



# Permeability Estimation in Heterogeneous Formations with Derivative-Free Optimization Based On Observed Data

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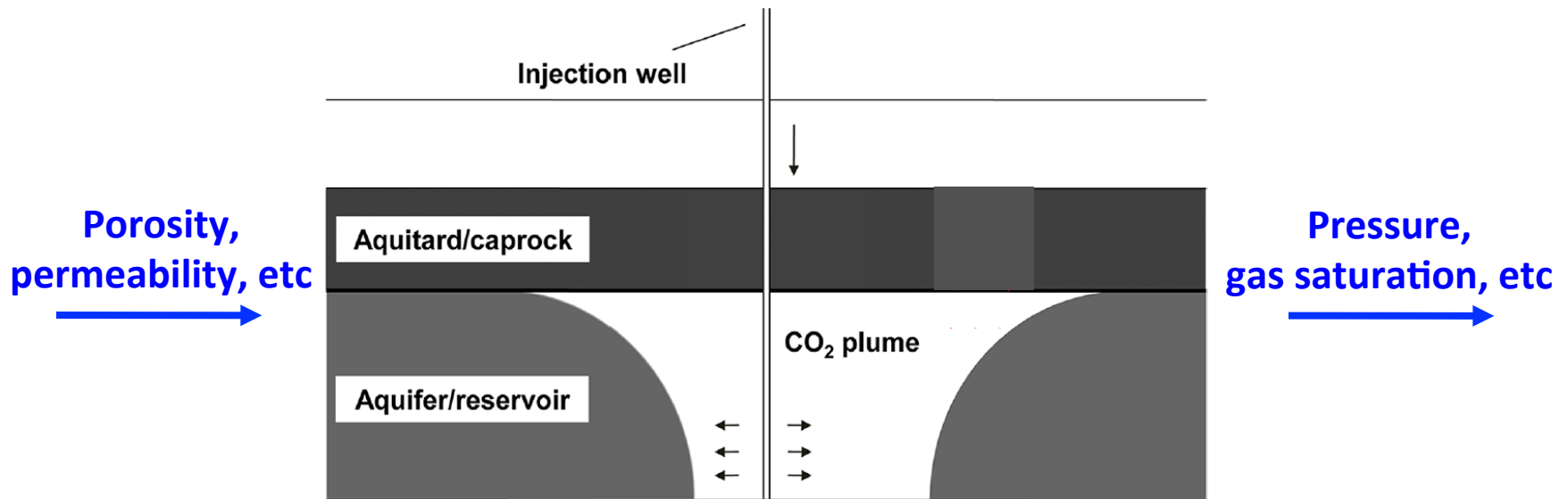
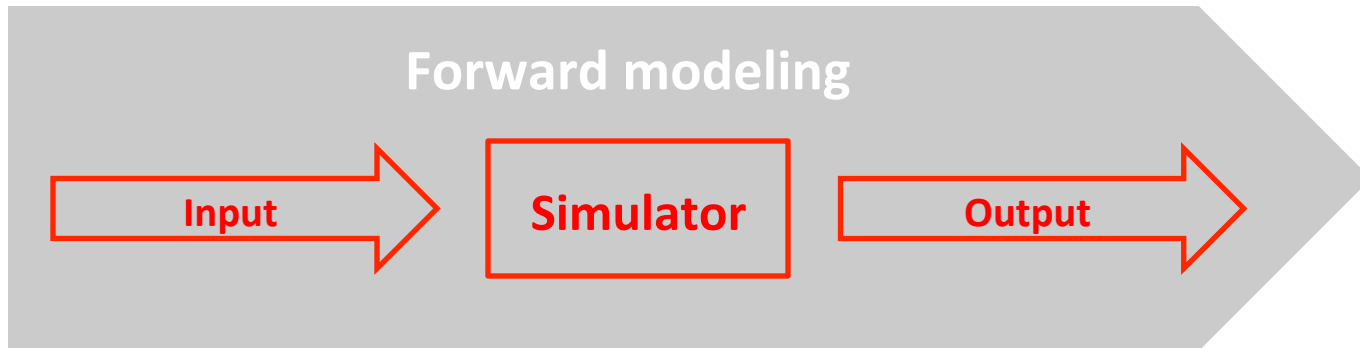
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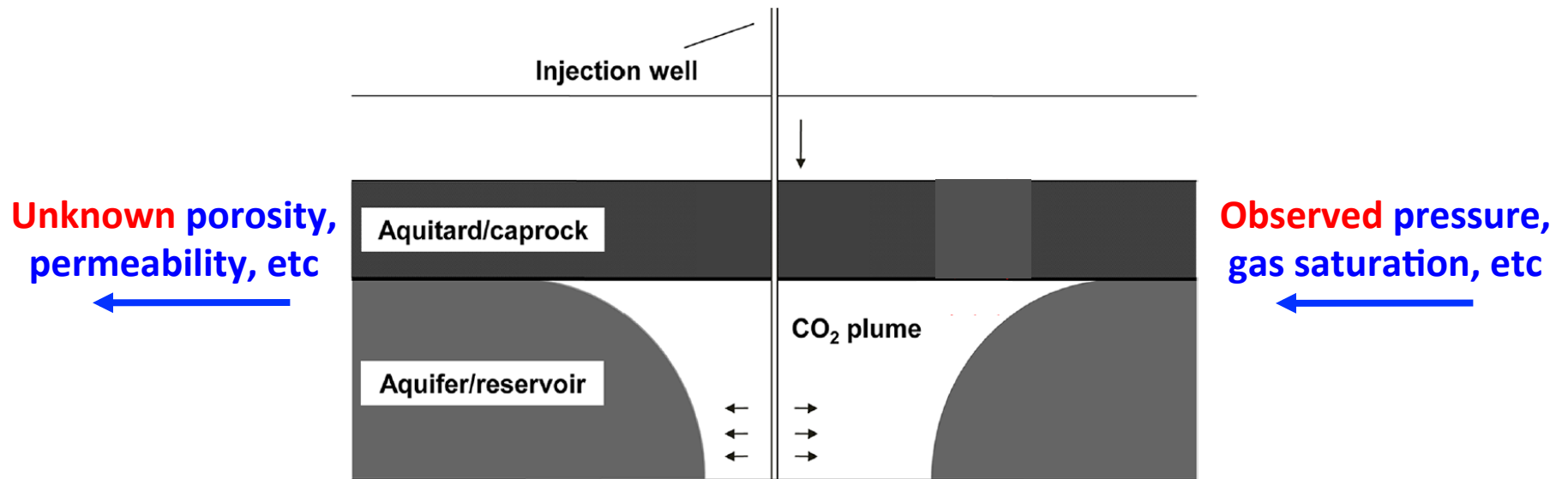
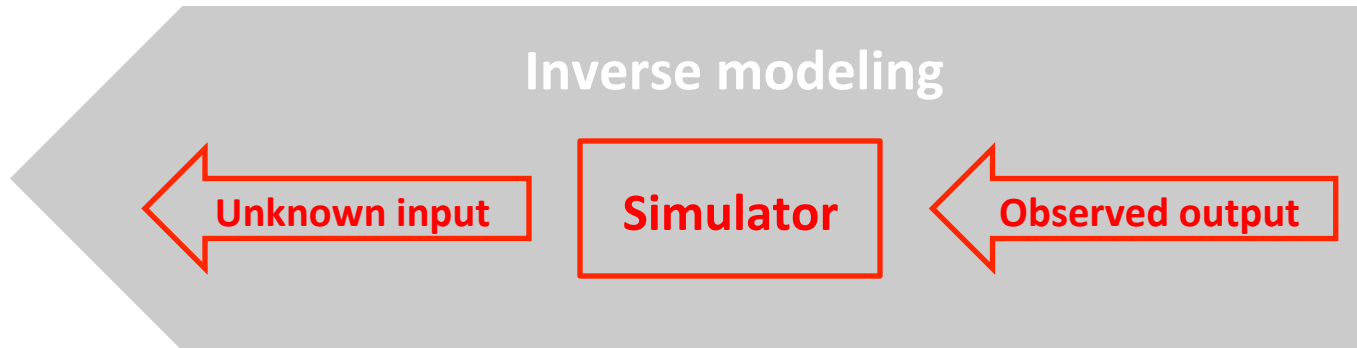
# Outline

- **Three key components of parameter estimation**
- **Work flow of parameter estimation**
- **Introduction to derivative-free optimization (DFO)**
- **Two case studies**
- **Conclusions**

# Three key components: System model



# Three key components: System model



# Three key components: Fitness measure

- **Least squared error:** ✓

– Mismatch between simulation and observation:  $\sum_i w_i \left( \frac{y_i^{\text{sim}}(p) - y_i^{\text{obs}}}{\sigma_i} \right)^2$

- **Maximum Likelihood**

– Likelihood of observation being present under parameter  $p$ :

$$f(y^{\text{obs}}|p) = \prod_i f_i(y_i^{\text{obs}}|p) \propto \exp \left\{ -\frac{1}{2} \sum_i \left( \frac{y_i^{\text{sim}}(p) - y_i^{\text{obs}}}{\sigma_i} \right)^2 \right\}$$

Simulation/black-box  
No algebraic form for gradient

- **Bayesian inference – posterior distribution**

– Prior probability distribution for  $p$ :  $f(p)$

– Posterior probability distribution for  $p$ :  $f(p|y^{\text{obs}}) = f(y^{\text{obs}}|p)f(p)$

# Three key components: Optimization algorithm

## Derivative-based or algebraic solvers

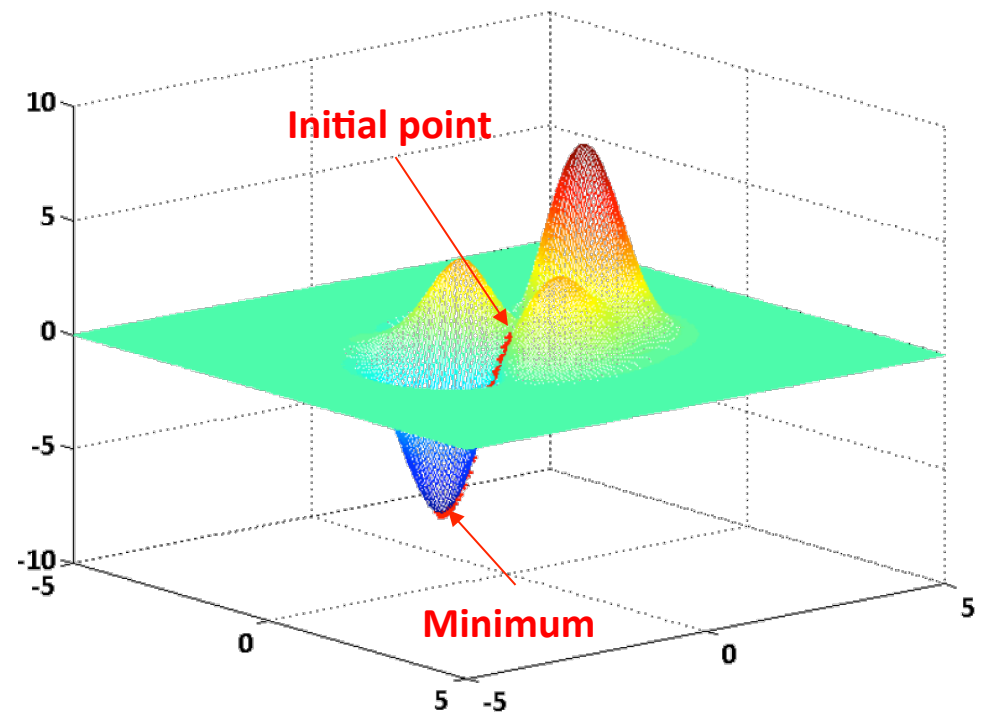
(BARON, CPLEX, IPOPT, CONOPT, etc.)

### Pros:

Fast, efficient solutions with provably optimal solutions

### Cons:

Need an algebraic model (access to derivative information)



Estimate gradient using central differencing

# Three key components: Optimization algorithm

## Derivative-free or black-box solvers

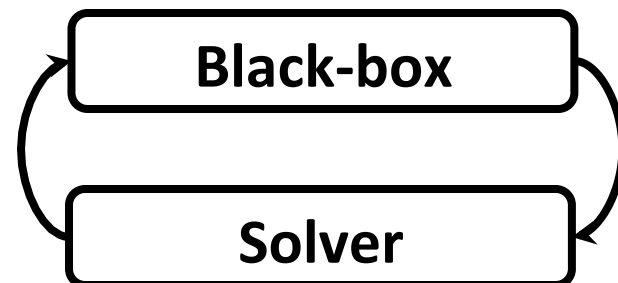
(Genetic algorithms, Matlab's `fminsearch()`, etc.)

### Pros:

Can solve problems where derivative information is unavailable, unreliable, or prohibitively expensive

### Cons:

Slow and little to no guarantees that you have an optimal solution in the end



# Three key components: Optimization algorithm

## Derivative-free or black-box solvers

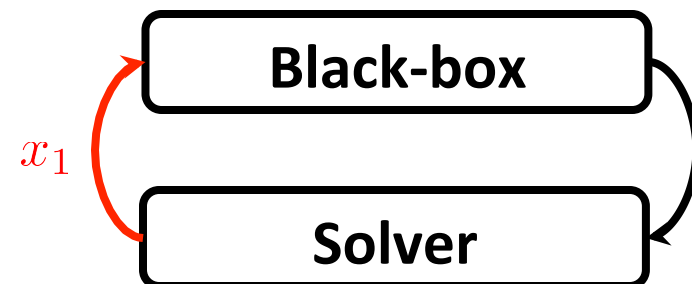
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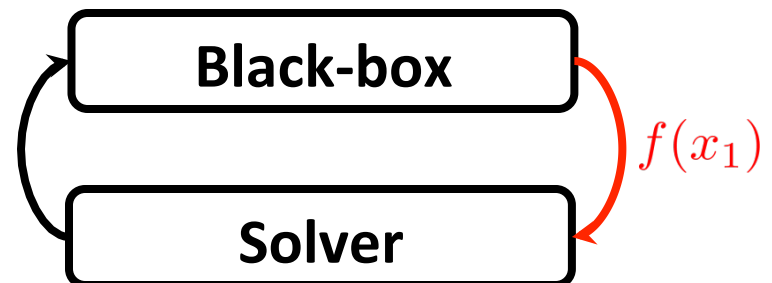
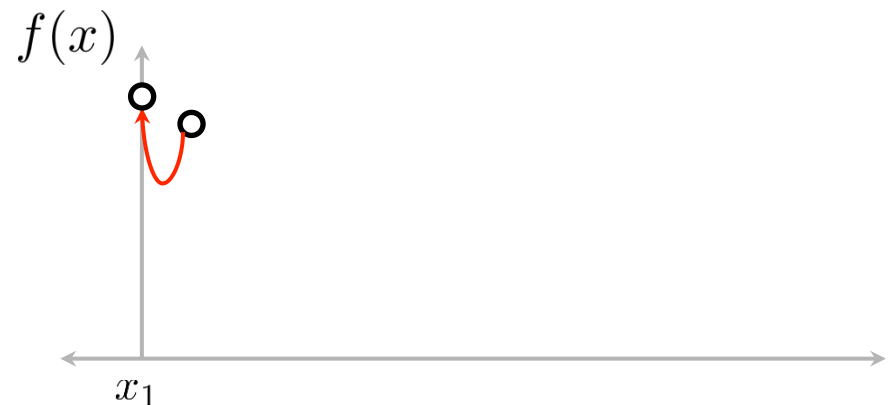
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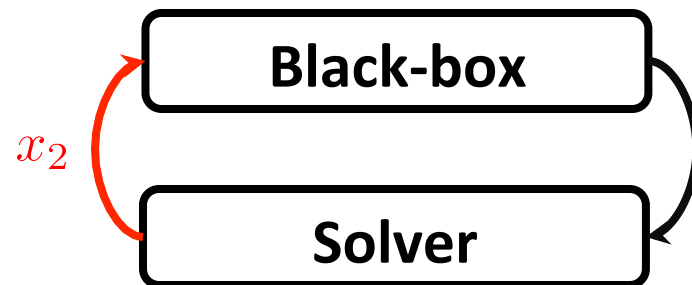
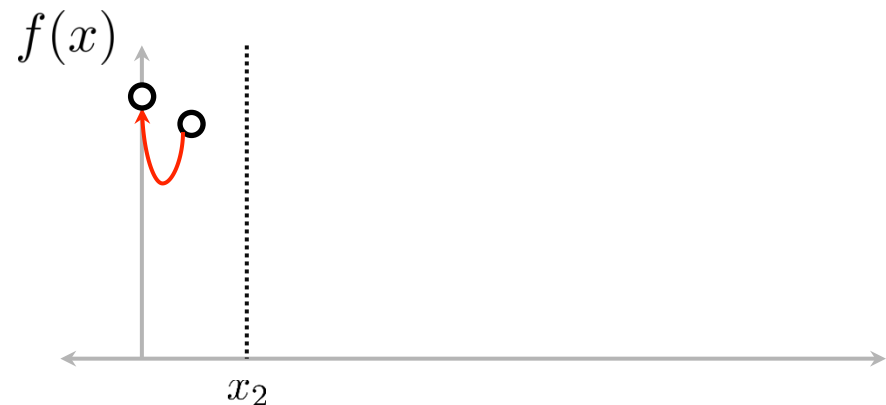
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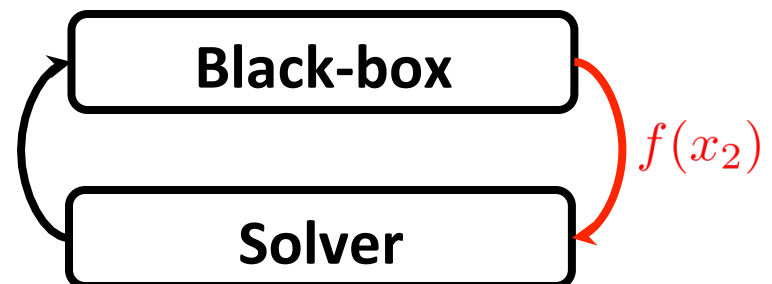
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# Three key components: Optimization algorithm

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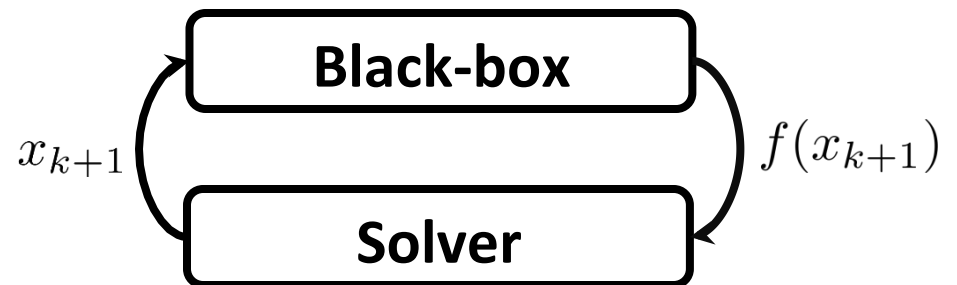
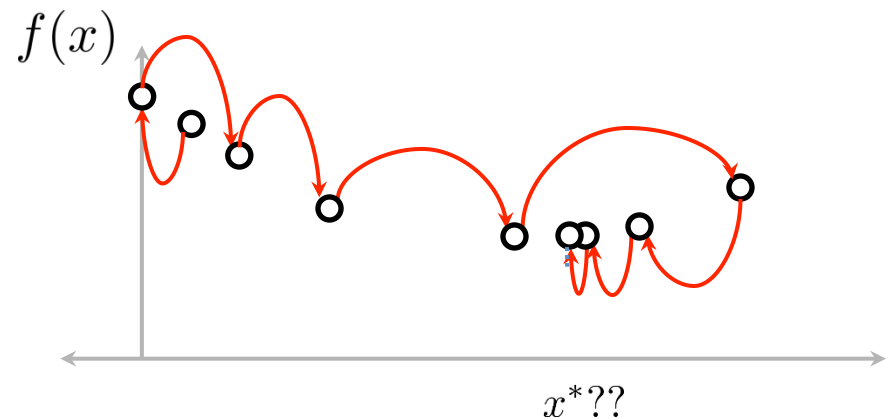
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### Pros:

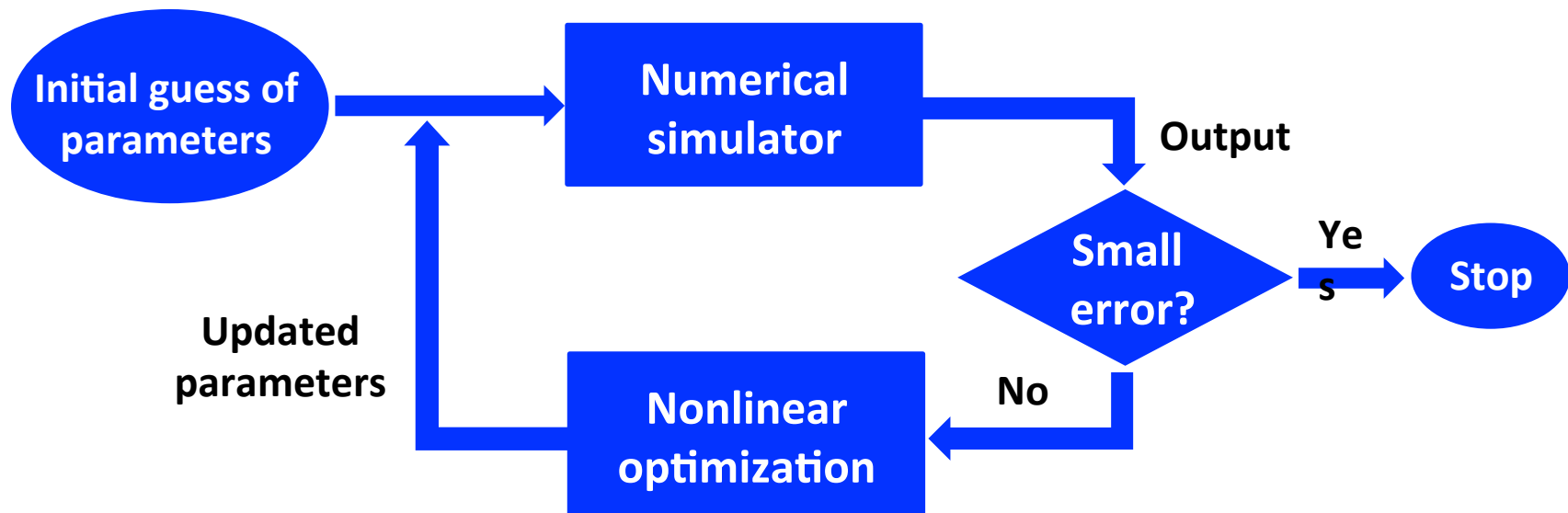
Can solve problems where derivative information is unavailable, unreliable, or prohibitively expensive

### Cons:

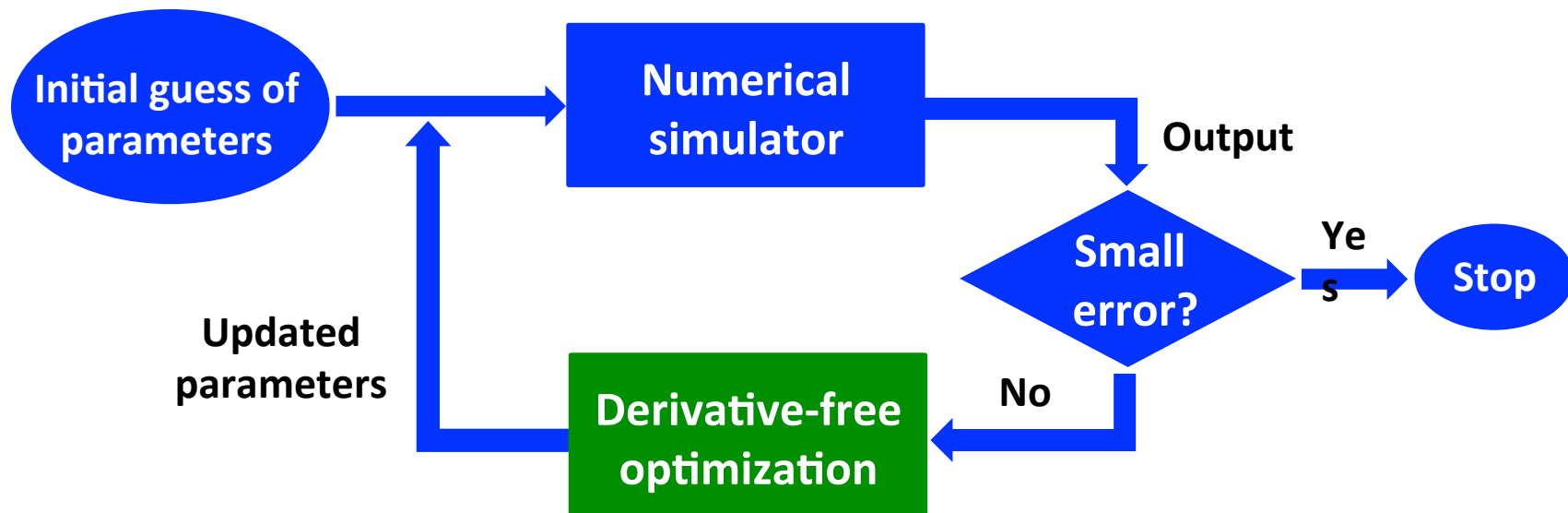
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# Procedure for estimating parameters

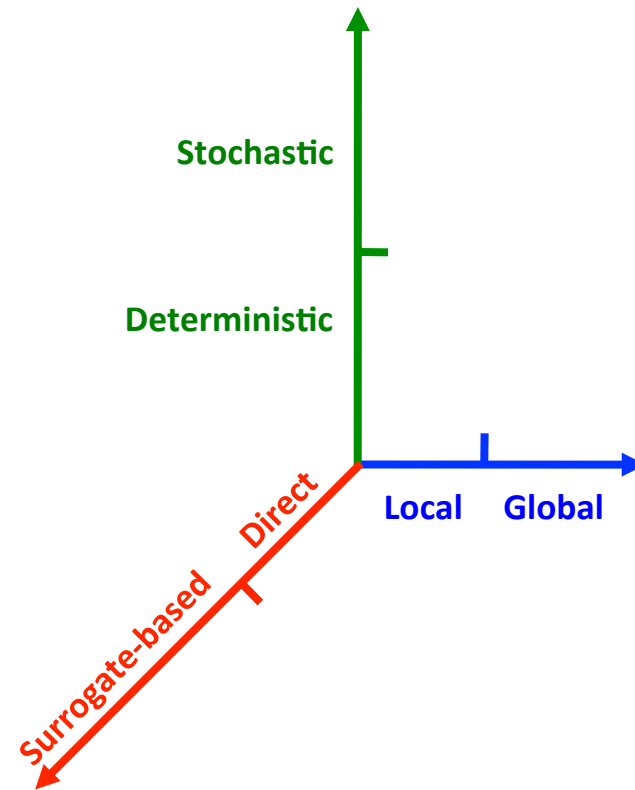
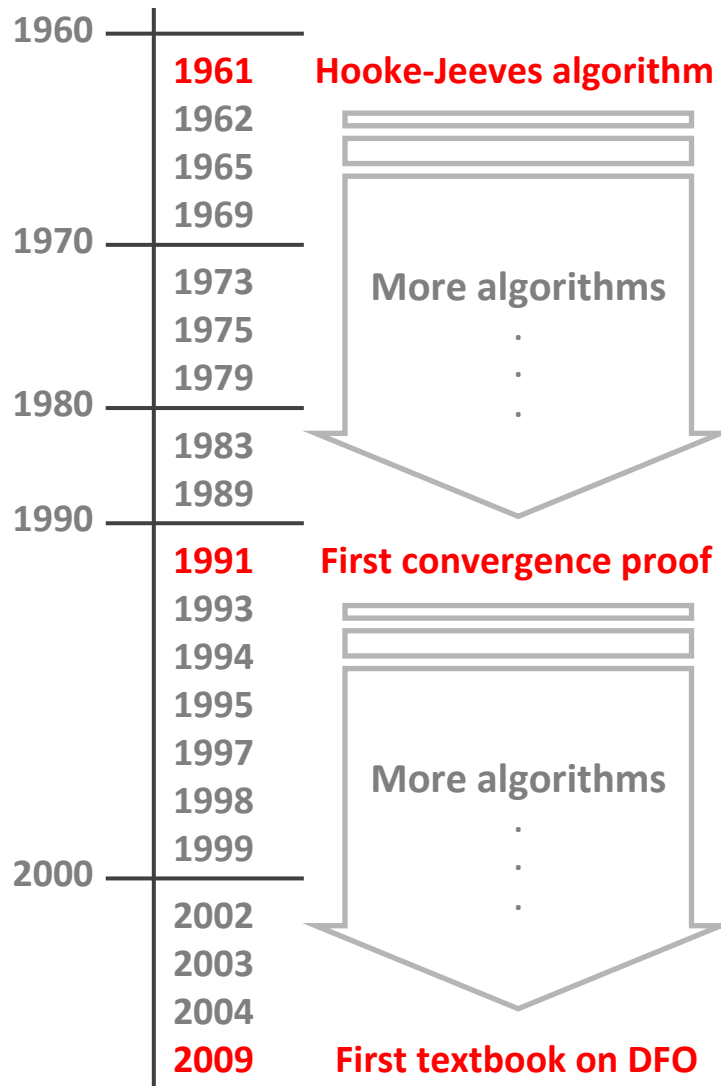


# Procedure for estimating parameters



- Performance of DFO solvers
- No systematic comparison of DFO solvers for parameter estimation

# Overview of Derivative-free optimization



# Local DFO algorithms and software

## Direct

- Nelder-Mead simplex algorithm — FMINSEARCH
- Generalized pattern search and generating search set
  - DAKOTA PATTERN
  - HOPSPACK
  - SID-PSM
  - NOMAD

## Surrogate-based

- Implicit filtering — IMFIL
- Trust-region methods
  - DFO
  - BOBYQA
  - NEWUOA



# Global DFO algorithms and software

## Direct

- **Deterministic**

- Lipschitzian-based partitioning
- Multilevel coordinate search

- **Stochastic**

- Hit-and-run
- Simulated annealing
- Genetic algorithms
- Particle swarm

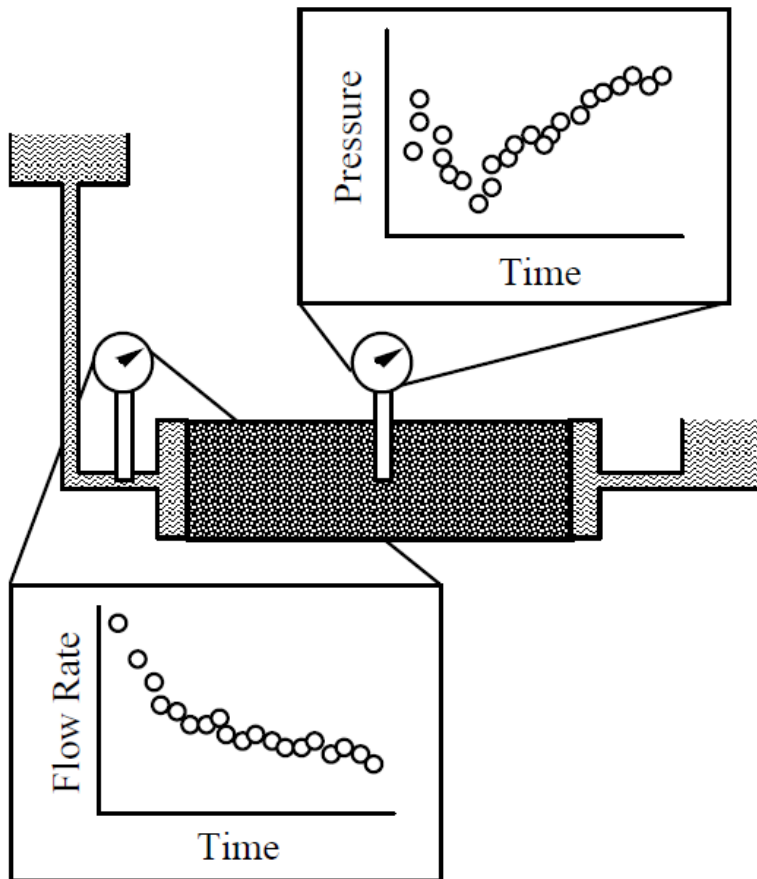
DAKOTA SOLIS-WETS  
DAKOTA DIRECT  
TOMLAB GLBSOLVE  
TOMLAB GLCSOLVE  
MCS  
ASA  
CMA-ES  
DAKOTA  
EA  
GLOBAL  
PSWARM

## Surrogate-based

- Response surface methods
- Branch-and-fit
- Surrogate management framework

TOMLAB EGO  
TOMLAB RBF  
SNOBFIT  
TOMLAB LGO

# Case study I: Three parameters to be estimated



Water is injected at constant pressure into a 1D column filled with partially saturated sand

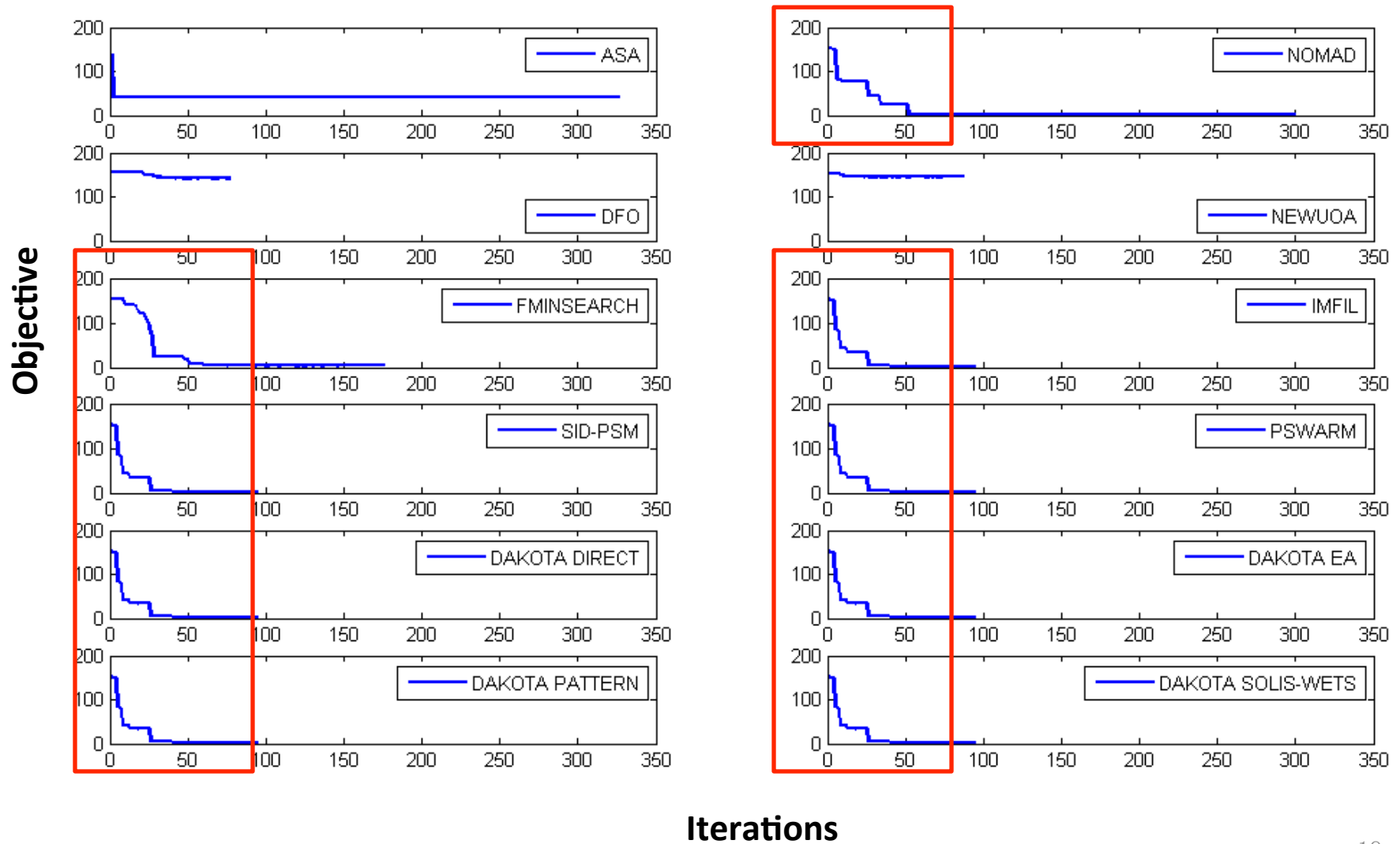
**Known:**

- Pressure profile
- Flow rate profile

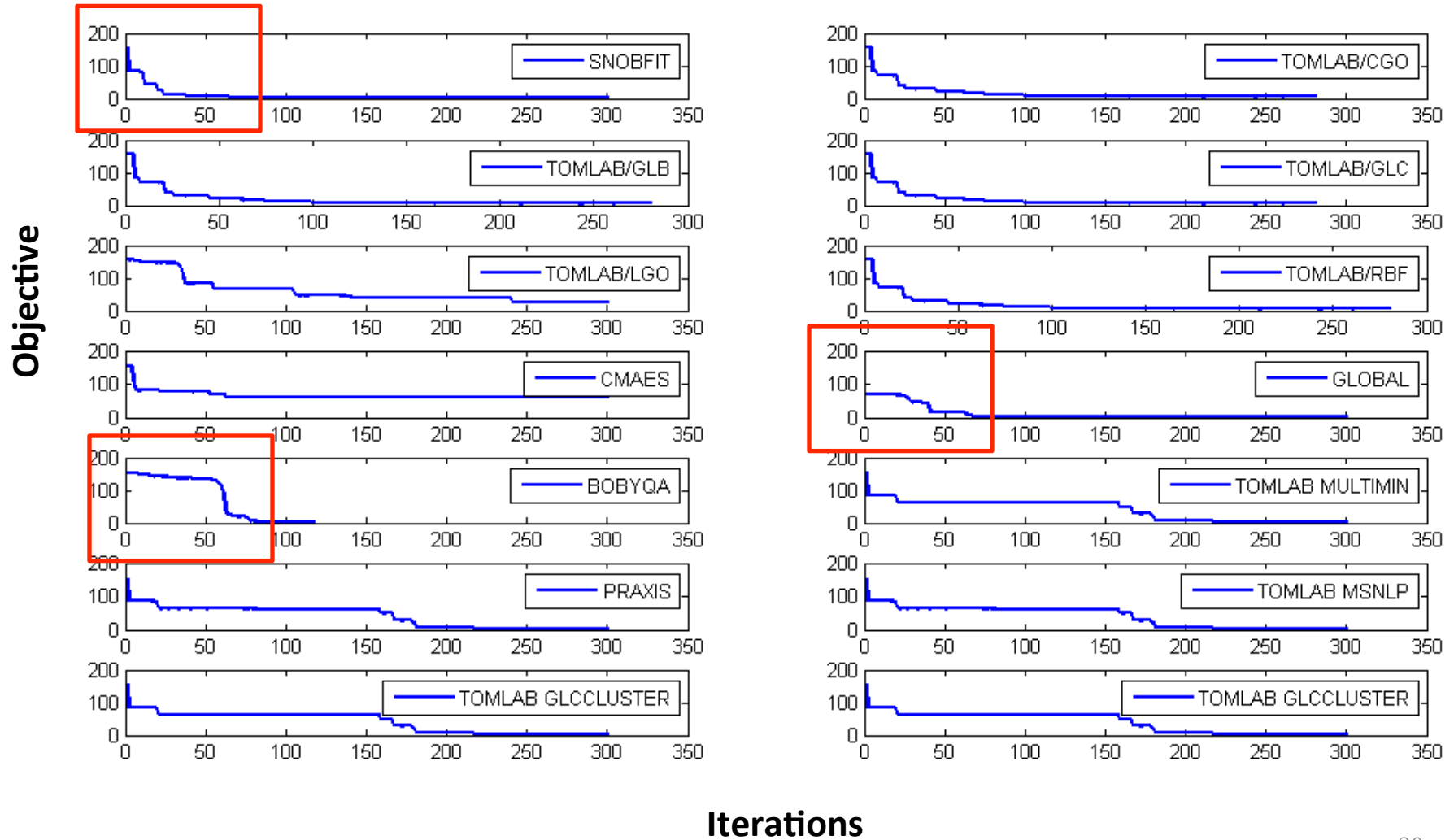
**Unknown:**

- Porosity
- Permeability
- Initial gas saturation

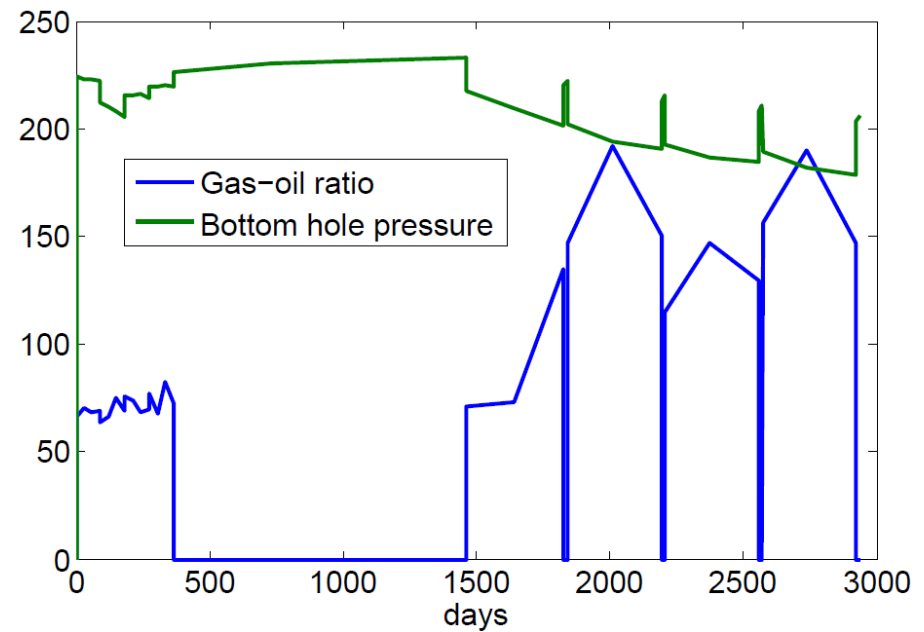
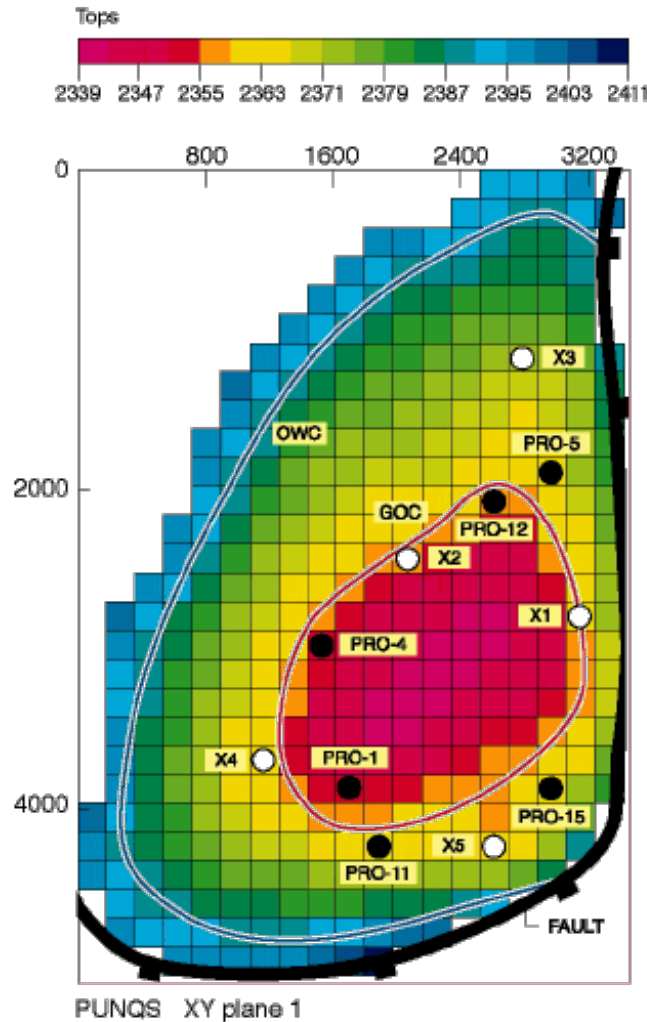
# Performance of DFO solvers



# Performance of DFO solvers-cont'd

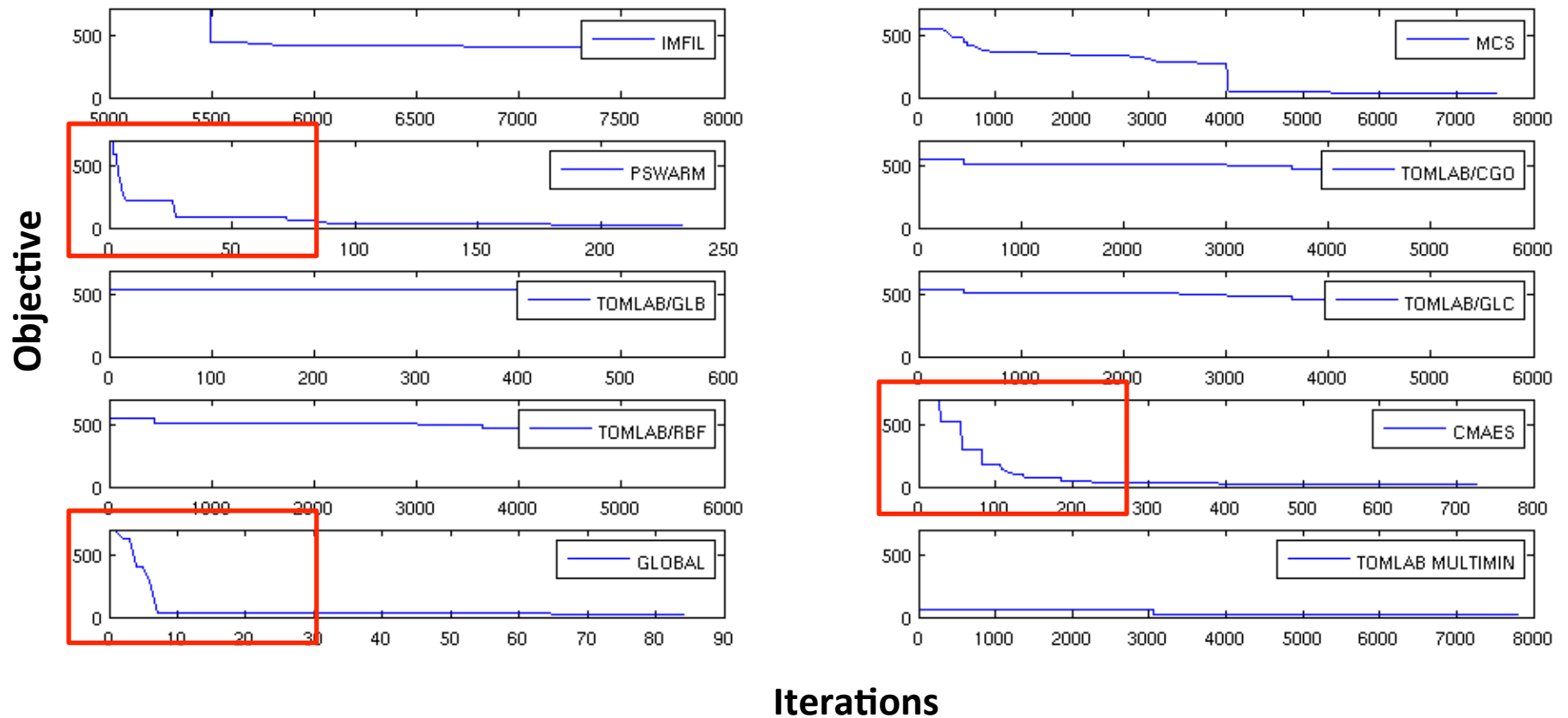


# Case study II: 2660 parameters to be estimated



- **Gridblocks:  $19 \times 28 \times 5 = 2660$**
- **2660 unknown porosities**
- **Permeability = function (porosity)**

# Performance of DFO solvers



# Conclusions and future work

- **Conclusions**

- Systematic comparison of current DFO solvers in inverse modeling
- DFO solver collection provides a robust package for inverse modeling
  - Small dimension problem: **FMINSEARCH, SID-PSM, NOMAD, DAKOTA, IMFIL, DFO, BOBYQA, NEWUOA**
  - Large dimension problem: **PSWARM, CMAES, GLOBAL**
- Performance depends on limits of computation resources such as CPU time and number of iterations

- **Future work**

- Test with different measure of fitness
- Apply DFO algorithms to permeability estimation of CO<sub>2</sub> sequestration in aquifer