From Buckets to Clouds: Building Better Environmental Models for Today's Decision-Making

Randy Hunt – Wisconsin Water Science Center
2010 Water Resources Discipline Lecture Series

John Doherty
Watermark Numerical Computing &
National Centre for Groundwater Research and Training

John Walker
Wisconsin WSC

Mike Fienen
Wisconsin WSC

My motivation for doing this tour:

Societal need is greater, stakes are higher – we can help

The basic premise:

- We are much more likely to find our work in a controversial setting (e.g., legal system) in the future
- We've learned a lot in the last 10 years, time to put this knowledge into practice
- The premier science agency for the US Gov't uses state-of-the-art tools
- We have a history, and we can't rest on our laurels…

John Wesley Powell

The Lecture Motivation: The question now is not whether to use these more sophisticated tools, but how to do it well

Path we’ll in today’s talk…

1) Understanding fundamental issues:
   - The cost of too complex
   - The cost of too simple

2) Constraining complexity

3) The last piece: How to finish solving a problem in something less than geologic time

Path we'll take for environmental models…

1) Understanding fundamental issues:
   - The cost of too complex
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Model Complexity

- "The Emperor" by Mary Anderson (1983)
- Freyberg (1988)
- Hunt and Zheng (1999) AGU Special Session report

guest editorial

GROUND-WATER MODELING – THE EMPEROR HAS NO CLOTHES[a]

by Mary P. Anderson[b]

The recent explosion of interest in ground-water modeling can be attributed largely to the urgent need for an objective, reliable way of predicting the movement of contaminants in ground water. Hence, those who follow the hydrogeologic literature will have noted a proliferation of both analytical and numerical solute transport models—all purporting to simulate contaminant movement in ground water under a variety of assumptions. In a few cases, contaminant transport models have been applied to field settings where there is information about an already existing contaminant plume. In this type of exercise the objective is to show that the model can reproduce the shape of the plume, so that the modeling attempt may be deemed a success. Unfortunately, success at this kind of modeling creates the notion that

GROUND WATER

FIELD REPORTS

AN EXERCISE IN GROUND-WATER MODEL CALIBRATION AND PREDICTION

by David L. Freyberg[a]

Abstract. For a classroom exercise, nine groups of graduate students calibrated a numerical ground-water flow model to a set of perfectly observed hydraulic head data for a hypothetical phreatic aquifer. All groups used exactly the same numerical model and identical sets of observed data. After calibration, the students predicted the hydraulic head distribution in the aquifer resulting from a modification in one boundary condition. A quantitative analysis of the results of this calibration-prediction exercise vividly demonstrates some of the difficulties in parameter identification for ground-water flow models. Group predictions differed significantly. Successful prediction was strongly correlated with successful estimation of conductivity values, and was essentially unrelated to successful estimation of aquifer bottom elevations or with the number of trial-and-error simulations required for calibration. Most importantly, success in prediction was unrelated to success in matching observed heads under premodification conditions. In this sense, good calibration did not lead to good prediction.

(often called calibration) to sophisticated, automated techniques that find parameter sets which optimize a multiobjective criterion characterizing the goodness of fit between simulated and observed head fields.

The nature of the inverse problem for ground-water flow has been studied extensively over the last twenty years. Yeh (1986) provides a useful review of this literature and the state of the art. Several well-known characteristics of the general parameter identification problem have dominated attempts to develop effective solution techniques. Neuman (1973) and Neuman and Yakowitz (1979) give clear descriptions of these characteristics. First, parameter estimates, particularly for hydraulic conductivity (or transmissivity), are highly sensitive to noise or errors in observed head data. Small observation errors can lead to large errors in estimated conductivity. Second, the solution to the inverse problem often, indeed typically, is nonunique. More than one parameter field may yield indistinguishably good fits to observed head

Eos, Transactions, American Geophysical Union, Vol. 80, No. 3, January 19, 1999, age 29

Debating Complexity in Modeling

Complexity in modeling would seem to be an issue of universal importance throughout the geosciences, perhaps throughout all science, if the debate last year among groundwater modelers is any indication. During the discussion the following questions and observations made up the heart of the debate.

As scientists trying to understand the natural world, how should our effort be apportioned? We know that the natural world is characterized by complex and interrelated processes. Yet do we need to explicitly incorporate these intricacies to perform the tasks we are charged with? In this era of expanding computer power and development of sophisticated preprocessors and postprocessors, are bigger machines making better models? Put another way, do we understand the natural world better now with all these advancements in our simulation ability? Today the public's patience for long-term projects producing indeterminate results is wearing thin. This increases pressure on the investigator to use the appropriate technology efficiently. On the other hand, bringing scientific

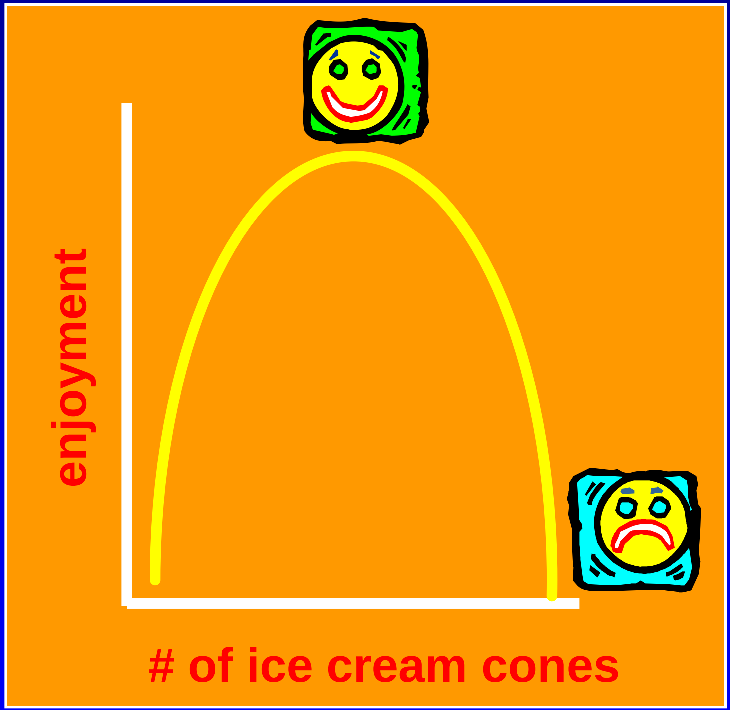
served that during the past 15 years problematic areas (for example, untrained modelers) have become less troublesome, but other conclusions from 1983 still hold. Field datasets commensurate to the model objective are still needed, and these data needs have become more demanding as models have become more complex. In that sense, it is not the amount but the quality of the clothes that is important. In addition, the amount of "clothes" (or complexity) the Emperor has is driven in many cases by the modeling objective.

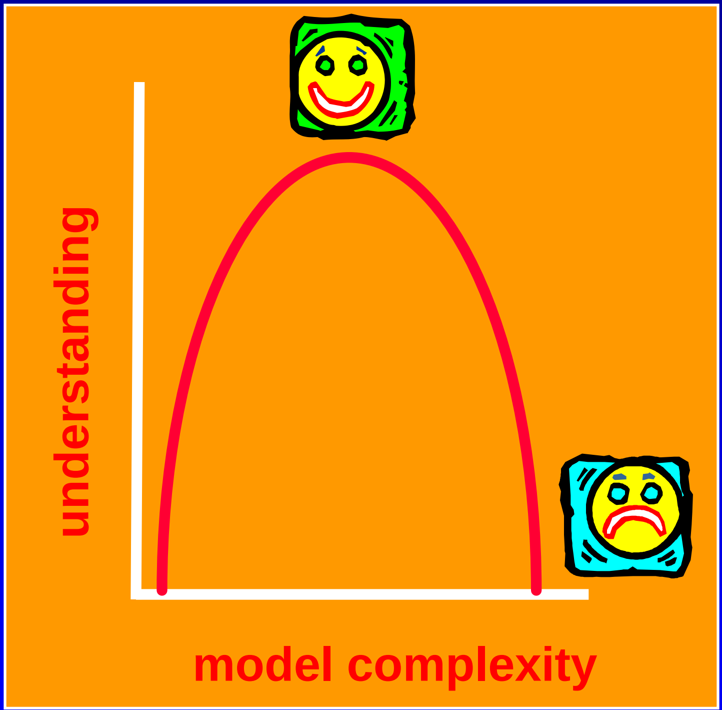
Three examples were provided in Anderson's talk: a parsimonious model constructed for water supply concerns, a research model developed to test a new lake package module for MODFLOW, and a model constructed by a company looking to obtain a permit to mine in an environmentally sensitive area. The mine model had the largest amount of regulatory and public involvement and also was the most complex. It was so complex, in fact, that the regulators relied on a simple two-dimensional model constructed after the complex model to

fractal scaling of hydraulic conductivity distributions by Fred Molz indicated an increasing degree of heterogeneity with decreasing measurement scale and a belief that fractal-type scaling may help determine appropriate measurement scale and level of complexity needed for transport modeling. An example provided by Ken Bradbury illustrated that a complex fractured rock setting could be simulated using the simple Wellhead Protection Area (WHPA) code if a well's zone of contribution was all that was desired. If the time of travel to the well was needed, however, only a much more complex, multilayer model would suffice. In addition, a case was presented by Glen Champion where a coupled lake-groundwater model was able to model drought and recovery of a lake district in northern Wisconsin, something not feasible using simpler techniques.

Others suggested ways to tame the complexity beast using approaches such as regression methods to determine supportable and desirable model complexity presented by Mary Hill; stochastic approaches to accommodate randomly occurring contaminant sources in deter-

Model Complexity: Law of Diminishing Returns? Hunt (1998)





The Upshot: Models too complex = non-unique (ill-posed / underdetermined), unstable, take longer to calibrate

1998 AGU Session Summary

"…we should feel comfortable resisting the *sirens of complexity* and construct simpler, less encompassing, models."

Hunt and Zheng (1999)

MODFLOW98 Keynote Address

Mary Anderson/Randy Hunt: "Complexity: Does the Emperor Have Too Many Clothes?"

John Doherty: "In Ground-water Modeling How Much Complexity is Too Much?"

ground water

Issue Paper/

Are Models Too Simple? Arguments for Increased Parameterization

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.

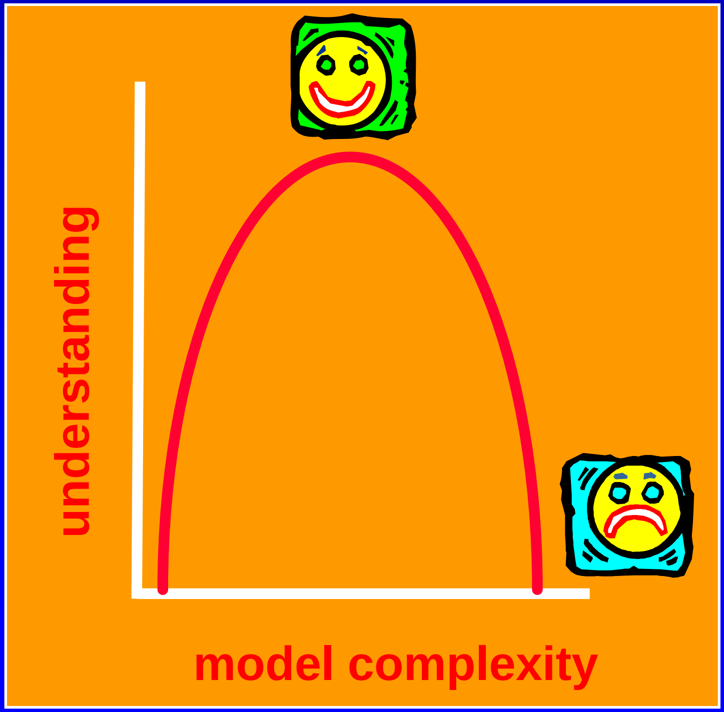
Path we'll take for environmental models…

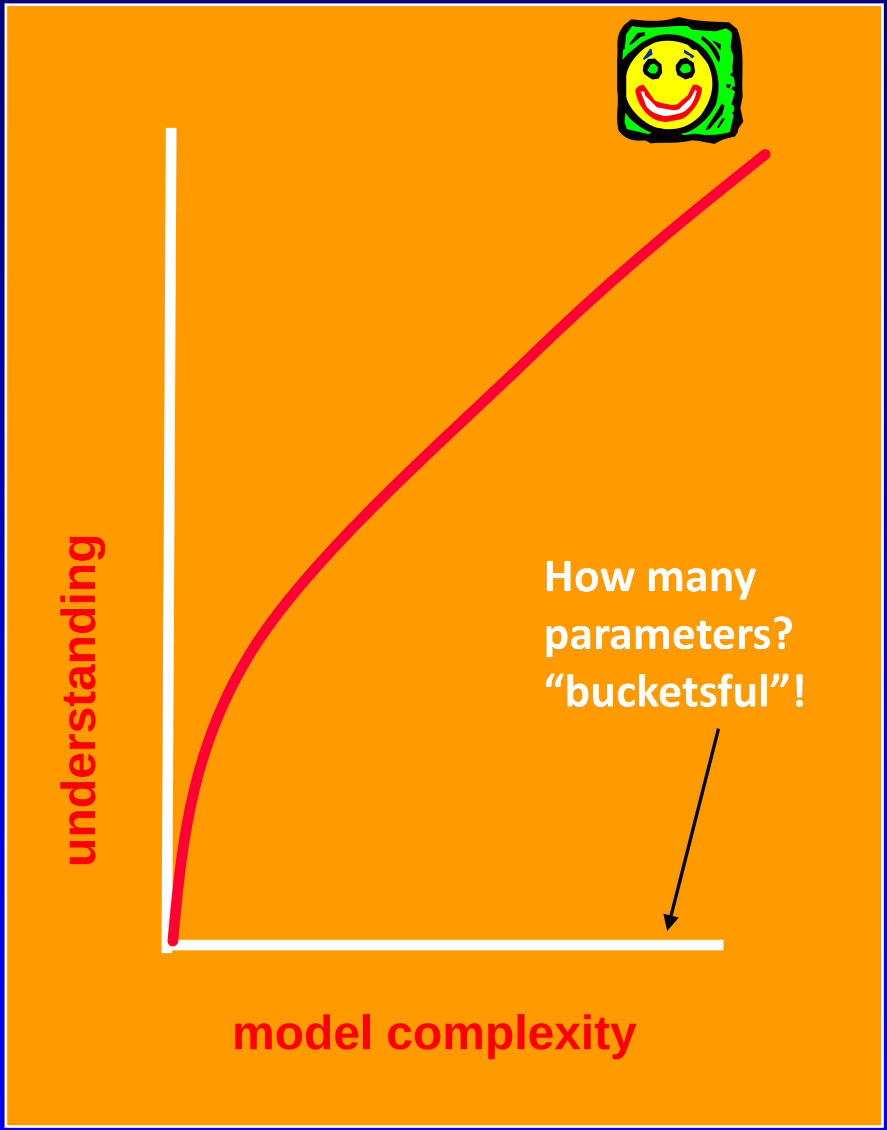
1) Understanding fundamental issues:
   - The cost of too complex
   - The cost of too simple

2) Constraining complexity

3) The last piece: How to finish solving a problem in something less than geologic time

John’s World


understanding
model complexity


understanding
How many
parameters?
“bucketsful”!
model complexity

Why should we add bucketsful?

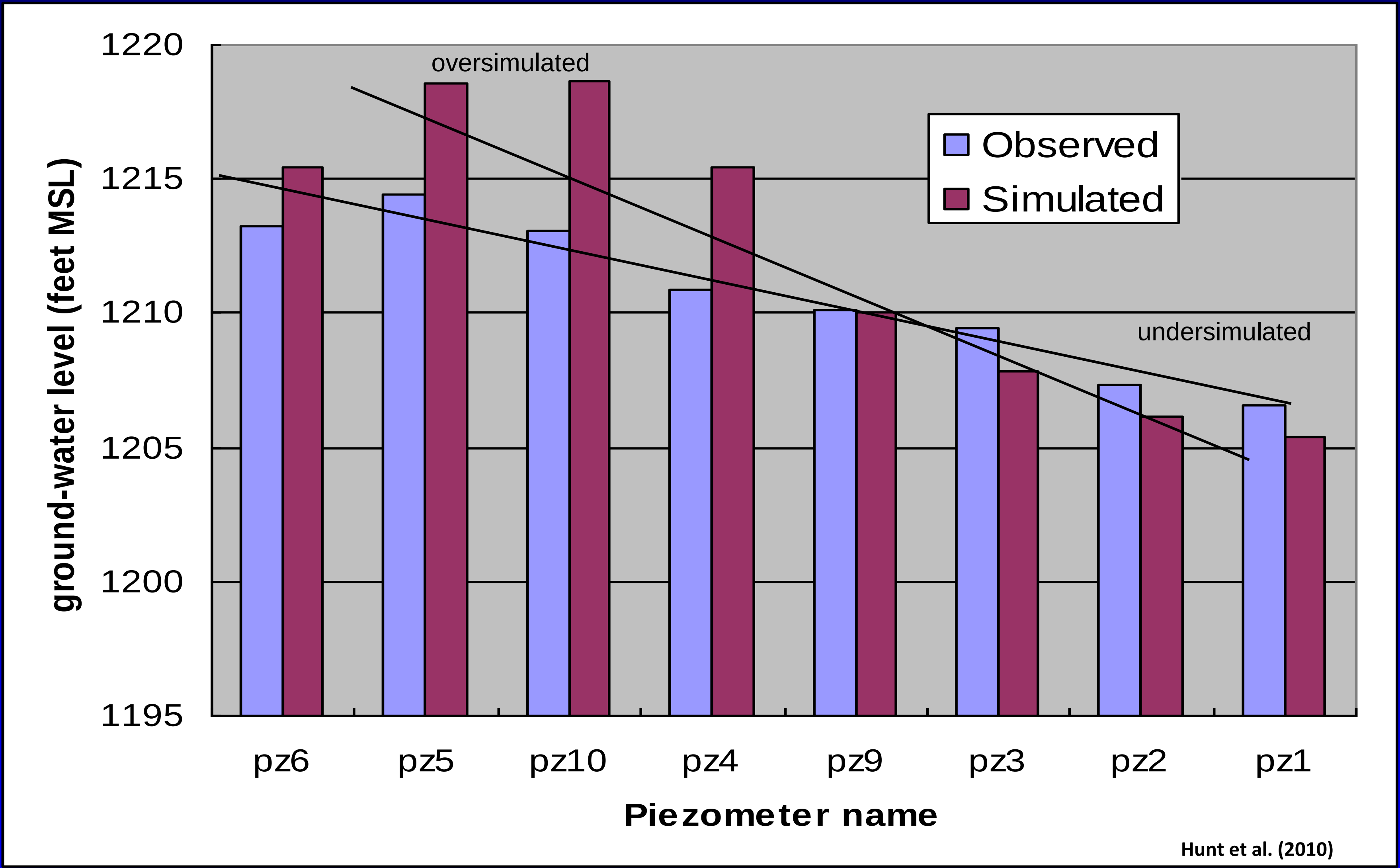
Reduce *structural error*

What is structural error?

The error introduced to a model by *oversimplification*

Oversimplification?

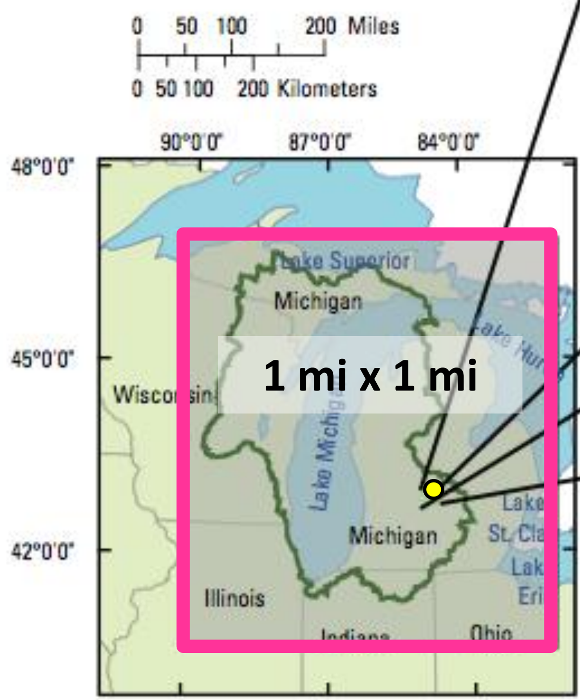
- It’s why today’s environmental models usually use numerical models instead of analytic solutions
- It’s why today’s environmental models usually use more than 1 zone for parameterization



A picture of structural error

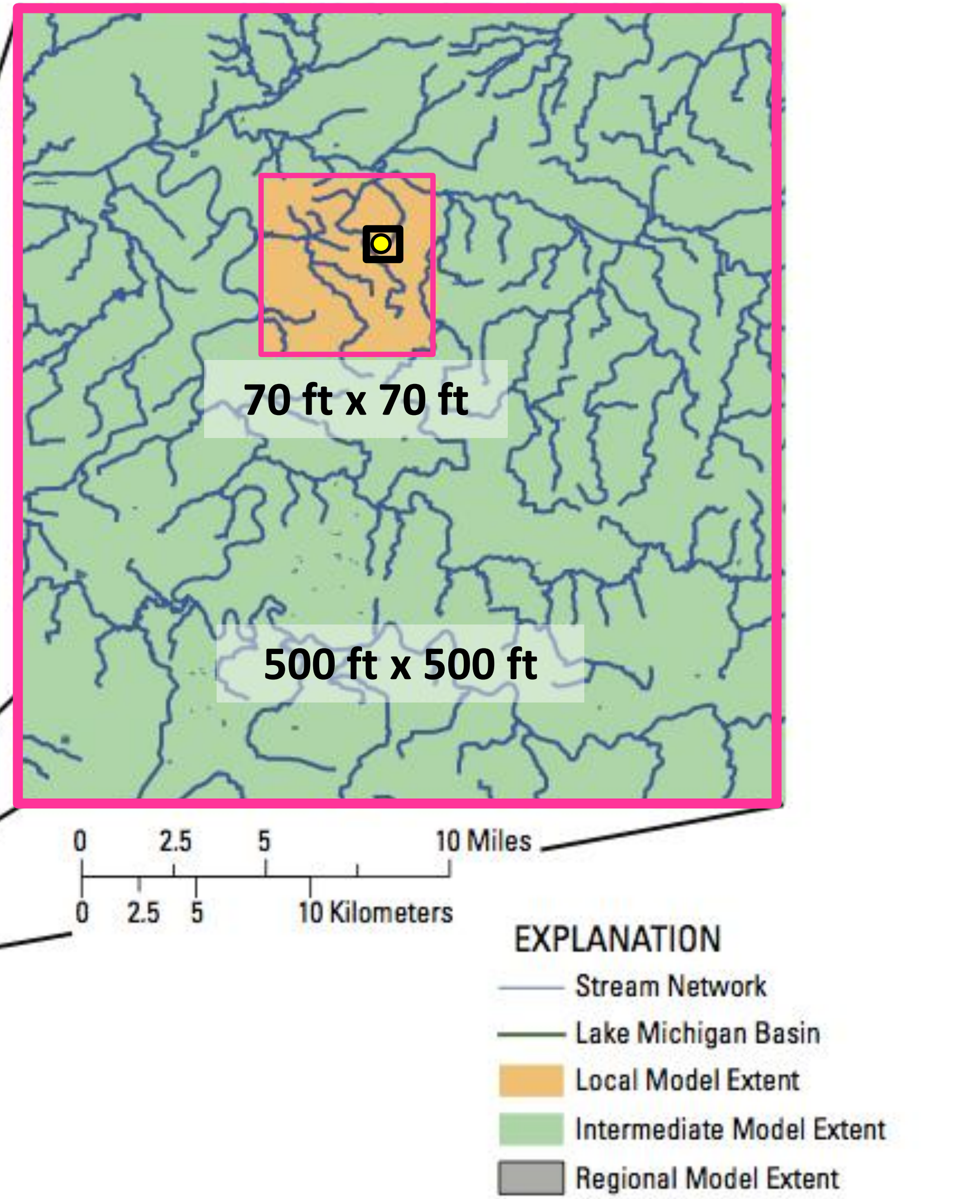
What was I thinking?!

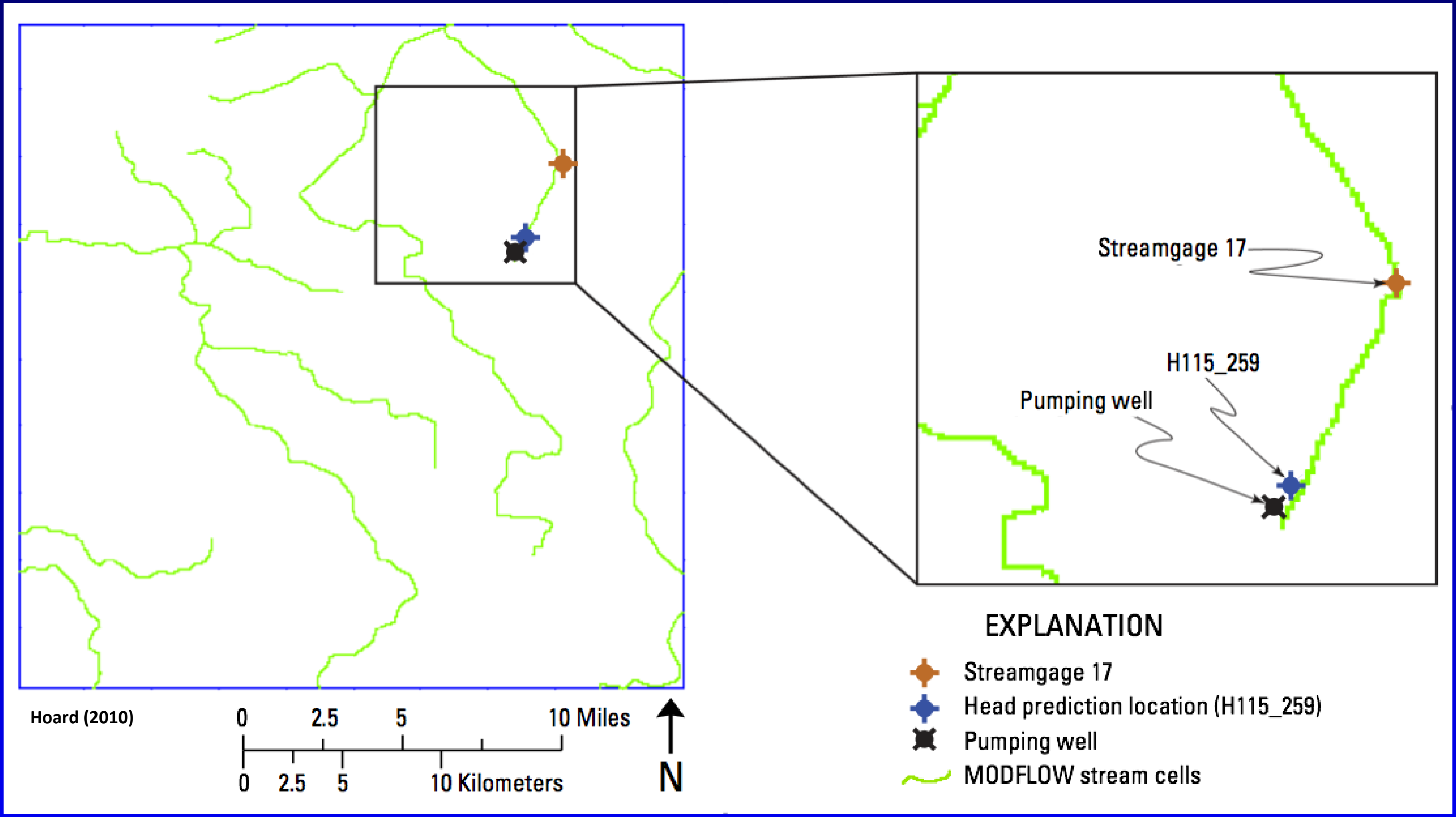
A well-understood example of the cost of too simple: The need to refine a grid (TMR)



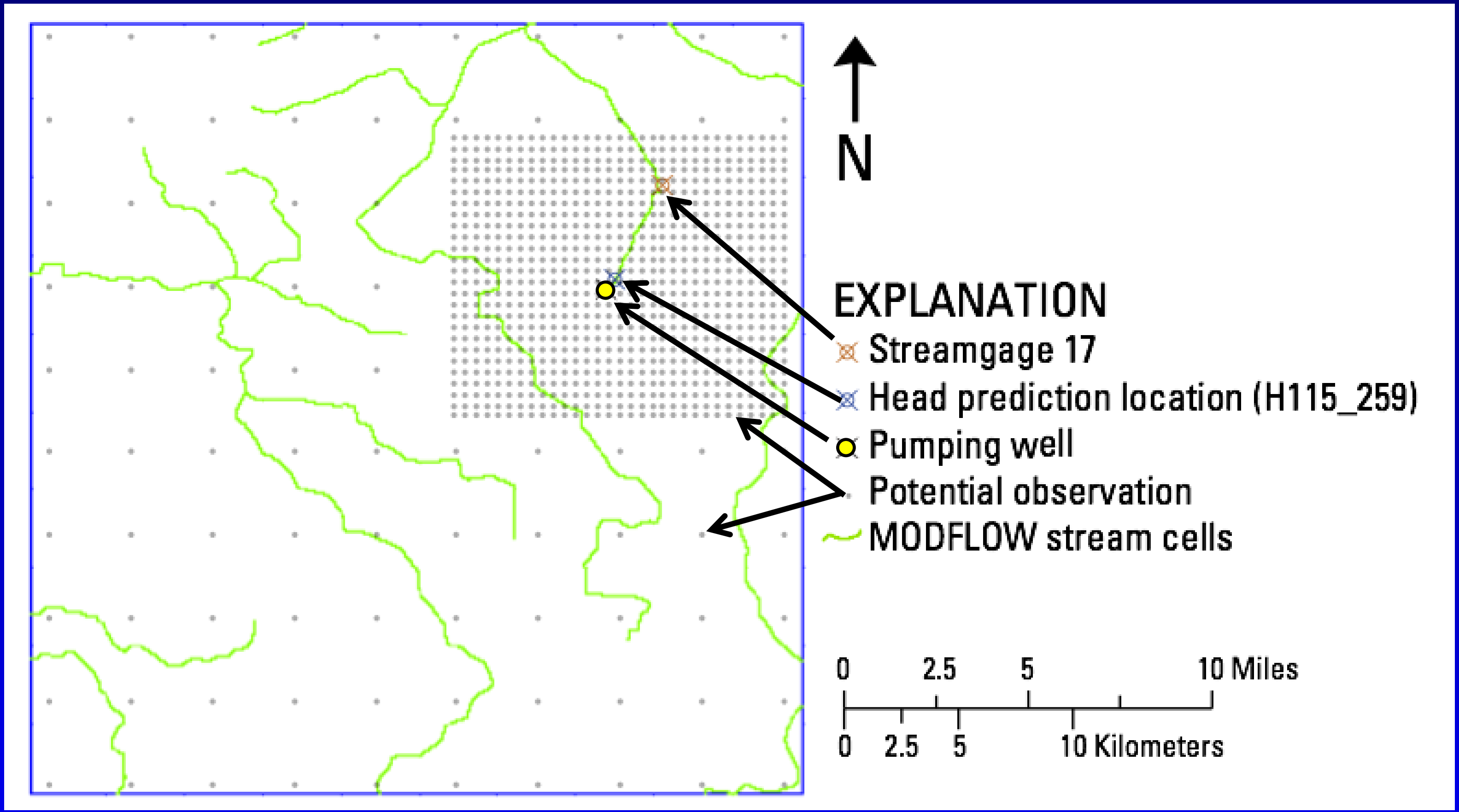
Feinstein and others (2010)

Hoard and others (2010)





Original objective: Using the TMR model for its more appropriate use – to assess effects of pumping on the stream headwaters

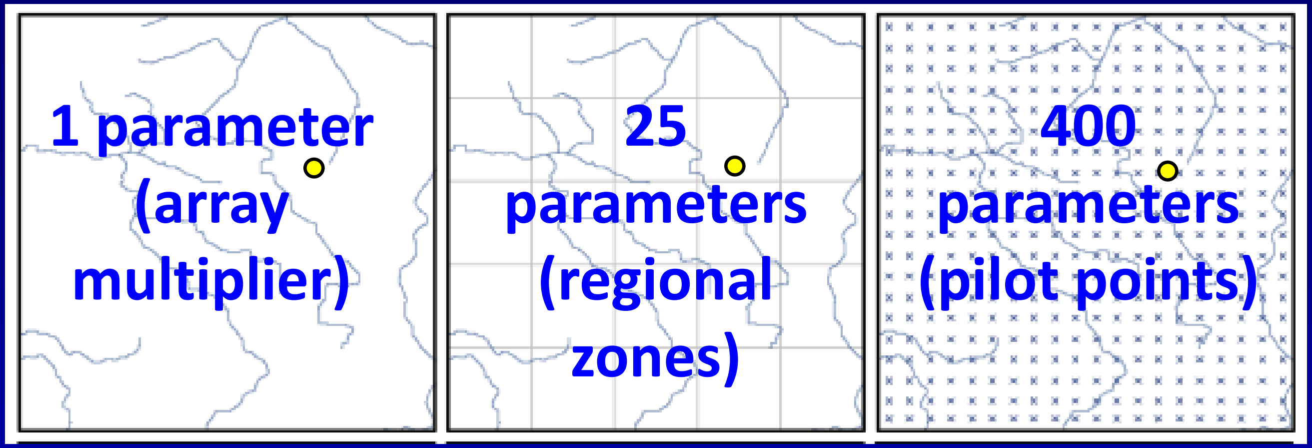


Fienen and others (2010)

New question: Where is the "bang for the buck" w.r.t. future data collection?

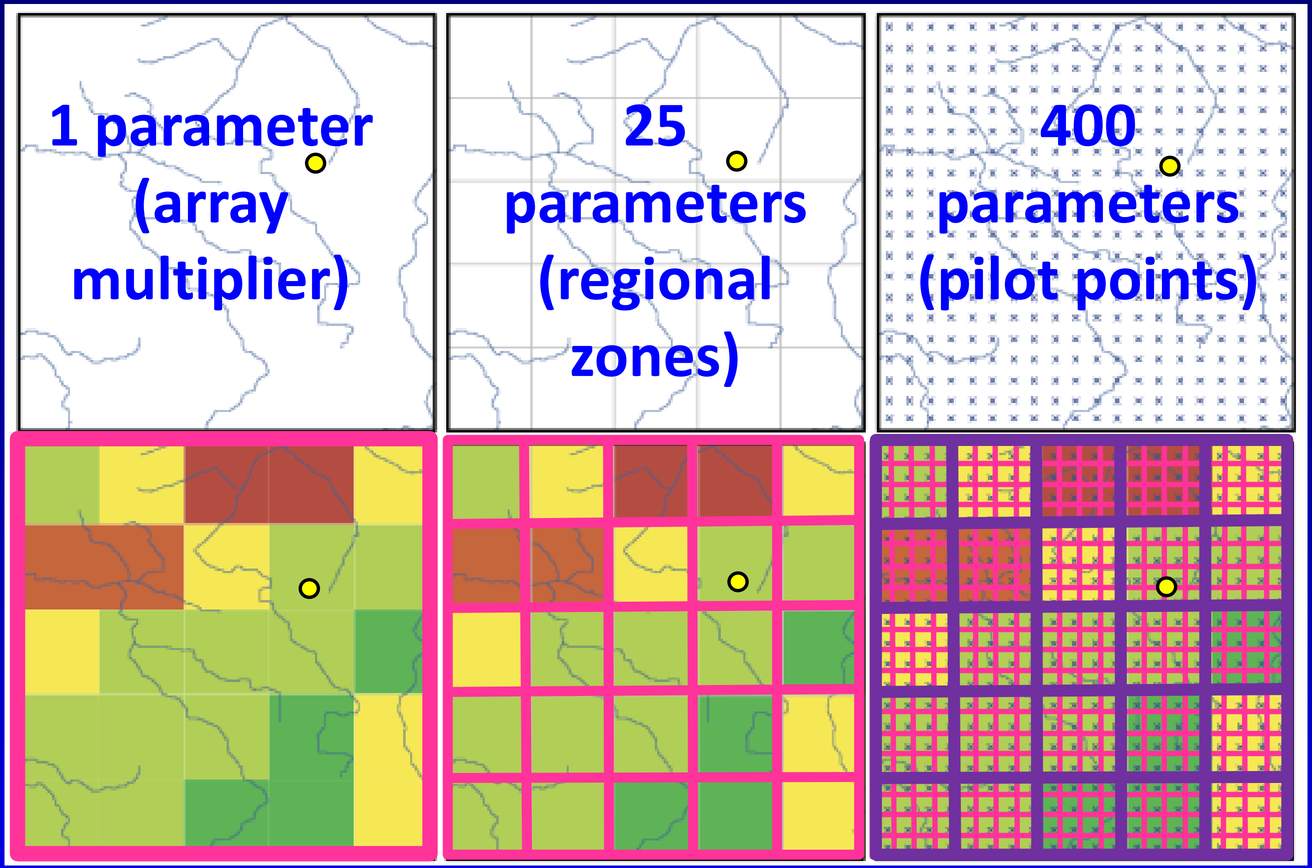
Is the old regional parameterization still appropriate?

TMR inset


1 parameter
(array
multiplier)
25
parameters
(regional
zones)
400
parameters
(pilot points)

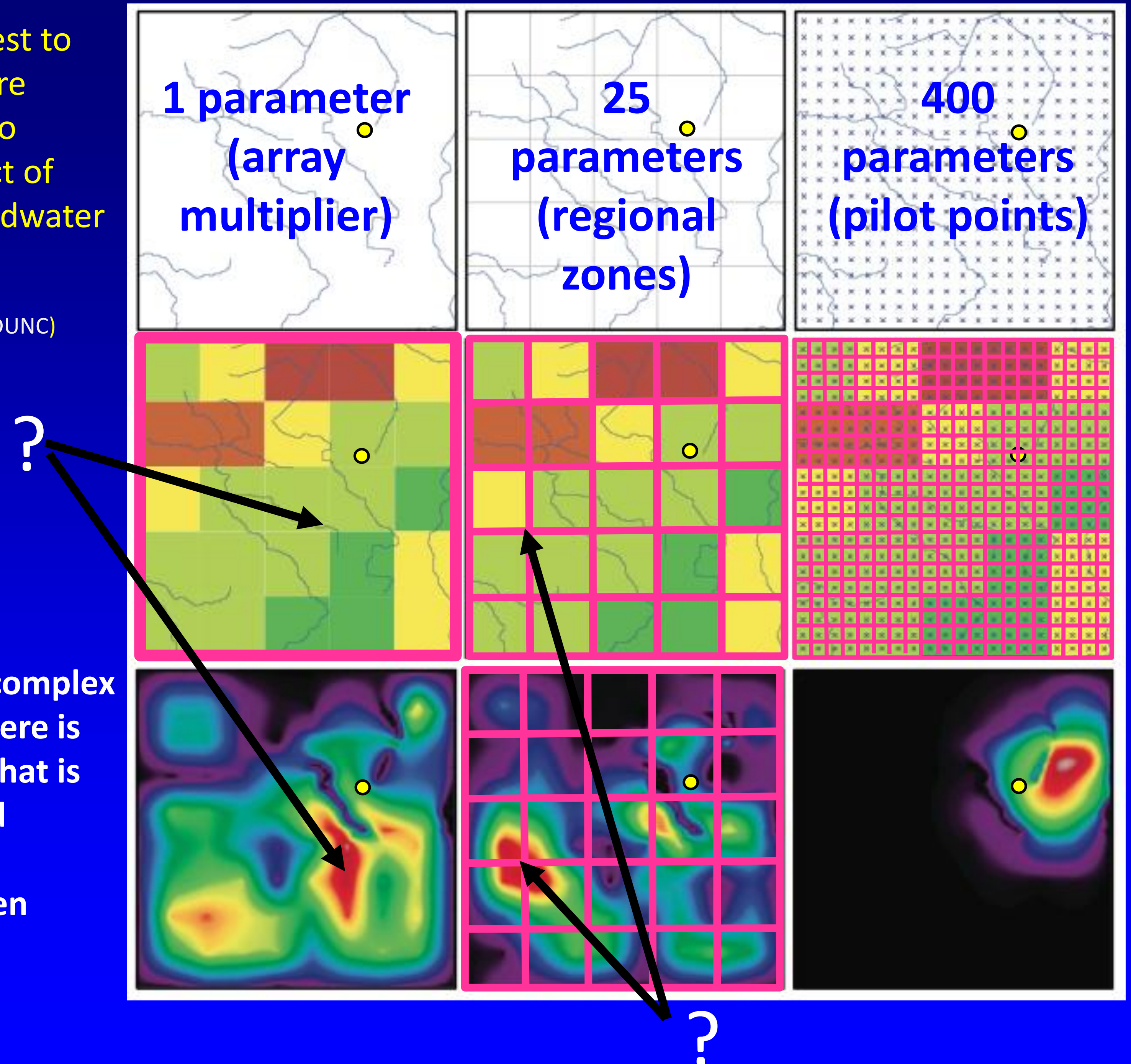
TMR inset

Picture of parameter *flexibility* in TMR (pink)



Where is best to collect future head data to assess effect of well on headwater stream?

(PEST utility PREDUNC)



"For every complex problem, there is an answer that is simple - and wrong."
H.L. Mencken

Why should would we add bucketsful?

Reduce Structural Error

What is structural error?

The error introduced to a model by oversimplification

Oversimplification?

- It's why today's environmental models usually use numerical models instead of analytic solutions
- It's why today's environmental models usually use more than 1 zone for parameterization

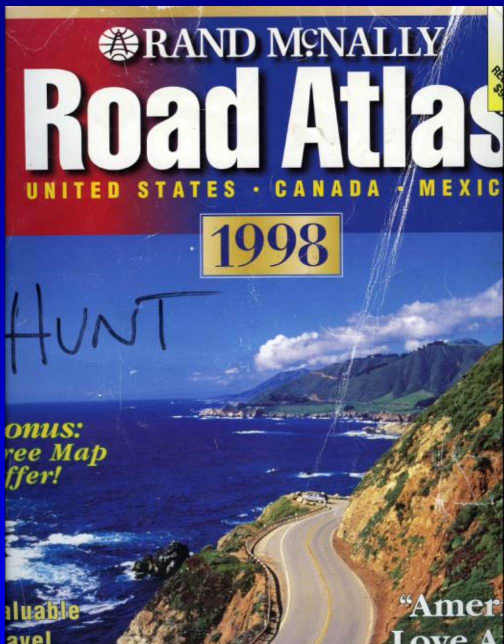
But how do we know when we've oversimplified *a priori*?

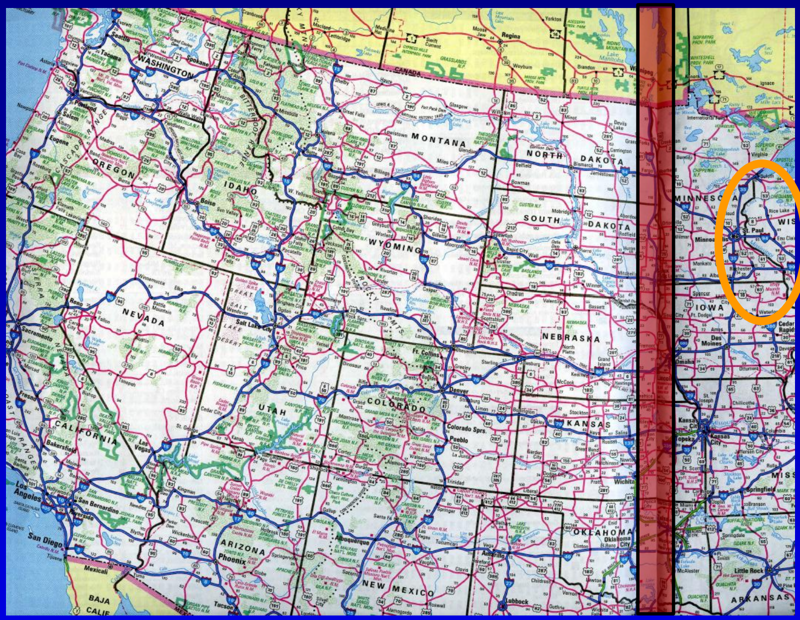
- **Aye, there's the rub….**

Thinking of the issue another way:

Model = Simplification of Reality

Model = Simplification of Reality = Try#1

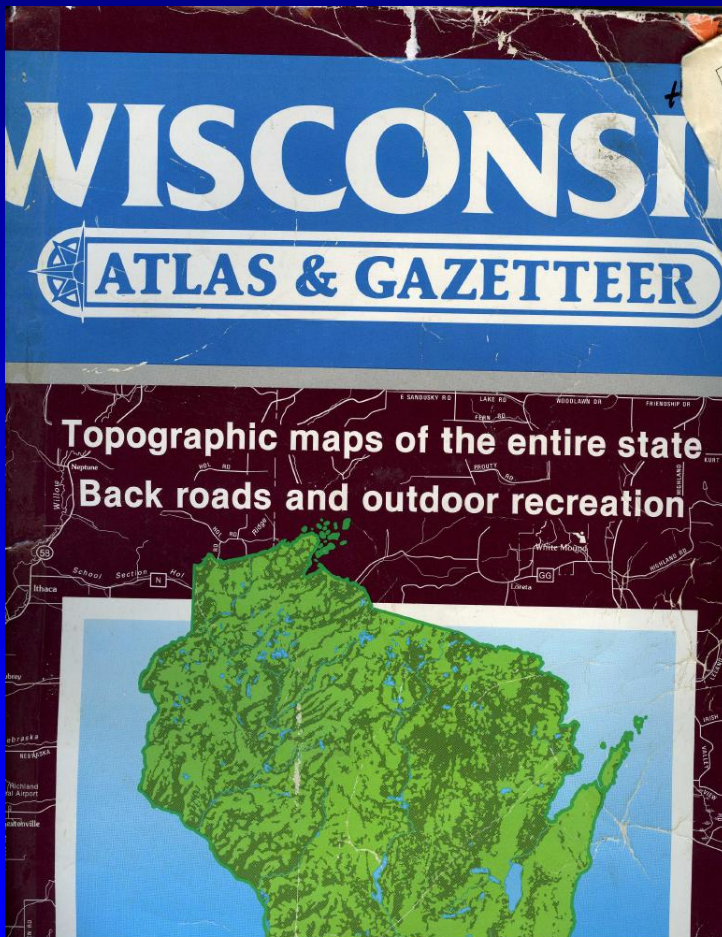


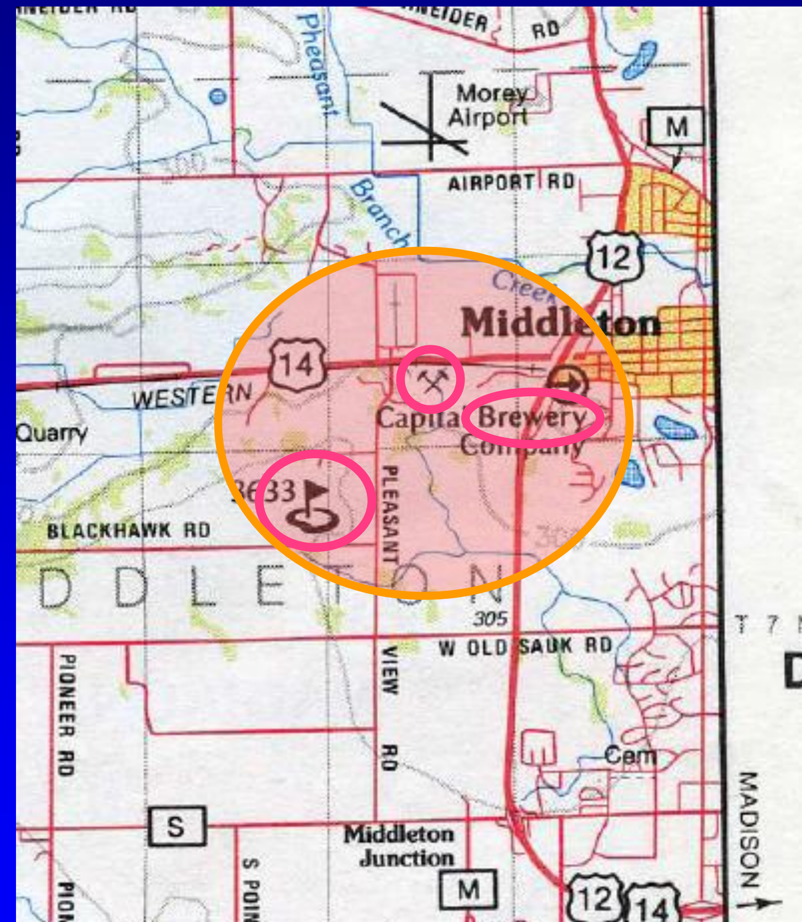


Okay for getting to Wisc but too coarse to get to Wisc WSC

Closer to appropriate simplification but still too coarse to get to Wisc WSC

Spend more $ on Model = Lesser Simplification of Reality = Try#2





Closer yet, but still this simplification still does not get us to the Wisc WSC…

Seems time to re-evaluate…

1) You've had 2 cracks at it using this traditional approach
   - 1st Try got to the state…but, couldn't reach the objective of the exercise
   - 2nd Try built on what was learned in the 1st Try but…cost 4 times the 1st!!

And, at the end of all this modeling, still have not reached the objective! Your credibility = ?

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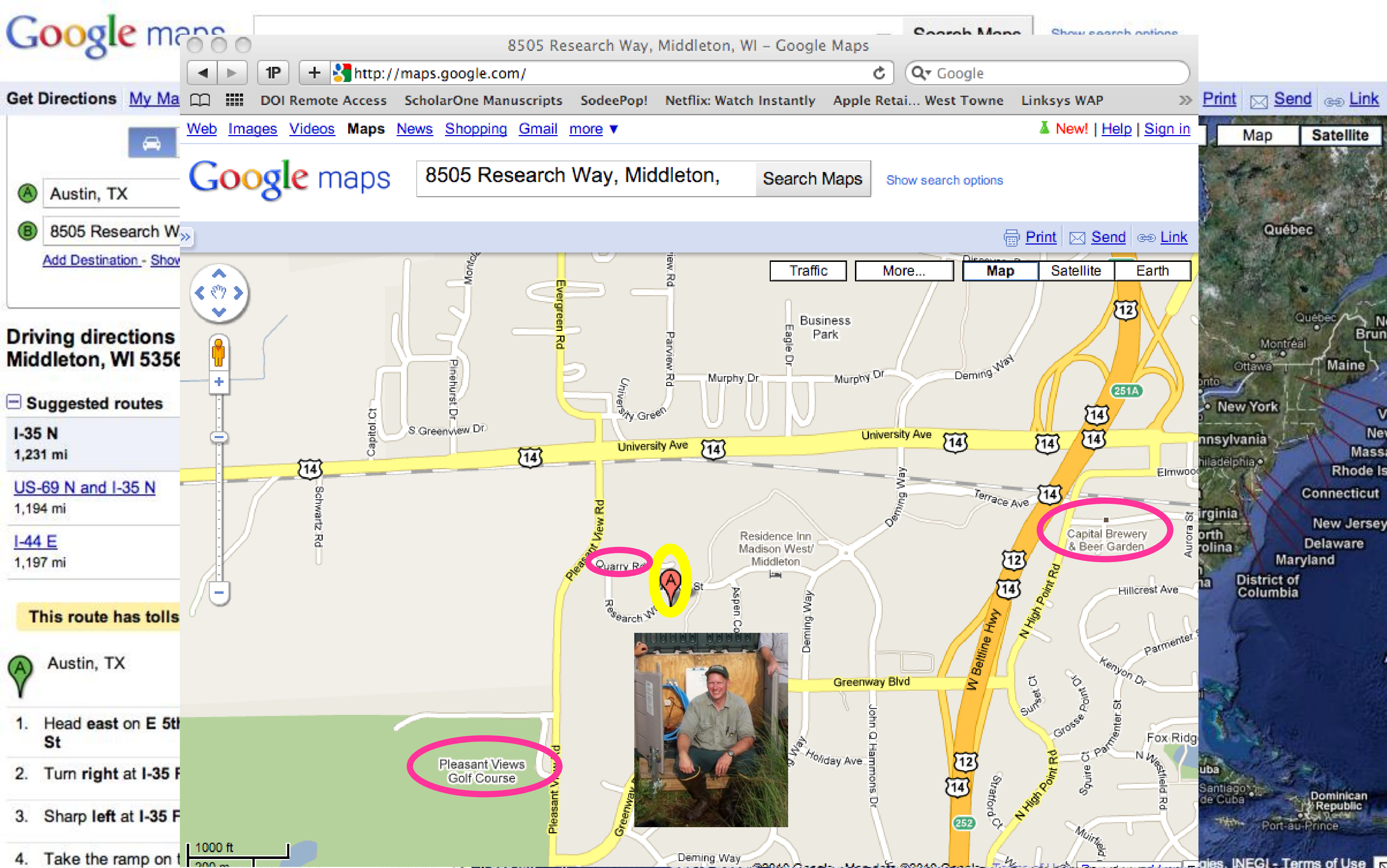
Simplification of Reality tuned for this objective

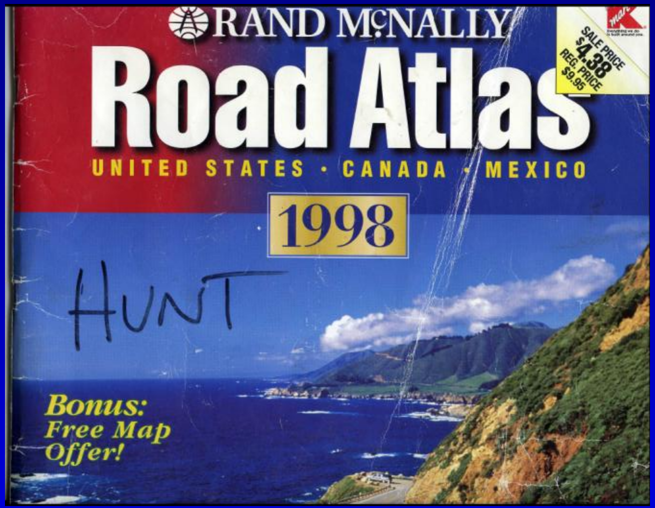


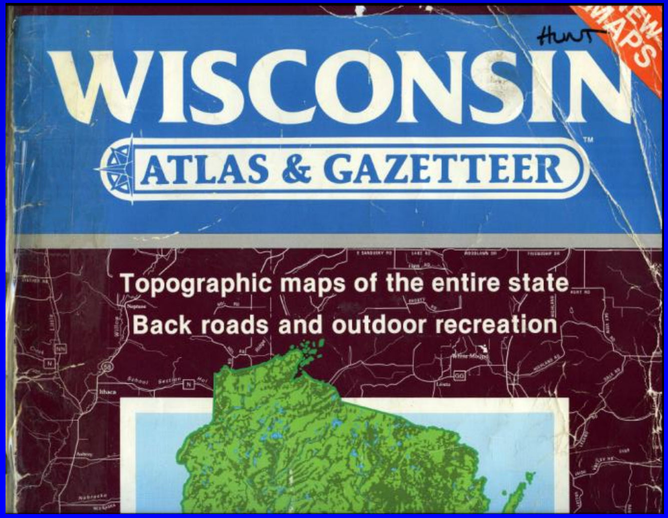
What did we just do?

- Used modern computing power
- Used modern software
- Used Cloud Computing (more on that later)
- Reached the objective quickly
- With reduced uncertainty
- User was in control the entire time (algorithm was not running amok)

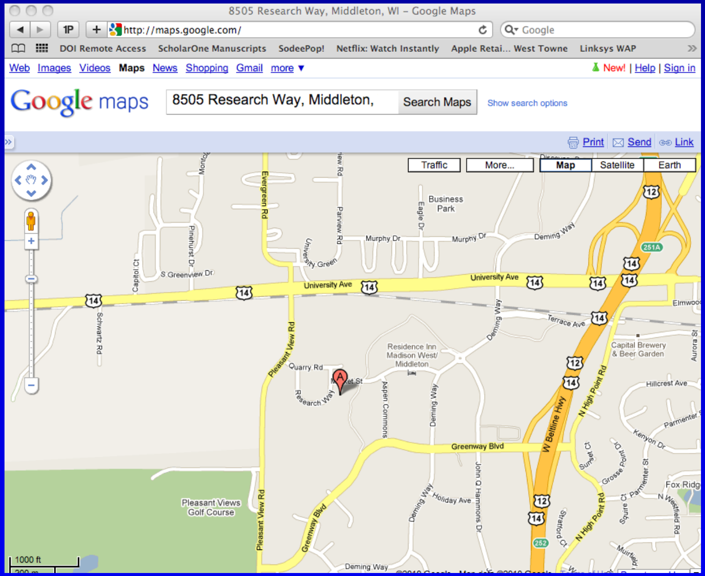
All are "models" of the real world, but not equal in their ability to meet the model objective

Old Way



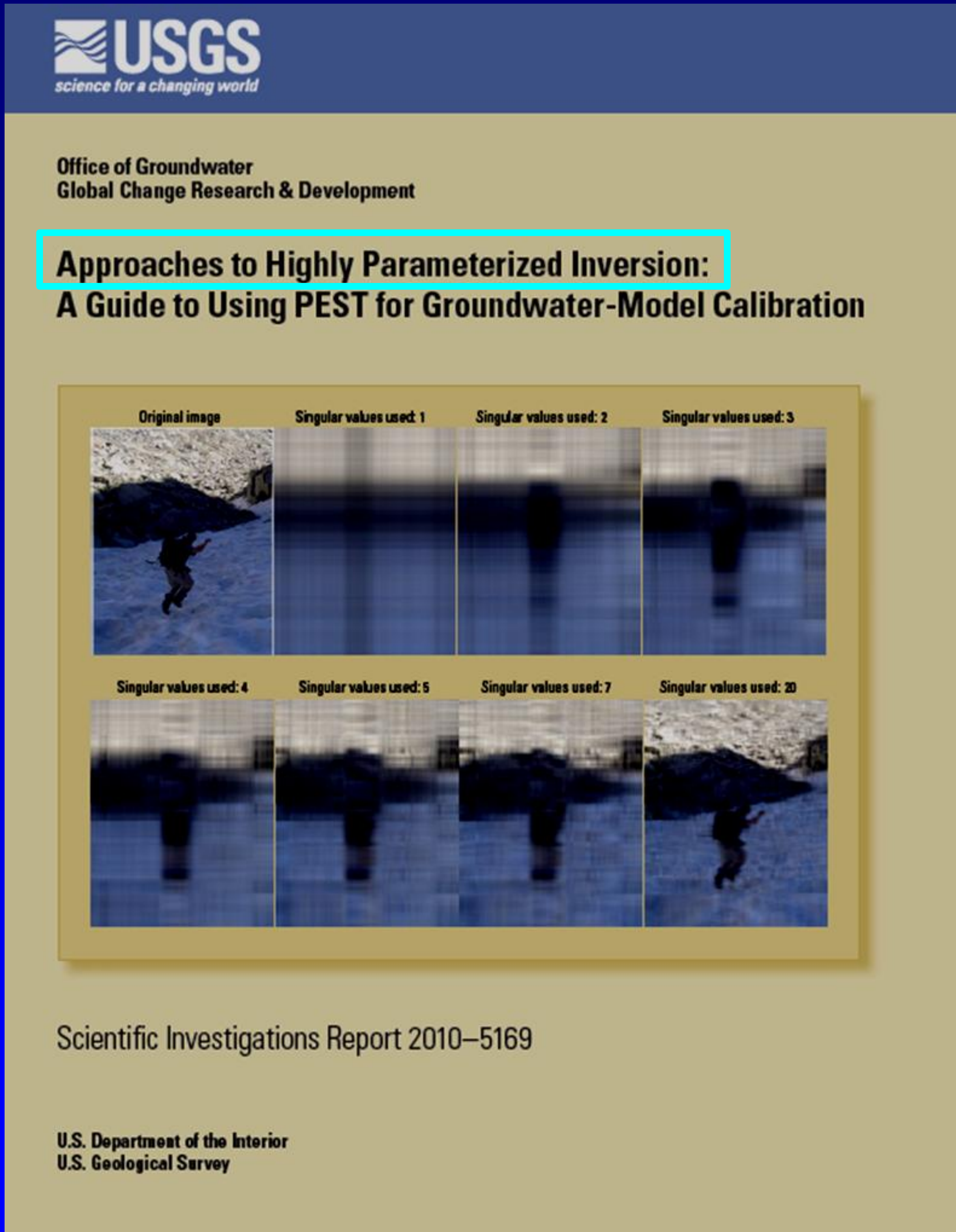


New Way



1) Starts out very flexible (use anywhere in the US)
2) Ends at optimal level of detail specified by the user

What if we could do the same for environmental models?

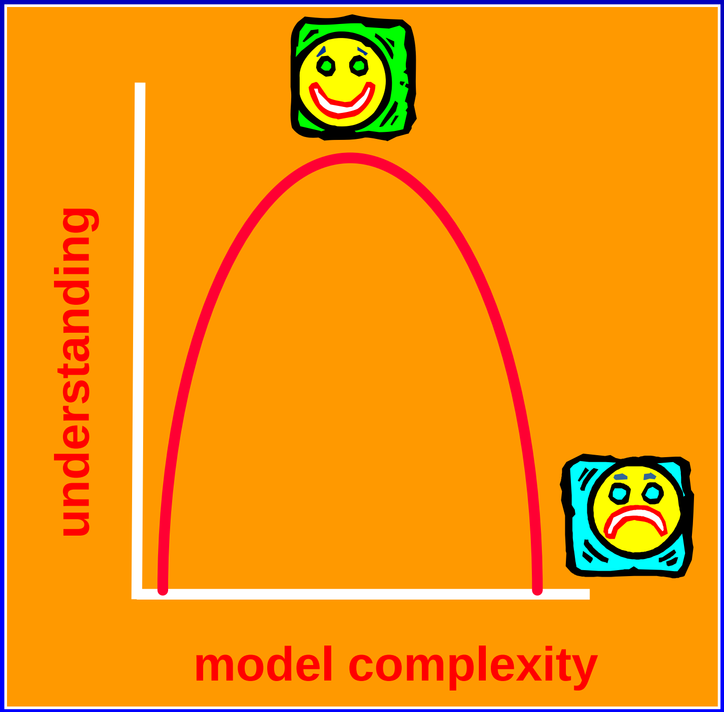


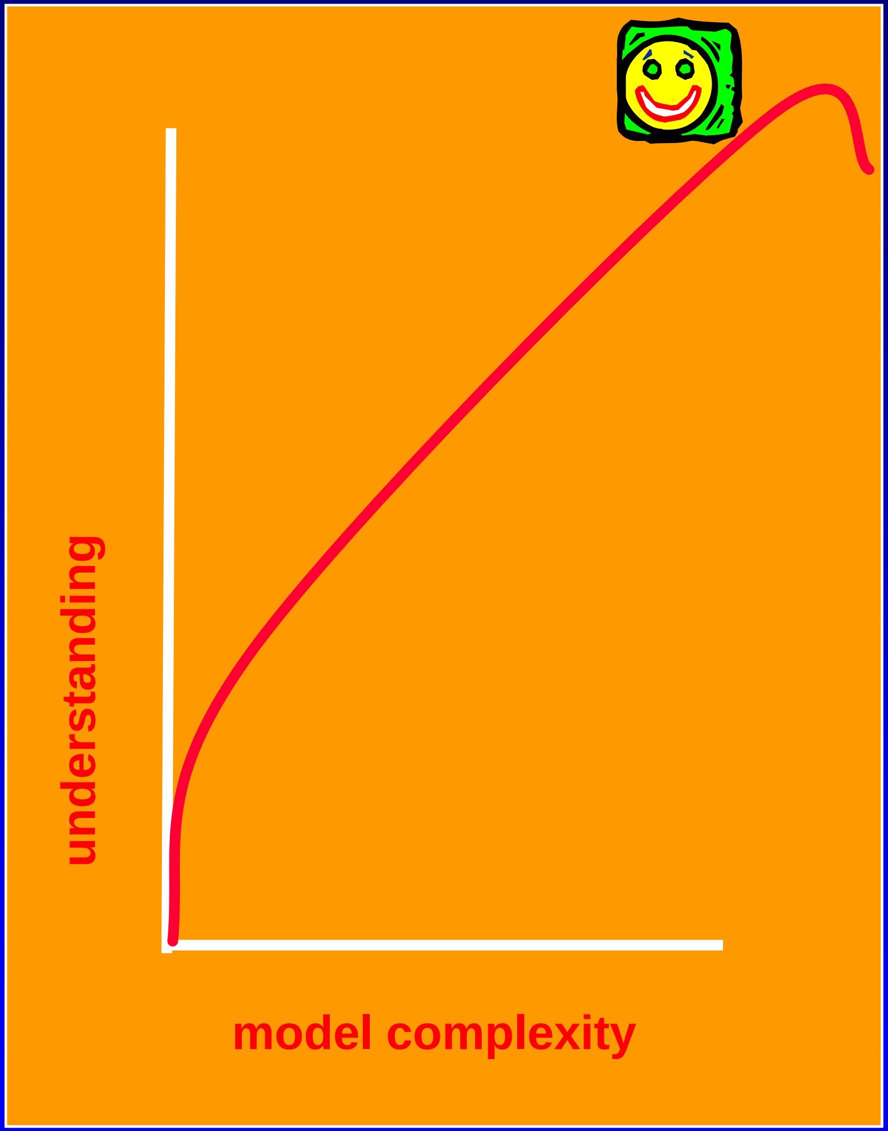
SIR 2010-5168
Pilot Points theory, guidelines, and future directions

SIR 2010-5169
A guide to using PEST for Groundwater-model calibration

SIR 2010-5211
A guide to using PEST for model-parameter and predictive-uncertainty analysis

John’s World


understanding
model complexity


understanding
model complexity

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

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

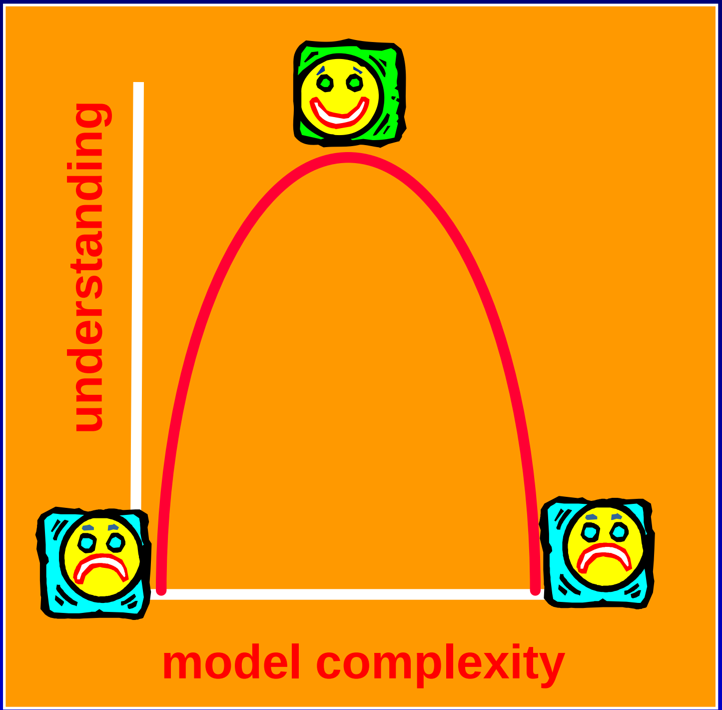
-are unstable

-take longer to calibrate (if they can be at all)

How to handle these ageless issues?

- 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)

"Parsimony"



"Simple as possible…

…but not simpler."

Thus zone based models *may not* be parsimonious!

Need to identify "sweet spot" on simplification

“Highly Parameterized”

Many (“bucketsful”) of parameters…

…but each optimal parameter is not necessarily a unique value.

Adding flexibility with more parameters does not mean high heterogeneity, parameter bullseyes, point-calibration and over-fitting

Soft-knowledge regularization forms the fallback

SVD

“Love it. Learn it.”

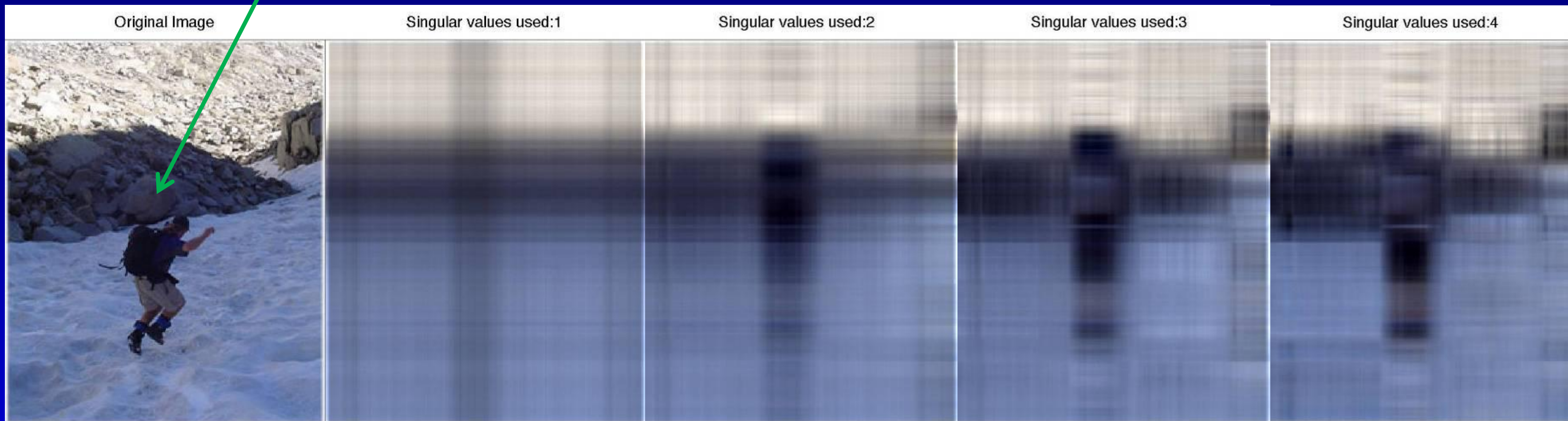
Mike Basial, CH2M Hill,

MODFLOW2008

Singular Value Decomposition

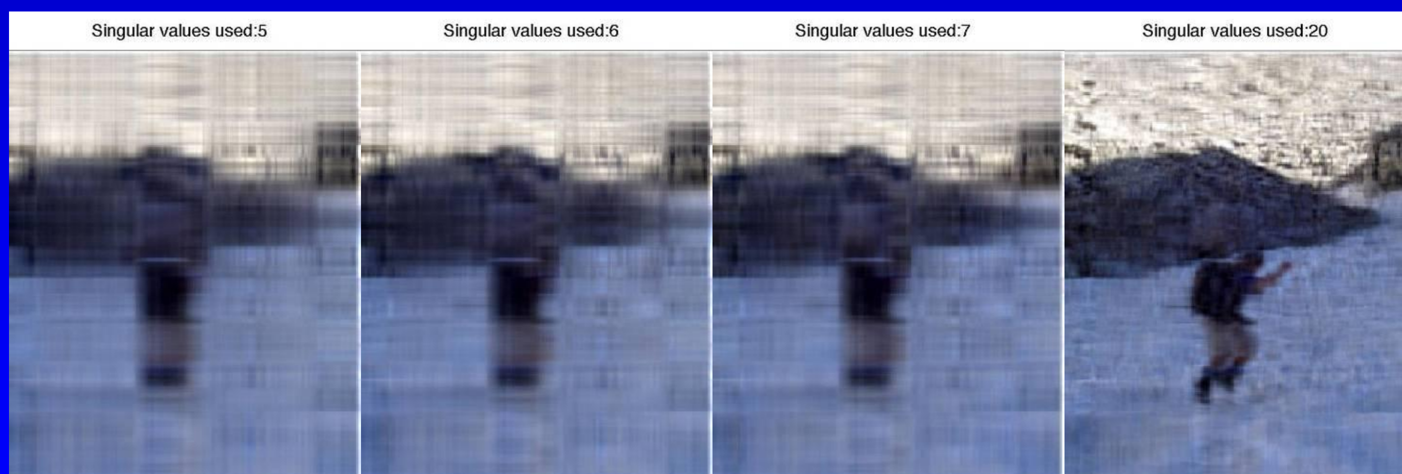
- SVD = subspace method algorithm whereby truncated linear combinations of parameters are solved for rather than base parameters (handles insensitivity and correlation)

If Mike Fienen was displayed in Google Earth…



Modeling Analogy:

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



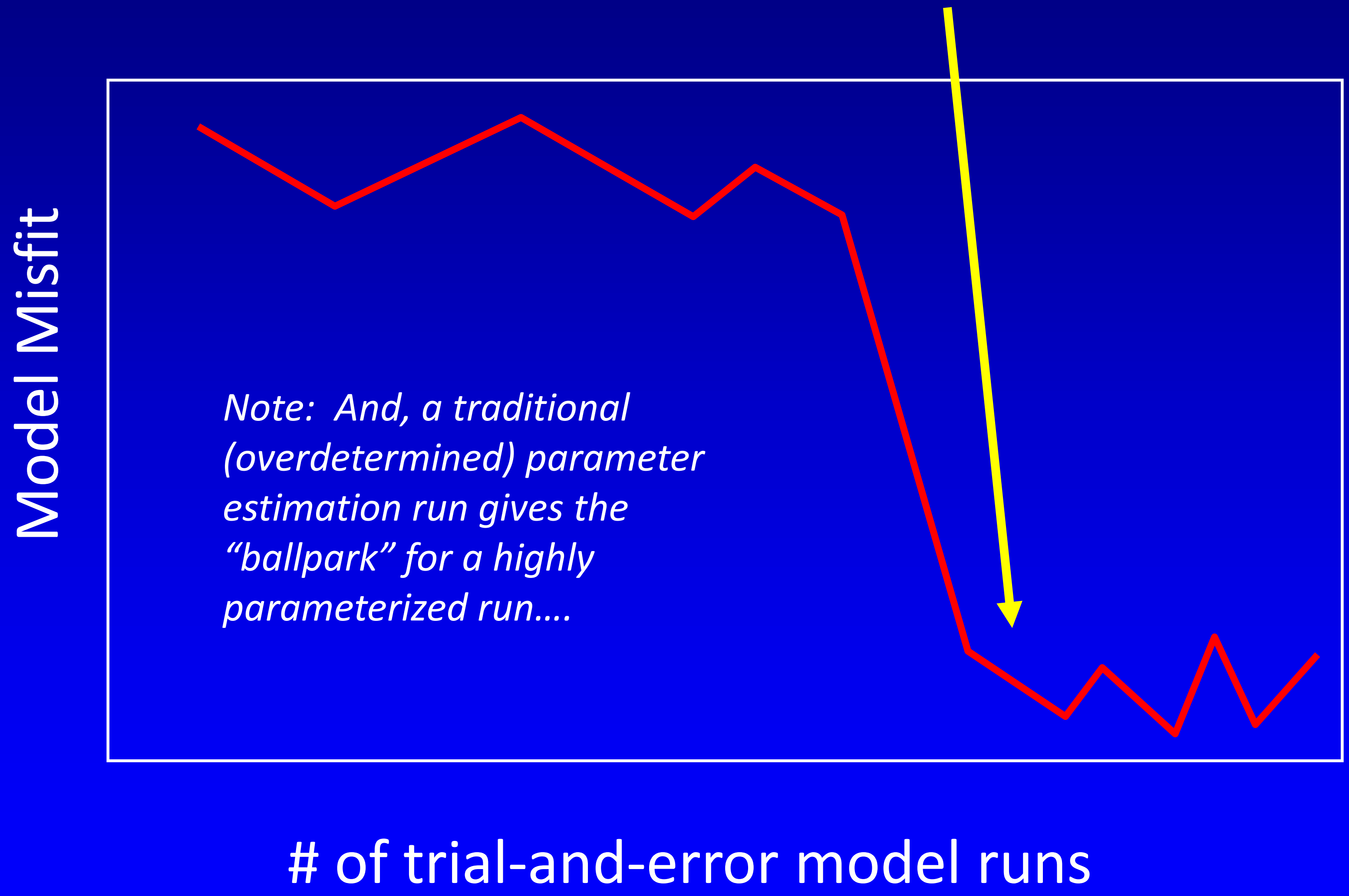
Last Thoughts about SVD – No Free Lunch

Highly parameterized problems are not as robust to bad guesses of initial values

- For Insensitive Parameters: SVD will put out optimal parameters = initial value
- For Correlated Parameters: SVD will put out optimal parameters with the same ratio as the initial values

Thus, initial values must be "in the ballpark" to avoid GIGO

Digression: Importance of trial-and-error calibration to get "in the ballpark"



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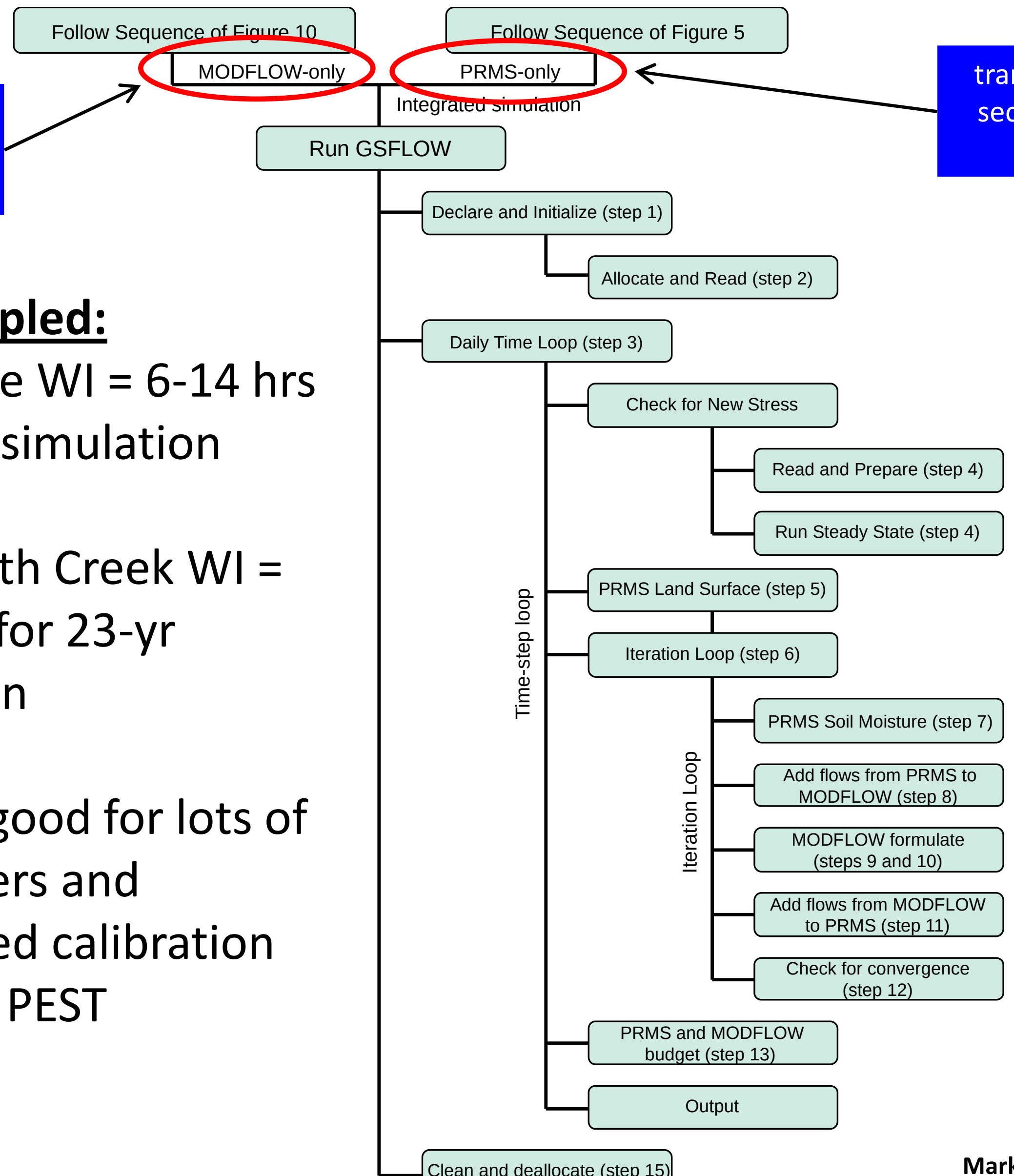
Thus, initial values must be "in the ballpark" to avoid GIGO

Worse yet, SVD *still* has as many model runs as traditional approaches!

GSFLOW and the need for speed

steady-state = seconds to run

transient = seconds to run



Markstrom et al. (2008)

Fully coupled:

Trout Lake WI = 6-14 hrs for 20-yr simulation

Black Earth Creek WI = 2-7 days for 23-yr simulation

…not so good for lots of parameters and automated calibration tools like PEST

Path we'll take for environmental models…

1) Understanding fundamental issues:
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Big Speedup: SVD-*Assist*

“Love it. Learn it.”

Mike Basial, CH2M Hill,

MODFLOW2008

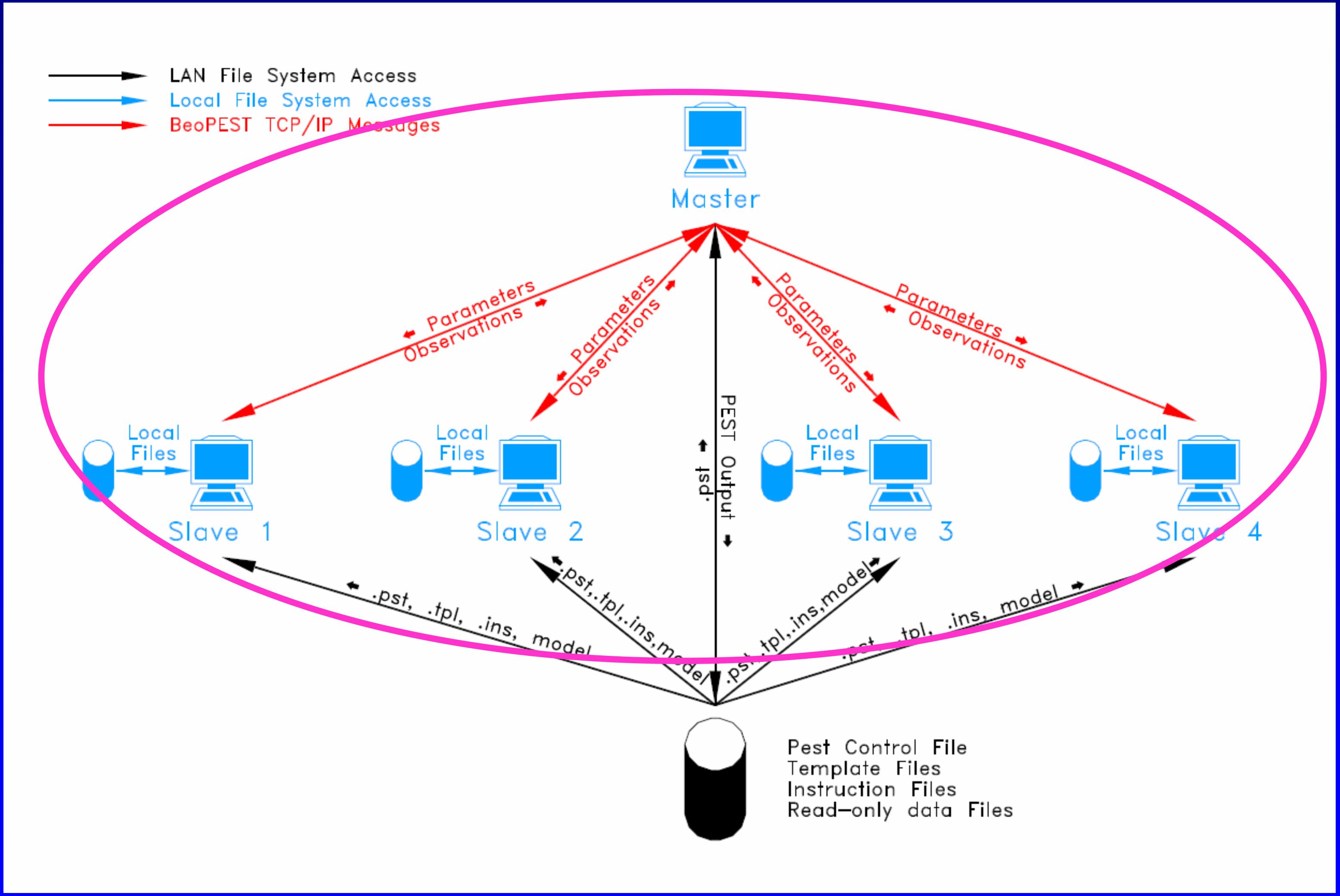
Singular Value Decomposition-Assist

Tonkin and Doherty (2005)

- SVD = subspace method whereby truncated linear combinations of parameters are solved rather than base parameters (handles insensitivity and correlation)
- Assist = Parameter estimation is done on "super parameters" calculated using sensitivities calculated at the initial values (reduces run times)

Upshot: Number of runs reduced 10X to 100X

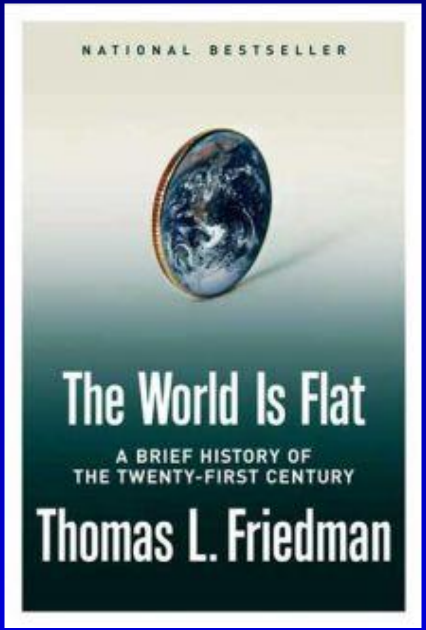
Bigger Speedup: "Big Iron" - Cheap CPUs & "Embarrassingly Parallel" Processing



Schreuder (2009)

The World Has Changed—Outsourcing/Collaboration

- "The World is Flat"
  - Discusses outsourcing in modern economy (importance of "value added")
  - Enabled by rapid communication and an inexpensive workforce
- Motivation for Collaboration
  - Increased complexity/effort of project
- Enabling of Collaboration
  - Digital nature of all aspects of our data
  - Ability to wrap up and send a model



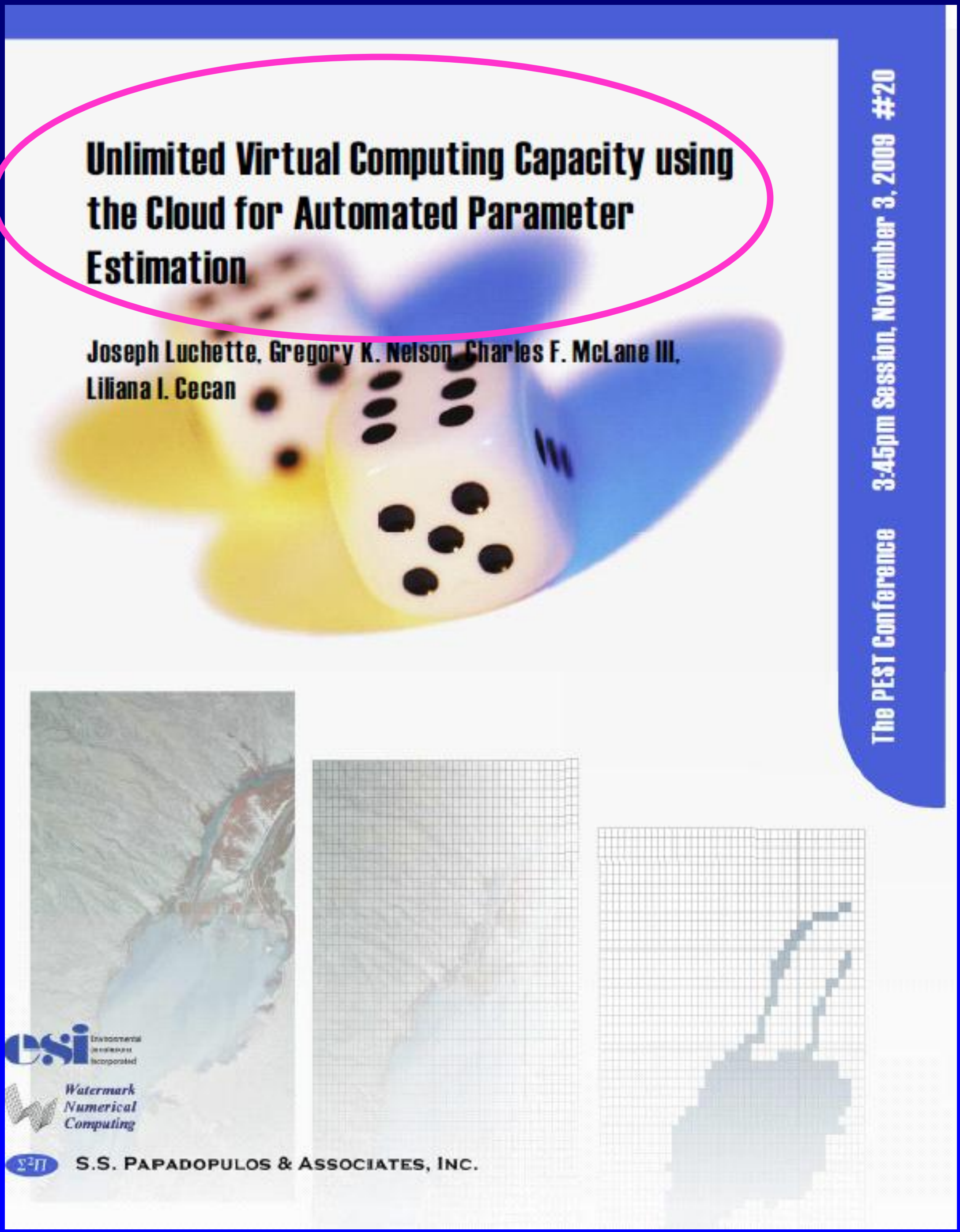
Thomas Friedman

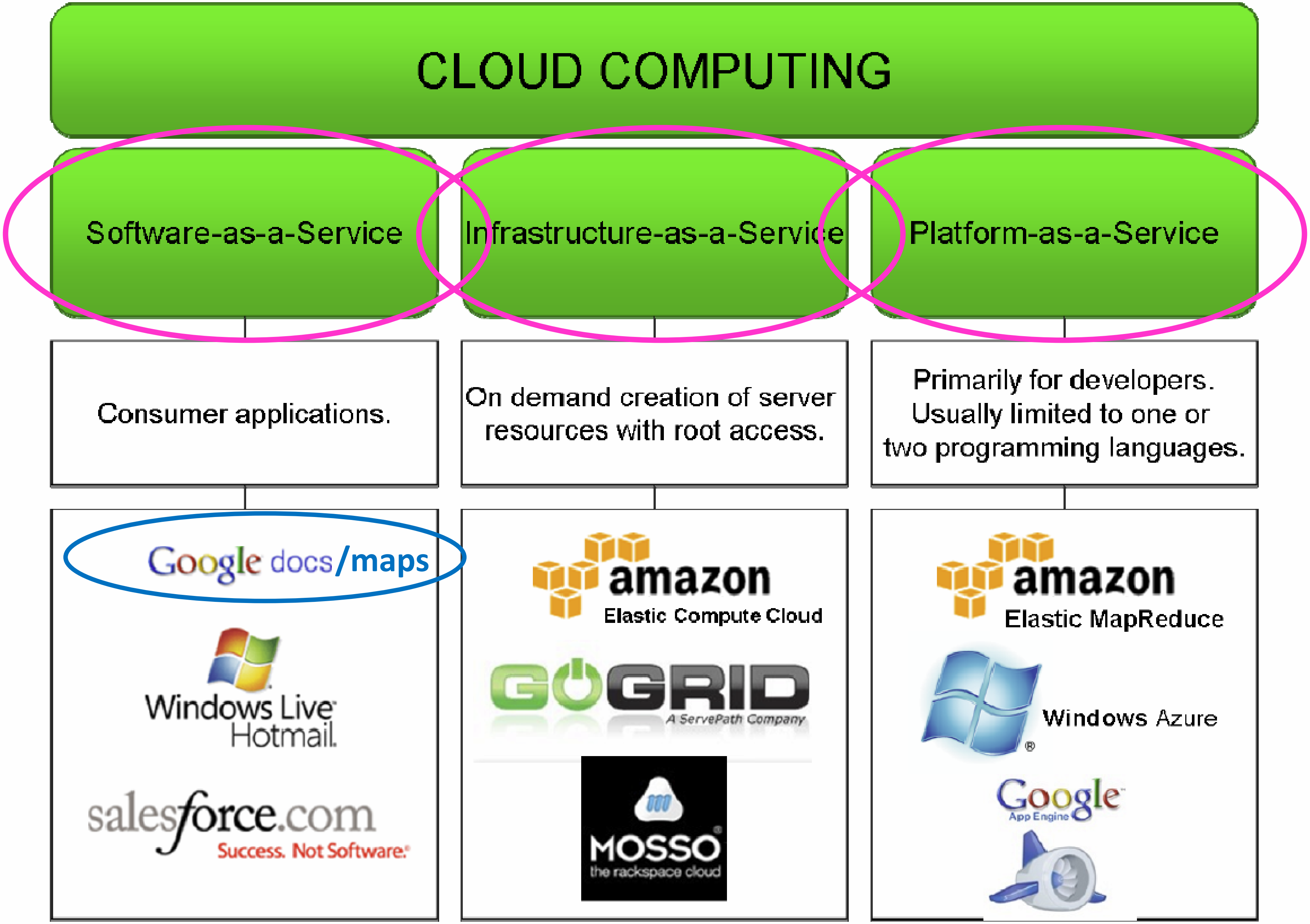
Taking advantage of the times: Cloud Computing

The PEST Conference
November 1-3, 2009
Potomac MD

Joe Luchette et al. (McLane and Assoc.)
Cloud Computing

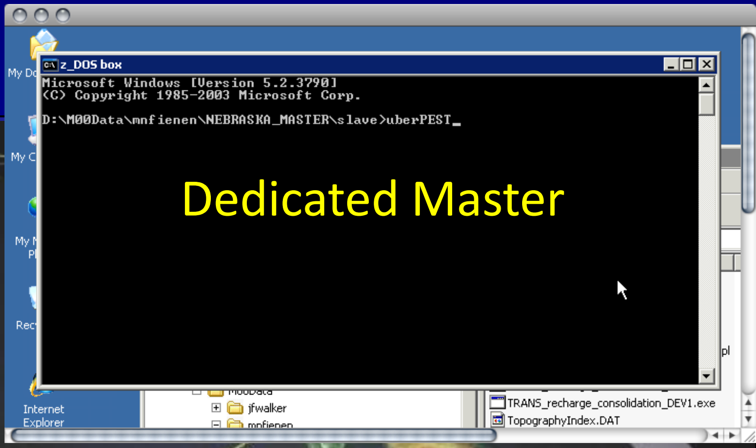
Willem Schreuder (Principia Mathematica)
BeoPEST



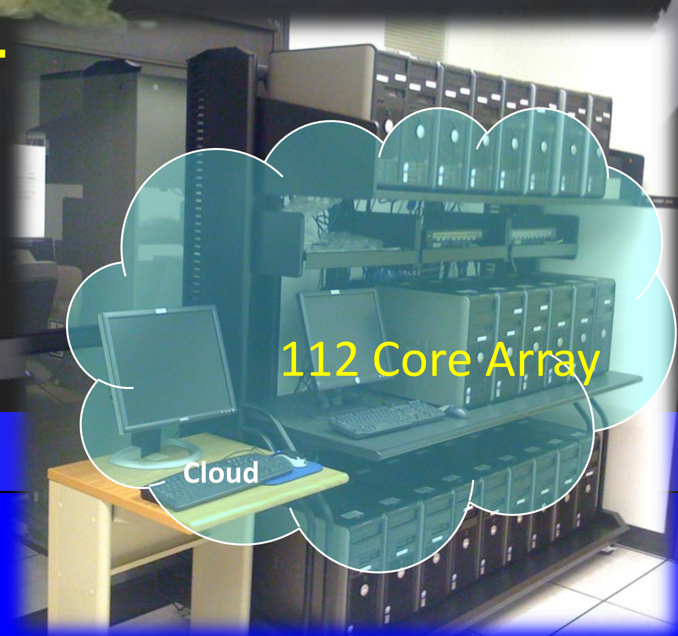

CLOUD COMPUTING
Software-as-a-Service
Infrastructure-as-a-Service
Platform-as-a-Service
Consumer applications.
On demand creation of server resources with root access.
Primarily for developers. Usually limited to one or two programming languages.
Google docs/maps
Windows Live Hotmail
salesforce.com
Success. Not Software.
amazon
Elastic Compute Cloud
GOGRID
A ServePath Company
MOSSO
the rackspace cloud
amazon
Elastic MapReduce
Windows Azure
Google
App Engine

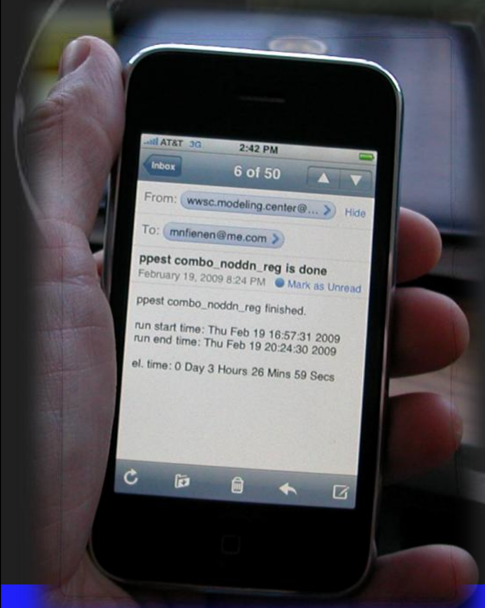
Wisconsin Water Science Center setup

Launch überPEST



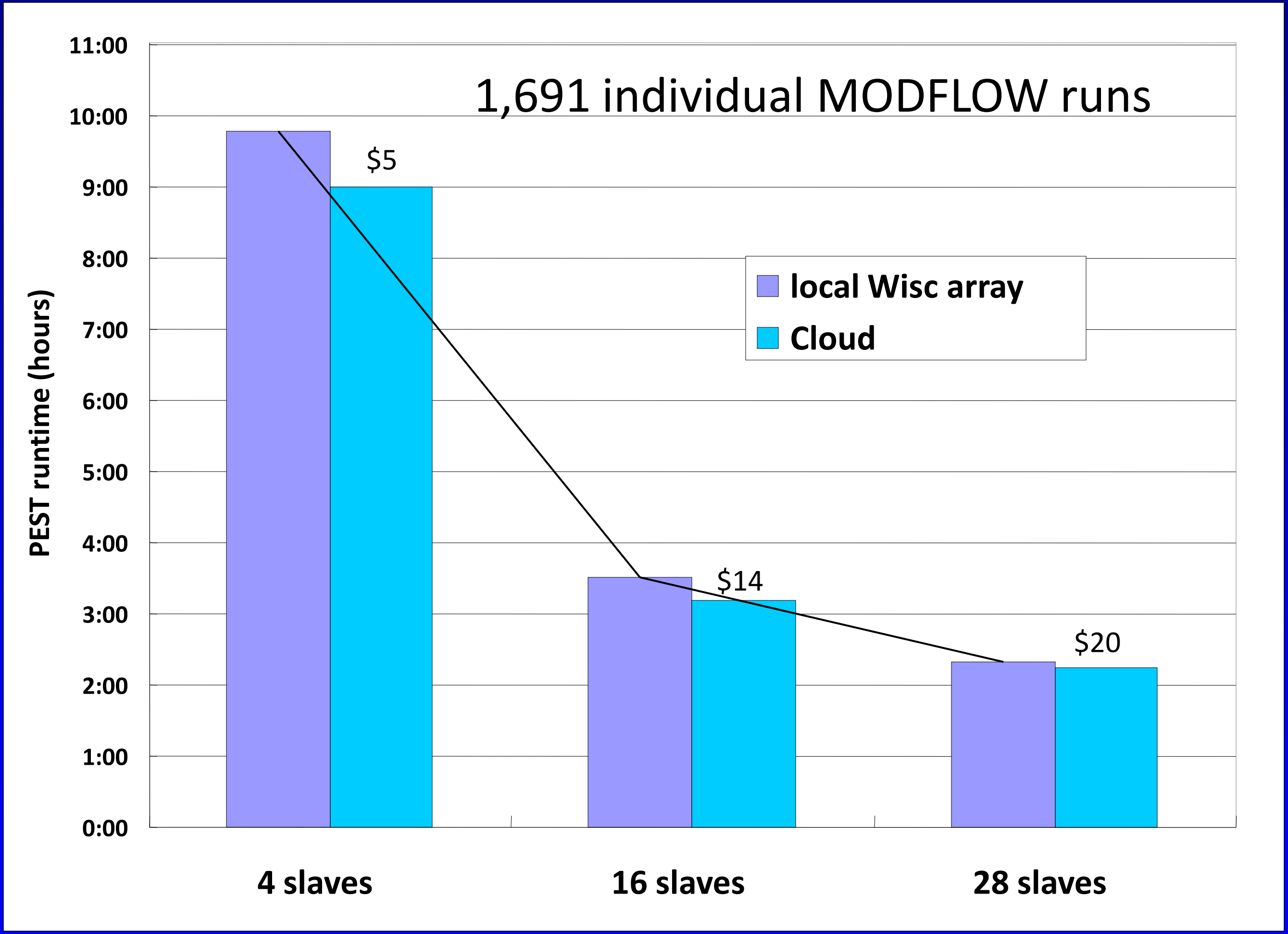
run ppest or BeoPEST





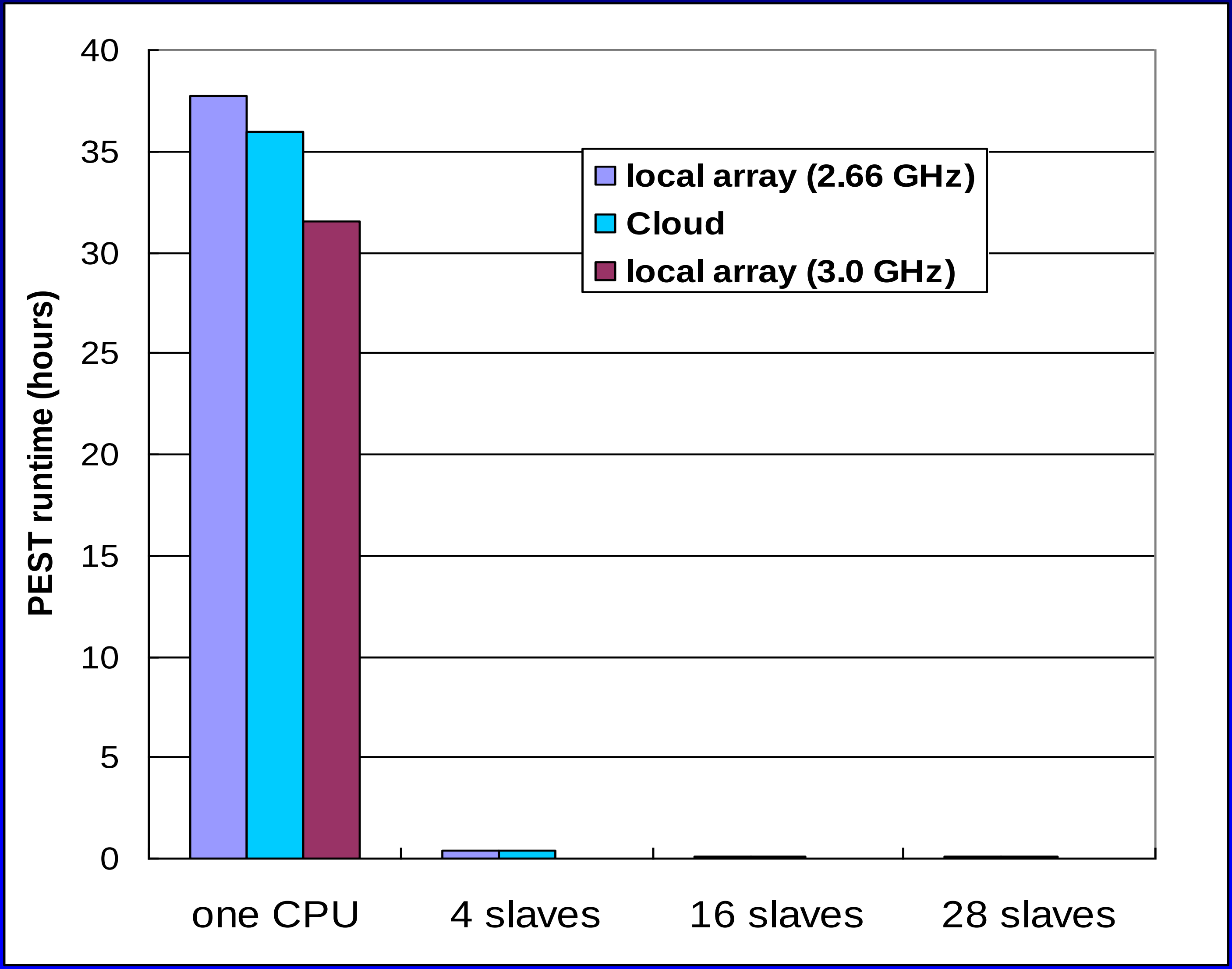
Post-process and send email on completion

Cloud vs. Wisconsin Local Array



Hunt et al. (2010)

Non-parallel vs. parallel



Rapid Communication for the journal Ground Water:

ground water

Rapid Communication/

Using a Cloud to Replenish Parched Groundwater Modeling Efforts

by Randall J. Hunt[1], Joseph Luchette[2], Willem A. Schreuder[3], James O. Rumbaugh[4], John Doherty[5,6], Matthew J. Tonkin[7], and Douglas B. Rumbaugh[4]

Abstract

Groundwater models can be improved by introduction of additional parameter flexibility and simultaneous use of soft-knowledge. However, these sophisticated approaches have high computational requirements. Cloud computing provides unprecedented access to computing power via the Internet to facilitate the use of these techniques. A modeler can create, launch, and terminate "virtual" computers as needed, paying by the hour, and save machine images for future use. Such cost-effective and flexible computing power empowers groundwater modelers to routinely perform model calibration and uncertainty analysis in ways not previously possible.

Introduction

Societal decision-making on water issues—both quantity and quality—requires science-based tools such as computer models. Numerical models are vital for inform- and alternate management scenarios with models—especially when performing model calibration and sensitivity analysis where the model is run many times.

At the November 2009 PEST (Parameter Esti-

Ground Water May-June 2010, vol. 48, no. 3, pages 360-365

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science for a changing world

“Buckets to Clouds” Approach in a nutshell

- Use modern computing power
- Use modern software
- Use Cloud Computing when it fits
- Target the objective and test quickly
- Give results with reduced uncertainty
- Require a user be in control of the process (algorithm not running amok)

Actual 1998 AGU Session Summary

"If models are kept in the context of their objective, we should feel comfortable resisting the *sirens of complexity* and construct simpler, less encompassing, models."

Hunt and Zheng (1999)

Updated for 2010's decision making:

But we should also feel free to use soft knowledge, mathematics, and enhanced computing capability to help us decide what is "*simple as possible, but not simpler*".