Automated Calibration with PEST-HP

GSSHA Model model Calibration in HPC

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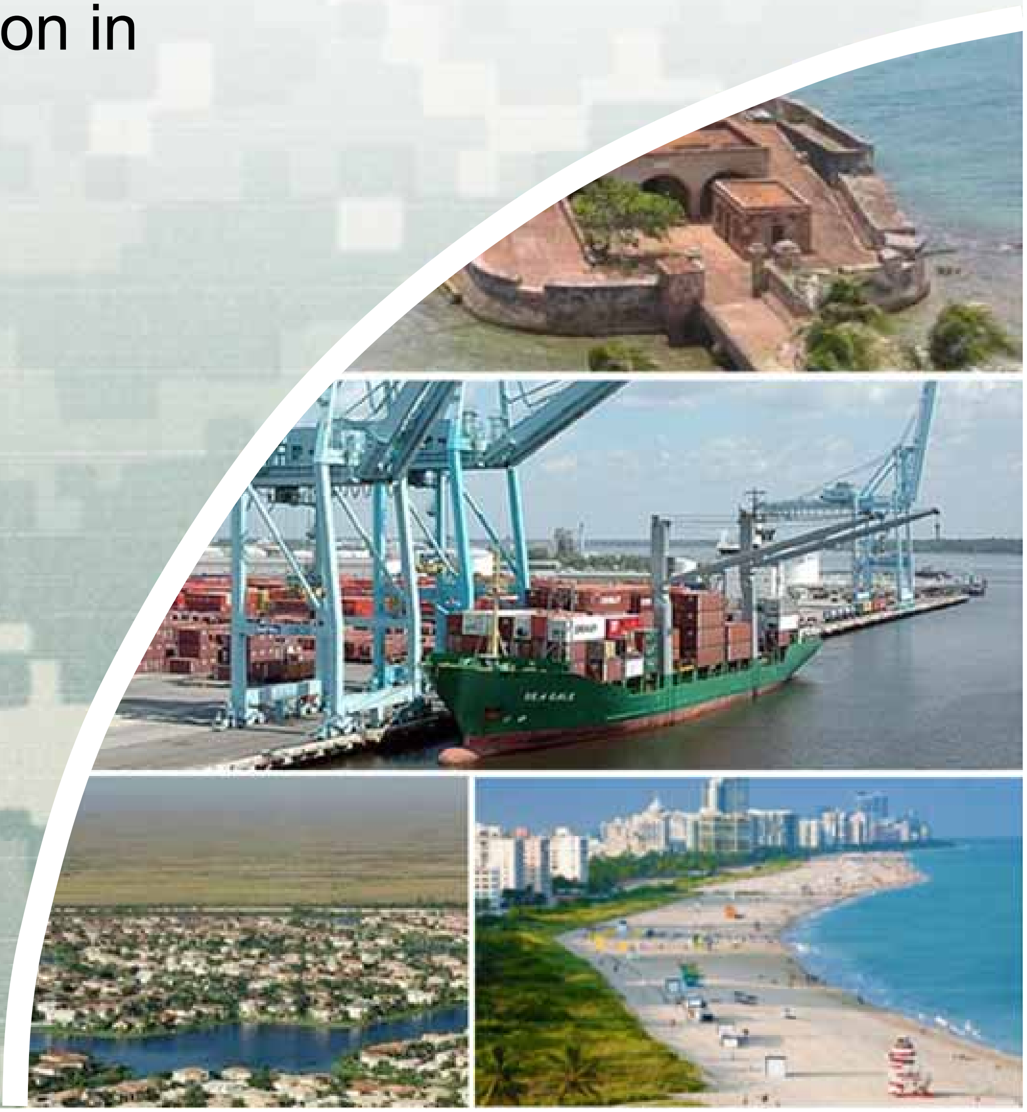

U.S.ARMY

US Army Corps of Engineers
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Inverse Problem / Calibration

Forward Model

Model Parameters

Predictions vs. Observations

Model Parameters

Predictions vs. Observations

Inverse/backward Model

Anatomy of the model

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As of:
POC:

What is PEST?

- 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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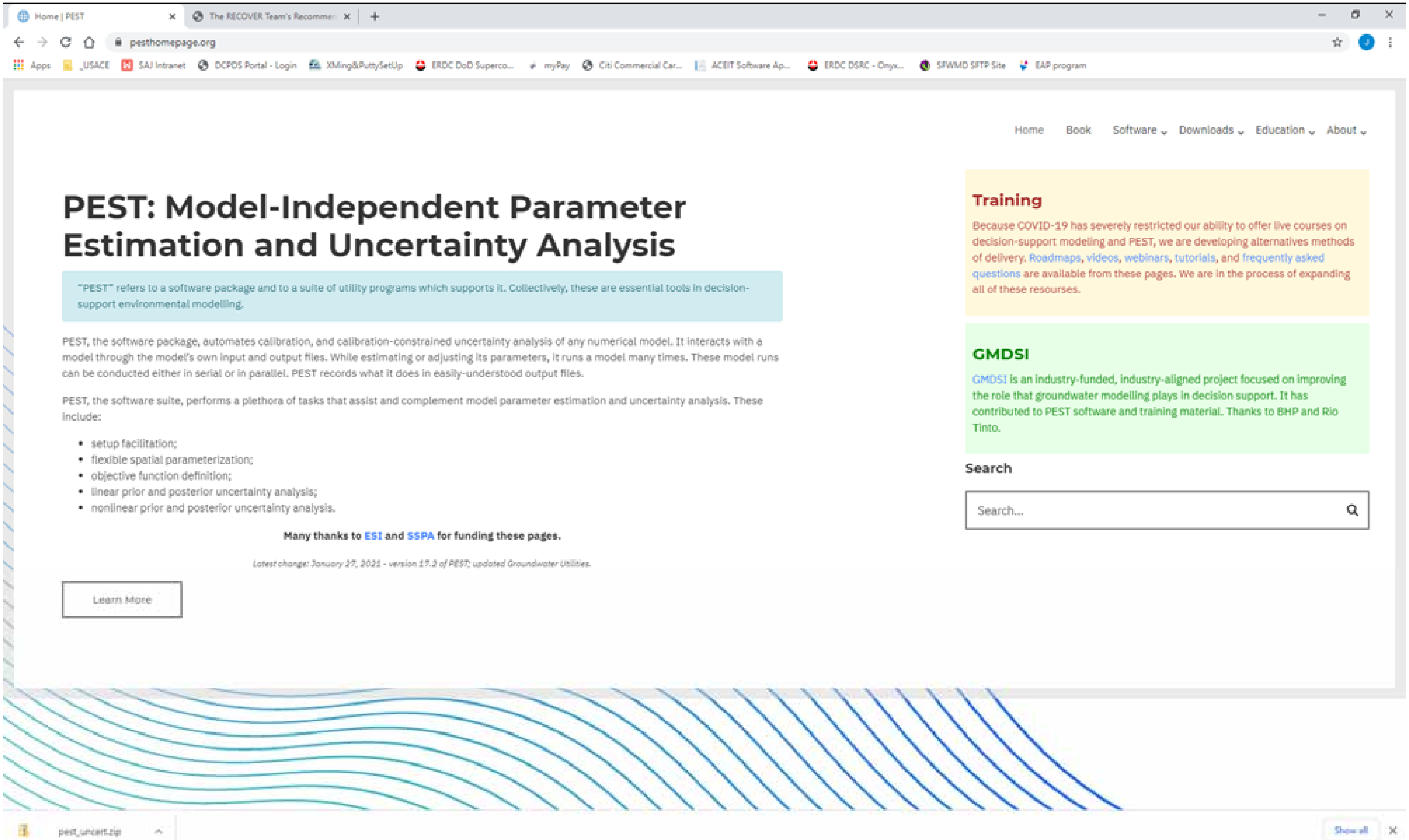

PEST - model independence …

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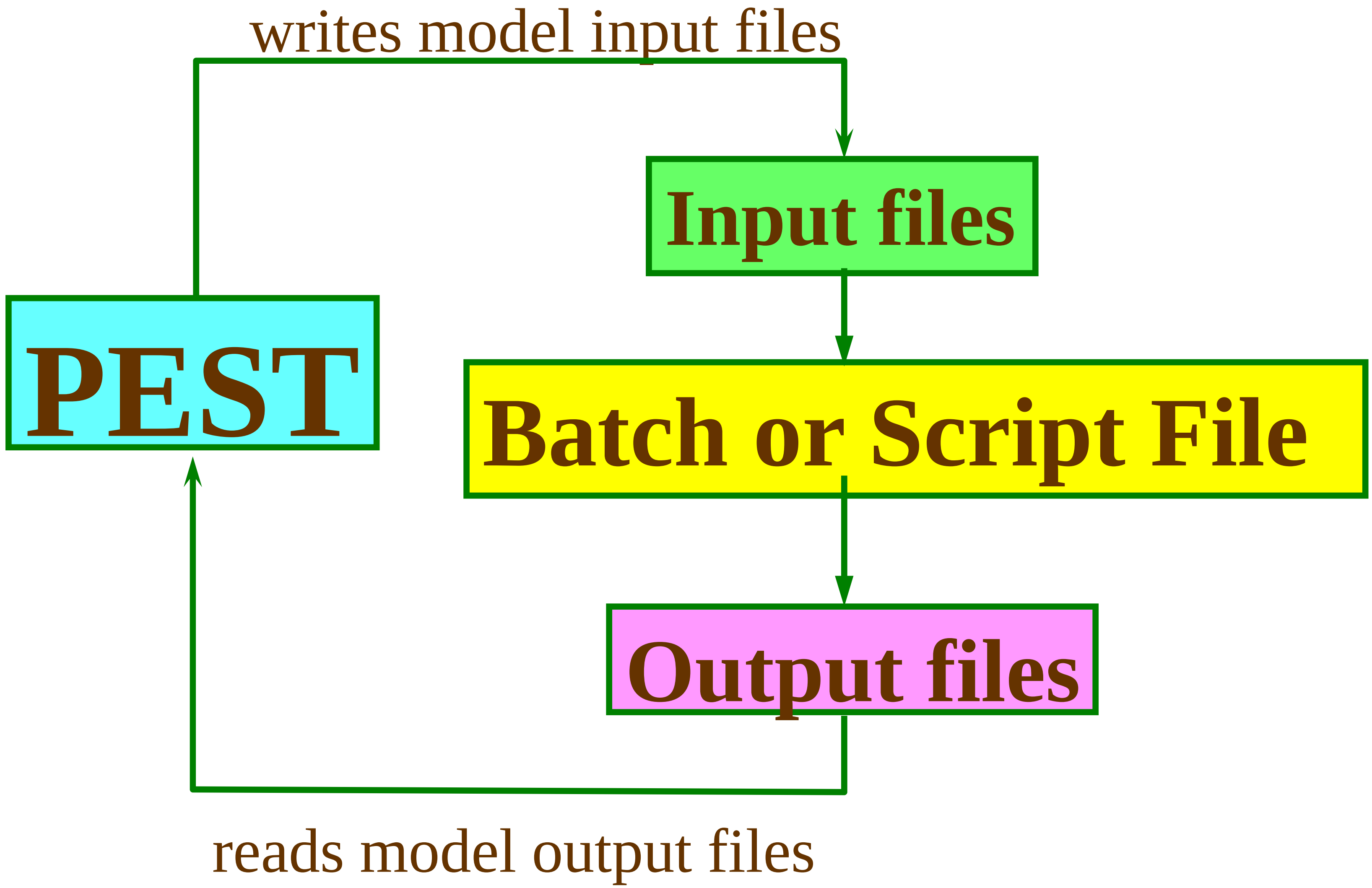


PEST toolbox

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

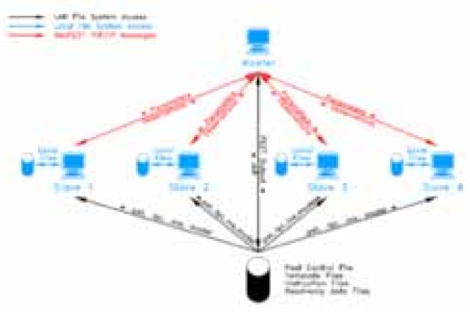
Optimization

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)

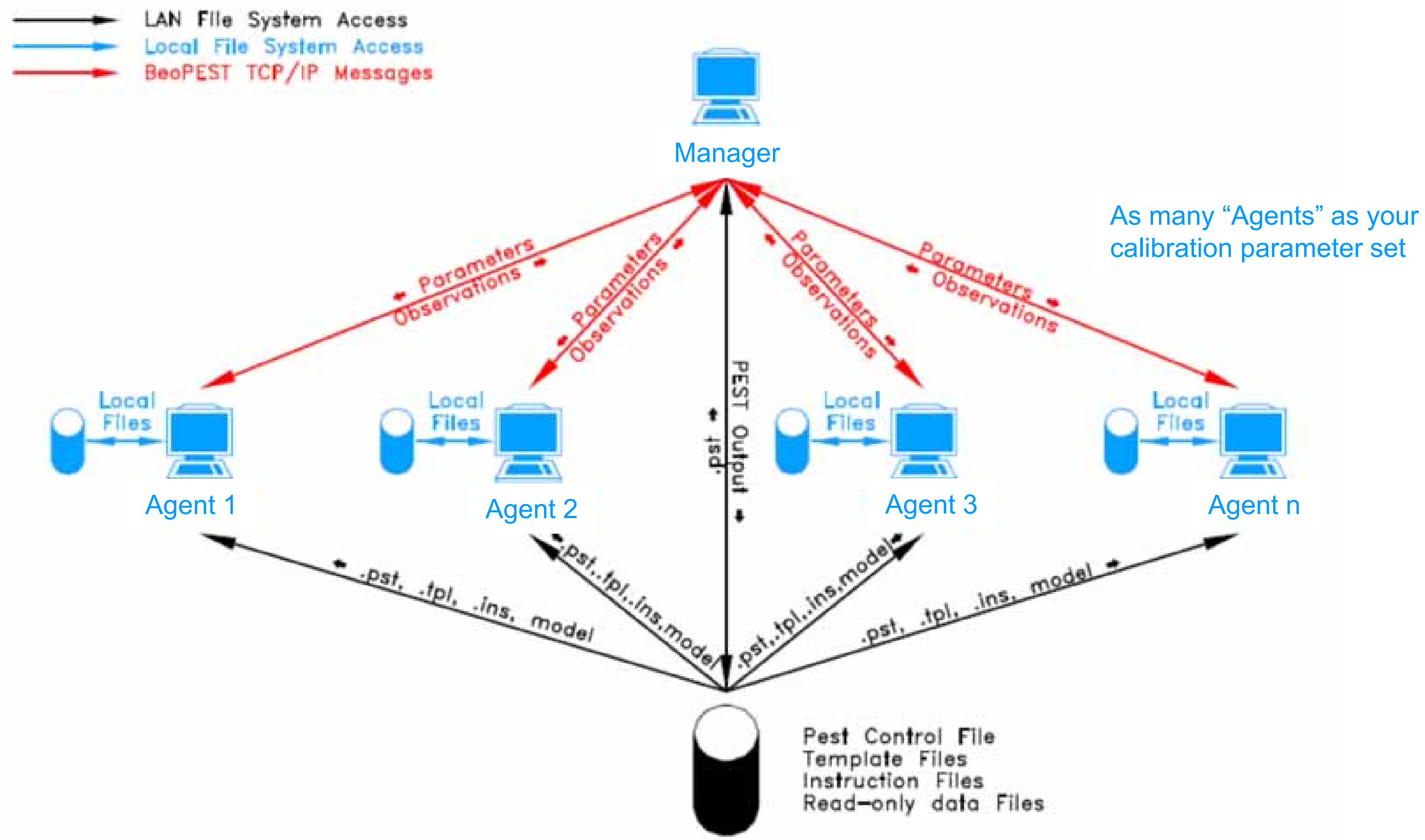
Improved Inversion algorithm for long model run times

Cannot run in "predictive analysis" mode

Other relevant alterations

Nomenclature change

PEST-HP



As many "Agents" as your calibration parameter set

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

- 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%
l2 !dum! !head2!
l3 !dum! !head3!
l6 !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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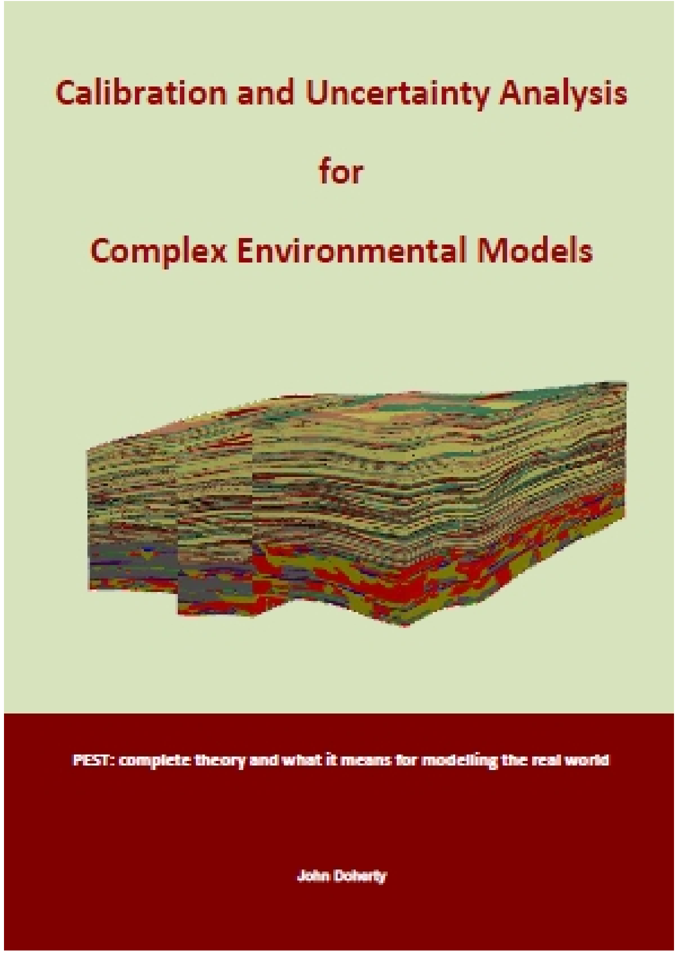

http://www.pesthomepage.org/PEST-The_Book.php

PEST Case

The Mendocino Example

Mendocino GSSHA Example

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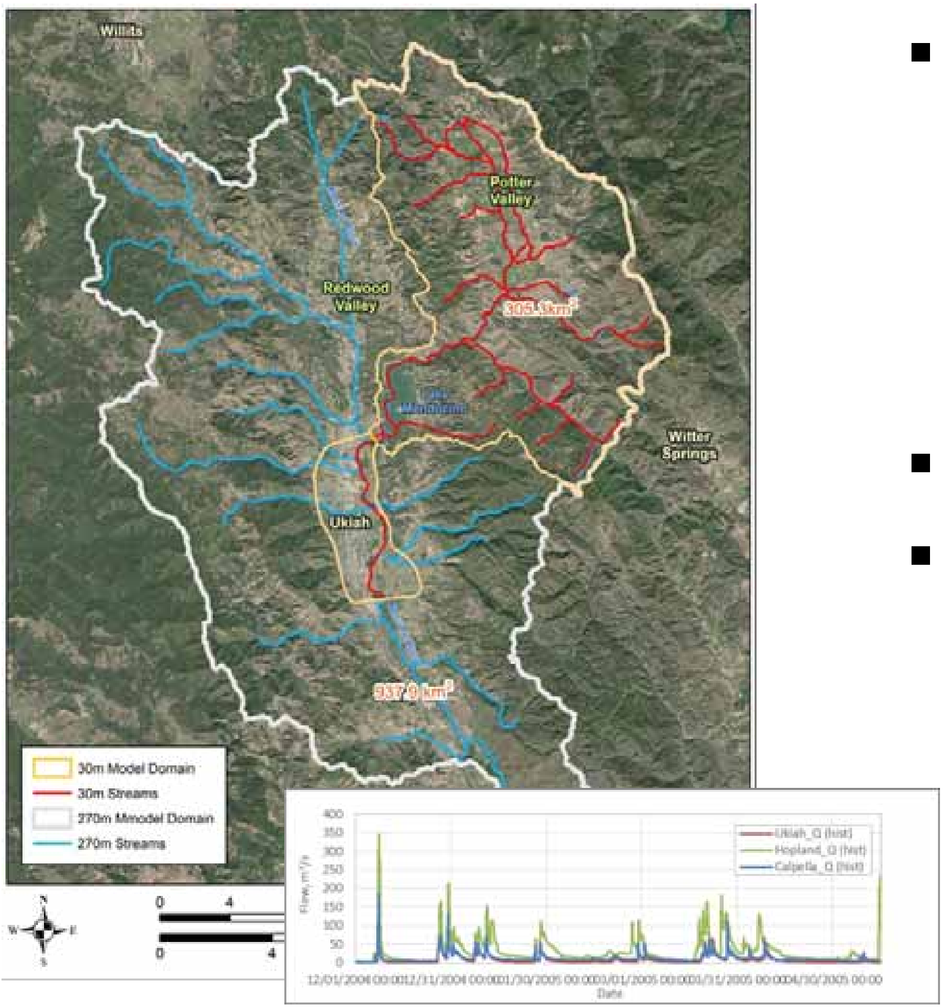

- Integrated GSSHA watershed model
  - ► Surface Water
  - ► Unsaturated Zone
  - ► Saturated Zone
- 39 Model parameters
- 560 observations of
  - ► daily flows at USGS gauging stations
  - ► event based flows and peak discharges

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Mendocino Inverse Problem

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

$$\left. + W_p^K \overbrace{\sum_{m=1}^{m=M} (EP_m^o - EP_m^s)_p^2}^{Event\ \ peaks\ \ at\ \ p} \right\}_p$$

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

PEST HP on ERDC's HPC

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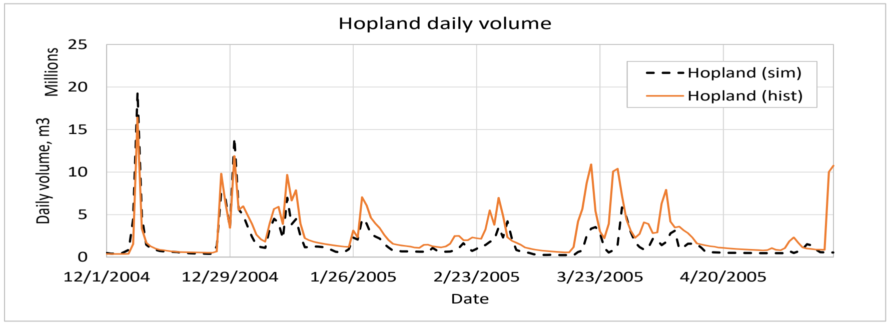
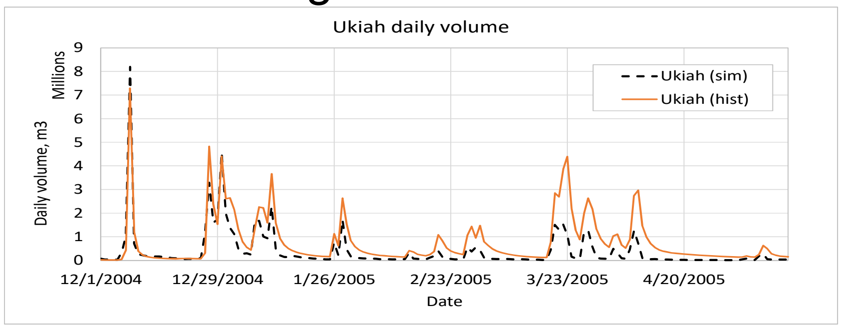
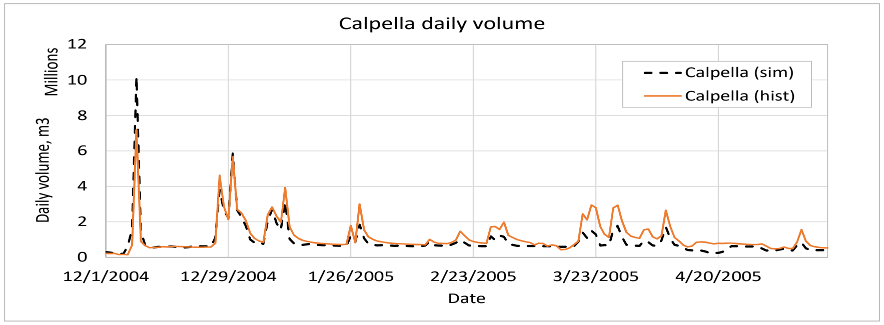
- Developed GSSHA models (ERDC's Team)
  - ► 3 grid resolutions
  - ► 2 temporal snapshots
- Develop PEST files (SAJ's team)
  - ► 40 nodes in Onyx
    - 1 "manager" node
    - 39 "agent" nodes
- PEST Outcome
  - ► ~ 2500 total model runs per scenario
- Calibration:







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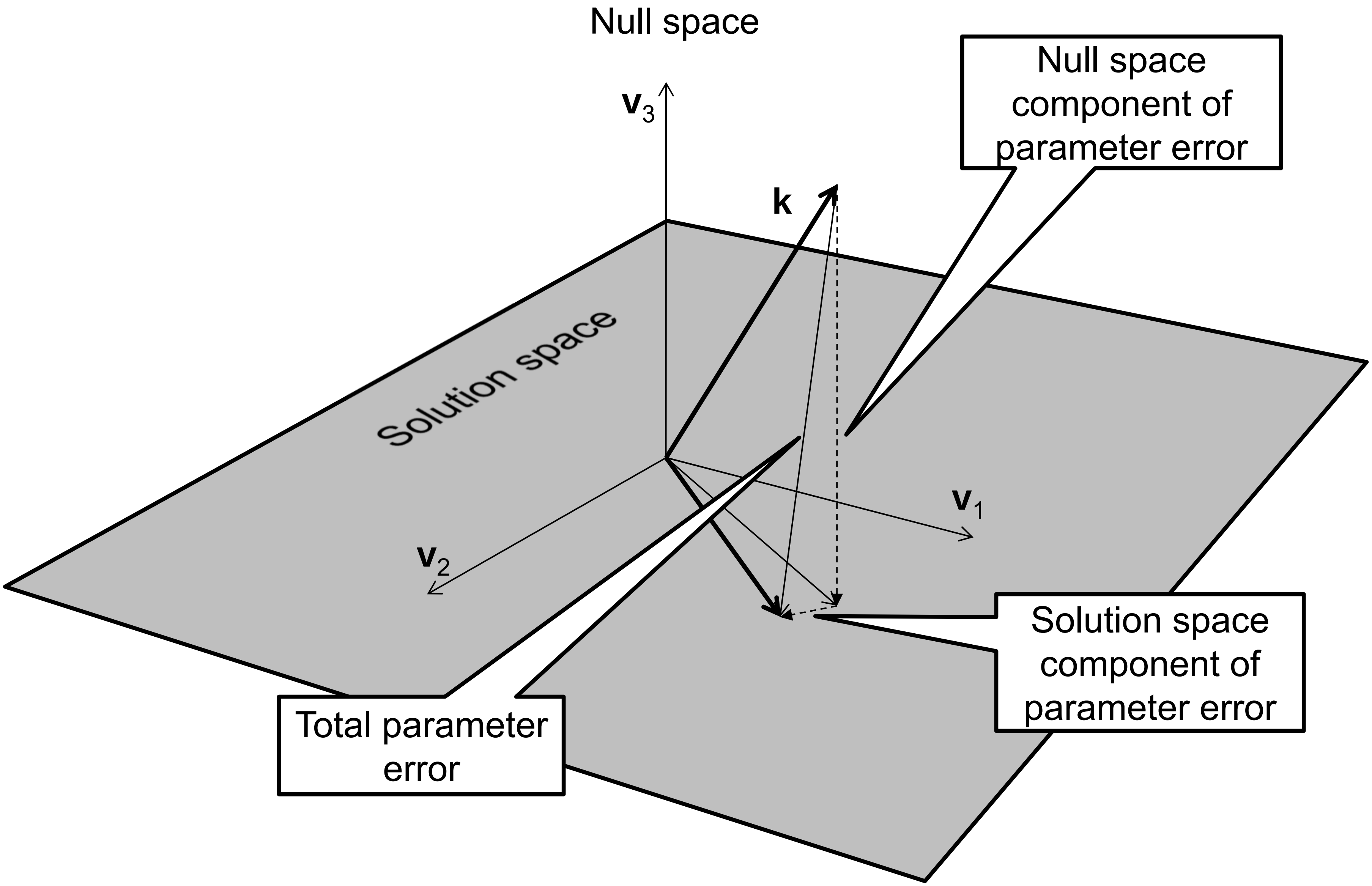
Null space
Null space component of parameter error
v3
k
Solution space
v1
v2
Solution space component of parameter error
Total parameter error

Null Space Monte Carlo

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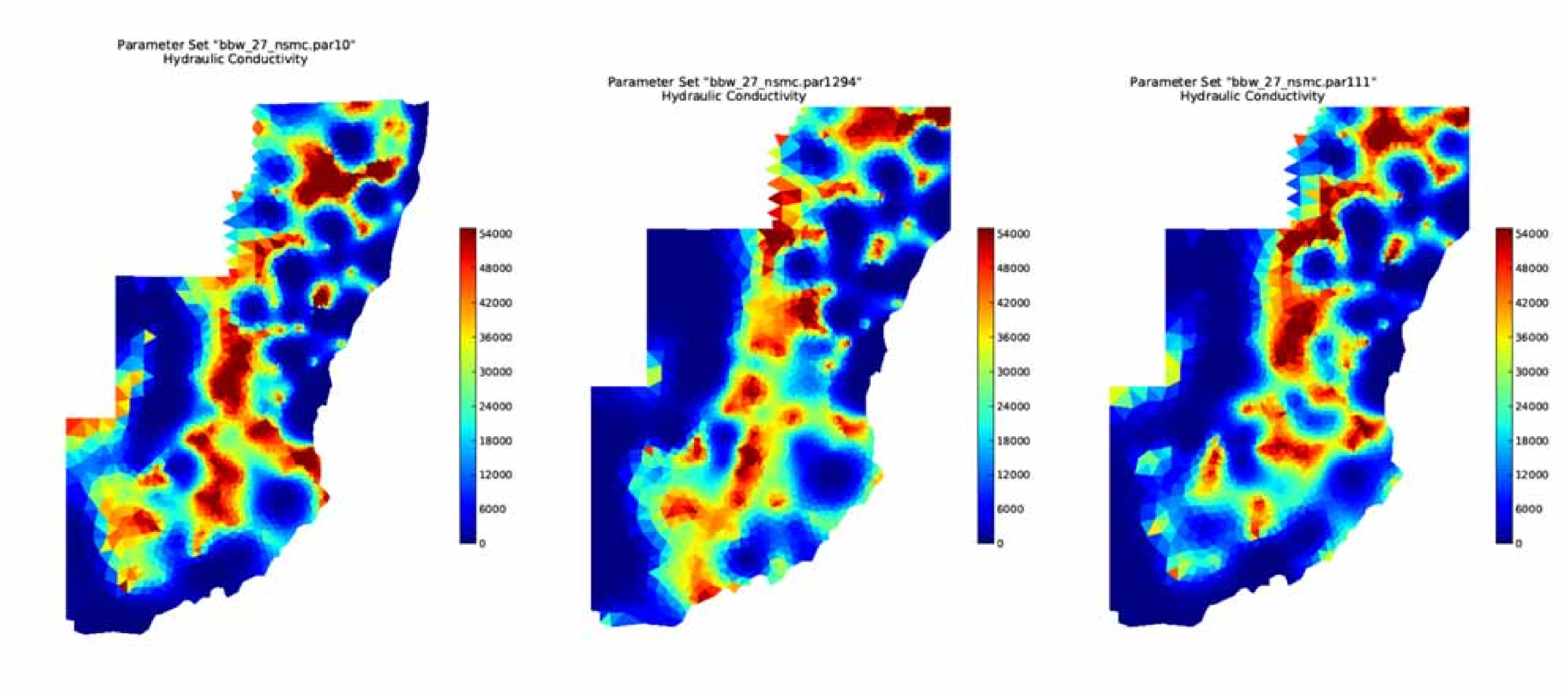
2700 Datasets that Calibrate the Model
and Respect the Parameter Bounds



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Don’t Get Lost in the Weeds

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