BERKELEY LAB
iTOUGH2
Short Course
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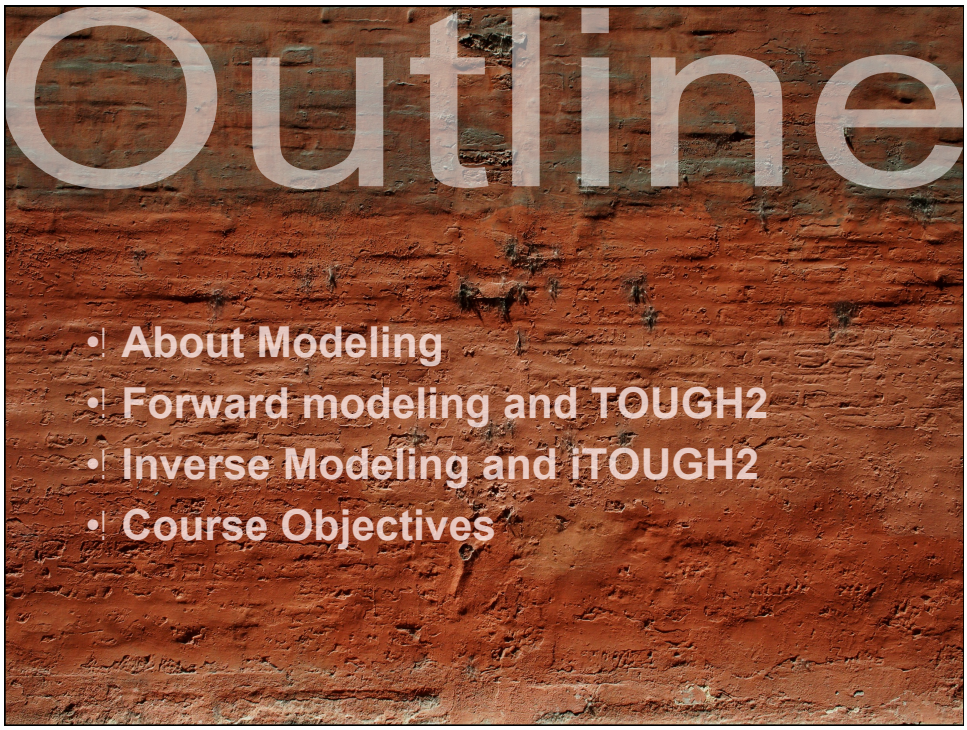
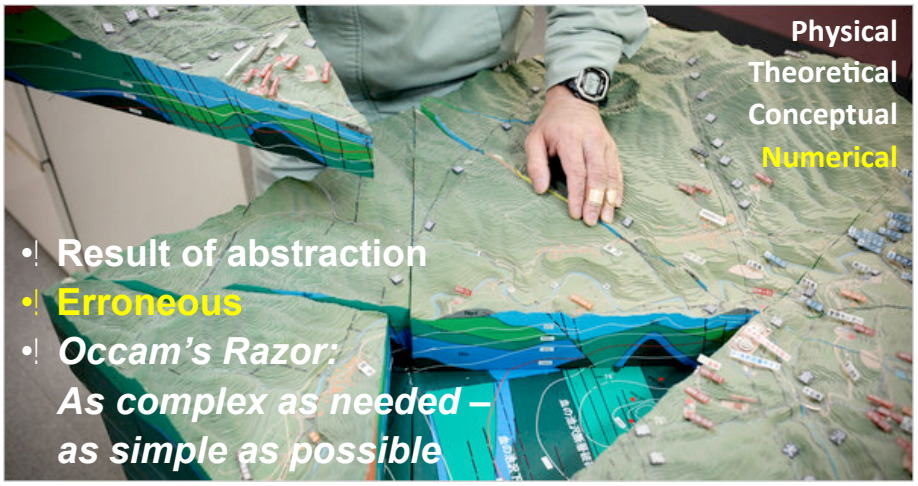

Outline
About Modeling
Forward modeling and TOUGH2
Inverse Modeling and iTOUGH2
Course Objectives

Subsurface models: then and now



"A model of the Yanaizu-Nishiyama geothermal plant. Japan's 18 geothermal plants account for only 0.3 percent of its electricity production."
A. Pollack, Japan's Nuclear Future in the Balance, *New York Times*, May 9, 2011.

A model is…

"… a *purposeful*, *simplified* representation of a real system"

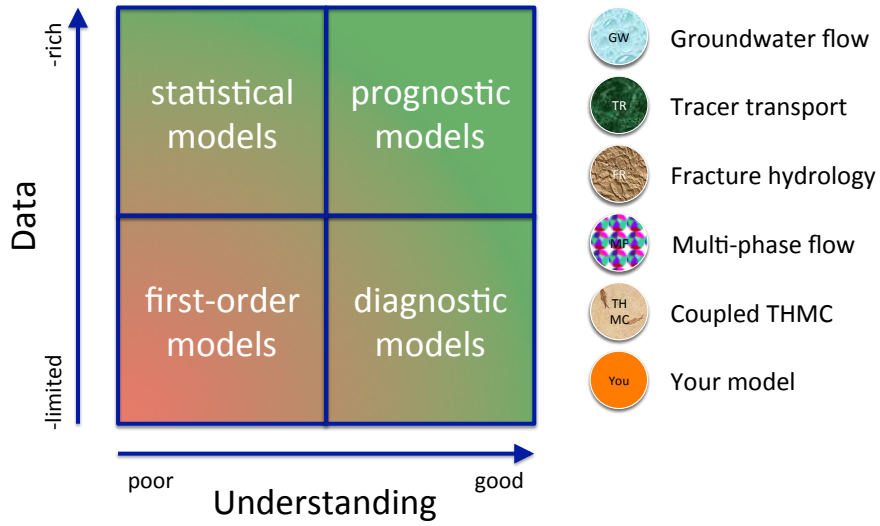
"… a simple worldview with an attitude"

"*simple and with purpose*":
The model is *simple* in that it contains only features of *primary importance* for the *intended use* of the model

Occam's razor
"Non sunt multiplicanda entia praeter necessitatem"

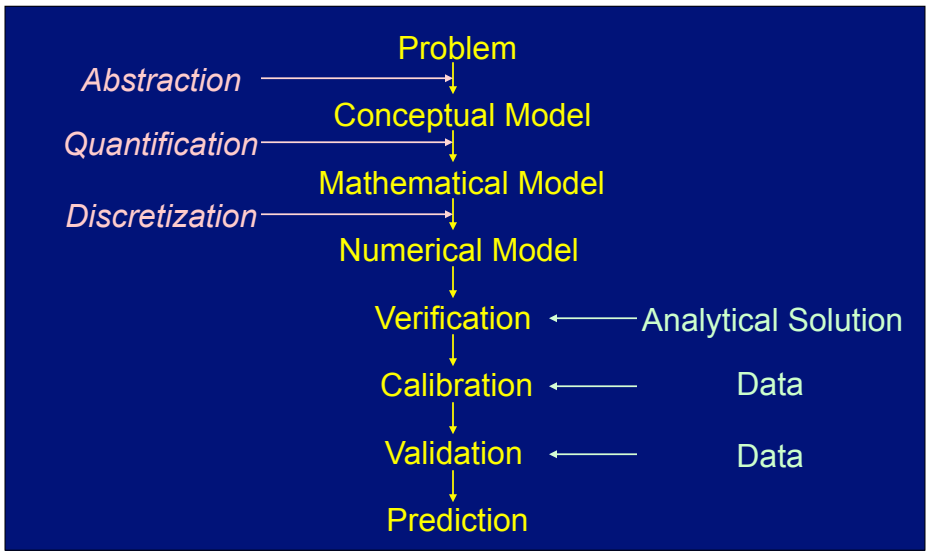
Make it as complex as needed, …
but *keep it as simple as possible!*

System understanding, data availability, and role of modeling



after Holling (1978)

Model Development



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Role of Mathematical Modeling

Improve process understanding — TOUGH2
- Understand nonlinearities/coupled processes
- Evaluate non-observable quantities
- What-if scenarios ("virtual sandbox")

iTOUGH2

Design experiments
- Identify experimental procedure yielding data that contain information about relevant properties

Analyze data
- Determine parameters from data
- Identify model structure

Decision support
- Risk assessment
- Sensitivity analysis

Make predictions
- Deterministic/probabilistic
- Sensitivity analysis

Uncertainty quantification — Optimization

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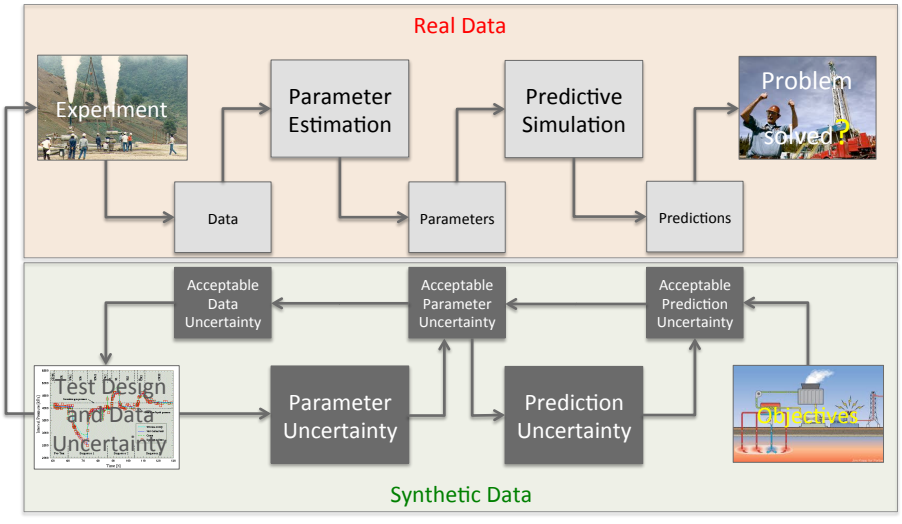
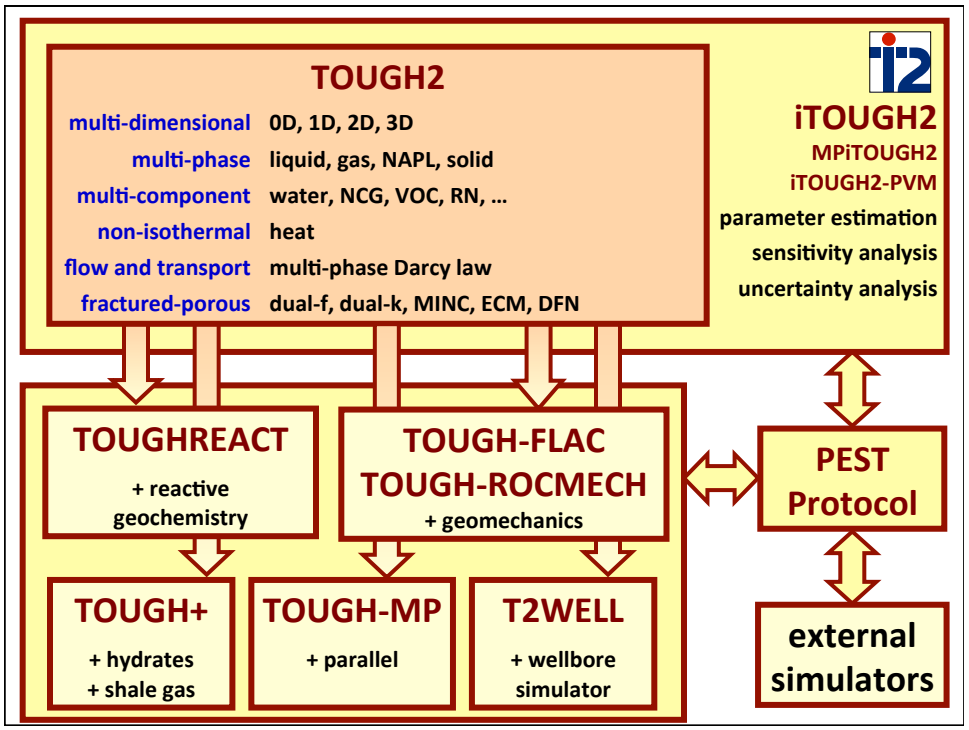
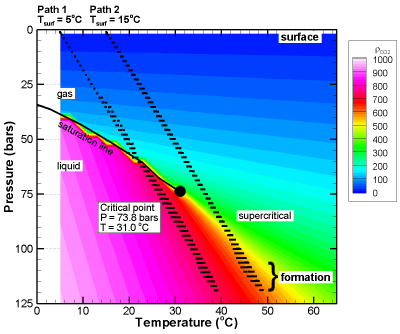
Uncertainty drives your modeling,…

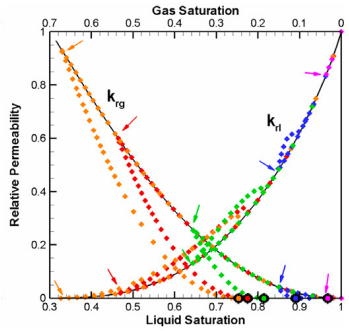


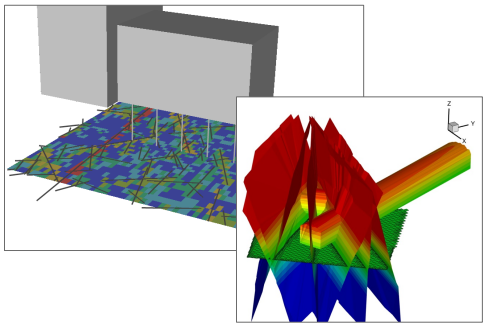
TOUGH
Suite of
Nonisothermal Multiphase Flow
and Transport Simulators


TOUGH2
multi-dimensional 0D, 1D, 2D, 3D
multi-phase liquid, gas, NAPL, solid
multi-component water, NCG, VOC, RN, …
non-isothermal heat
flow and transport multi-phase Darcy law
fractured-porous dual-f, dual-k, MINC, ECM, DFN
iTOUGH2
MPiTOUGH2
iTOUGH2-PVM
parameter estimation
sensitivity analysis
uncertainty analysis
TOUGHREACT
+ reactive geochemistry
TOUGH-FLAC
TOUGH-ROCMECH
+ geomechanics
PEST Protocol
TOUGH+
+ hydrates
+ shale gas
TOUGH-MP
+ parallel
T2WELL
+ wellbore simulator
external simulators

Components κ	Phase β			
	Solid	Fluid		
		Liquid		Gas
		Aqueous	NAPL	
Water	Ice	Liquid water	Water dissolved in NAPL	Water vapor
NCG	-	NCG dissolved in liquid water	NCG dissolved in NAPL	Non-condensible gas
VOC	-	VOC dissolved in liquid water	VOC in NAPL phase	Chem. vapor
Minerals	Grains	Dissolved, Colloids	Dissolved, Colloids	-



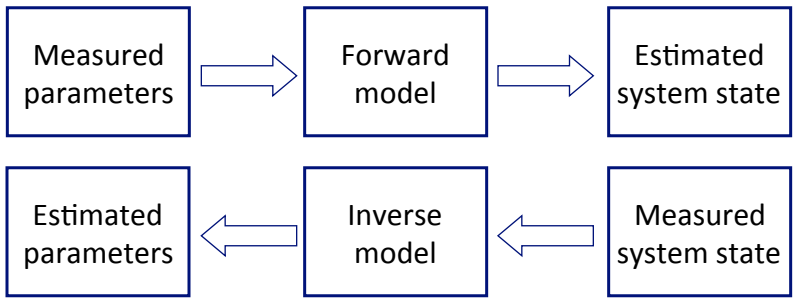




Forward Modeling

p* contains *n* measured parameters (prior information)

z contains calculated system response at *m* calibration points



r contains *m* residuals (**z*** - **z**)

p contains *n* parameters to be estimated

z* contains observations at *m* calibration points

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- Mathematical model G relates parameters **p** to observations **z** $G(\mathbf{p}) = \mathbf{z}$
- Observations have noise:

$$\mathbf{z} = G(\mathbf{p}) + \varepsilon = \mathbf{z}_{true} + \varepsilon$$

- Forward problem: find **z** given **p**
- Inverse problem: find **p** given **z**

$$\mathbf{p} = G^{-g}(\mathbf{z})$$

- Model identification problem: find G given examples of **p** and **z**
- Discrete inverse problem: **z** is a vector of observations at discrete points in space and time ("calibration points")

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- Inverse modeling ≈ parameter estimation ≈ model calibration ≈ history matching ≈ curve fitting ≈ regression (≈ optimization ≈ filtering)
- distinction is largely irrelevant
- preferred terms in different disciplines:
  - inverse problem: generally many parameters; ill-posed; geophysics; imaging; applied mathematics
  - parameter estimation: generally few parameters; well-posed; hydrogeology
  - model calibration: process modeling
  - history matching: reservoir engineering
  - curve fitting: data analysis
  - regression: statistics

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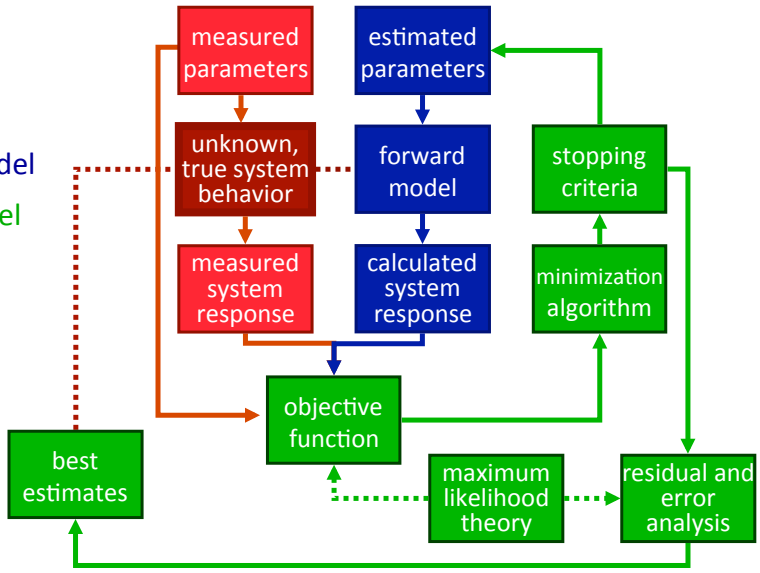
iTOUGH2 flowchart

True system

Data

Forward model

Inverse model



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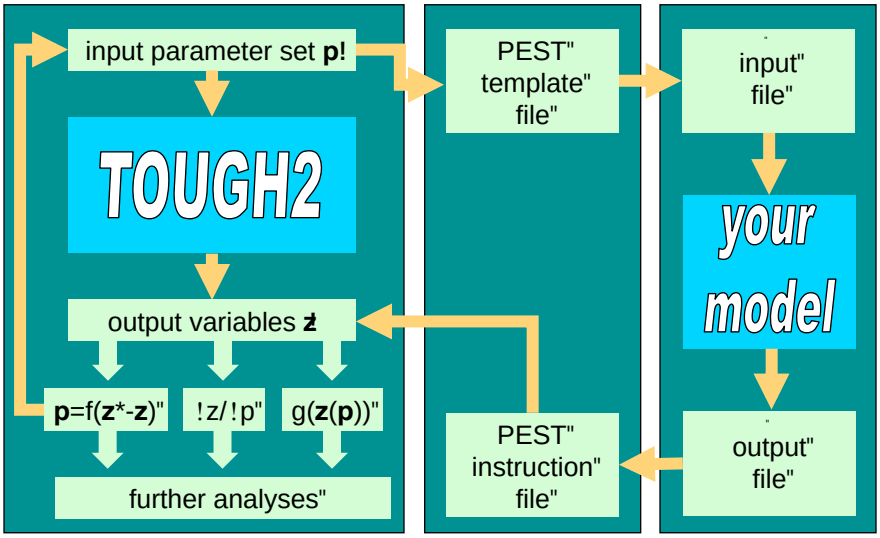
Running TOUGH2 once is tough; running it many times is iTOUGH2



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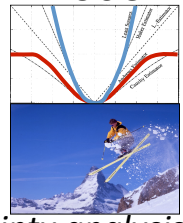
Inverse modeling ingredients

- Parameters **p** — Parameterization
- Data **z*** — Joint inversion
- Forward operator **z**(**p**) — TOUGH2
- Objective function S(**z***-**z**(**p**))
- Minimization algorithm min S(**p**)
- Sanity check S_{min}, σ_p, σ_z *uncertainty analysis*

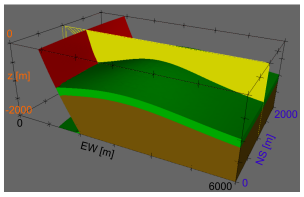


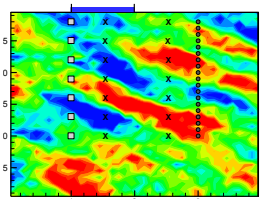
ingredient #1:

parameters

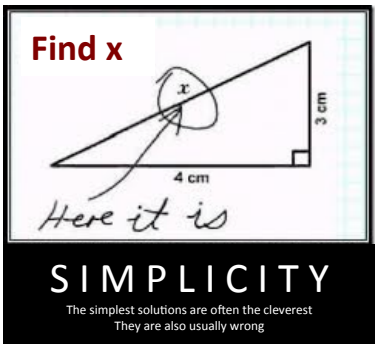
So many parameters…so little (CPU) time!

- Parameterization
  - Properties
  - Structure
  - Forcing terms
  - Conceptual errors
  - Joint estimation of properties, structure, forcing terms, errors





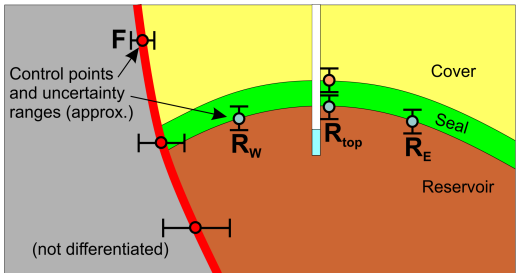
- Occam's razor
  - *as complex as needed – as simple as possible*
  - Start simple and add complexity
  - Start complex and simplify
- Parameter selection
  - Sensitivity
  - Independence
  - Superparameters

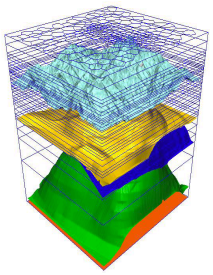


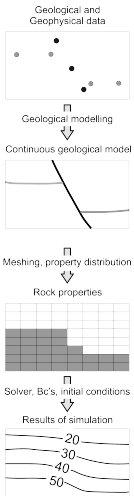
Different models created by different geologists for the same region (Courrioux et al., Experience from 3D cartography training sessions. Implication for uncertainty factors identification. 34th International Geological Congress, August 5-10, 2012, Brisbane, Australia)

Joint analysis of structural and property data reduces estimation and prediction bias

Wellmann et al., *C&G* (2014)







- Parameterize geologic structure at control points
- Develop integrated workflow from structural geologic data to discretized reservoir model
- Jointly estimate structural geometry and reservoir properties

Want more parameters?
Give me more data!

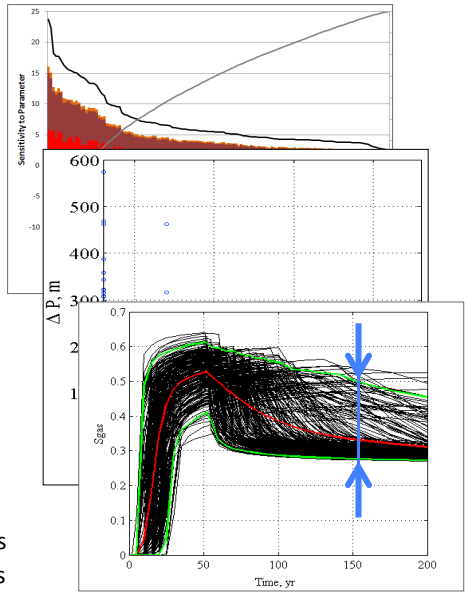
The more
high-quality,
sensitive,
complementary,
consistent
data, the better

mixing ingredients #1 and #2:

sensitivity analysis

Going global with sensitivity analysis

- Local sensitivity analysis
  - Requires (only) *n*+1 (parallel) runs
  - By-product of derivative-based minimization algorithms
  - Many useful composite measures on parameter influence and data worth
- Morris One-At-A-Time
  - Requires *r*(*n*+1) runs
  - Identifies influential and non-influential parameters
  - Identifies nonlinearity and interaction effects
- Sobol'/total sensitivity indices
  - variance/sampling based
  - Identifies contribution of uncertain parameter to prediction uncertainty
  - Fix one parameter – vary all the others
  - Vary one parameter – fix all the others

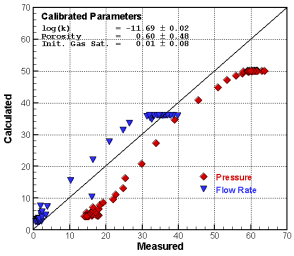


ingredient #3:

objective function

heteroscedastic

$$\tilde{z}(z;\,!) = \begin{cases} \dfrac{(z' \,!\, 1)}{!\;\; g'^{!1}} & \text{if } ! \neq 0 \\ g\;\ln(z) & \text{if } ! = 0 \end{cases}$$

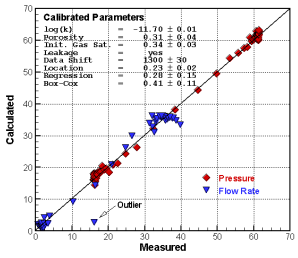


autocorrelated

$$\tilde{r}_i = \begin{cases} r_1\sqrt{(1 \,!\, !^2)} & \text{if } i = 1 \\ r_i \,!\, ! \;\; r_{i!1} & \text{if } i = 2, \ldots, m \end{cases}$$

skewed and heavy-tailed

$$p(r_i \mid !,\;\;) = \frac{2\#_{\,!}}{! + !^{-1}} \quad \exp\left\{-c_\beta \left| r_{i,t} \right|^{2/(1+\beta)}\right\}$$



concurrently estimate *statistical* parameters
β, λ, ρ, ξ

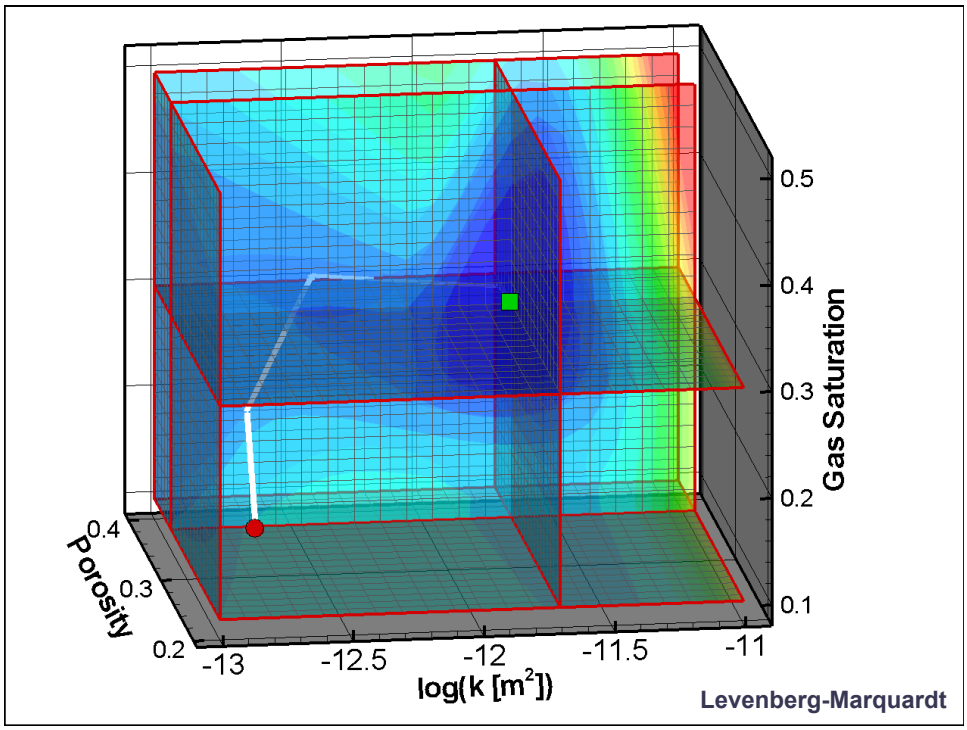
Schoups and Vrugt, *WRR*, 2010; Finsterle and Zhang, *C&G*, 2011

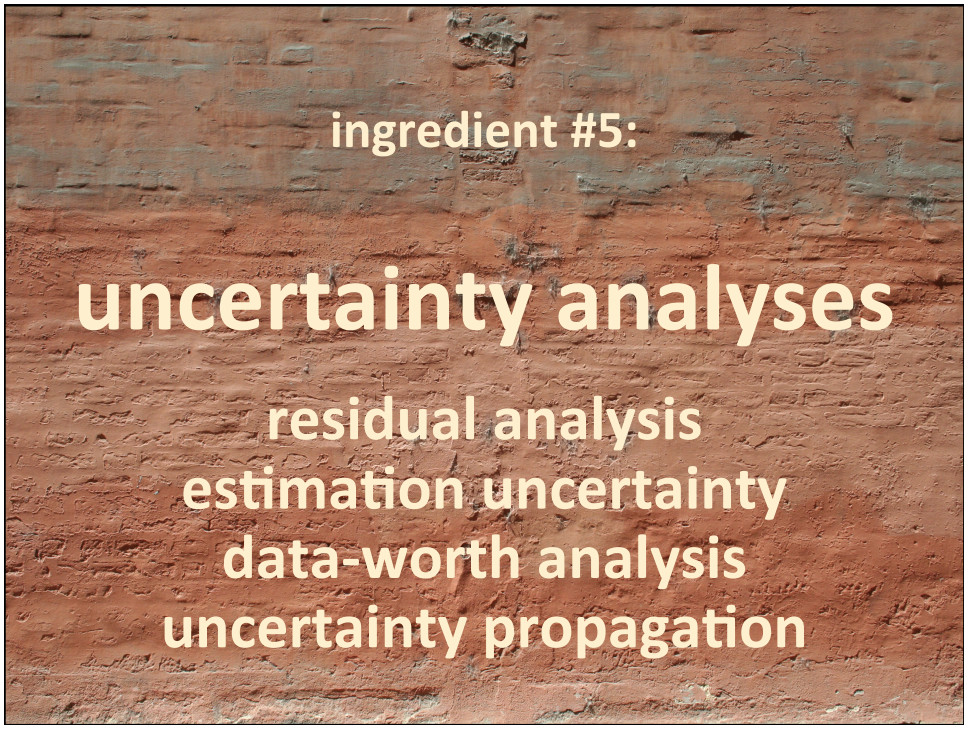
ingredient #4:

minimization algorithm

Derivative-Based Minimization Algorithms

Harmony Search
Swarm Optimization
Evolutionary Algorithms
Simulated Annealing


0.5
0.4
0.3
0.2
0.1
Gas Saturation
0.4
0.3
0.2
Porosity
-13
-12.5
-12
-11.5
-11
log(k [m²])
Levenberg-Marquardt



Why residual and uncertainty analysis?

- Parameter estimates may be worthless if:
  - Model does not match the data, i.e., is an unlikely representation of the true system
    goodness-of-fit, Fisher Model Test
  - Estimates are biased by systematic errors or outliers in the data
    residual analysis
  - Estimation uncertainty is large
    C_{pp}, *correlation coefficients*
  - Solution is *non-unique* or *unstable*
  - Predictions are highly *uncertain*

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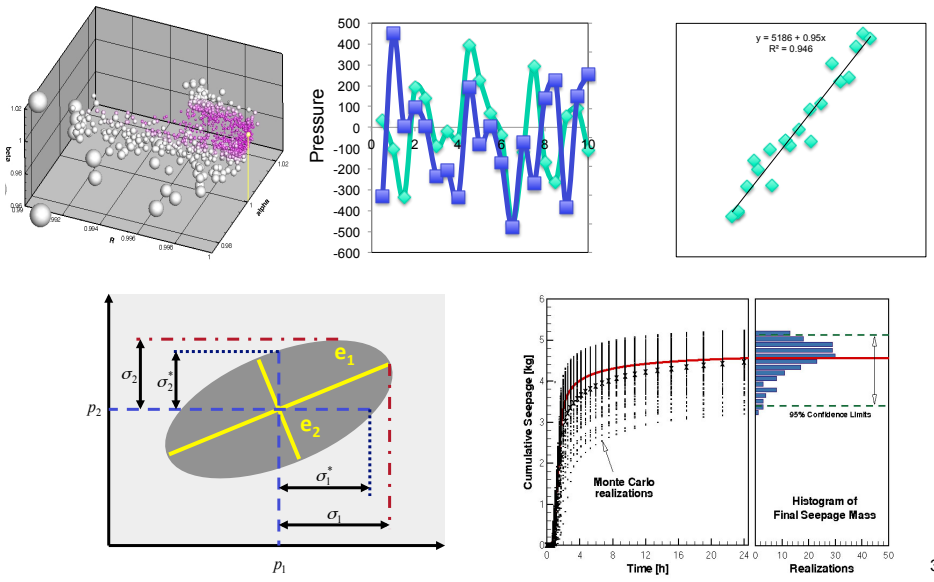
Residual and Uncertainty Analysis



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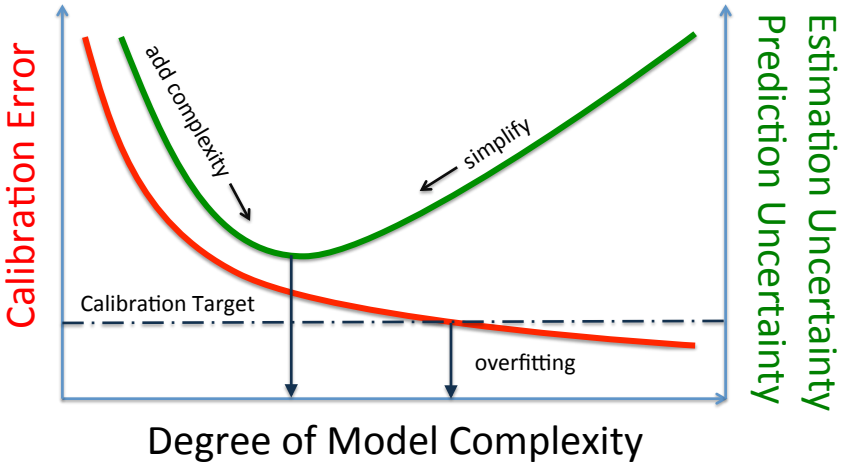
Occam's Razor - sharpened!



Success Criteria

- Captures salient features of system behavior (expert judgment)
- Acceptable match (goodness-of-fit criteria)
- Acceptable estimation uncertainty (determinant of estimation covariance matrix)
- Ability to make acceptable predictions (validation acceptance criteria)
- Combination (model identification criteria)

➢ Depends on study objectives

➢ Use as criteria for test design!

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Textbooks

- Aster et al., *Parameter Estimation and Inverse Problems*, 2nd, Ed., Academic Press, 2013.
- Hill and Tiedeman, *Effective Groundwater Model Calibration, With Analysis of Data, Sensitivities, Predictions, and Uncertainty*, Wiley, 2007.
- Saltelli et al., *Global Sensitivity Analysis, The Primer*, Wiley, 2008.
- …

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Course Objectives

- **General:** Provide participants with *conceptual understanding*, *theoretical background*, and *practical experience* in solving simulation-*optimization* problems in geosciences and engineering using *iTOUGH2*.
- **Lectures:** Understand optimization and uncertainty quantification:
  - Fundamental concepts
  - Theoretical basis
  - Practical approaches
  - Interactive discussions
- **Computer Exercises:** Gain experience using iTOUGH2
- **Course Project:** Define and develop a simulation-optimization problem of interest to you

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iTOUGH2 Short Course

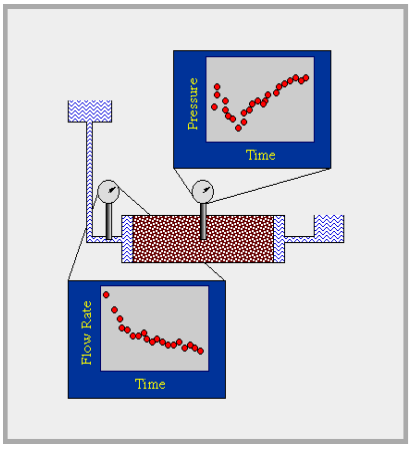
Lawrence Berkeley National Laboratory
Earth Sciences Division
Berkeley, California

Computer Exercises: Overview

Darcy
Polynomial
CO_2 Injection Test Design
Five-Spot Geothermal Injection-Production
Standard Test Set
Project

Tutorial Problem: Darcy

- Objectives:
  - Understand main iTOUGH2 concepts
  - Get familiar with key iTOUGH2 input blocks
  - Get familiar with iTOUGH2 output file
  - Examines impact of measurement noise on estimates
  - Requires some knowledge of TOUGH2 simulator
- Parameter Estimation Problem:
  - Estimate 3 parameters…
  - …based on transient pressure and flow-rate data…
  - …using Levenberg-Marquardt minimization algorithm



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Variations of Darcy Problem

- darcy1i: run forward problem
- darcy2i: inversion with perfect data (*nonoise.dat*)
- darcy3i: inversion with noisy data (*noisy.dat*)
- darcy4i: explore
- darcy5i: grid search
- darcy6i: Morris global sensitivity analysis
- darcy7i: Saltelli/Sobol' global sensitivity analysis
- darcy8i: Monte Carlo (LHS) uncertainty quantification

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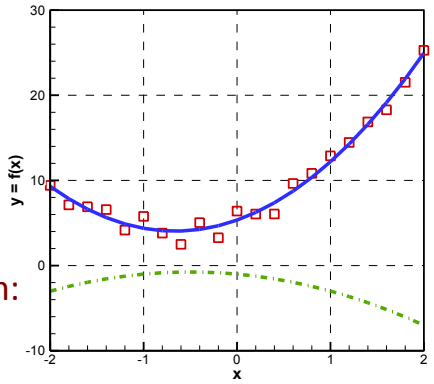
iTOUGH2-PEST Tutorial Problem: Polynomial

- Objectives:
  - Understand main iTOUGH2 concepts
  - *Get familiar with PEST protocol*
  - Get familiar with key iTOUGH2 input blocks
  - Get familiar with iTOUGH2 output file
- Parameter Estimation Problem:
  - Estimate coefficients of polynomial…
  - …using Levenberg-Marquardt minimization algorithm

$$y(x) = \sum_{i=0}^{n} a_i \cdot x^i$$



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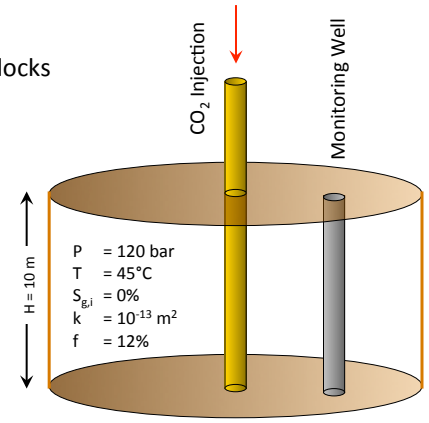
Tutorial Problem: CO_2 Injection

- Objectives:
  - Understand main iTOUGH2 concepts
  - Get familiar with key iTOUGH2 input blocks
  - Get familiar with iTOUGH2 output file
  - Requires some knowledge of TOUGH2 simulator (module ECO2N)
- Analyses performed:
  - Forward simulation
  - Sensitivity analysis
  - Data inversion
  - Uncertainty propagation analysis



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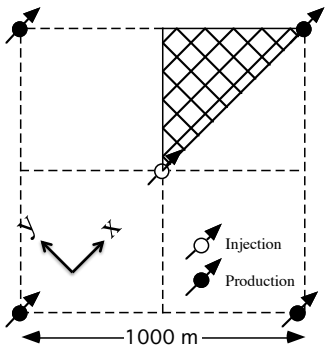
Five-Spot Geothermal Injection-Production Problem

- Objectives:
  - Understand main iTOUGH2 concepts
  - Get familiar with key iTOUGH2 input blocks/ commands and output files
  - Requires some knowledge of TOUGH2 simulator (module EOS1)
- Exercises:
  1. TOUGH2 simulation with iTOUGH2
  2. Generation of synthetic data
  3. Defining parameters and performing sensitivity analysis
  4. Inversion of synthetic data
  5. Uncertainty propagation analysis
  6. Explore



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Standard iTOUGH2 Samples and Installation Test Cases

- sample1-7: see report *iTOUGH2 Sample Problems*
- sampleLOCAL: local minimization algorithms
- sampleGLOBAL: global minimization algorithms
- sampleGS: user-specified sets (eos7c)
- sampleGSLIB: geostatistics
- sampleMOAT: Morris global sensitivity analysis
- samplePARALLEL: parallel execution
- samplePARETO: Pareto frontier using iTOUGH2-PEST
- sampleREGION: Permeability region

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Formulate Optimization Problems

Parameters	Observations	Objective Function
Problem A:		
Problem B:		

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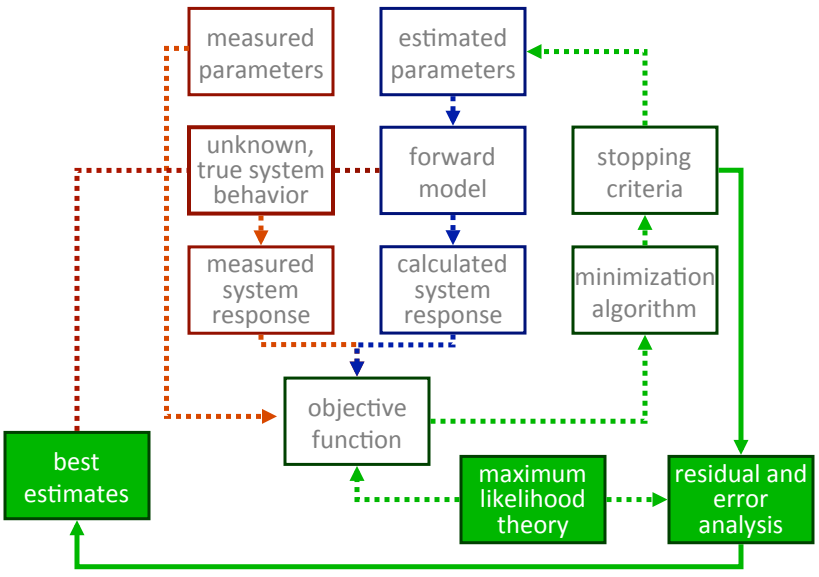
Residual Analysis

1



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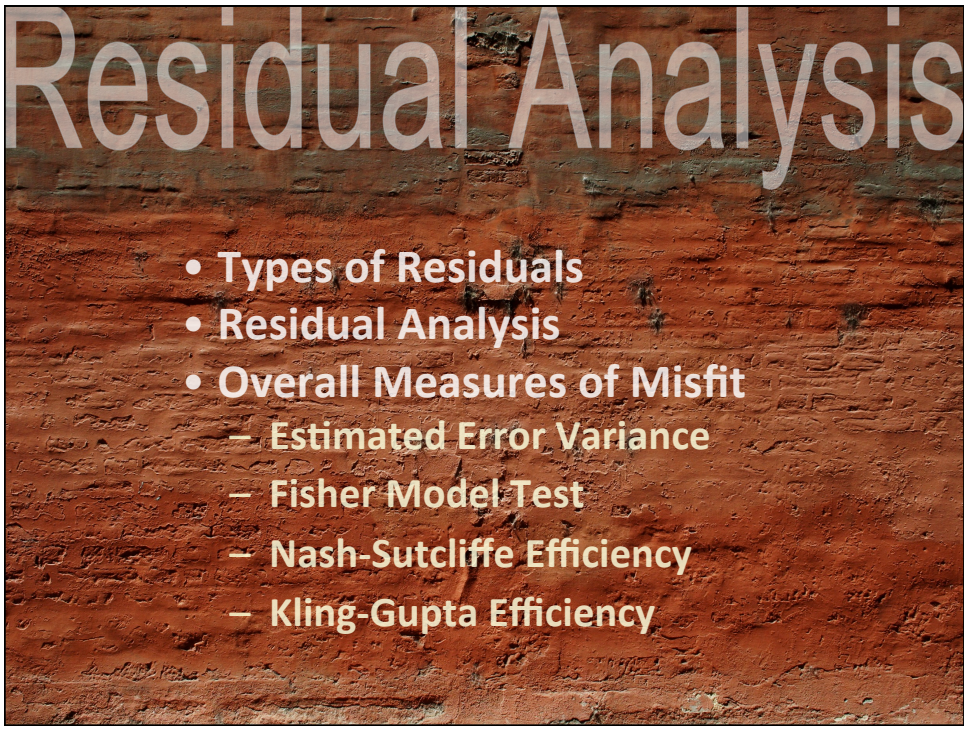
Why Residual and Uncertainty Analysis?

- Parameter estimates may be worthless if:
  - Model with optimized parameter does not match the data, i.e., it is an unlikely representation of the true system
    goodness-of-fit, Fisher Model Test
  - Estimates are biased by systematic errors or outliers in the data
    residual analysis
  - Estimation uncertainty is large
    C_{pp}, *correlation coefficients*
  - Solution is *non-unique* or *unstable*

3



Type of Residuals: Systematic

- Systematic error in data:
  - Data conversion error: factor, shift, drift
  - Experimental error: leak, forcing term
- Systematic error in model:
  - Inadequate process description
  - Inadequate parameterization
  - Inadequate model structure
- *Contain information* about parameters of interest
  - A function of parameters.
- *Inconsistency* between real system and its model representation
- If systematic residuals persist *after* inversion, adjust experiment *or* model!

5

Type of Residuals: Random

- Errors in stochastic model
  - Distributional assumption
  - Heteroscedasticity: non-uniform variance
  - Correlations
- Reducing errors in stochastic model
  - Analyze residuals
  - Use appropriate transformations
  - Include correlations
  - Use robust estimators

$$\tilde{z}(z;\lambda)=\begin{cases}\dfrac{(z^{\lambda}-1)}{\lambda\cdot g^{\lambda-1}} & \textbf{if } \lambda\neq 0\\ g\cdot\ln(z) & \textbf{if } \lambda=0\end{cases}$$

$$\tilde{r}_i=\begin{cases}r_1\sqrt{(1-\rho^2)} & \textbf{if } i=1\\ r_i-\rho\cdot r_{i-1} & \textbf{if } i=2,\ldots,m\end{cases}$$

$$\hat{r}=\begin{cases}1-\cos(\tilde{r}/c) & \textbf{if } |\tilde{\mathbf{r}}|\leq \mathbf{c}\pi\\ 2 & \textbf{if } |\tilde{r}|>\mathbf{c}\pi\end{cases}$$

6

Steps of Residual Analysis

① Plot the residual
→ look for randomness

② Standard statistics (mean, median, skewness, kurtosis)
→ look for symmetry

③ Regression analysis on measure vs. calculated
→ look for zero intercept, unit slope, and unit Pearson's *R* (coefficient of determination)

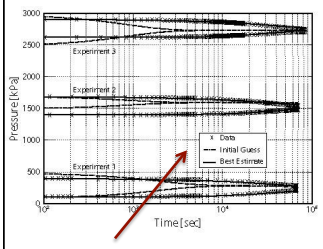
④ Fisher, Nash-Sutcliffe and Kling-Gupta efficiency criteria
→ close to 1

⑤ Runs statistics
→ Statistically tests number of positive and negative runs in residuals

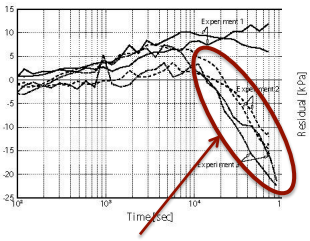
7

Remedies

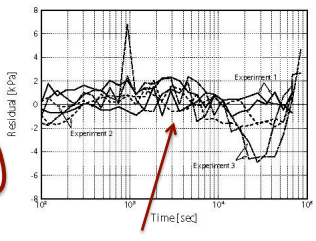
- Residuals should be *random*
- Trends and patterns in residuals indicate *systematic errors*
- Try to *remove systematic errors* by:
  - Refining the functional model
  - Correcting systematic data errors
  - Parameterizing and estimating conceptual model elements
  - Parameterizing and estimating measurement errors



Perfect match between data and model



Systematic errors from gas leakage



Random residuals after gas leakage is explicitly modeled

8

Covariance Matrices

- *A priori* error variance (assumed 1.0): σ_0^2
- *A priori* covariance matrix of observations: $\mathbf{C}_{zz} = \sigma_0^2 \cdot \mathbf{V}_{zz}$
- *A posteriori* error variance: $s_0^2 = \frac{\mathbf{r}^T \mathbf{C}_{zz}^{-1} \mathbf{r}}{m-n}$
- Covariance matrix of estimated parameters:

$$\mathbf{C}_{pp} = s_0^2 \left(\mathbf{J}^T \mathbf{C}_{zz}^{-1} \mathbf{J} \right)^{-1}$$

- Covariance matrix of calculated observation: $\mathbf{C}_{\hat{z}\hat{z}} = \mathbf{J}^T \mathbf{C}_{pp} \mathbf{J}$
- Covariance matrix of residuals: $\mathbf{C}_{rr} = \mathbf{C}_{zz} - \mathbf{C}_{\hat{z}\hat{z}}$
- *i*th diagonal element of covariance matrix: $\sigma_{z_i}^2, \sigma_{\hat{z}_i}^2, \sigma_{r_i}^2$

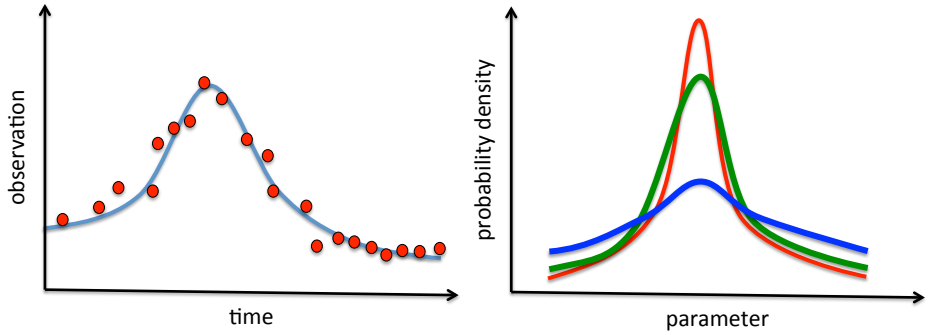
9

Residual Analysis Output in iTOUGH2

- The following are tabulated in the output file (*.out).
  - `RESIDUAL:` $r_i = z_i^* - z_i$
  - `C.O.F.:` Relative contribution [%] to objective function
  - `STD. DEV.:` *A posteriori* standard deviation of calculated system response $\mathbf{C}_{\hat{z}\hat{z}} = \mathbf{J}^T \mathbf{C}_{pp} \mathbf{J}$
  - `Yi:` Local reliability or influence ➔ $y_i = 1 - \left(\sigma_{\hat{z}_i} / \sigma_{z_i} \right)^2$
    Observations with y_i < 0.25 are poorly controlled
  - `Wi:` Studentized residual ➔ $w_i = r_i / \sigma_{r_i}$
    Potential outlier if $\text{abs}(w_i) > u(0.95) = 1.96$
  - `IOD:` Relative impact [%] of omitting observation based on D-optimality criterion (“data-worth analysis”)

10

Evaluate the worth of data points
- without having data!



$$\text{rel. data worth} = \frac{\det(\mathbf{C}_{pp}) - \det(\mathbf{c}_{pp})}{\det(\mathbf{C}_{pp})}$$

$$\mathbf{C}_{pp} = s_0^2 \left(\mathbf{J}^T \mathbf{C}_{zz}^{-1} \mathbf{J} \right)^{-1}$$

$$\mathbf{c}_{pp} = s_0^2 \left(\mathbf{j}^T \mathbf{c}_{zz}^{-1} \mathbf{j} \right)^{-1}$$

Example: darcy3i

```
*********************
 RESIDUAL ANALYSIS
*********************

[ … Description for the columns of the table … ]

------------------------------------------------------------------------
   #  OBSERVATION    AT TIME [min]     MEASURED     COMPUTED     RESIDUAL
------------------------------------------------------------------------
   1  log(abs. perm.)             -0.12000E+02 -0.11687E+02 -0.31333E+00 }
   2  Porosity                     0.25000E+00  0.37257E+00 -0.12257E+00 } prior info
   3  Initial gas sat              0.10250E+02  0.10291E+02 -0.41477E-01 }
   4  Pressure 1/2    0.50000E+00  0.10370E+06  0.10367E+06  0.35837E+02
   6  Pressure 1/2    0.10000E+01  0.10317E+06  0.10327E+06 -0.10851E+03  [cont...]
   8  Pressure 1/2    0.15000E+01  0.10257E+06  0.10291E+06 -0.33246E+03

[ … Repeated for all observations … ]
```

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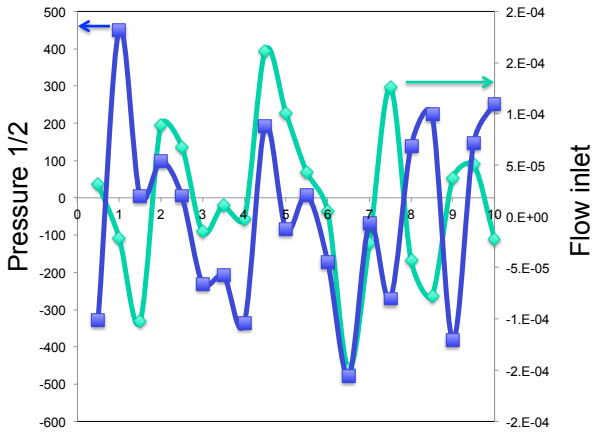
Example: darcy3i



Appear random, with no clear trend in the data

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Summary Statistics

- `MEAN`: mean of the residual (should be close to zero)
- `STD. DEV.`: standard deviation (should be consistent with stochastic model, i.e., *a priori* defined standard deviations)
- `M/S`: Ratio of mean and standard deviation; indicates whether mean (bias) is significant (should be small)
- `SKEWNESS`: Degree of asymmetry of residuals (should be 0)
- `KURTOSIS`: Relative peakedness of distribution (should be 0)

$$SKEW = \frac{1}{m}\sum_{i=1}^{m}\left(\frac{r_i - \bar{r}}{SDEV}\right)^3 \qquad KURT = \frac{1}{m}\sum_{i=1}^{m}\left(\frac{r_i - \bar{r}}{SDEV}\right)^4 - 3$$

Note: statistical measures may not be robust for small data sets

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Summary Statistics

- `MEDIAN`: median of the residuals (should be close to 0)

$$\hat{r} = \begin{cases} r_{(m+1)/2} & \text{odd } m \\ 0.5r_{m/2} + r_{m/2+1} & \text{even } m \end{cases}$$

- `AVE. DEV.`: Mean absolute deviation (should be close to 0)

$$ADEV = \frac{1}{m}\sum_{i=1}^{m}\left|r_i - \hat{r}\right|$$

- Large differences between median and mean and between standard deviation and average deviation indicate robustness issue

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Example: darcy3i

```
Summary of Residual Analysis
----------------------------
Max weighted residual at observation    :             28
Max weighted residual                   :    -0.2300E+01
Max residual                            :    -0.4600E+03
Number of poorly controlled observations:              0
Number of large normalized residuals    :              3
Max normalized residual at observation  :             28
Max normalized residual                 :           2.40
Probable size of maximum error          :     0.5021E+03

[ ... Some iteration statistics ... ]

Control Measures
----------------
Trace (P*QLL) : n   =   3               :     0.3000E+01
Sum   (Yi)    : m-n =  37               :     0.3700E+02

Objective Function                                        C.O.F.
------------------
Initial value of objective function     :     0.5208E+03    1210.52 %
Minimum value of objective function     :     0.4303E+02     100.00 %
```

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Example: darcy3i

[… Summary statistics for each dataset …]

```
========================================================================
DATASET              DATAPOINTS          MEAN       MEDIAN    STD. DEV.
------------------------------------------------------------------------
Pressure 1/2      [Pa]       20    -0.137E+02   -0.287E+02    0.210E+03
Flow inlet        [kg/sec]   20    -0.708E-06    0.628E-05    0.898E-04
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
ALL RESIDUALS     WEIGHTED   43    -0.359E-01   -0.000E+00    0.101E+01
========================================================================
```

Consistent with measurement noise added to data in *nonoise.dat* to create *noise.dat*

[… Summary statistics for each datatype …]

```
========================================================================
DATATYPE             DATAPOINTS          MEAN       MEDIAN    STD. DEV.
------------------------------------------------------------------------
PRESSURE          [Pa]       20    -0.137E+02   -0.287E+02    0.210E+03
FLOW RATE         [kg/sec]   20    -0.708E-06    0.628E-05    0.898E-04
========================================================================
```

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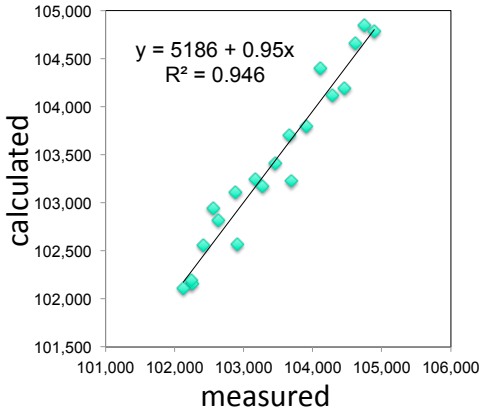
Linear Regression Analysis

- INTERCEPT (should be 0)
- SLOPE (should be 1)
- R: coefficient of determination (should be 1)
- NSE: Nash-Sutcliffe Efficiency (should be 1)
- KGE: Kling-Gupta Efficiency (should be 1)
- GAMMAi: Contribution of correlation error, variability error and bias error to the total error



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Nash-Sutcliffe Efficiency (*NSE*)

- A normalized model performance criterion, with observed mean as baseline

$$NSE = 1 - \frac{\sum_{i=1}^{m}(z_i - z_i^*)^2}{\sum_{i=1}^{m}(z_i^* - \mu_{obs})^2} = 1 - \frac{(\mathbf{r}^T\mathbf{r})/m}{\sigma_{obs}^2}$$

- Popular criterion in hydrology
- *NSE* ≤ 1; ideal value: *NSE* = 1
  → *NSE* can be used as objective function to be maximized
- If *NSE* ≤ 0, the model is not a better predictor than using the observed mean
- Decomposition: *NSE* = *A* – *B* – *C*

$A = R^2$: Correlation between *z*(**p**) and *z**

$B = [R - (\sigma_{calc}/\sigma_{obs})]^2$: Variability

$C = [(\mu_{calc} - \mu_{obs})/\sigma_{obs})]^2$: Bias

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Nash-Sutcliffe Efficiency (*NSE*)

- Decomposition helps examine the different components of the residuals
- Murphy (1988) : $NSE = A - B - C$

  $A = R^2$: Correlation between *z*(**p**) and *z**

  $B = [R - (\sigma_{calc}/\sigma_{obs})]^2$: Conditional bias

  $C = [(\mu_{calc} - \mu_{obs})/\sigma_{obs})]^2$: Unconditional bias

- Gupta (2009) : $NSE = 2\alpha R - \alpha^2 - \beta^2$

  R : Correlation between *z*(**p**) and *z**

  $\alpha = (\sigma_{calc}/\sigma_{obs})$: Relative variability

  $\beta = (\mu_{calc}/\mu_{obs})$: Relative bias

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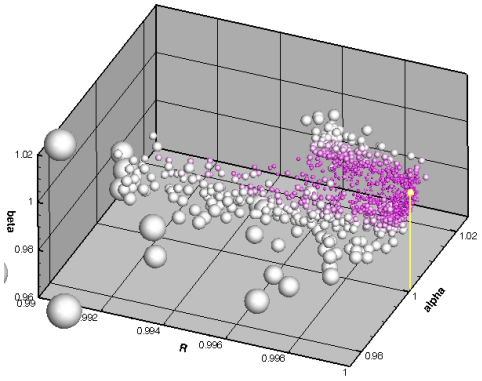
Kling-Gupta Efficiency (*KGE*)

- Reweights different components derived from the decomposed *NSE*
- Measures Euclidian distance from ideal point:
  $R = 1, \quad \alpha = 1, \quad \beta = 1$
- *KGE* ≤ 1
  ideal value: *KGE* = 1
  → *KGE* can be used as a multi-objective calibration criterion to be maximized

$$KGE = 1 - \sqrt{(R-1)^2 + (\alpha-1)^2 + (\beta-1)^2}$$



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Kling-Gupta Efficiency (*KGE*)

- Relative contribution of the 3 components:

$$\Gamma_i = \frac{G_i}{G_1 + G_2 + G_3}$$

where

$$G_1 = (R-1)^2$$
$$G_2 = (\alpha-1)^2$$
$$G_3 = (\beta-1)^2$$

- For more information:
  Gupta et al., *Journal of Hydrology*, *377*, 80 - 91, 2009

22

Example: darcy3i

```
Linear Regression Analysis of Calculated Versus Observed Data ...
-------------------------------------------------------------

============================================================
DATASET              DATAPOINTS     INTERCEPT       SLOPE
------------------------------------------------------------
Pressure 1/2      [Pa]       20     0.506E+04   0.951E+00
Flow inlet        [kg/sec]   20    -0.884E-05   0.985E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
ALL               WEIGHTED   40     0.366E+00   0.100E+01
============================================================


=====================================================================
       R      NSE          KGE      GAMMA1      GAMMA2      GAMMA3
---------------------------------------------------------------------
0.973       0.943       0.964       0.590       0.410       0.000
0.869       0.755       0.824       0.554       0.446       0.000
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1.000       1.000       1.000       0.000       0.512       0.488
=====================================================+===============
```

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Estimated Error Variance s_0^2

- The *estimated error variance*
  - a posteriori error variance
  - an aggregate measure of *goodness-of-fit*
  - represents the *mean weighted residual*

$$s_0^2 = \frac{\mathbf{r}^T \mathbf{C}_{zz}^{-1} \mathbf{r}}{m - n}$$

r : residual
$\mathbf{C}_{zz}$: observation covariance matrix
m : number of observations
n : number of parameters

- If *a priori* assumptions about the residuals (expressed through matrix $\mathbf{C}_{zz}$) were reasonable, then s_0^2 / σ_0^2 is close to 1: Fisher Model Test
- Recall: Solving a weighted least-squares problem minimizes the estimated error variance

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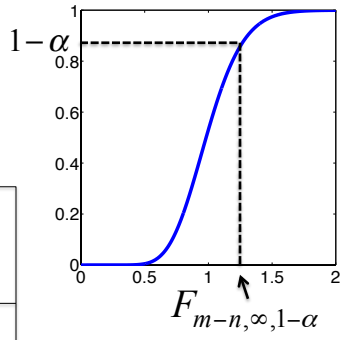
Fisher Model Test

- The ratio s_0^2/σ_0^2 is a random variable following an *F*-distribution
- $F_{m-n,\infty,1-\alpha}$ is the inverse of the cumulative *F*-distribution for 1-α



$s_0^2/\sigma_0^2 > F_{m-n,\infty,1-\alpha}$

Error in functional or stochastic model

$1 \le s_0^2/\sigma_0^2 \le F_{m-n,\infty,1-\alpha}$

Model test passed!

$s_0^2/\sigma_0^2 \le 1$

Error in stochastic model or "overfitting"

- Only meaningful if a reliable stochastic model is available

25

Example: darcy3i vs. darcy4i

```
Fisher Model Test
-----------------
```

noisy.dat

```
Root mean square error              : 0.1078E+01
Estimated error variance            : 0.1163E+01
Variance used for error analysis    : 0.1187E+01 (a posteriori variance)
Nash-Sutcliffe efficiency criterion :     1.0000
Degree of freedom                   :         37 (no prior information)
Confidence level (1-alpha)          :       95.0 [%]
Lucky you                           : Model test successful!
                                      --> Estimated error variance is used!
Fisher model test criterion         :       1.41 (F-distribution)
Factor for confidence bands         :       2.03 (t-distribution)
Factor for confidence regions       :       2.91 (chi-square distribution)
```

noisier.dat

```
Root mean square error              : 0.3183E+01
Estimated error variance            : 0.1013E+02
Variance used for error analysis    : 0.1013E+02 (a posteriori variance)
Nash-Sutcliffe efficiency criterion :     0.9999
Degree of freedom                   :         37 (no prior information)
Confidence level (1-alpha)          :       95.0 [%]
Warning                             : Model test failed!
                                      --> Estimated error variance is used!
Fisher model test criterion         :       1.41 (F-distribution)
Factor for confidence bands         :       2.03 (t-distribution)
Factor for confidence regions       :       2.91 (chi-square distribution)
```

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Model Identification Criteria

- Criteria to allow comparison of different inversions
  - Different data sets, parameters, or conceptual models
- Goodness of fit (s_0)
  - Not appropriate since adding more parameters always improves the fit (risk of overparameterization)
- Optimality criteria: A: trace($\mathbf{C}_{pp}$) E: max eig($\mathbf{C}_{pp}$) D: det($\mathbf{C}_{pp}$)
- Akaike Information Criterion

$$AIC = (m-n)s_0^2 + \ln|\mathbf{C}_{zz}| + m\ln(2\pi) + 2n$$

- Akaike's Bayesian Information Criterion

$$AIC = (m-n)s_0^2 + \ln|\mathbf{C}_{zz}| + m\ln(2\pi) + \ln|\mathbf{J}^T\mathbf{C}_{zz}^{-1}\mathbf{J}|$$

- Kashyap Criterion

$$d_k^* = (m-n)s_0^2 + \ln|\mathbf{C}_{zz}| + m\ln(2\pi) + n\ln(m/2\pi) + \ln|\mathbf{J}^T\mathbf{C}_{zz}^{-1}\mathbf{J}|$$

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Example: darcy3/4i

$$c_{ij}^* = \frac{c_{ij}}{p_i p_j}$$

```
Optimality Criteria  [noisy.dat]              unscaled          scaled
-------------------
D-optimality = det(Cpp)              :      0.2622E-12      0.1306E-15
A-optimality = trace(Cpp)            :      0.5905E-03      0.2072E-02
E-optimality = max eigenvalue        :      0.5323E-03      0.2129E+00
Log-likelihood ln(L)                 :      0.2362E+02
Akaike  =-2ln(L)+2n                  :     -0.4123E+02
ABIC    =-2ln(L)+ln|F|               :     -0.2168E+02
Kashyap =-2ln(L)+ln|F|+n*ln(m/2Pi)   :     -0.1591E+02
```

negative log-likelihood to be minimized

```
Optimality Criteria [noisier.dat]            unscaled          scaled
-------------------
D-optimality = det(Cpp)              :      0.1493E-09      0.1139E-12
A-optimality = trace(Cpp)            :      0.4288E-02      0.1812E-01
E-optimality = max eigenvalue        :      0.3789E-02      0.1601E+00
Log-likelihood ln(L)                 :     -0.1423E+03
Akaike  =-2ln(L)+2n                  :      0.2906E+03
ABIC    =-2ln(L)+ln|F|               :      0.3081E+03
Kashyap =-2ln(L)+ln|F|+n*ln(m/2Pi)   :      0.3139E+03
```

All criteria have lower values for noisy.dat because of higher data quality, making it the preferred model

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Questions Residual Analysis

1. The *a posteriori* error variance s_0^2 turns out to be significantly greater than the *a priori* error variance σ_0^2.
   - What does "significantly" mean?
   - What does that result indicate?
2. What are you looking for when evaluating residuals?

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iTOUGH2 Short Course

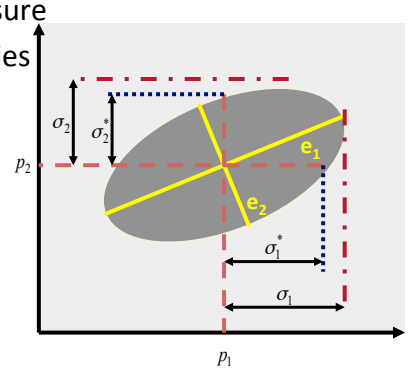
Lawrence Berkeley National Laboratory
Earth Sciences Division
Berkeley, California

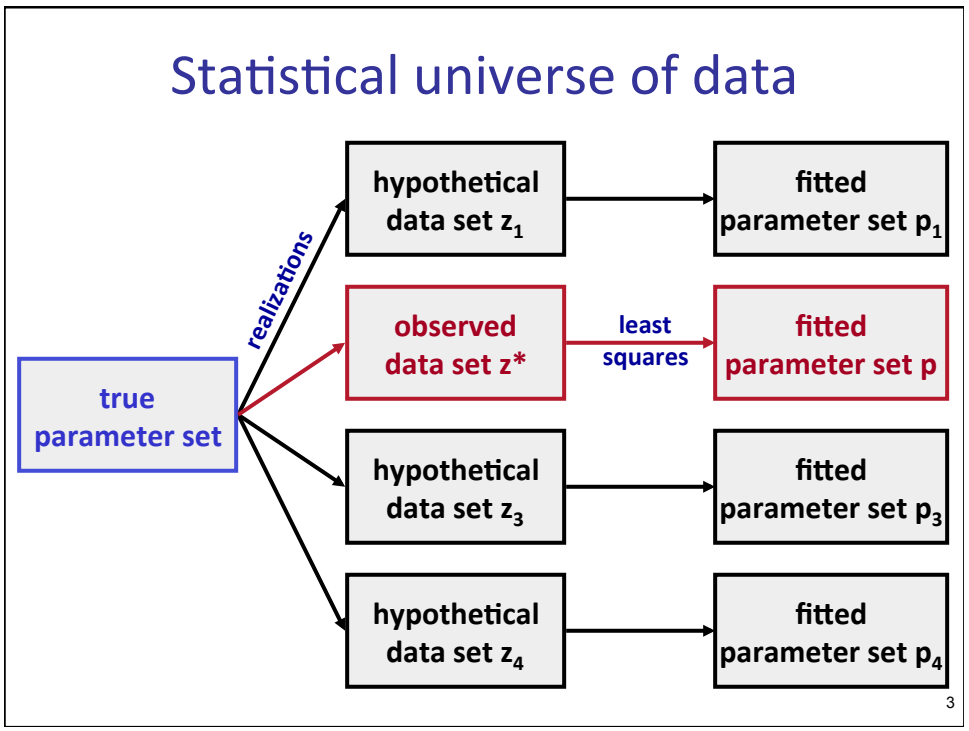
Uncertainty Analysis

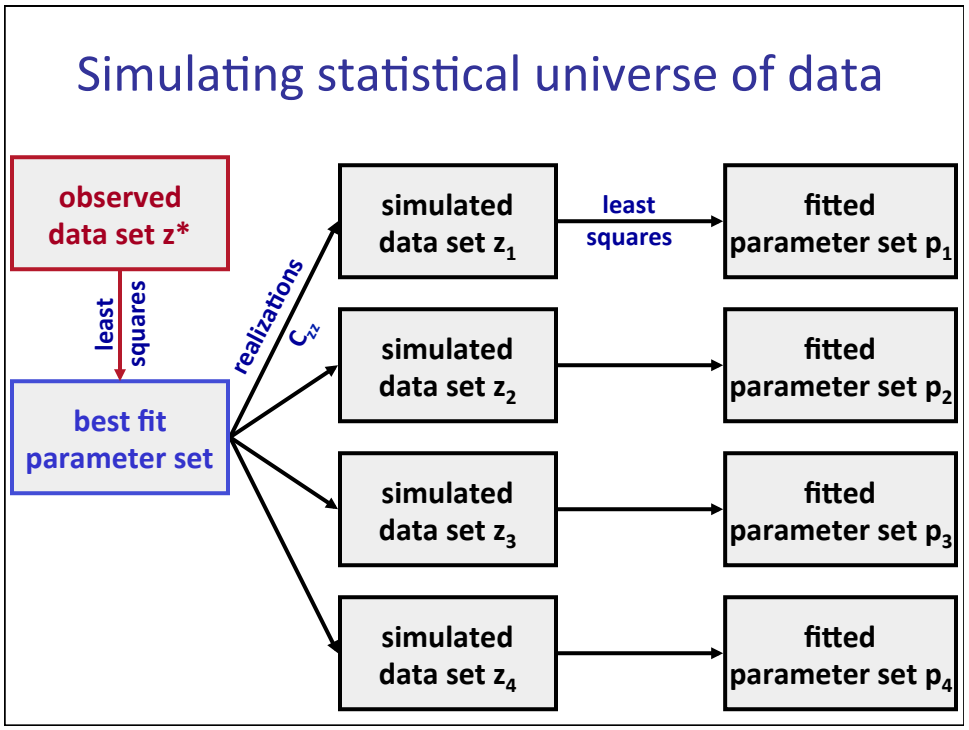
Covariance Matrix of Estimated Parameters C_{pp}
Uncertainty Propagation Analysis

Parameter uncertainty analysis in

- Covariance/correlation matrix
- Correlation chart
- Direct (pairwise) parameter correlations
- Conditional estimation uncertainties
- Overall parameter correlation measure
- Improvement over prior uncertainties
- Eigenanalysis of covariance matrix
- Correction for nonlinearities

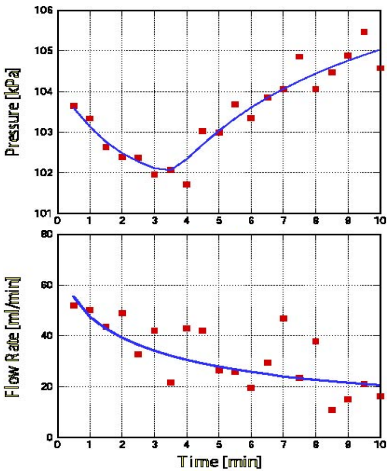



Statistical universe of data
hypothetical data set z_1
fitted parameter set p_1
realizations
observed data set z*
least squares
fitted parameter set p
true parameter set
hypothetical data set z_3
fitted parameter set p_3
hypothetical data set z_4
fitted parameter set p_4
3

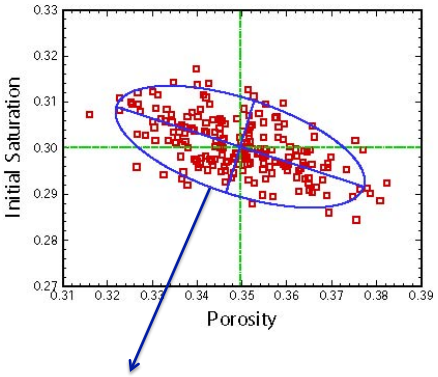

Simulating statistical universe of data
observed data set z*
least squares
best fit parameter set
realizations
C_{zz}
simulated data set z_1
least squares
fitted parameter set p_1
simulated data set z_2
fitted parameter set p_2
simulated data set z_3
fitted parameter set p_3
simulated data set z_4
fitted parameter set p_4

Simulating estimation uncertainty

200 realizations of hypothetical pressure and flow rate data



200 best estimates of porosity and initial gas saturation



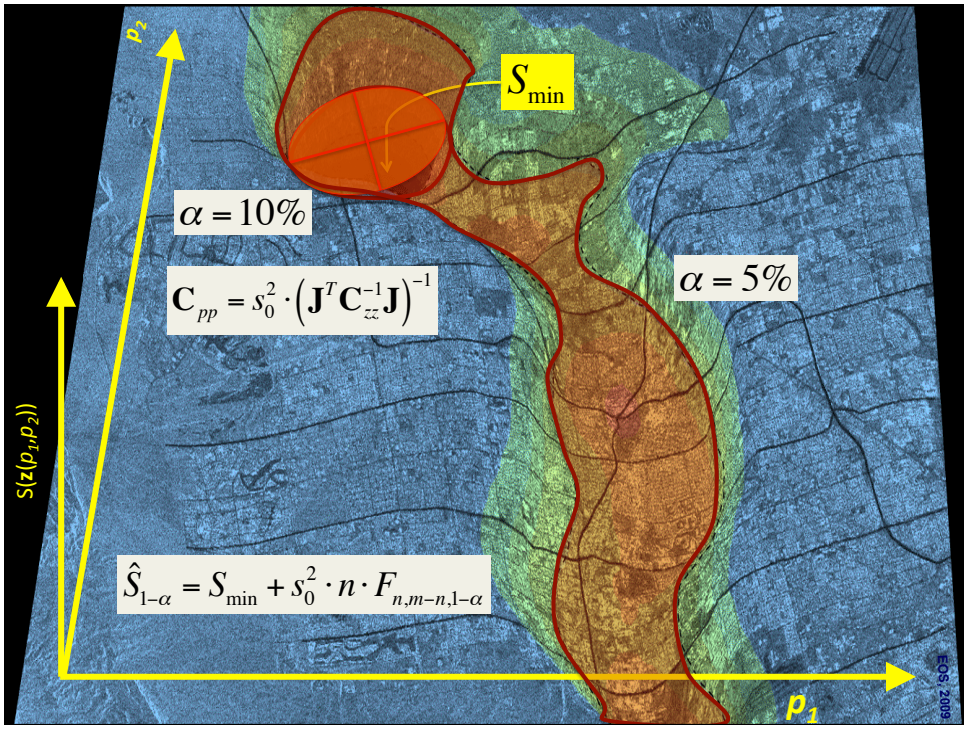
$\mathbf{C}_{pp}$ gives reasonable estimate of uncertainty region

5

Confidence Region

- The contours of the objective function visualize:
  - Confidence region
  - Correlation structure
  - Appropriateness of linearity assumption
  - Appropriateness of normality assumption
  - Well-posedness of inverse problem

6



Confidence Region

- The probability that the true parameter set lies within the ellipsoidal confidence region represented by $\mathbf{C}_{pp}$ is (1-α).
- The true confidence region is bounded by the contour line of the objective function at level:

$$S_{\min} + s_0^2 \cdot n \cdot F_{m-n,\infty,1-\alpha}$$

- The confidence region increases with decreasing α.
- $\mathbf{C}_{pp}$ is only a good representation of actual confidence region if linearity and normality assumptions are not violated.

8

Covariance Matrix of Estimated Parameters $\mathbf{C}_{pp}$

- The covariance matrix $\mathbf{C}_{pp}$ is an estimate of the uncertainty of the estimated parameters:

$$\mathbf{C}_{pp} = s_0^2 \left(\mathbf{J}^T \mathbf{C}_{zz}^{-1} \mathbf{J} \right)^{-1}$$

- $\mathbf{C}_{pp}$ is an approximation of the actual parameter uncertainty; it is based on a normality and linearity assumption
- $\mathbf{C}_{pp}$ is proportional to goodness-of-fit (s_0^2)
- $\mathbf{C}_{pp}$ is inversely proportional to sensitivity matrix ($\mathbf{J}$)
- $\mathbf{C}_{pp}$ is proportional to measurement uncertainty ($\mathbf{C}_{zz}$)

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Estimation Uncertainty

- Decreases with improvement of fit
  - *Use good data and good model*
- Decreases with increasing sensitivity
  - *Use sensitive data*
- Decreases with decreasing correlations
  - *Use data that allow for independent determination of each parameter*
  - *Avoid overparameterization*
- Design tests accordingly!

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Covariance Matrix
Correlation Matrix

- The diagonal of $\mathbf{C}_{pp}$ contains variances σ_{ii}^2 of estimated parameters.
- Off-diagonal elements are covariances c_{ij} between pairs of parameters.
- Off-diagonal elements are "normalized" to yield *correlation coefficients* r_{ij}:

$$-1 < r_{ij} = \frac{c_{ij}}{\sqrt{\sigma_{ii}^2 \cdot \sigma_{jj}^2}} < 1$$

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Correlation Coefficients

- A correlation coefficient of *zero* indicates that the two parameters can be estimated *independently*.
- A correlation coefficient of *–1 or 1* indicates *non-uniqueness*.
- A negative correlation coefficient indicates that a statistically similar match can be obtained by increasing one parameter and decreasing the other.
- If correlations exist, the uncertainty in one parameter affects the uncertainty in the other parameters.
- Design experiment as to minimize correlations.

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Example: darcy3i

```
****************
 ERROR ANALYSIS
****************

Error analysis is based on >>> a posteriori <<< variance:  1.1628577E+00

Covariance(L+D)/Correlation(U) Matrix of Estimated Parameters
------------------------------------------------------------
                  log(abs. perm.)        Porosity  Initial gas sat

log(abs. perm.)       2.77543E-04           0.843           -0.259
Porosity              2.35163E-04      2.80104E-04           -0.490
Initial gas sat      -1.74370E-05     -3.32081E-05      1.63676E-05


Matrix of Direct Correlations
-----------------------------
                  log(abs. perm.)        Porosity  Initial gas sat
log(abs. perm.)             1.000           0.851           0.331
Porosity                    0.851           1.000          -0.525
Initial gas sat             0.331          -0.525           1.000
```

Correlation coefficient, r_{ij}

σ_p^2

covariance, c_{ij}

Indicates degree to which a change in one parameter can be compensated by another

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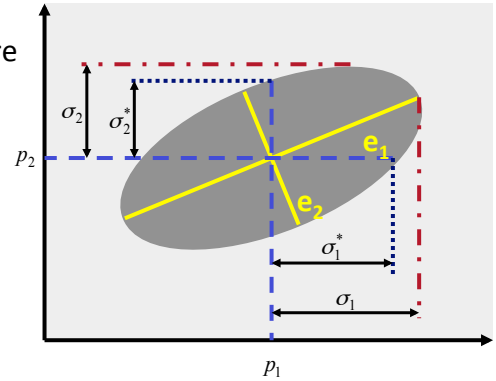
Overall Correlation

- The *conditional* standard deviation σ^* is the estimation uncertainty assuming that all other parameters are perfectly known.
- C_{pp} holds the *marginal* standard deviations σ.
- The ratio σ^*/σ is a measure of overall correlation.
- The ratio σ^*/σ should be close to 1.



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Example: darcy3i

Arrange in order of decreasing independence (C/M)

Square root of the diagonal of C_{pp}

```
Standard Deviations
-------------------
[ ... description of the column ... ]

PARAMETER        BEST ESTIMATE A PRIORI CONDITIONAL    MARGINAL   C/M 1-M/P
Initial gas sat    1.02915E+01    N/A   3.32706E-03 4.04569E-03 0.822 1.000
log(abs. perm.)   -1.16866E+01    N/A   8.44619E-03 1.66596E-02 0.507 1.000
Porosity           3.72609E-01    N/A   7.65512E-03 1.67363E-02 0.457 1.000
```

Specified only if used to weight parameters in objective function

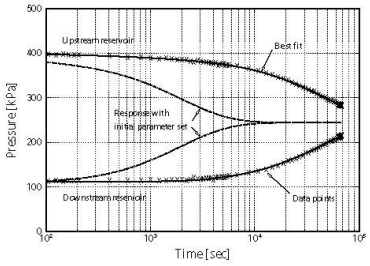
Measure of how much is learned from inversion compared to a priori uncertainty

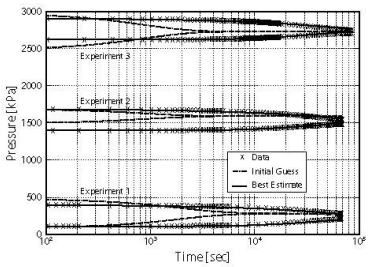
```
Correlation Chart
-----------------

-0.6    -0.4    -0.2   0.0                0.0     0.2     0.4     0.6     0.8
|-------|-------|-------|    PARAMETER      |-------|-------|-------|-------|
     |--------|---------|  Initial gas sat
     |        |
     |        |---------|  log(abs. perm.)  |--------------------------------|
     |                                                                       |
     |------------------|     Porosity      |--------------------------------|
```

Correlation between gas saturation and porosity

Reducing Correlations: Example





Add experiments on different pressure levels and invert jointly

	log(*k*)	log(*b*)	ϕ
log(*k*)	1.67	-0.99	-0.87
log(*b*)	-0.99	2.16	0.87
ϕ	-0.87	0.87	0.003

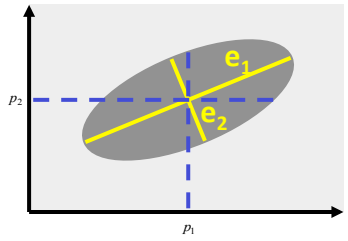
	log(*k*)	log(*b*)	ϕ
log(*k*)	1E-4	-0.52	-0.12
log(*b*)	-0.52	4e-4	-0.02
Φ	-0.12	-0.02	0.01

Example: darcy3i

```
Eigenanalysis of Covariance Matrix (R-Mode Factor Analysis)
------------------------------------------------------------
Performance index       :  3.25365122E-02
Condition number        :  5.07978268E+01

Eigenvalues
-----------
                                  1               2               3
  1 Eigenvalue     :        4.7286641E-05   5.1655936E-04   1.0168926E-05

Eigenvectors
------------
                                  1               2               3
  1 log(abs. perm.)        6.9034965E-01   7.0218708E-01  -1.7421439E-01
  2 Porosity              -6.5282457E-01   7.0839235E-01   2.6832882E-01
  3 Initial gas sat        3.1182918E-01  -7.1509271E-02   9.4744340E-01
```



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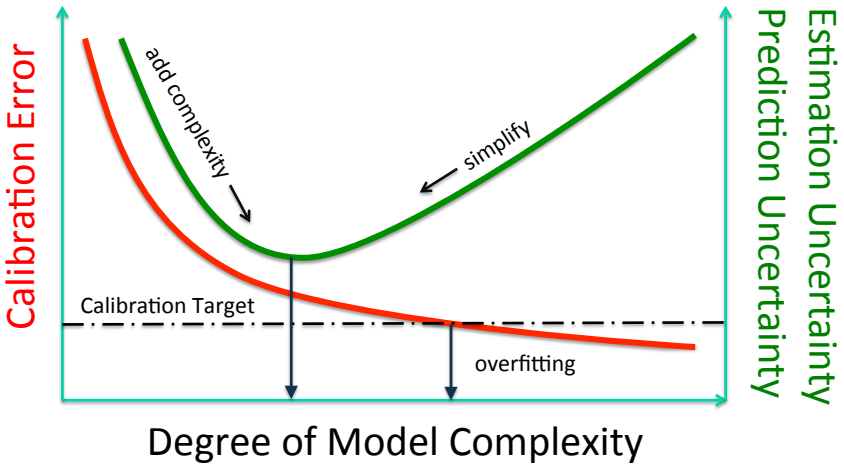
Under- and overparameterization: Occam's Razor



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Overparameterization

- A match can *always* be improved by adding more parameters to **p**.
- Adding new parameters increases correlations and thus *increases estimation uncertainty*.
- Check $\mathbf{C}_{pp}$ for large variances, correlation coefficients close to –1 or 1, and large condition numbers.
- Add parameters only if the fit can be *significantly improved* without introducing strong parameter correlations.
- *Avoid over- **and** under-parameterization*

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Uncertainty Analysis: Questions

1. Discuss

$$\mathbf{C}_{pp} = s_0^2\left(\mathbf{J}^T\mathbf{C}_{zz}^{-1}\mathbf{J}\right)^{-1}$$

2. Under which conditions is $\mathbf{C}_{pp}$ a good approximation of the actual confidence region?
3. How can you reduce estimation uncertainty?

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Uncertainty Analysis: Questions

4. Discuss "underparameterization" and "overparameterization".

5. $\mathbf{C}_{zz} = \sigma_0^2 \mathbf{V}_{zz}$ is the *a priori* observation covariance matrix.

   If all elements of $\mathbf{C}_{zz}$ were multiplied by a factor of 4, how would this affect:

   - The value of the objective function S?
   - The estimated parameter set $\mathbf{p}$?
   - The estimated error variance s_0^2?
   - The uncertainty of the estimated parameters $\mathbf{C}_{pp}$?
   - The outcome of the Fisher Model Test?

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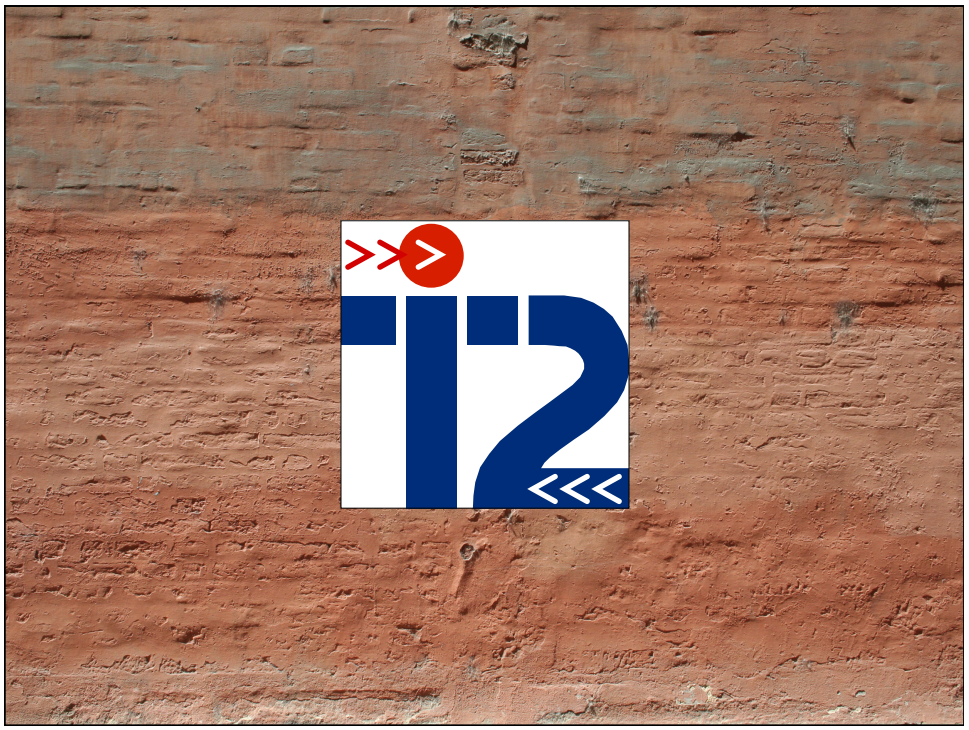

iTOUGH2 Commands

```
> COMPUTATION
  >> ERROR
     >>> ALPHA: alpha          significance level
     >>> A PRIORI              use σ0²
     >>> A POSTERIORI          use s0²
     >>> let FISHER model test decide
     >>> check LINEARITY assumption
```

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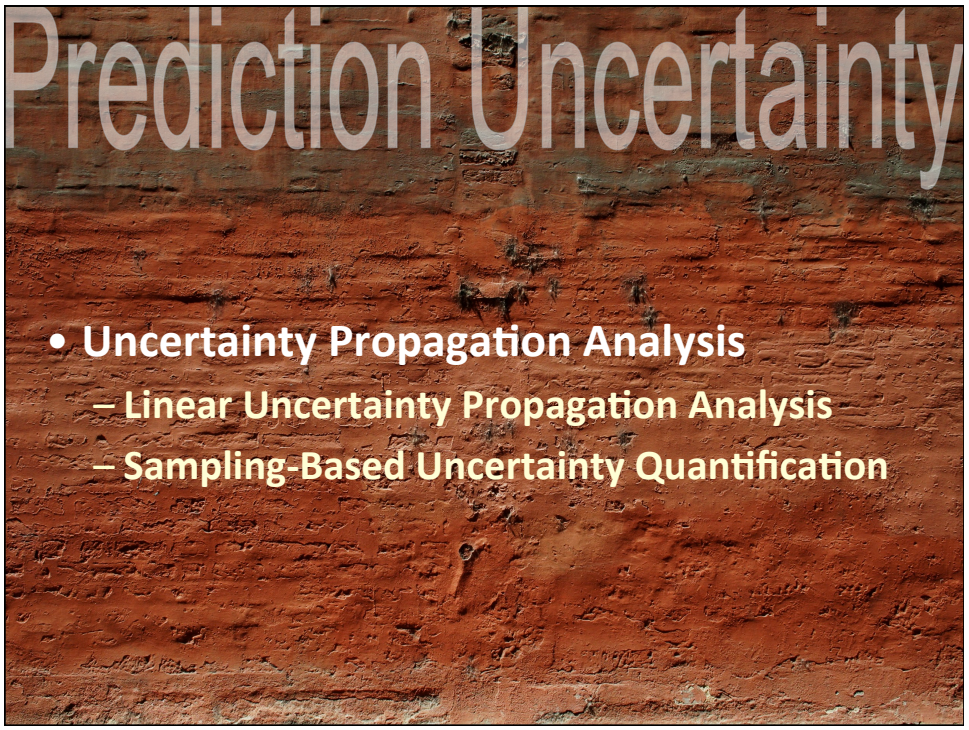

Uncertainty Propagation Analysis

- Calculate prediction uncertainty as a result of parameter uncertainty.
- *Linear analysis* (First-Order Second-Moment)
  - Fast (*n*+1 forward runs)
  - Easy to report (mean and covariance matrix)
  - Based on linearity and normality assumption
- *Monte Carlo simulations*
  - Expensive (many forward runs)
  - Difficult to report
  - Full distribution
  - No distributional assumptions

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Linear Error Propagation Analysis (First-Order-Second-Moment)

- *Assumptions*
  - Change in model prediction Δz can be approximated by a linear function of the parameter changes Δp
  - Δp is (log-)normally distributed

$$\mathbf{C}_{\hat{z}\hat{z}} = \mathbf{J}\mathbf{C}_{pp}\mathbf{J}^T$$

- Error band is *symmetric*, representing (log-) normally distributed prediction errors
- May assign certain probability to *unphysical* system behavior

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Monte Carlo Simulations

- Run many simulations with randomly selected parameter combinations drawn from the given probability density function.
- Provides *full distribution* of prediction uncertainty (histogram), which can be analyzed statistically.
- *Nonlinearities* are automatically taken into account.
- Results are always *physically reasonable*.
- Experimental designs: *Latin Hypercube Sampling*.
- Parameter *correlations* may be included.

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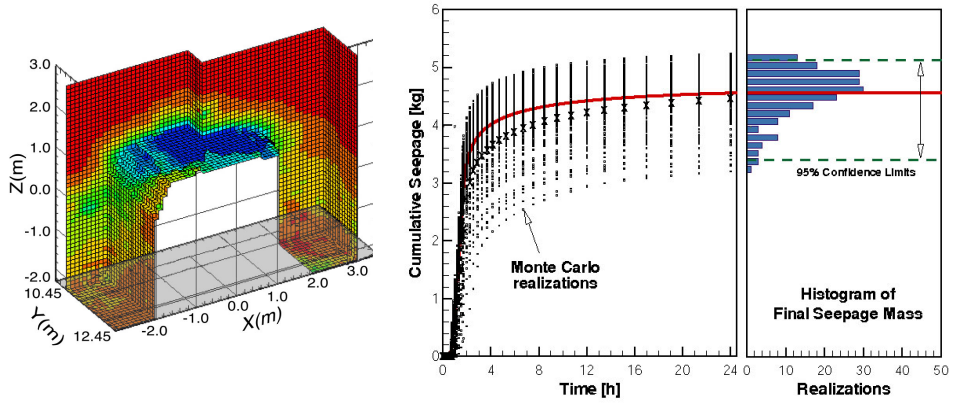
Monte Carlo Simulations



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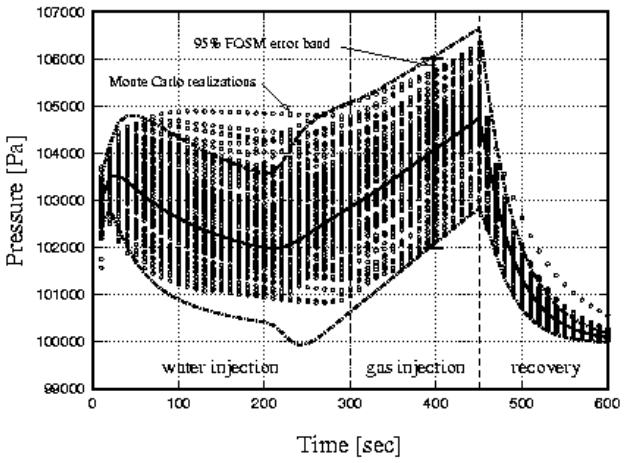
Comparison FOSM-MC



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Uncertainty Analysis: Questions

6. Describe the main differences between FOSM and Monte Carlo simulations.
7. Assume you have to estimate the (hopefully small) probability that the TCE concentration at a drinking water well does not exceed a certain level.
   - Which uncertainty propagation analysis method would you choose?
   - Justify your choice.
   - Describe the procedure.

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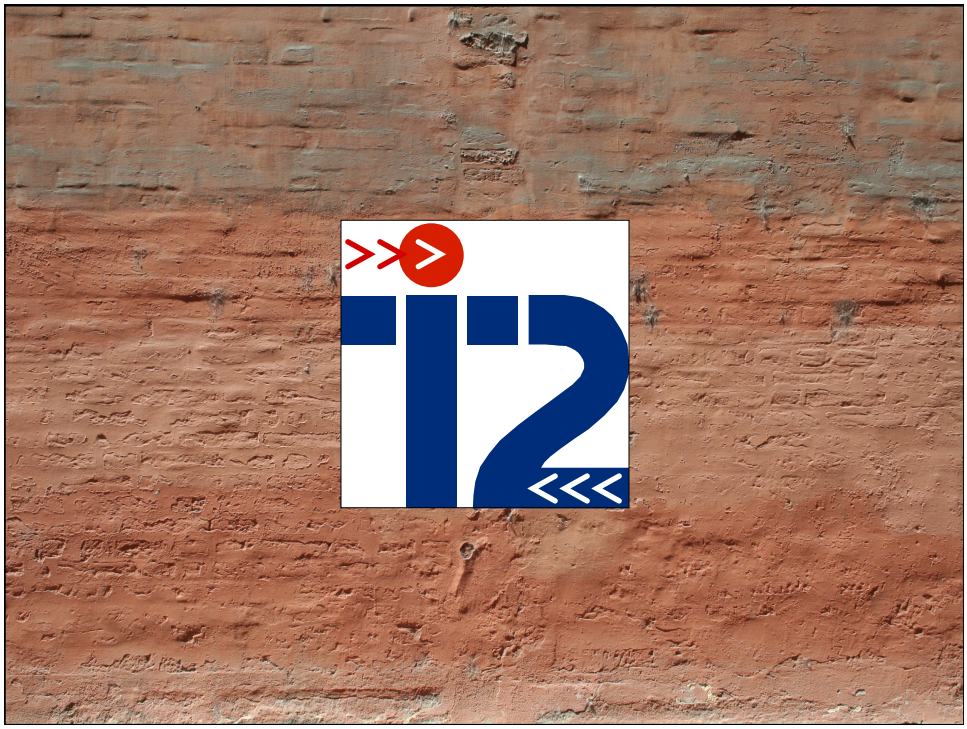

Uncertainty Propagation

Specify uncertainties in input parameters in block
> PARAMETERS or provide covariance matrix of estimated parameters using one of several formats

```
> COMPUTATION
  >> ERROR
     >>> FOSM
```

```
> COMPUTATION
  >> STOP
     >>> number of MC SIMULATIONS: 1000
     <<<
  >> ERROR
     >>> MONTE CARLO SEED: 9999 GENERATE
     >>> LATIN HYPERCUBE SAMPLING
     >>> EMPIRICAL ORTHOGONAL FUNCTION
```

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