Simplified Access to the Power of PEST through PEST++ and keyPEST

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Friday Cleanup - AWRA

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http://pubs.usgs.gov/tm/tm7c5/

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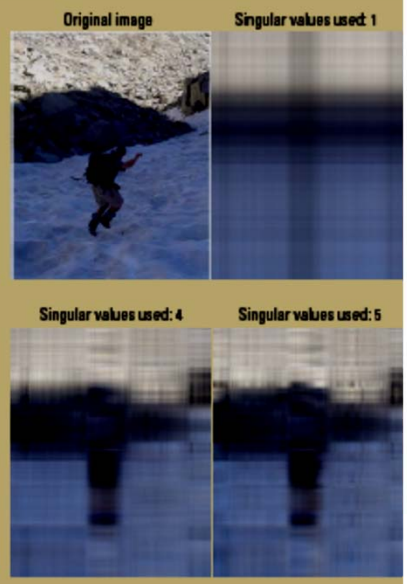
Approaches to Highly Param
A Guide to Using PEST for Gr



Scientific Investigations Report 201

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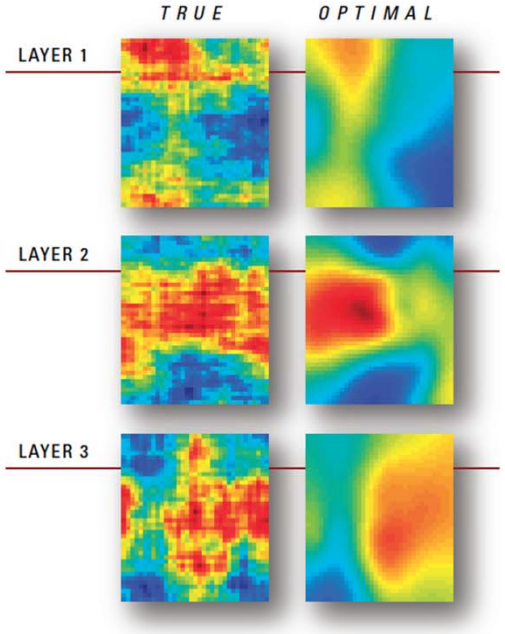
Approaches in Highly Parameterized Inversion: bgaPEST, a Bayesian Geostatistical Approach Implementation with PEST—Documentation and Instructions



Techniques and Methods, Book 7, Section C9

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es in Highly Parameterized Inversion:
General Time-Series Processor
n Model Calibration and
nmarization

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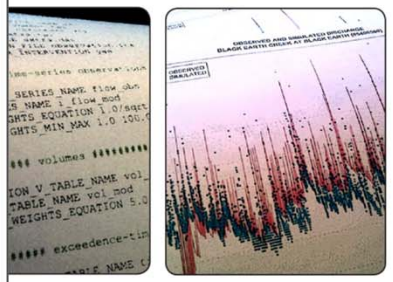

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Approaches in Highly Parameterized Inversion:
PESTCommander, a Graphical User Interface
or File and Run Management Across Networks

echniques and Methods Book 7, Chap. C8

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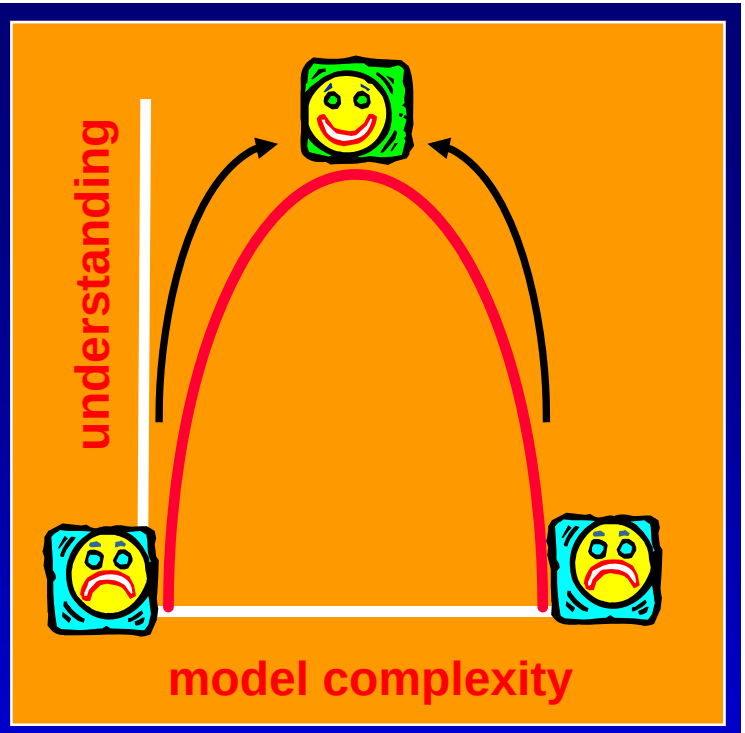
Goal of all models = "Parsimony"

"Simple as possible…

…but not simpler."



Thus oversimplified models *are not* parsimonious!

Need to identify "sweet spot" on simplification

ground water

PE-methods

Pointy-headed?

Are ~~Models~~ Too ~~Simple?~~ Arguments for Increased ~~Parameterization~~

User-friendly Software

by Randall J. Hunt[1], John Doherty[2], and Matthew J. Tonkin[3,4]

Abstract

The idea that models should be as simple as possible is often accepted without question. However, too much simplification and parsimony may degrade a model's utility. Models are often constructed to make predictions; yet, they are commonly parameterized with a focus on calibration, regardless of whether (1) the calibration data can constrain simulated predictions or (2) the number and type of calibration parameters are commensurate with the hydraulic property details on which key predictions may depend. Parameterization estimated through the calibration process is commonly limited by the necessity that the number of calibration parameters be smaller than the number of observations. This limitation largely stems from historical restrictions in calibration and computing capability; we argue here that better methods and computing capabilities are now available and should become more widely used. To make this case, two approaches to model calibration are contrasted: (1) a trad-

2007 Ground Water 43(3): 254-262.

No free lunch, all models of the nat'l world:

-are non-unique (ill-posed/underdetermined)

-are unstable

-take longer to calibrate/run uncertainty

What approaches are robust (=90% of problems)?

- *Don't* artificially limit numbers of parameters (=reduce model structural error)
- *Add soft-knowledge* as fallback-position to constrain inestimable parameters (= Tikhonov Regularization)
- *Reduce* model *dimensionality* (= Singular Value Decomposition)
- Run the model on *lots of machines* (= Parallel Processing)

[edit]

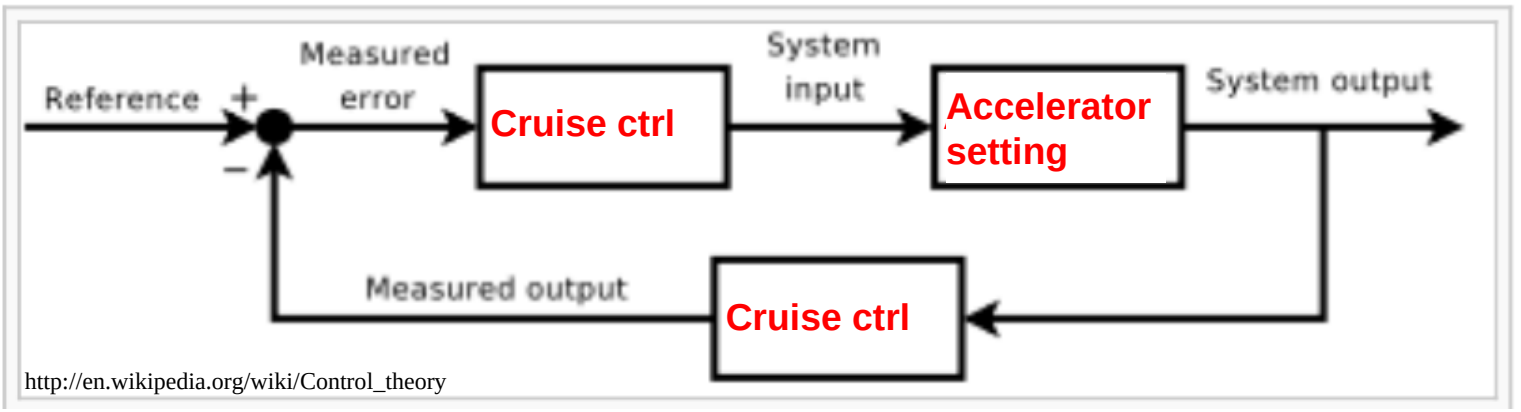
nce value *r(t)*. The controller *C*
puts *u* to the system under
r feedback controller.

-Multi-Output) systems, with more
ctors instead of simple scalar
l (typically functions).

t (i.e., elements of their transfer
d using the Laplace transform on

Solving for *Y*(*s*) in terms of *R*(*s*) gives:

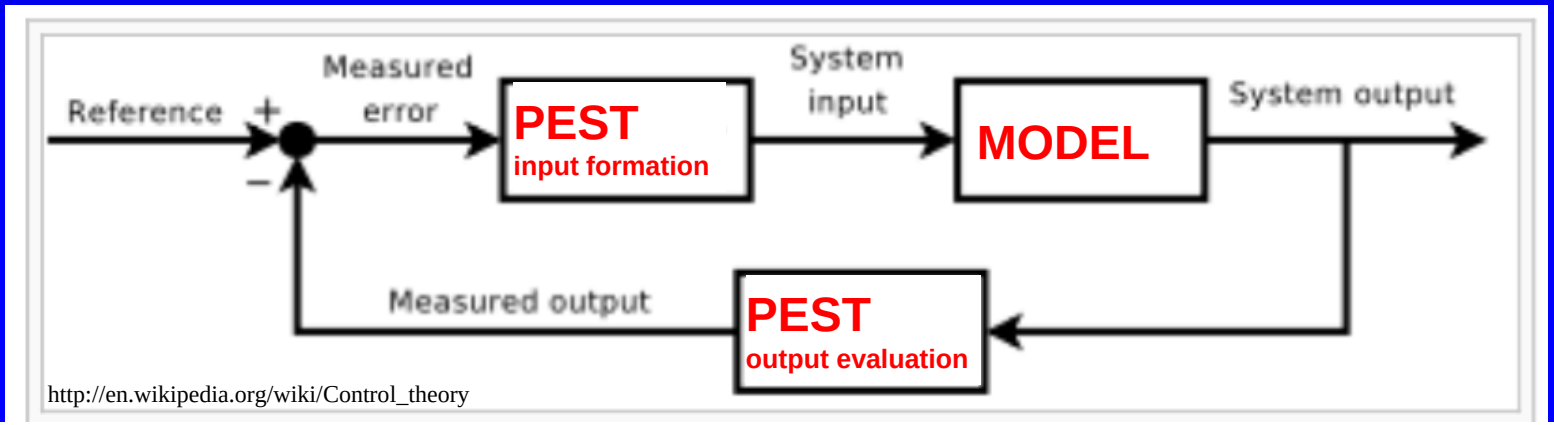
$$\left(\qquad P(s)C(s) \qquad \right)$$



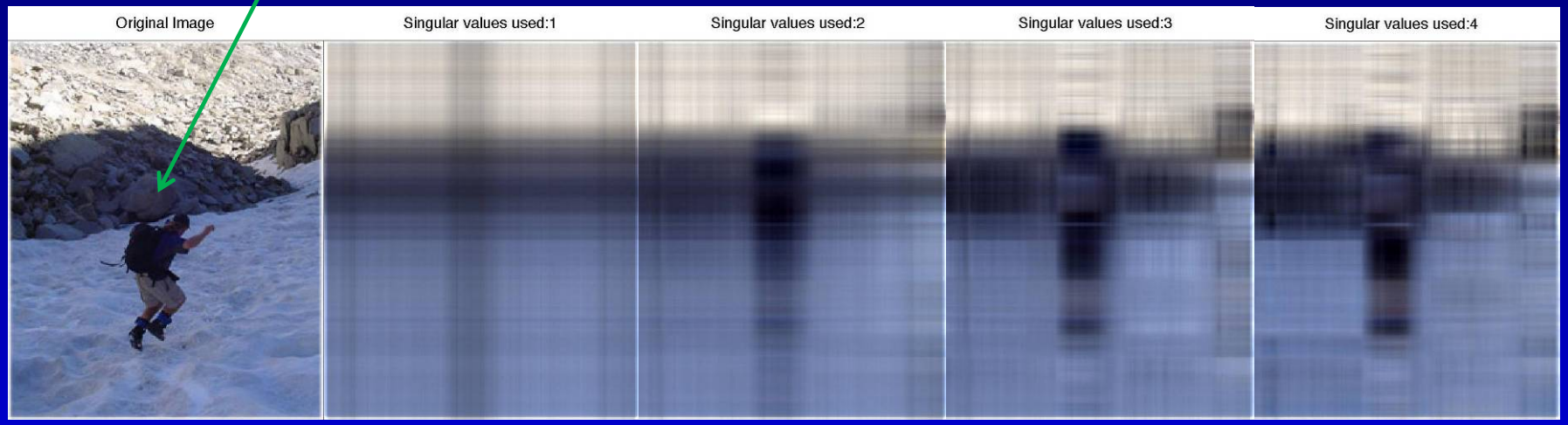
http://en.wikipedia.org/wiki/Control_theory

Bad Analogy?
"Cruising" to calibration?

At this speed?

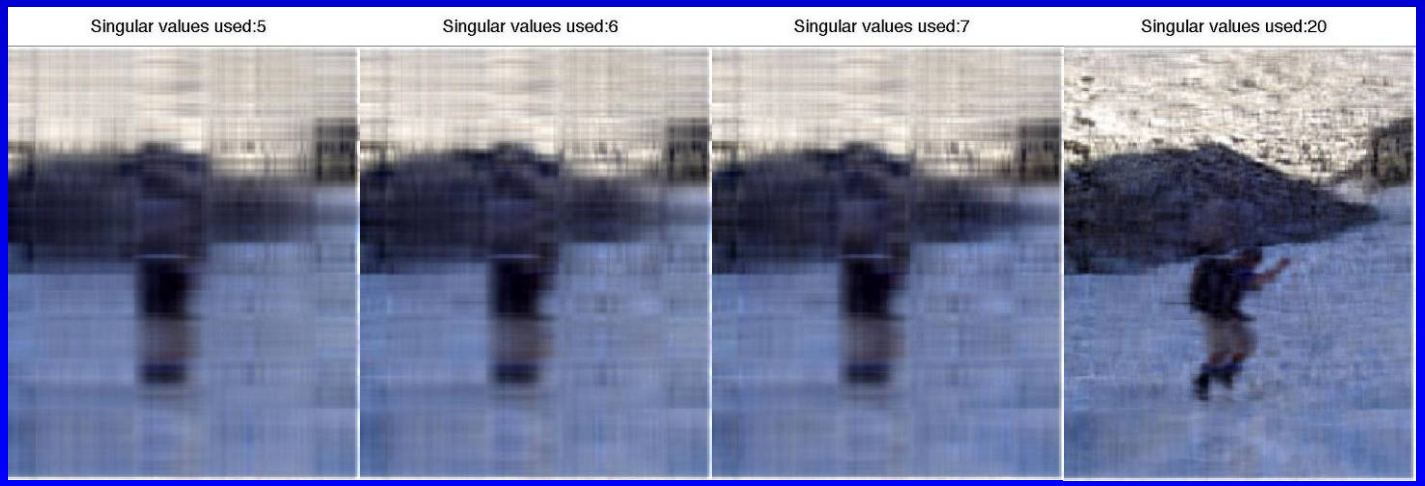


If Mike Fienen was displayed in Google Earth…



Modeling Analogy:

If you use too few = degrade fit and increase structural error



What to remember

- SVD allows you to “move directly to calibration and collect $200”.
- But, recognize what the SVD cruise control is doing:
  - For Insensitive Parameters: outputs optimal parameters = initial value (same as you would)
  - For Correlated Parameters: outputs optimal parameters with the same ratio as the initial values (same as you would)

Therefore - highly parameterized problems are not as robust to bad guesses of initial values

Why PEST++? (POINTY HEAD ALERT)

PEST++ extends SVD and replaces GML (see Appendix 3)

PEST++ speeds up SVD via PROPACK

PEST++ automatically switches between SVD-Assist and SVD

Perturbation of singular values adjusted by highest base parameter (helps avoid bounds, normalize perturbation across singular values)

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Approaches in Highly Parameterized Inversion: PEST++, a Parameter ESTimation Code Optimized for Large Environmental Models

Techniques and Methods, Book 7, Section C5

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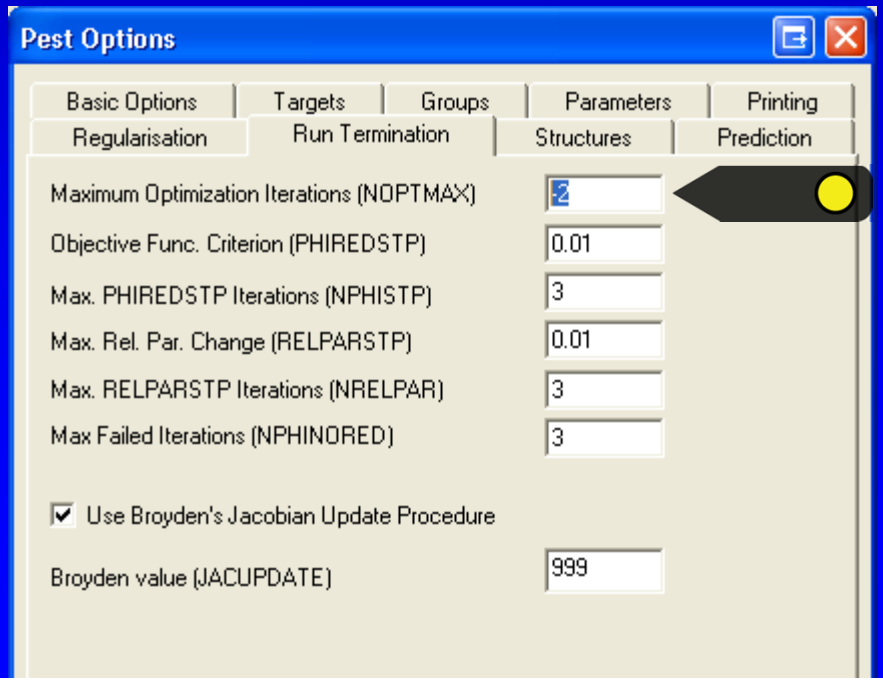
What the user needs to know to invoke these enhancements:

Why keyPEST? Typical PEST Control File:

```
pcf
* control data
restart estimation
1  283  1  0  1
1  1  single  point  1  0  0
1.000000e+001  2.000000e+000  3.000000e-001  1.000000e-002  7 999
1.000000e+001  1.000000e+001  1.000000e-003
1.000000e-001 noaui
-2  1.000000e-002  3  3  1.000000e-002  3
0  0  0
```

Set NOPTMAX to -2:
(all we need is the Jacobian Matrix **.jco* file to do SVD)



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PEST++ Control File: CONTROL DATA SECTION

```
pcf
* control data
restart estimation
1  283  1  0  1
1  1  single  point  1  0  0
1.000000e+001  2.000000e+000  3.000000e-001  1.000000e-002  7 999
1.000000e+001  1.000000e+001  1.000000e-003
1.000000e-001 noaui
-2  1.000000e-002  3  3  1.000000e-002  3
0  0  0
```

Set NOPTMAX to -2:

(all we need is the Jacobian Matrix **.jco* file to do SVD)

NECESSARY FOR SEAMLESS HANDOFF TO PEST for the problems that are not the 90%

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keyPEST input:

```
begin control_data KEYWORDS
        noptmax = -2
KEYWORDS
```

Magic!

All other values are either:

1. calculated by keyPEST (all the NPAR, NOBS, etc.)
2. have been assigned default values by keyPEST or
3. are optional

Fienen, M.N., Hunt, R.J., and White., J.T., in prep, Approaches in Highly Parameterized Inversion: keyPEST, A Keyword Input Reader for PEST++ and PEST, USGS Techniques and Methods Report

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Your mission, if you choose to accept it….

Help us beta test these new tools! Drop us a line at:

rjhunt@usgs.gov

mnfienen@usgs.gov