

Automated Calibration with PEST-HP

GSSHA Model model Calibration in HPC

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Inverse Problem / Calibration



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Forward Model

Model Parameters



Predictions vs. Observations

Model Parameters



Predictions vs. Observations

Inverse/backward Model



Anatomy of the model



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What is PEST?



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- PEST: Model-Independent Parameter Estimation and Uncertainty Analysis
 - ▶ Automates Calibration
 - ▶ Calibration Constrained Uncertainty Analysis
 - ▶ Interaction with any model through I/O files
- PEST also
 - ▶ setup facilitation
 - ▶ flexible spatial parameterization
 - ▶ objective function definition
 - ▶ sensitivity analysis
 - ▶ linear and non-linear uncertainty analysis



www.pesthomepage.org



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Home | PEST

The RECOVER Team's Recommen...

pesthomepage.org

Apps _USACE SAI Intranet DCPDS Portal - Login XMing&PuttySetUp ERDC DoD Superco... myPay Citi Commercial Car... ACEBIT Software Ap... ERDC DSRC - Onyx... SFWMD SFTP Site EAP program

Home Book Software Downloads Education About

PEST: Model-Independent Parameter Estimation and Uncertainty Analysis

"PEST" refers to a software package and to a suite of utility programs which supports it. Collectively, these are essential tools in decision-support environmental modelling.

PEST, the software package, automates calibration, and calibration-constrained uncertainty analysis of any numerical model. It interacts with a model through the model's own input and output files. While estimating or adjusting its parameters, it runs a model many times. These model runs can be conducted either in serial or in parallel. PEST records what it does in easily-understood output files.

PEST, the software suite, performs a plethora of tasks that assist and complement model parameter estimation and uncertainty analysis. These include:

- setup facilitation;
- flexible spatial parameterization;
- objective function definition;
- linear prior and posterior uncertainty analysis;
- nonlinear prior and posterior uncertainty analysis.

Many thanks to [ESI](#) and [SSPA](#) for funding these pages.

Latest change: January 27, 2021 - version 17.2 of PEST; updated Groundwater Utilities.

Learn More

Training

Because COVID-19 has severely restricted our ability to offer live courses on decision-support modeling and PEST, we are developing alternatives methods of delivery. [Roadmaps](#), [videos](#), [webinars](#), [tutorials](#), and [frequently asked questions](#) are available from these pages. We are in the process of expanding all of these resources.

GMDSI

GMDSI is an industry-funded, industry-aligned project focused on improving the role that groundwater modelling plays in decision support. It has contributed to PEST software and training material. Thanks to BHP and Rio Tinto.

Search

pest_uncert.zip

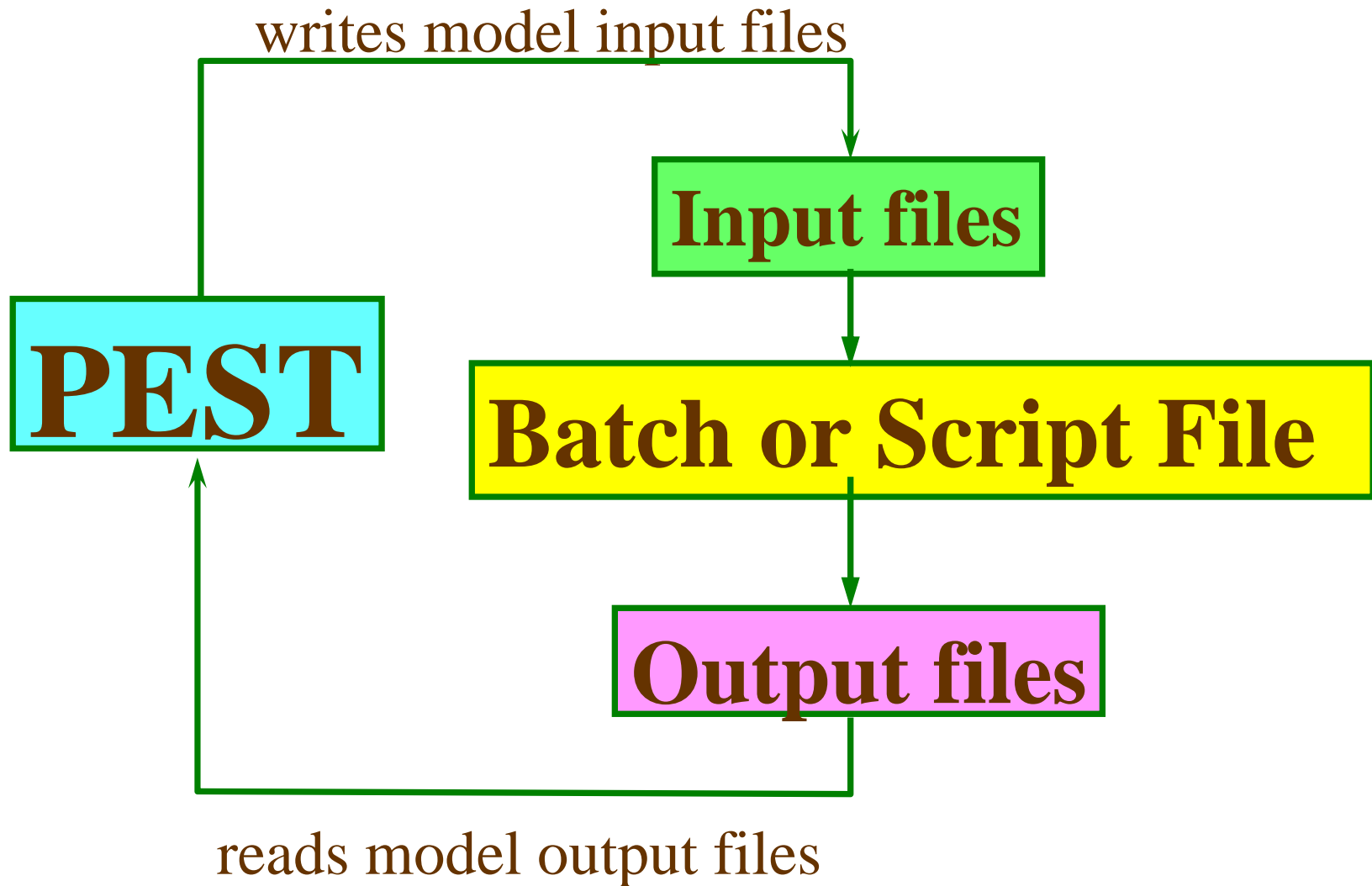
Show all



PEST - model independence ...



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PEST toolbox



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PEST

Inverse Modeling
Levenberg-Marquardt
Method
CMA_ES
SCEUDA

Uncertainty Analysis
Linear Analysis
Null Space Monte Carlo
Pareto

Parallel Run Managers

PEST++

Inverse Modeling
Levenberg-Marquardt Method
Differential Evolution
Particle Swarm
Ensemble Smoother

Uncertainty Analysis
Linear Analysis

Global Sensitivity Analysis
Method of Morris
Sobol's Method

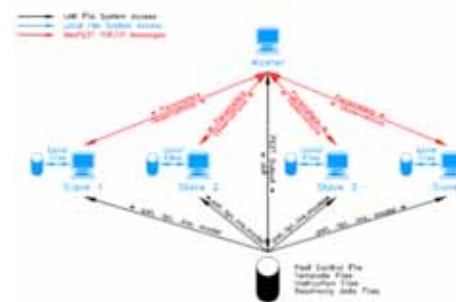
Optimization

Parallel Run Managers

BeoPEST

Similar to PEST and Parallel Pest
design to work with computer
clusters

Can be run across the internet



PEST-HP

Similar to BeoPEST but
optimized for Highly
Parallelized Computing
Environments (e.g.
ERDC's HPC)

Improved Inversion
algorithm for long model
run times

Cannot run in
"predictive analysis"
mode

Other relevant
alterations

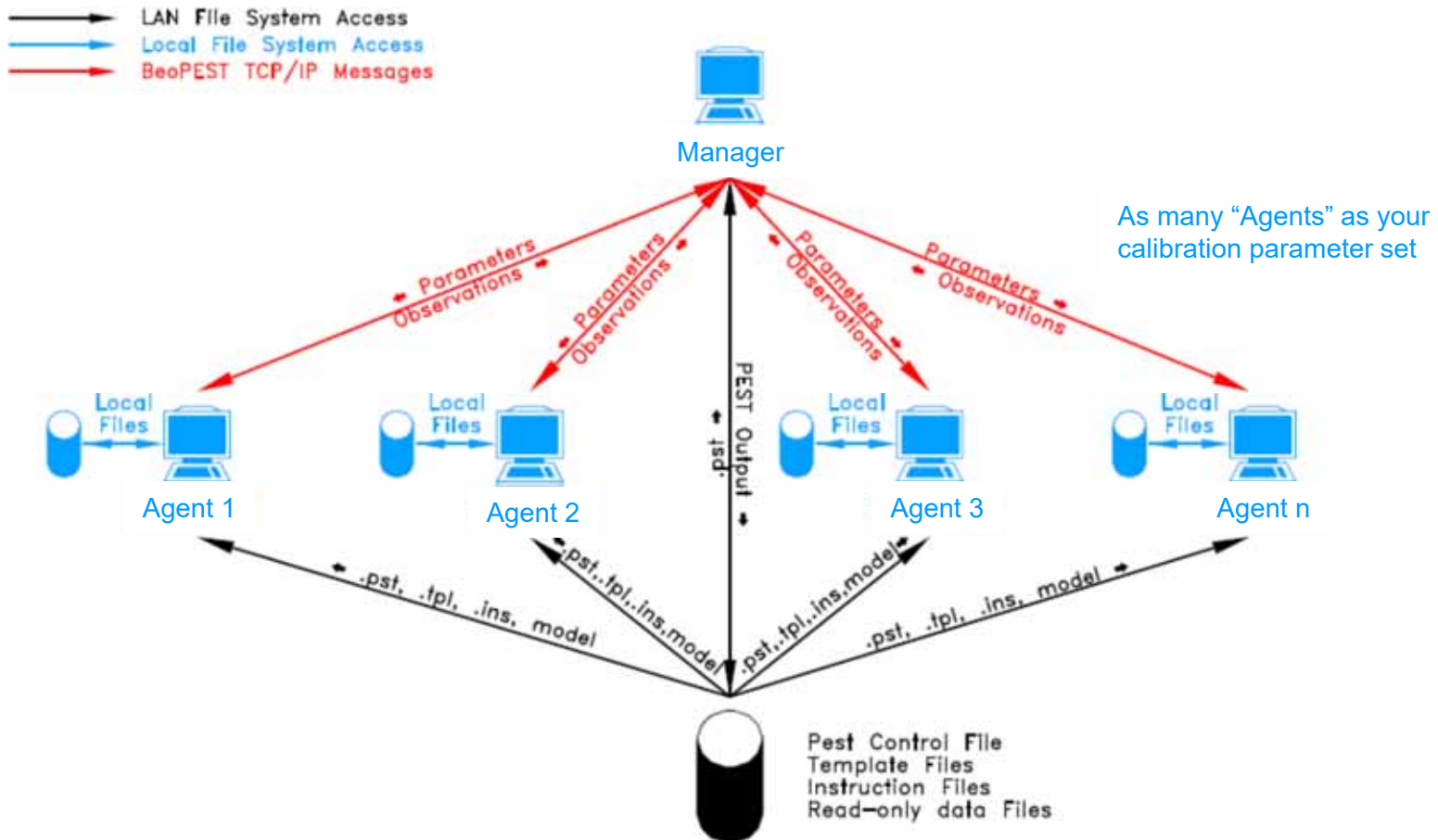
Nomenclature change



PEST-HP



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Model Independence

Model Input and Pest Template File



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■ Model Input

```
`case number as453'
4.68943    4.45663    5.44356    line 1 of input
4.54356                                line 2 of input
4                                line 3 of input
5.467543    5.544352    } parameter line 1
6.524532    7.433797    } parameter line 2
5.45E+03    5.613435    } parameter line 3
5.43E-05    6.544524    } parameter line 4
6
1.0
1.2
1.6
1.7
2.4
4.3
```

■ Pest Template File

```
ptf #
`case number as453'
4.68943    4.45663    5.44356    line 1 of input
4.54356                                line 2 of input
4                                line 3 of input
# top1#    # top2#    parameter line 1
# base1#    # base2#    parameter line 2
# hcond1#    # hcond2#    parameter line 3
# stor1#    # stor2#    parameter line 4
6
1.0
1.2
1.6
1.7
2.4
4.3
```



Model Output and PEST Instruction Files



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■ Model Output File

TIME = 4.54 DAYS ----->

SOLUTION CONVERGENCE TO 1.430E-5
NO STABILITY THRESHOLDS EXCEEDED

RESULTS:-

OBSERVATION PT	HEAD
1	3.432425
2	5.654356
3	10.54234
4	14.54432
5	30.65542
6	65.43562
7	14.54332
8	34.45234

■ PEST Instruction File

```
pif %  
%HEAD%  
12 !dum! !head2!  
13 !dum! !head3!  
16 !dum! !head6!
```

Instructs PEST how and
where to look for simulated
outcomes in output file



PEST Control File



```
pcf
*control data
restart estimation
8 3 2 0 1
3 2 single point 1 0 0
20.0 -2.0 0.3 0.03 10 999 LAMFORGIVE
5.0 5.0 0.001 0
0.1 0 0.005 3 3 0.01 3
1 1 1 1
* singular value decomposition
2
250 1.0e-7 1
* parameter groups
elev relative 0.05 0 switch 2 parabolic
gwnt relative 0.05 0 switch 2 parabolic
* parameter data
top1 log factor 1.12E-01 0.01000 0.300 rough 1.0 0 1
top2 log factor 1.12E-01 0.01000 0.300 rough 1.0 0 1
base1 log factor 1.12E-01 0.01000 0.300 rough 1.0 0 1
base2 log factor 1.12E-01 0.01000 0.300 rough 1.0 0 1
...
*observation groups
HEADS
* observation data
head2 5.500 0.30 HEADS
head3 10.100 0.20 HEADS
head6 68.000 0.50 HEADS
...
```



PEST Control File



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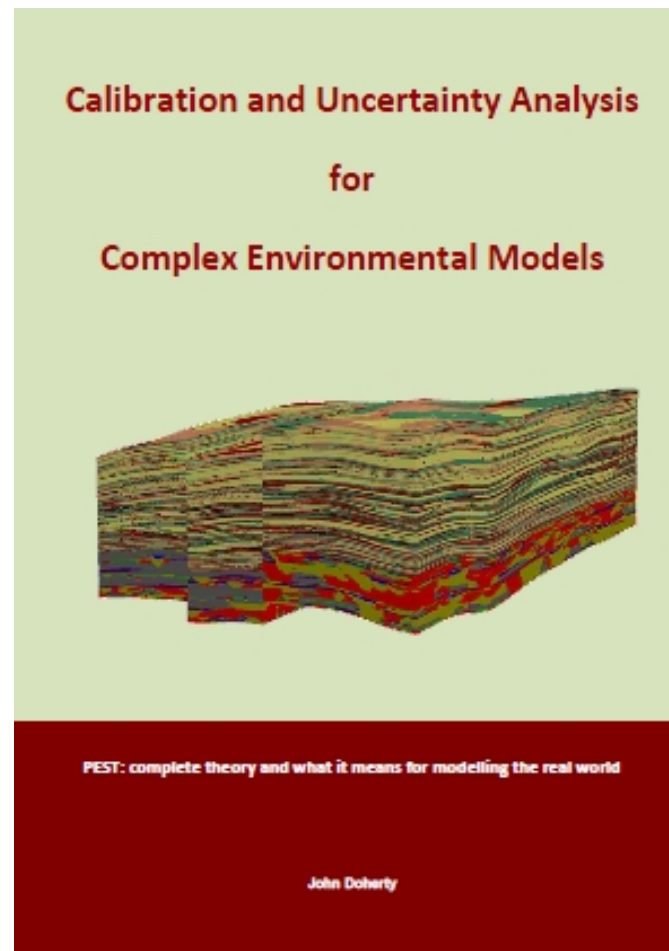
```
* model command line
./MendocinoPEST.sh
* model input/output
CalibrationTable.cmt.tpl CalibrationTable.cmt
CalibrationChannelInput2018.cif.tpl CalibrationChannelInput2018.cif
mendocino_100m_2018.prj.tpl mendocino_100m_2018.prj
Mendocino.ins1 ./DailyVols.csv
Mendocino.ins2 ./EventSummary.csv
*prior information
++ AUTO_NORM(4)
```



Reference / Theory



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http://www.pesthomepage.org/PEST-The_Book.php



PEST Case



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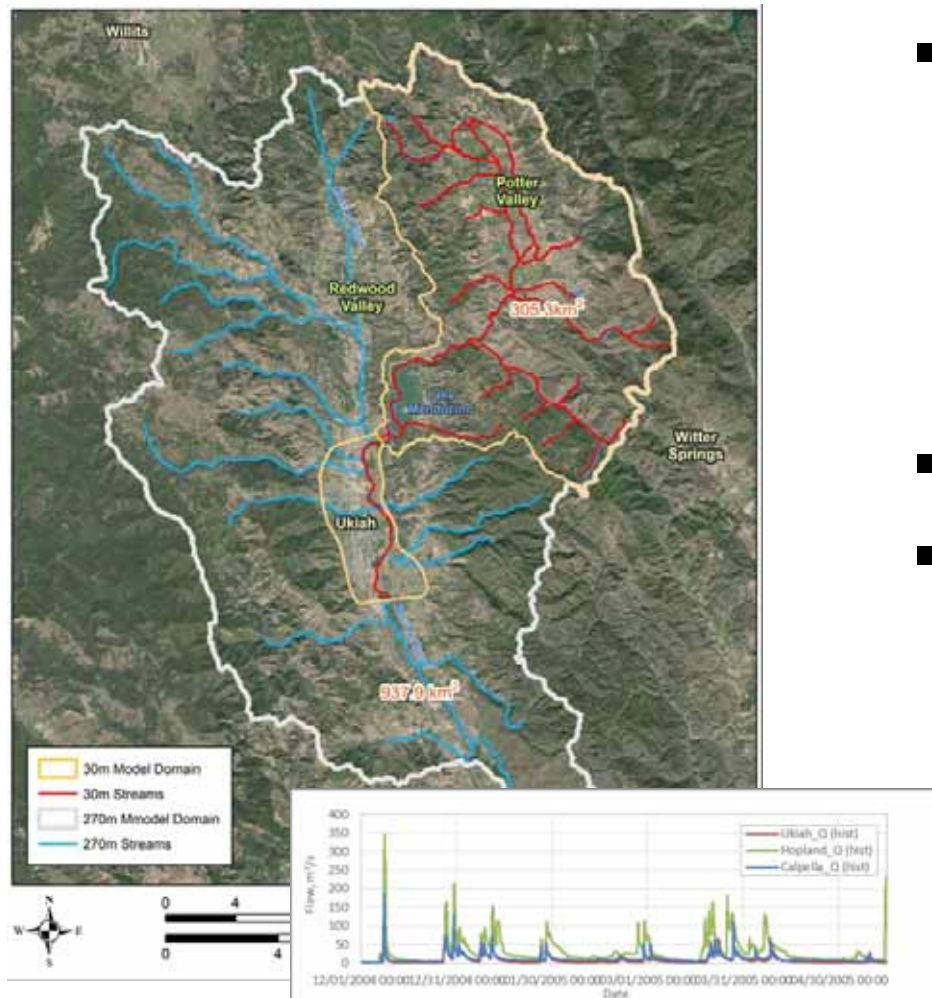
The Mendocino Example



Mendocino GSSHA Example



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- Integrated GSSHA watershed model
 - ▶ Surface Water
 - ▶ Unsaturated Zone
 - ▶ Saturated Zone
- 39 Model parameters
- 560 observations of
 - ▶ daily flows at USGS gauging stations
 - ▶ event based flows and peak discharges



Mendocino Inverse Problem



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$$\varphi = \sum_{p=1}^{p=P} \left\{ \overbrace{W_p^Q \sum_{i=1}^{i=T} (Q_i^o - Q_i^s)_p^2}^{\text{Daily Flows at } p} + \overbrace{W_p^V \sum_{m=1}^{m=M} (EV_m^o - EV_m^s)_p^2}^{\text{Event Vols at } p} + \underbrace{W_p^K \sum_{m=1}^{m=M} (EP_m^o - EP_m^s)_p^2}_{\text{Event peaks at } p} \right\}_p$$

- Minimize differences wrt
 - ▶ Daily flows
 - ▶ Event Volumes
 - ▶ Event peaks
- Weighed per
 - ▶ metric
 - ▶ location



PEST HP on ERDC's HPC



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- Developed GSSHA models (ERDC's Team)

- ▶ 3 grid resolutions
- ▶ 2 temporal snapshots

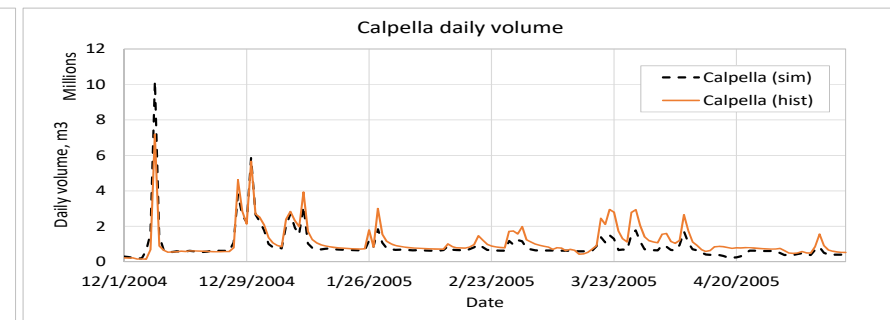
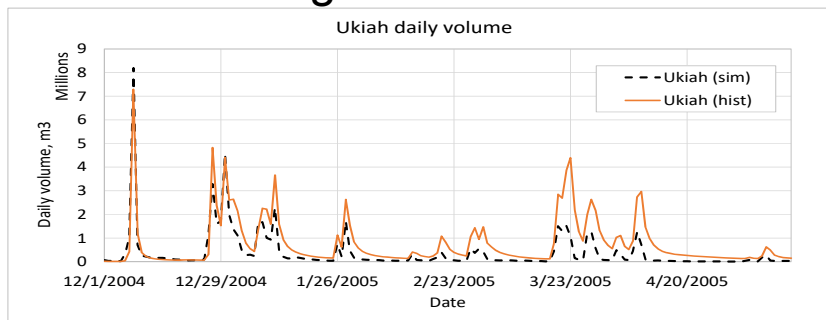
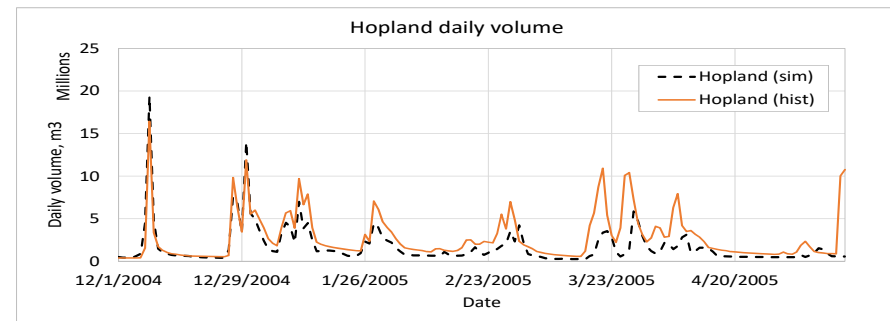
- Develop PEST files (SAJ's team)

- ▶ 40 nodes in Onyx
 - 1 "manager" node
 - 39 "agent" nodes

- PEST Outcome

- ▶ ~ 2500 total model runs per scenario

- Calibration:



Null space

\mathbf{v}_3

\mathbf{k}

Null space
component of
parameter error

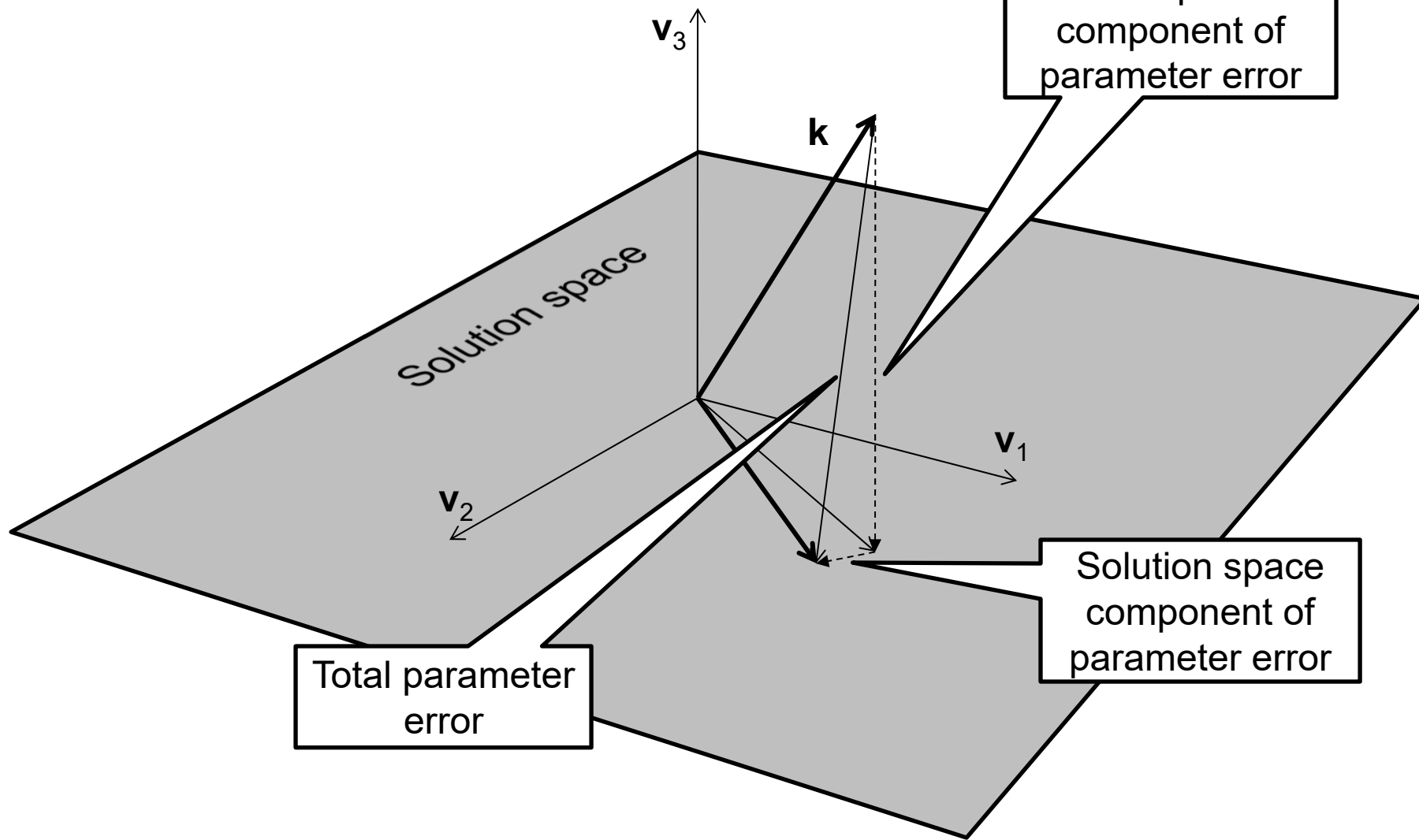
Solution space

\mathbf{v}_1

\mathbf{v}_2

Solution space
component of
parameter error

Total parameter
error



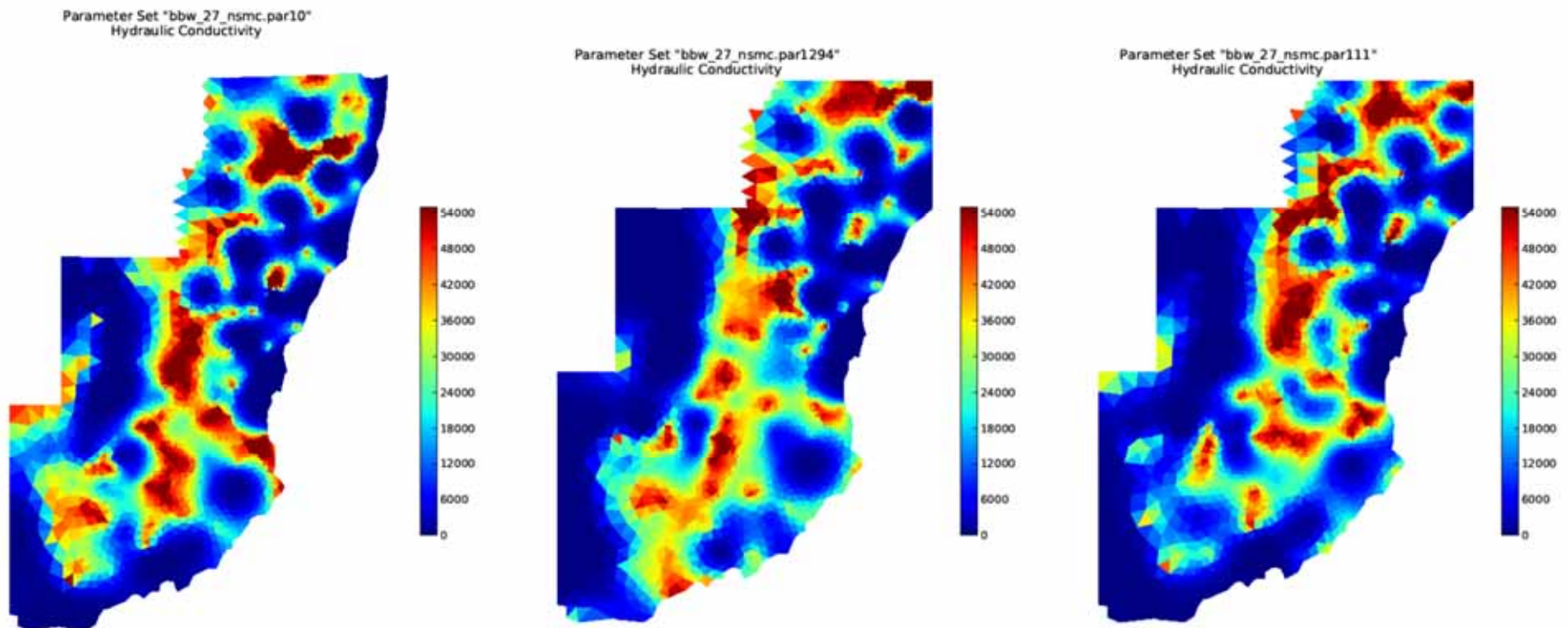


Null Space Monte Carlo



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2700 Datasets that Calibrate the Model
and Respect the Parameter Bounds





Don't Get Lost in the Weeds



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