SAND2008-1917P

Deterministic Site Characterization Tool

Multi-Model Ranking and Inference

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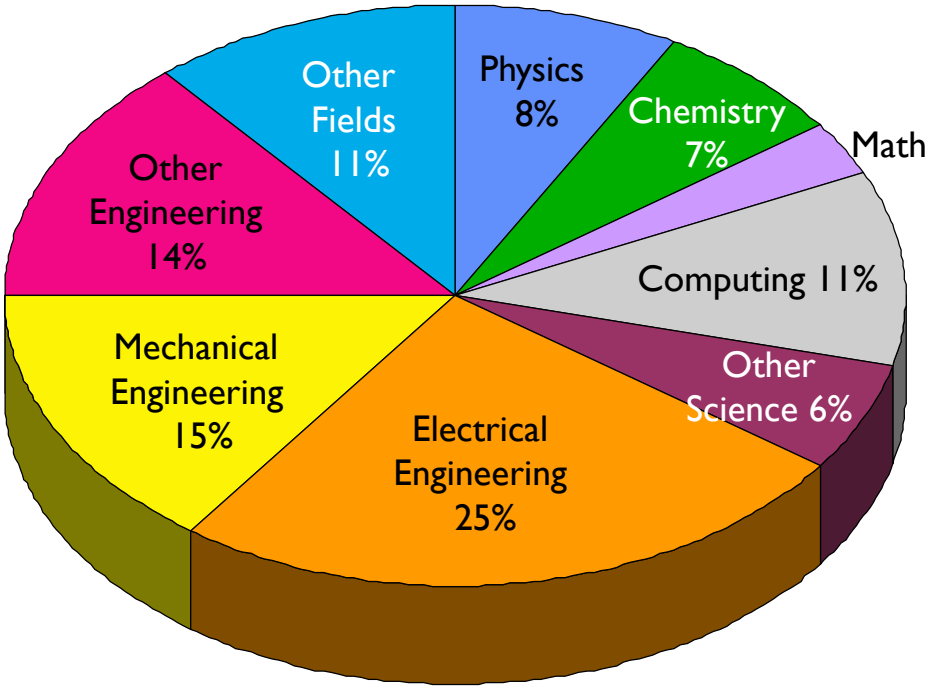
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

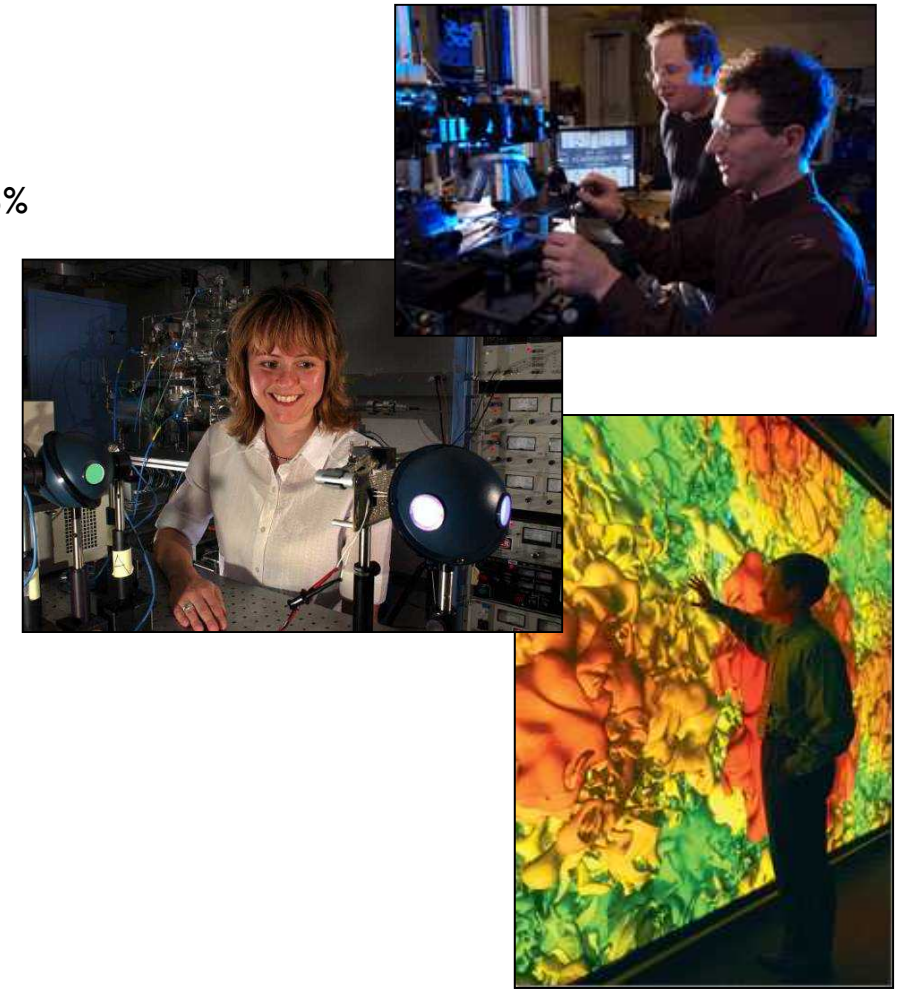
Introduction

- Sandia National Laboratories
- Decision making in the face of uncertainty
- Model development as part of site characterization
- Model ranking
- Model averaging
- Experimental approach
- Simple model application

Sandia National Laboratories

Sandia is a Multidisciplinary Science and Engineering Laboratory



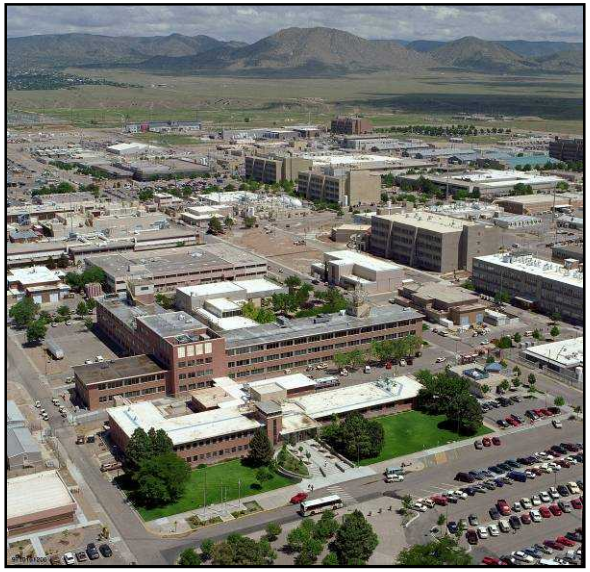


- ***Over 8,500 full-time employees***
- ***Over 1,500 Ph.D.s***
- ***Over 2,500 MS/M***

US Department of Energy

Sandia National Laboratories

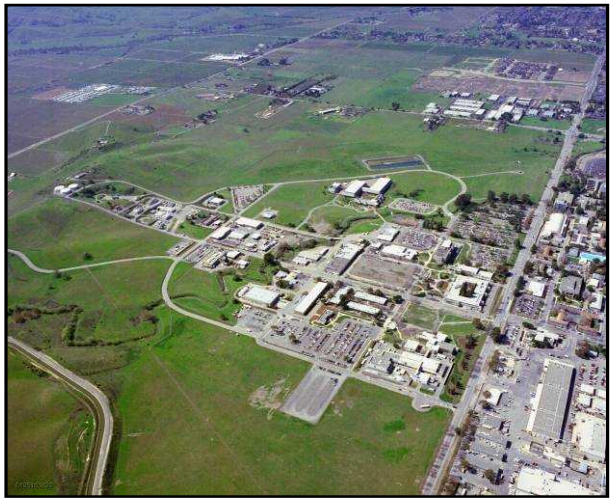
Sandia National Laboratories is Geographically Distributed



Albuquerque, New Mexico

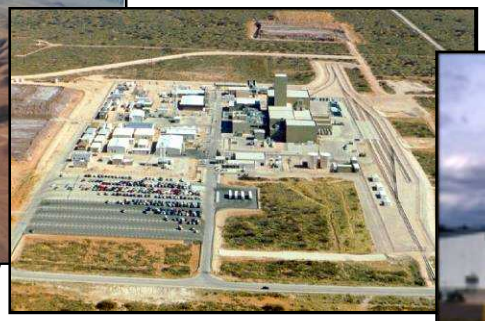
Tonopah Test Range, Nevada

Kauai Test Facility Hawaii



Livermore,California

Nevada



WIPP, New Mexico

Pantex, Texas

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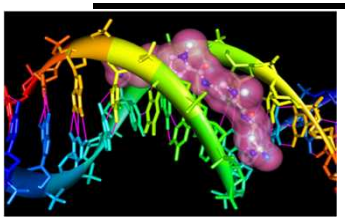
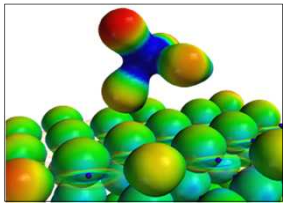
Eight Science and Technology Councils



Bio Science & Technology

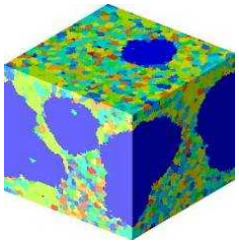
Engineering Sciences



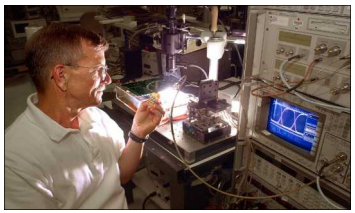
Chemical & Earth Sciences

Manufacturing Sciences

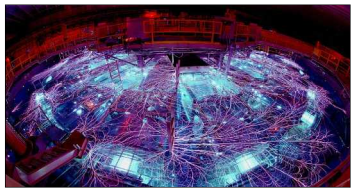
Computer & Information Science



Materials Sciences



Electronics



Pulsed Power Science

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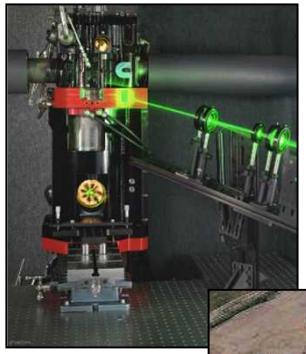
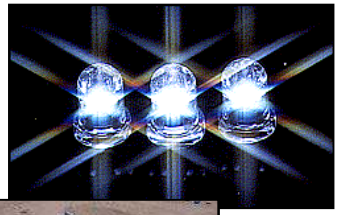
Energy, Resources, and Nonproliferation Strategic Management Unit

Fuel and Water Systems

Nuclear Energy

Science Underpins and Enables Technology for the Energy, Resource, and Global Security Missions





Science and Technology

Global Security

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Repository Science

- Yucca Mountain
  - Office of Civilian Radioactive Waste Management (OCRWM) lead laboratory for repository systems
    - Strong centralized leadership for its science program
    - Management and integration for all Yucca Mountain scientific programs – including budget allocation
    - Increase OCRWM's technical credibility with the scientific community, as well as the project's regulators and stakeholders
    - Support OCRWM 's license application and its defense in the Nuclear Regulatory Commission's review process
      - Define scientific program to support License Application
      - Develop and defend Total System Performance Assessment and underlying technical bases
- Waste Isolation Pilot Plant – TRU Waste
  - Chief scientific advisor to DOE
    - Performance, compliance, and impact assessment
    - Sensitivity analysis and scientific investigations
    - Monitoring and data analyses
    - Computer modeling
    - Technical review and expert elicitations

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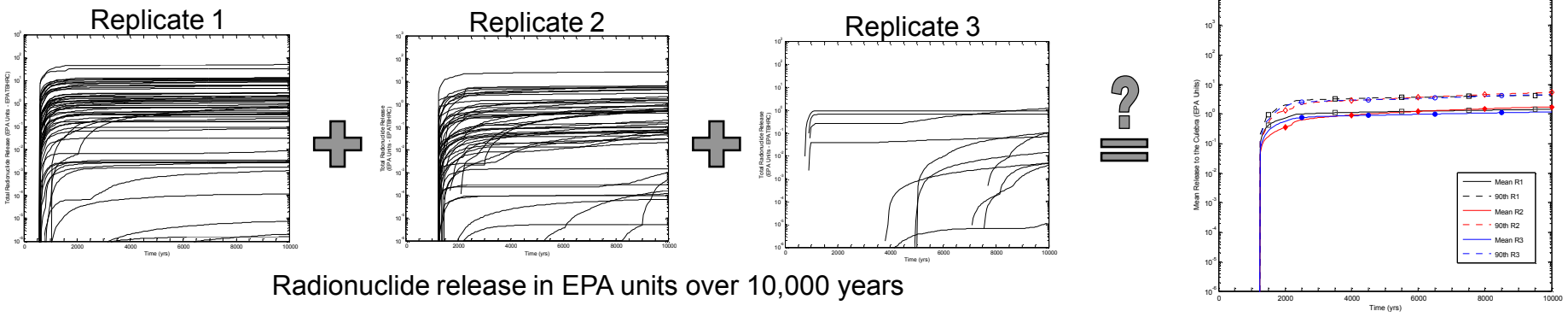
This Project

Deterministic Site Characterization Tool Using Multi-Model Ranking and Inference

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Site Characterization is About Decision Making

- **Risk Assessment**
  - **Reduces performance uncertainty**
  - **Reduces time, effort, and costs**
  - **Increases reliability**
  - **Increases public trust**



Radionuclide release in EPA units over 10,000 years

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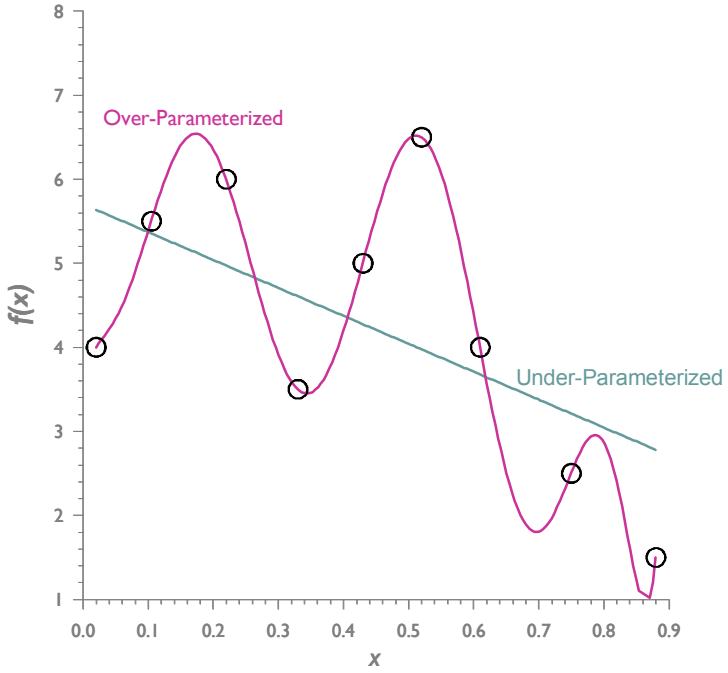
Characterizing the Sub-surface

- Multiple models can fit existing data
  - Different conceptualizations
  - Different parameterization
  - Same data set



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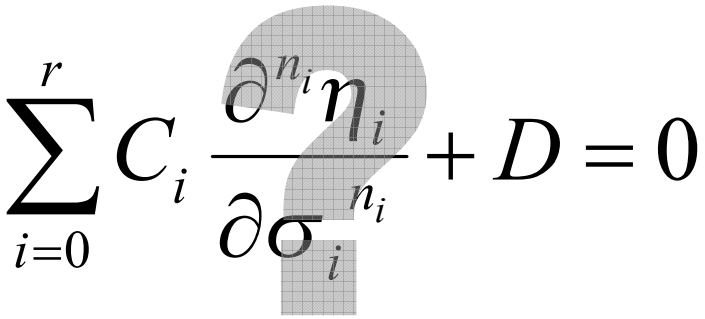
Characterizing the Sub-surface

- Under these conditions, how can we:
  - Find the 'best' model?
    - Understand risk
    - Prediction
  - Guide future data gathering efforts?
  - Infer possible processes, structures, and features?



Modeling

"One of the most insidious and nefarious properties of scientific models is their tendency to take over, and sometimes supplant, reality. They often act as blinders, limiting attention to an excessively narrow region. No application of logic can prove a model to be true, though its lack of plausibility can often be demonstrated easily. The extravagant reliance on models has contributed much to the contrived and artificial character of large portions of current research."

Chargaff, E., 1978, Heraclitean Fire: Sketches from a Life before Nature, The Rockefeller University Press, N.Y., 252 p.

Heraclitean: of or pertaining to Heraclitus or his philosophy.

Heraclitus: Early Greek philosopher who maintained that strife and change are the natural conditions of the universe.

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Modeling

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Need to define 'true' in a manner that is consistent with the problem at hand.

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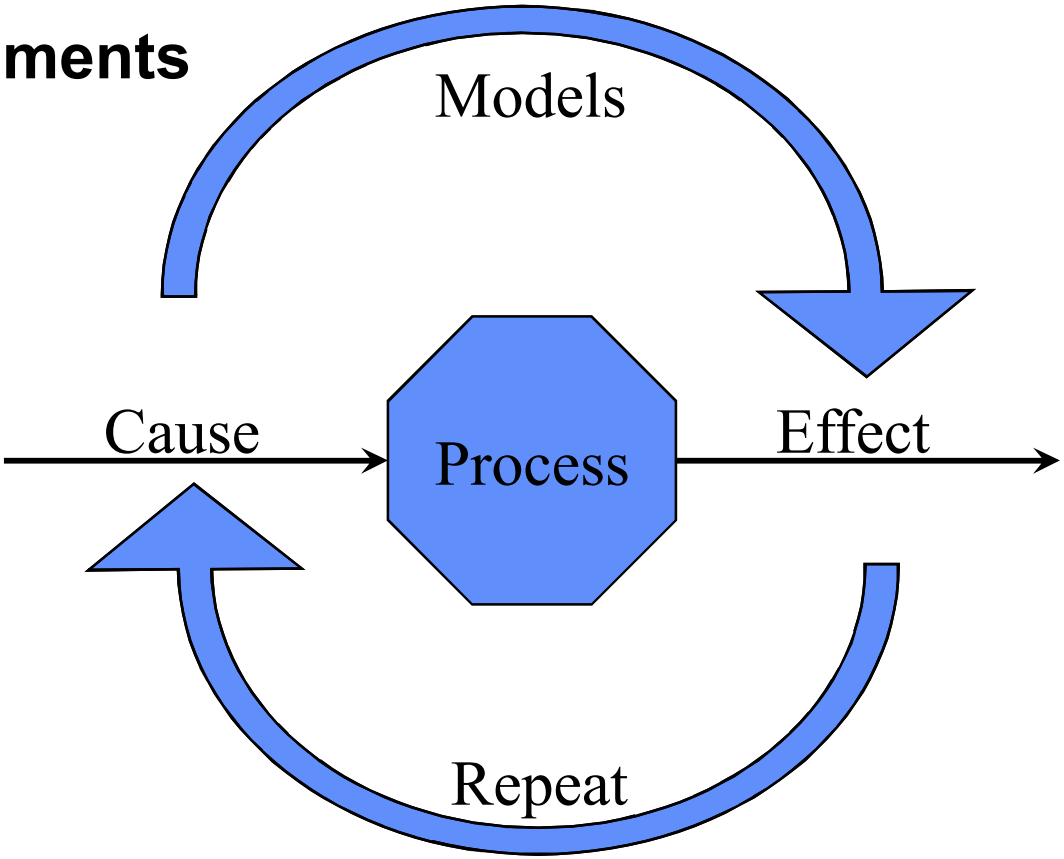
‘Best’ Groundwater Models

- No spatial and/or temporal bias
- Calibrates to reasonable estimated parameter values
- Has good fit statistics while maintaining parsimony
  - Trade-off between bias and variance
  - Trade-off between underfit and overfit
- Considerable expertise, training, and experience is necessary to define a set of reasonable models

Modeling and Scientific Understanding

- **Experiments**



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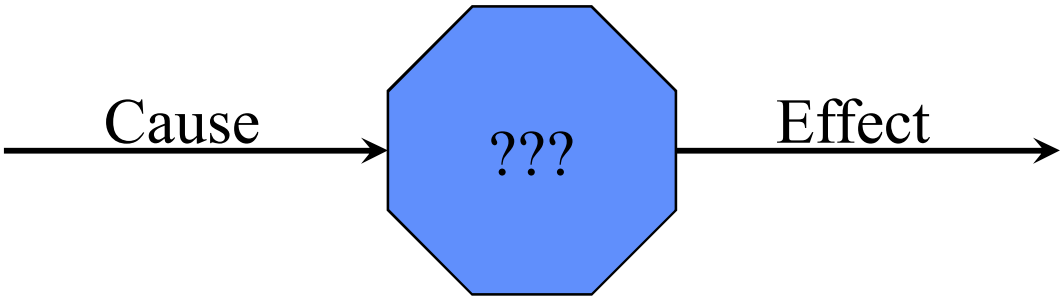
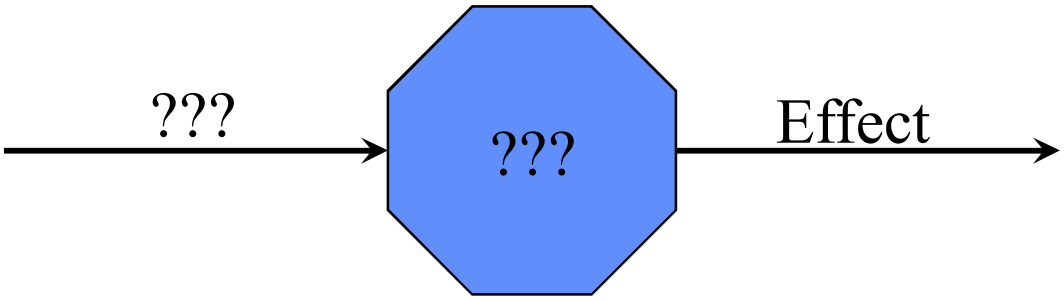
Modeling and Scientific Understanding

- **Groundwater**



Modeling and Scientific Understanding

- **Groundwater**



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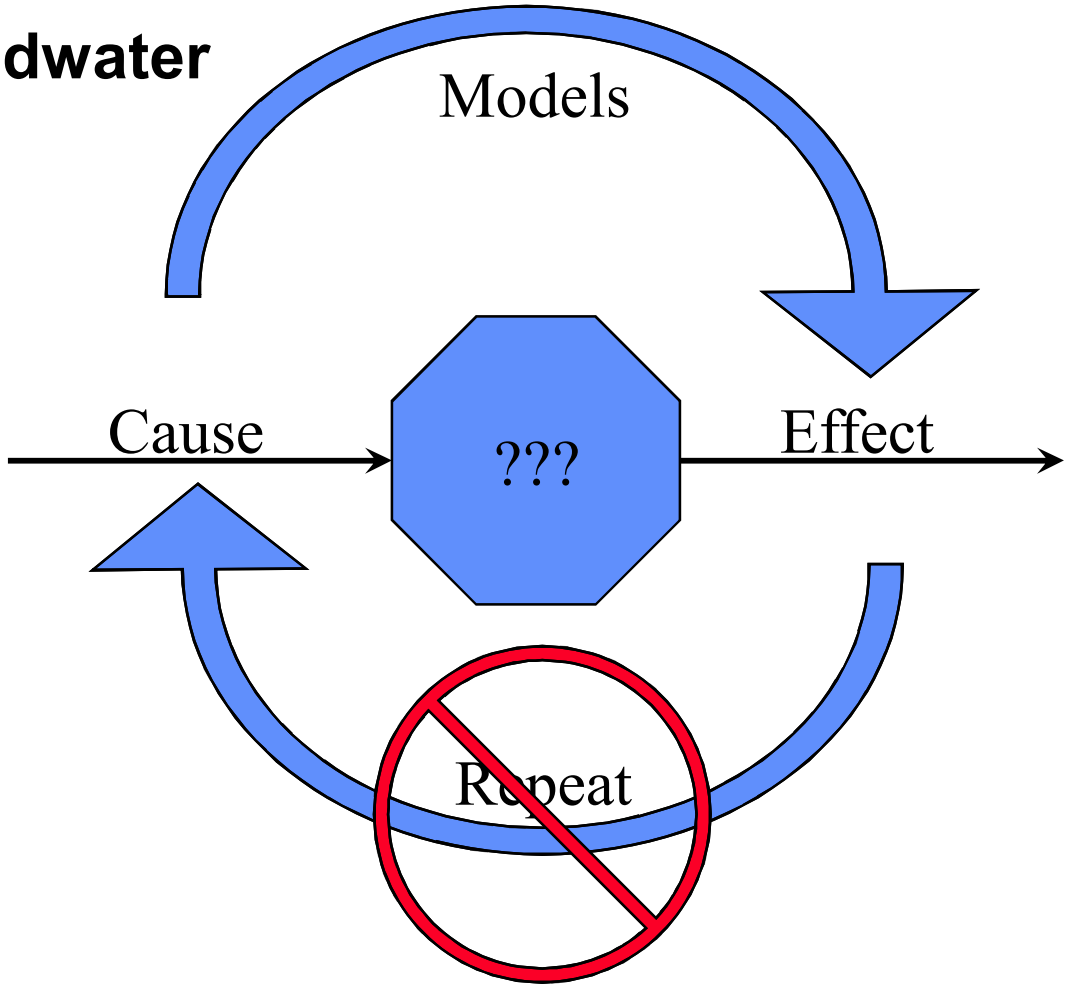
Modeling and Scientific Understanding

- **Groundwater**



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How To Model

- Hydrologist
  - Observes and measures
  - Applies knowledge and expertise
  - Forms conceptual models (hypotheses)
    - Multiple working hypotheses
- Conceptual models are converted to numerical models
- Models are fit to observational data
- ‘Best’ model is picked to make predictions

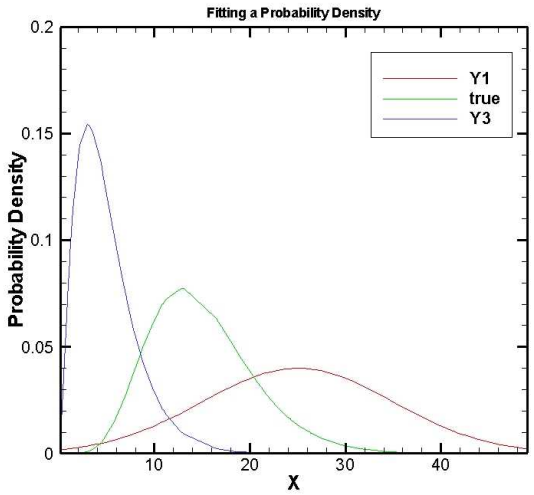
How To Model

Inverse Problem

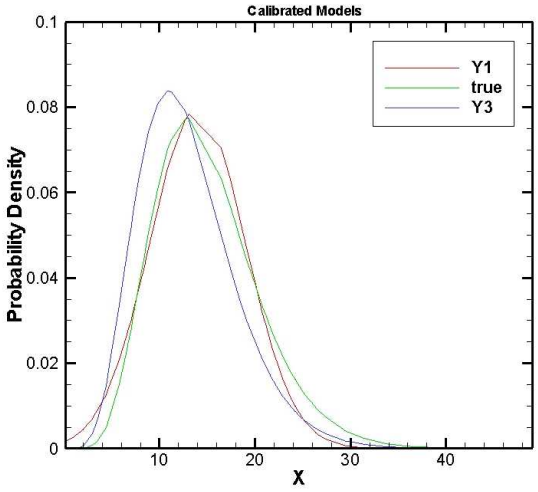
Develop a conceptual model → Calibrate model → Decide if fit is 'good enough' → Make predictions →

Acquire more data

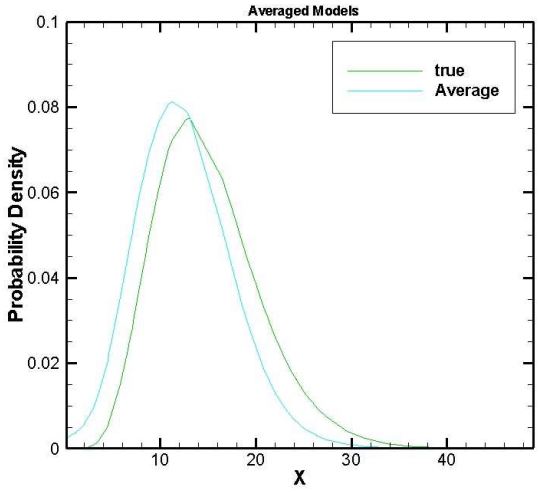
Multiple Models



Calibrated Models



Averaged Models



Kullback-Leibler (K-L) Information

- **K-L information is the information, *I*, that is lost when a model, *g*, is used to simulate a true condition, *f*.**

$$f = g + I$$

  - **However, in groundwater, we do not know *f*, and thus we cannot know *I***
  - **Akaike Information Criteria, AICc**

Akaike Information Criteria

$$AICc = n\log(\sigma^2) + 2k + \left(\frac{2k(k+1)}{n-k-1}\right)$$

n = # of observations; σ^2 = residual variance = $WSSR/n$; k = # of parameters

- **Estimates relative expected estimated K-L information loss**
- **Accounts for number of estimated parameters and the number of observations**
- **Typically for groundwater, $n/k < 40$**

Ranking

- **Simple Difference:**

$$\Delta_i = AICc_i - AICc_{\min}$$

$\Delta_i < 2$: very good
$4 < \Delta_i < 7$: less support
$\Delta_i > 10$: dismissed from consideration

Burnham, K.P., and D.R. Anderson. 2002. Model Selection and Multi-Model Inference: A Practical Information-Theoretic Approach. New York: Springer-Verlag

- **Model Probabilities:**

$$w_i = \frac{\exp(-0.5\Delta_i)}{\sum_{j=1}^{R} \exp(-0.5\Delta_j)}$$

Posterior model probability:
w_i is the weight of evidence in favor of model I having the least K-L information loss.

- **Evidence Ratios:**

$$\frac{w_i}{w_j}$$

There is w_i / w_j times more evidence supporting the best model, i.

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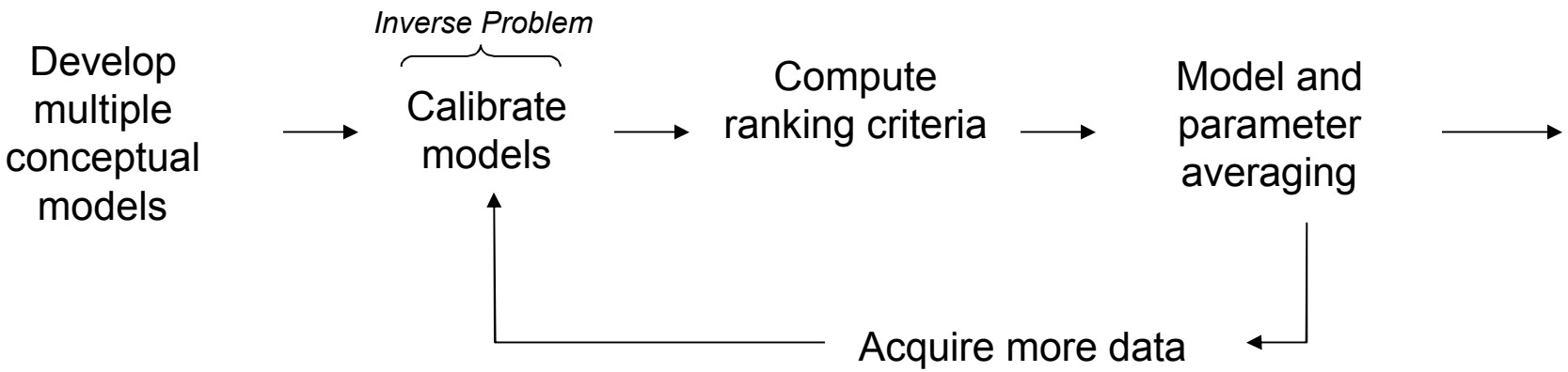
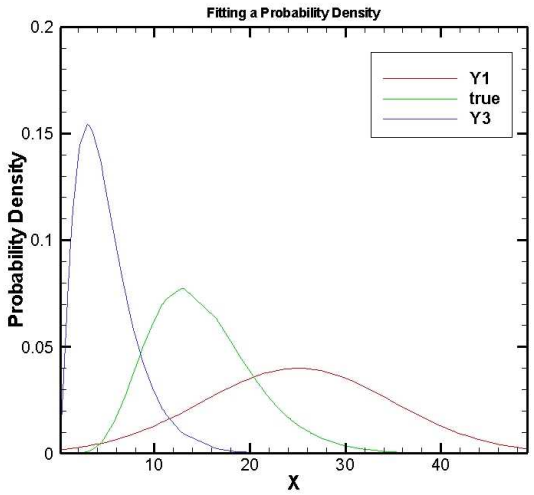
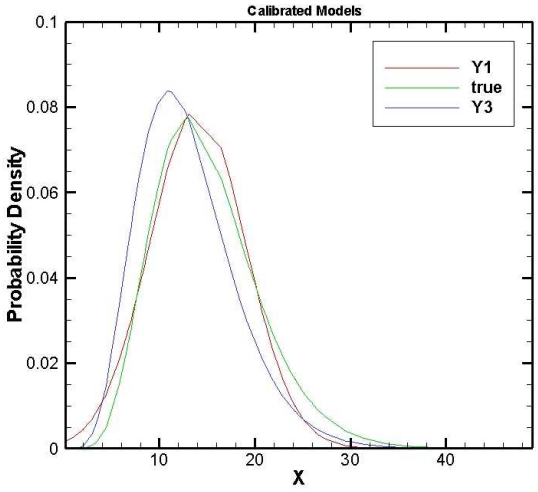
Ranking and Inference Process



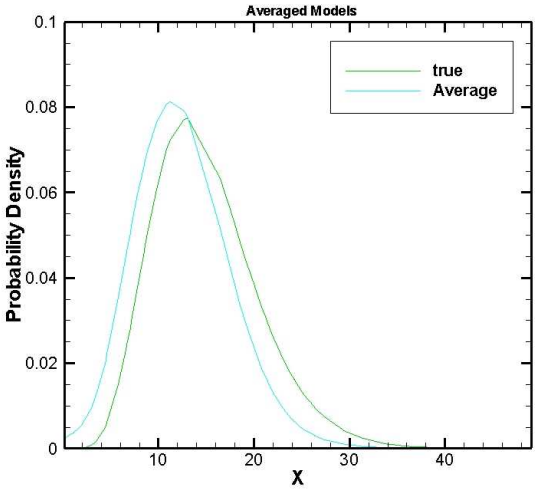
Multiple Models



Calibrated Models



Averaged Models



Questions

1. What if one model is not overwhelmingly best?
2. What if all models show high variability around a prediction?

Then using the best model can result in erroneous predictions

Answer: Multi-model averaging

Multi-Model Averaging

- Compute an estimate of the predicted and parameter values by weighting the model predictions:

$$\hat{\hat{y}} = \sum_{i=1}^{R} w_i \hat{y}_i \qquad \hat{\hat{\beta}}_j = \sum_{j=1}^{R'} w'_j \hat{\beta}_{j,i}$$

- Allows estimation of optimal parameter values and predictions from multiple models
- Can predict multi-model variance
  - Provides bounds on possible parameter values
  - Can compute confidence intervals

Benefits

- Creates a connection between the site characterization and performance assessment teams
- Provides defensible confidence in site understanding and model prediction
- Links data collection with model development
- Lowers investigation and data collection costs
- More efficient (e.g. faster) identification and understanding of the key site structures and processes
- Extensible throughout the entire characterization process

Sandia National Laboratories

Our Team

Thomas Lowry
Scott James
Bill Arnold
Genetha Gray
Matt Grace
Ricardo Garcia
Zach Pickett
Matthew Parno
Michael Ahlman
Joe Kanney

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Simple Example

Excel Example of Thermometer Calibration