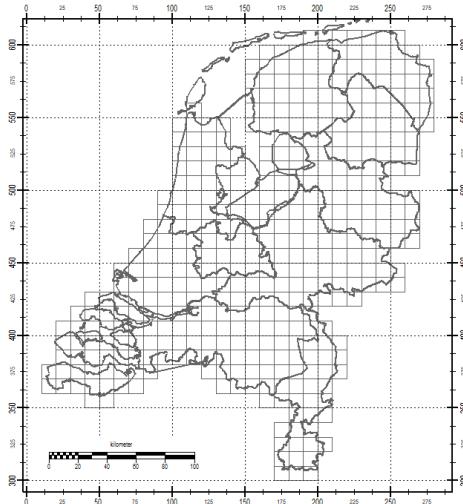
No. Computers=4

NCPU=3



Conclusions

- Applying submodels in optimization yields high efficiencies from the beginning
- Optimization process is able to focus and restart on particular areas (submodels)
- Insight in parameter adjustments per submodel
- Two or three outer cycles are often enough



Contact

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