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Research Center at the University of Tübingen
Department for Applied Geology
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Implementation and performance of selected evolutionary algorithms

... for the tuning of groundwater remediation systems

Accelerating Site Closeout – Improving Performance – & Reducing Costs Through
OPTIMIZATION
June 15 – 17, 2004
Dallas, Texas

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NEWS

- **Advective control**: heuristic optimization of particle tracking problems

- **Binary** and **real coded** decision parameters: SGA vs. **DES**

- Hydraulic/economic optimization of **Pump-and-Treat** and **Funnel-and-Gate** systems

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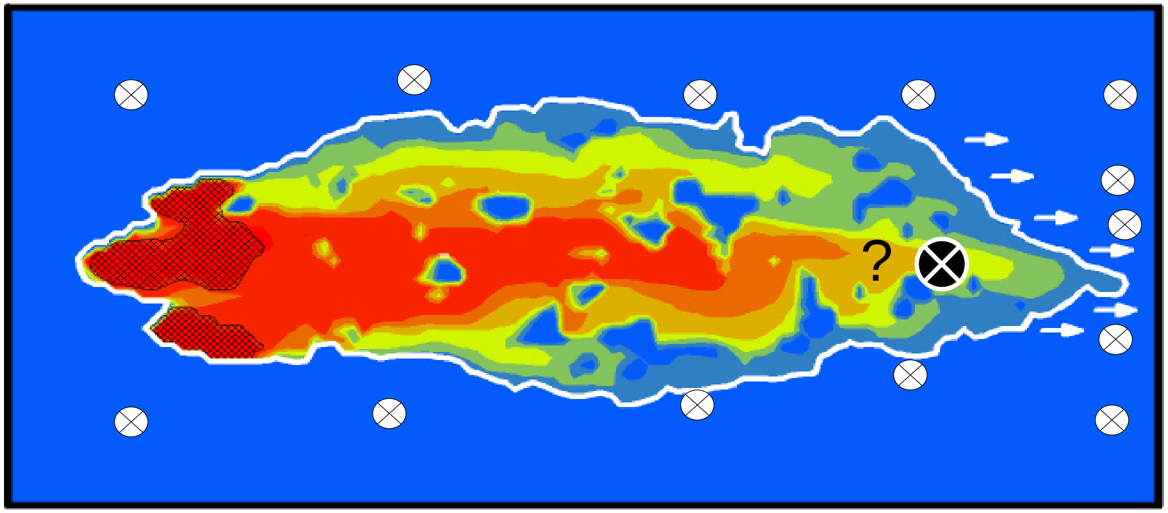
Capture zone evaluation criteria for pump-and-treat

(cp. *Mulligan & Ahlfeld 1999)*



´´Concentration control´´

- (Accurate) Transport model of contaminant site required.

- Evaluation of system performance by logging contaminant concentrations at compliance areas or at hypothetical monitoring wells

- Adaptation of contaminant pumping wells: minimum pumping rate, minimum operation time.

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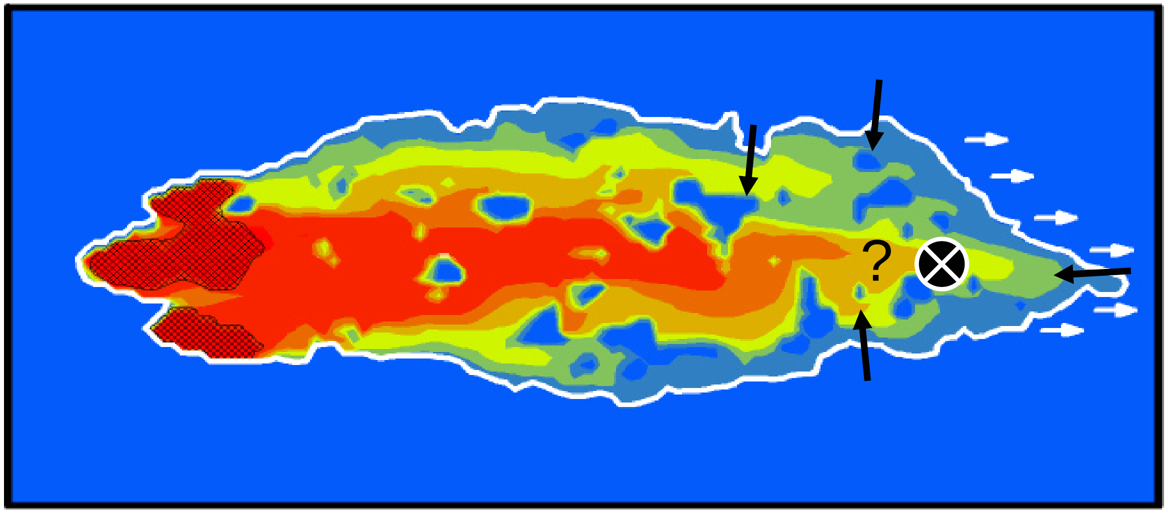
Capture zone evaluation criteria for pump-and-treat

(cp. *Mulligan & Ahlfeld 1999)*



´´Hydraulic control´´

- Hydraulic and/or transport model of contaminant site required.
- Evaluation of system performance by ensuring gradient/velocity constraints at selected control points (pre-definition of optimal capture zone, downgradient control hardly possible).
- Adaptation of contaminant pumping wells: minimum pumping rate, minimum operation time.
- Relatively fast method.

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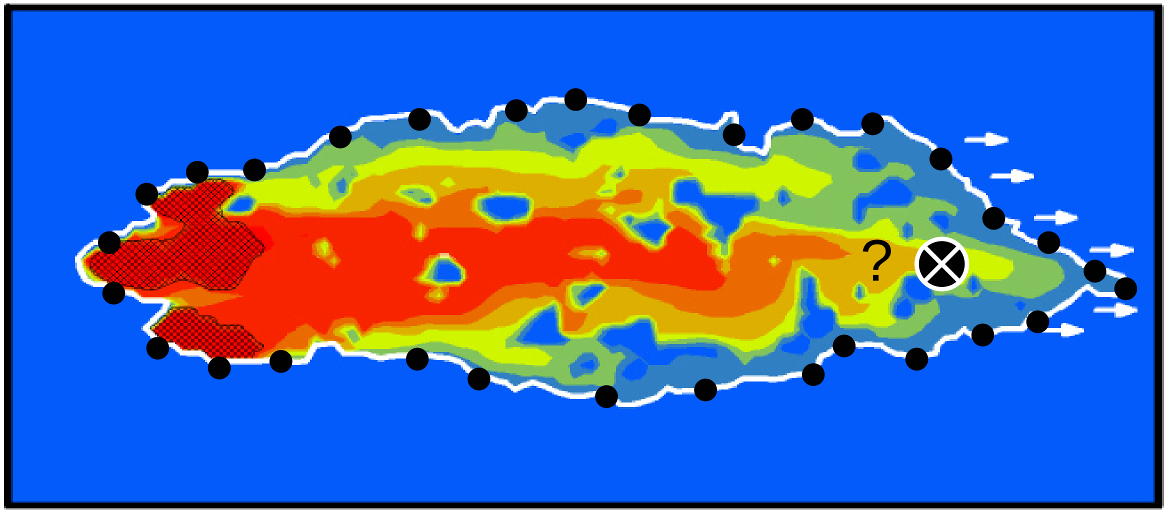
(cp. *Mulligan & Ahlfeld 1999)*



´´Advective control´´

- Hydraulic model of contaminant site required.
- Evaluation of system performance by tracking particles at selected control points.
- Adaptation of contaminant pumping wells: minimum pumping rate.
- Relatively fast method.

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Advective control vs. alternative methods

→ Only direct method, optimal well configuration not predefined.

→ Source of uncertainty: hydraulic description, delineation of contaminated zone.

→ Can also be used for optimization of wells with time-related capture zones or recharge areas

Problem: natural heterogeneous aquifers lead to highly nonlinear relationship between well positions, pumping rates and the ´degree´ of capture.

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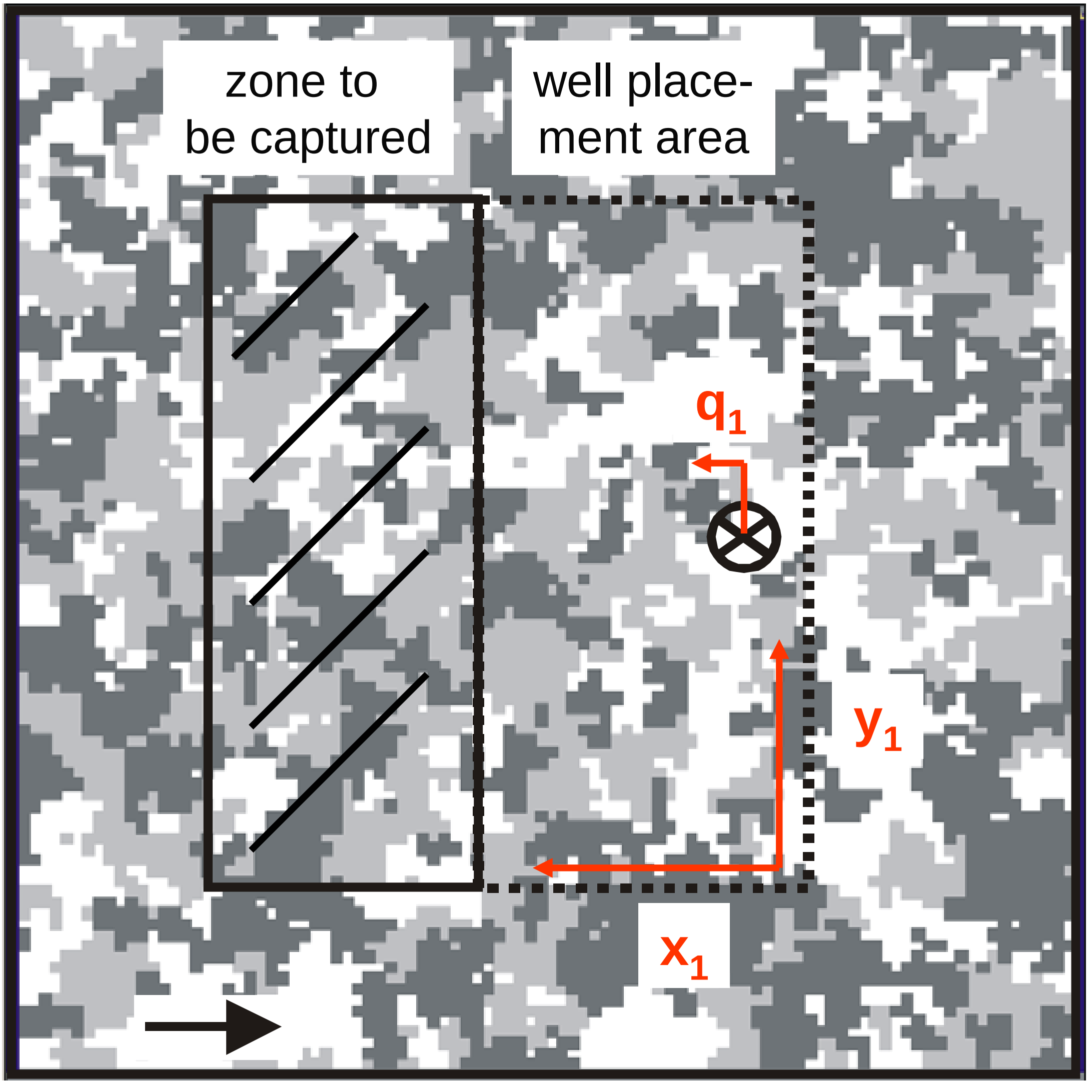
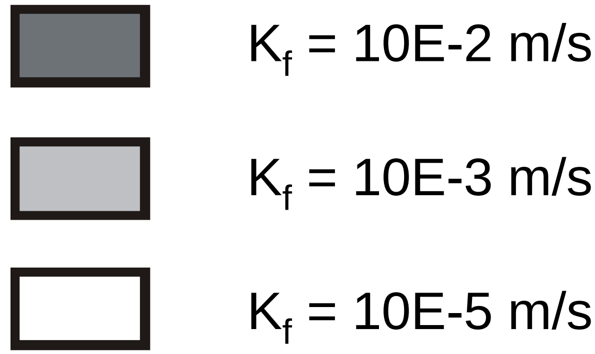
Example problem: heterogeneous aquifer, 1 well



hydr. conductivity distribution



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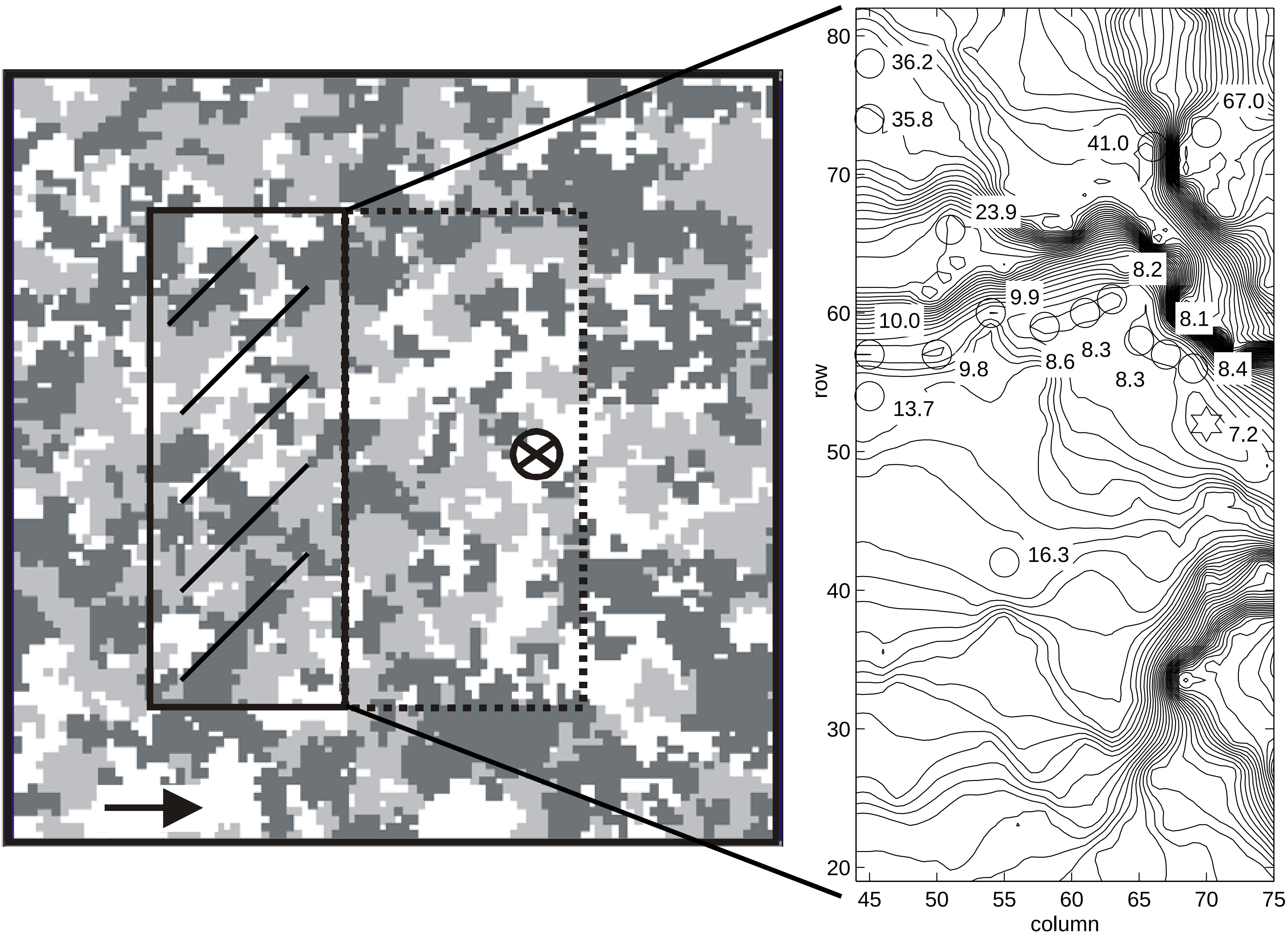
Minimum pumping rate distribution (1 well)



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Explicit formulation of multi-criterion objective function

$$J = \min f(q_{1..N}, x_{1..N}, y_{1..N})$$

$$f = f_q(q_{1..N}) \cdot p\,(q_{1..N}, x_{1..N}, y_{1..N})$$

´cost term´ **´penalty term´**

calculation by (non)linear/economic model

containment ?
computation by numerical model

$$p = \nu(q_{1..N}, x_{1..N}, y_{1..N})$$

ν : relative number of captured particles

$$p = 10^{100\nu}$$

e.g., exponential penalty term

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Objective function solver: requirements

! Objective function is not differentiable

! Objective function is supposed to have various local optima

! Flexible applicability to high dimensional problems (e.g. 4 wells: D = 12)

Heuristic techniques:

- solve problems with rules-of-thumb or common sense rules
- typically transformed from another science field

Evolutionary algorithms
analogies to evolutionary processes

Simulated annealing
simulation of heating and cooling of metal

Tabu search
Inspired by random elements of human behavior

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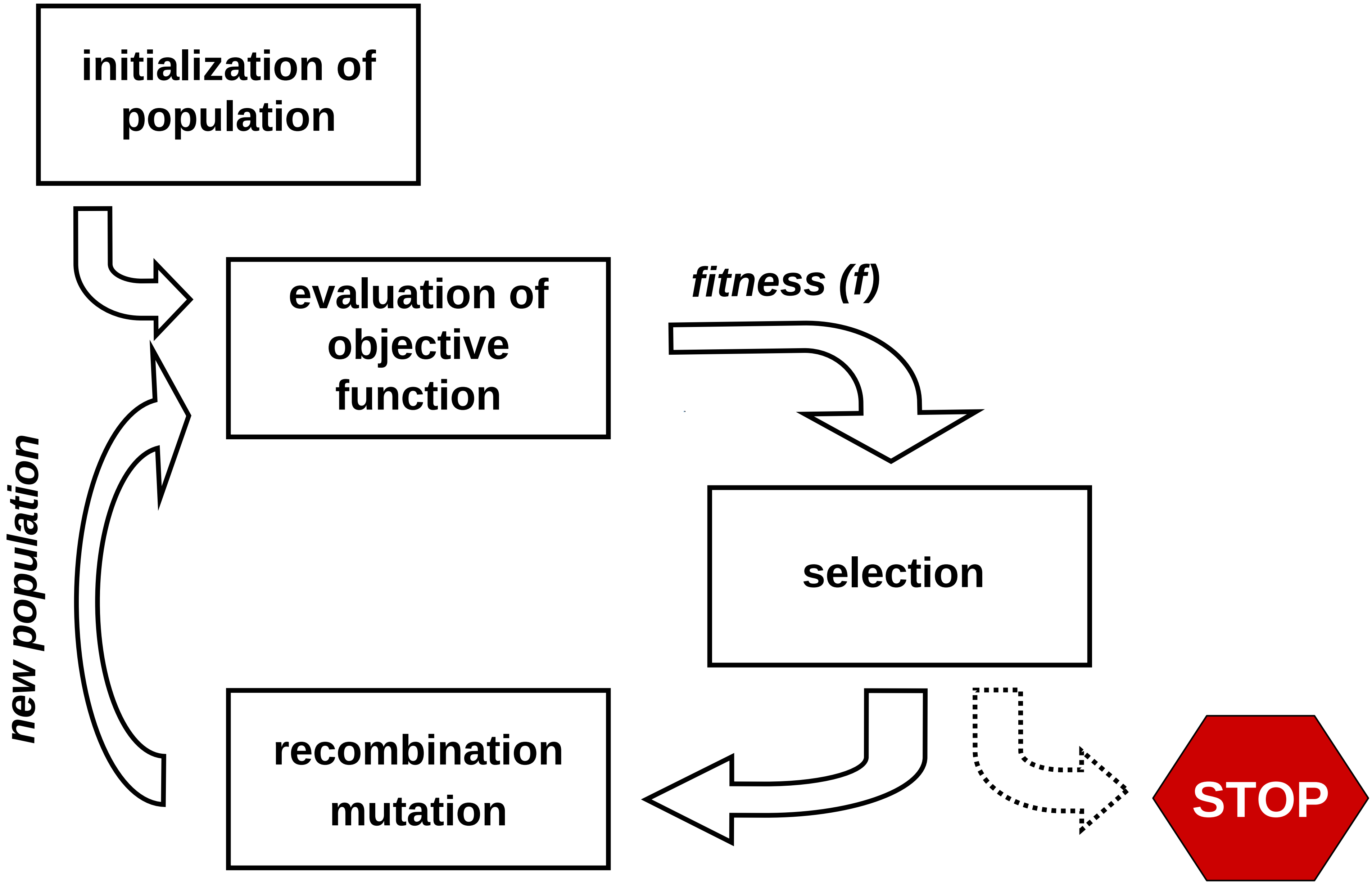
Evolutionary algorithms: operators



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Two variants: Representation

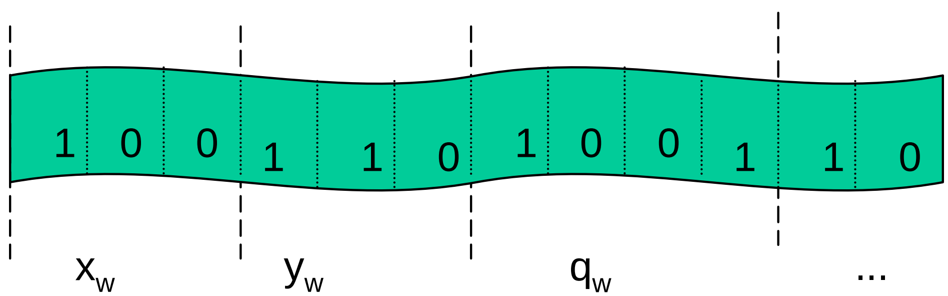
GENETIC ALGORITHM

(SGA)

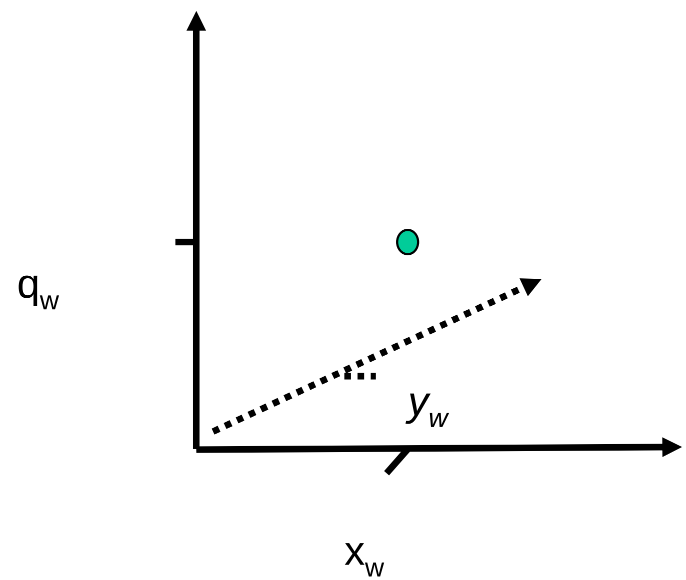
EVOLUTION STRATEGY

(DES)

binary



real valued



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Two variants: Mutation

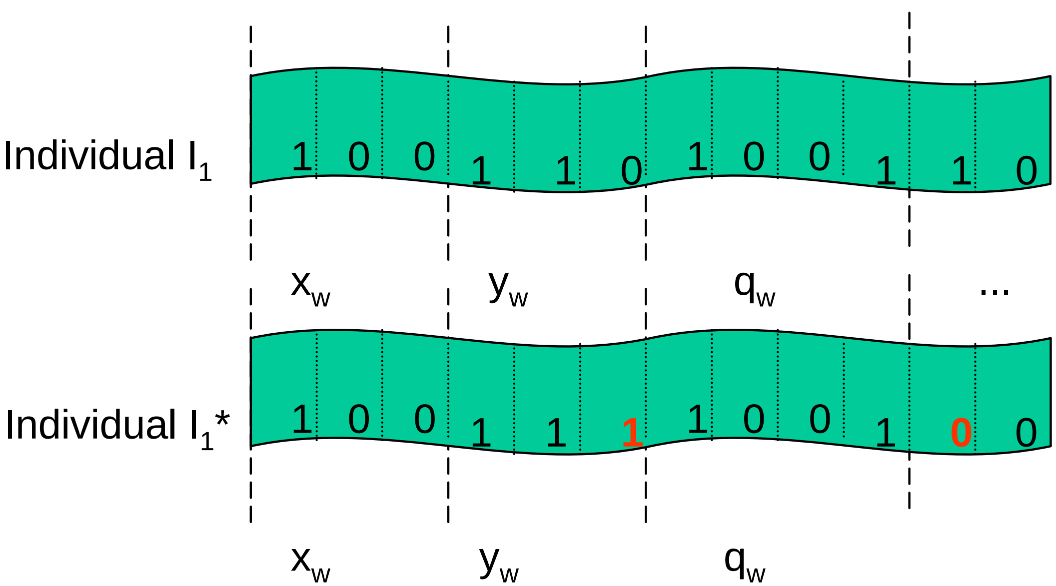
GENETIC ALGORITHM

(SGA)

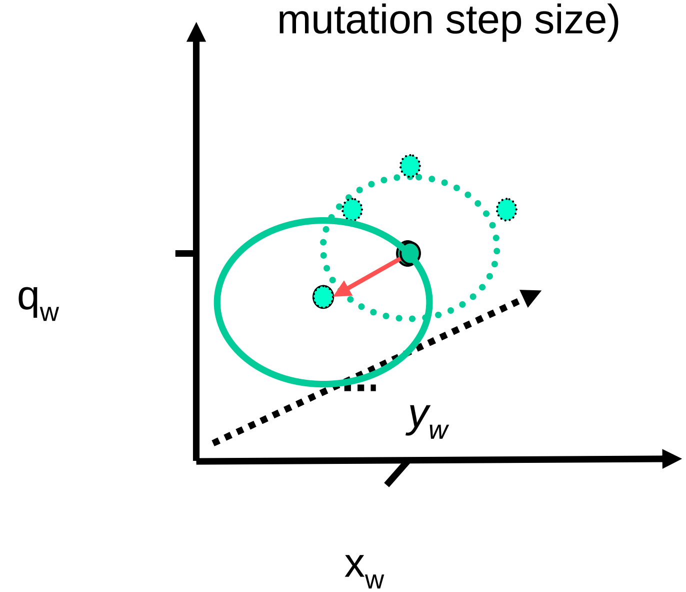
EVOLUTION STRATEGY

(DES)

flipping bits



Mutation follows n-dimensional probability density function with adapted standard derivation (= mutation step size)



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Two variants: Recombination

GENETIC ALGORITHM

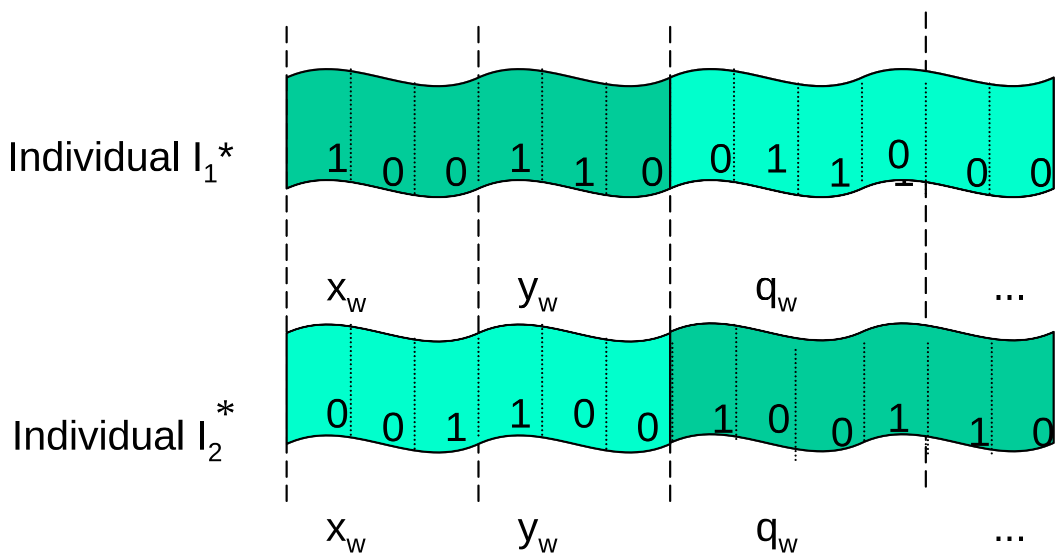
(SGA)

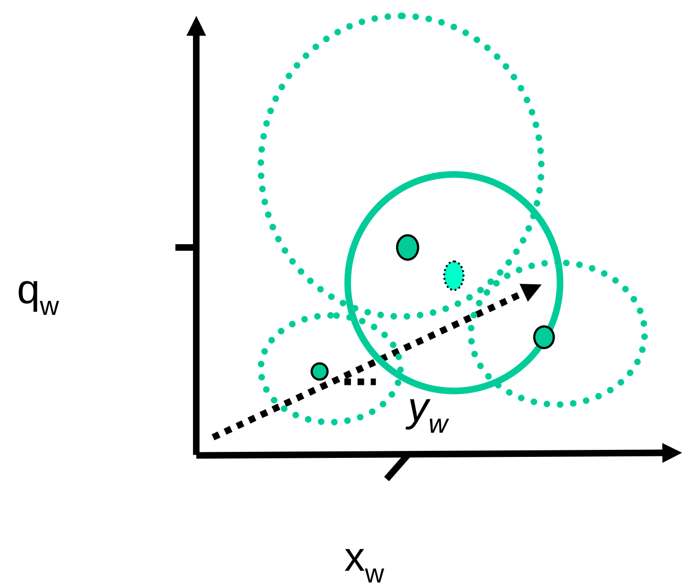
EVOLUTION STRATEGY

(DES)

binary

real valued, multi-parent





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Derandomized Evolution Strategies

(cp. *Hansen & Ostermeier 2001; Hansen et al. 2003*)

- **Features:** Self-adaptive mutative step size control; weighted/intermediate multi-parent recombination, \`cumulation\`; \`CMA\`

- **Applicability:** Efficient for non-linear, badly scaled, high dimensional problems

- **Questions:** Suitable for advective control problem with both discrete & real valued object parameters? Maximum number of iterations? Stop criterion?

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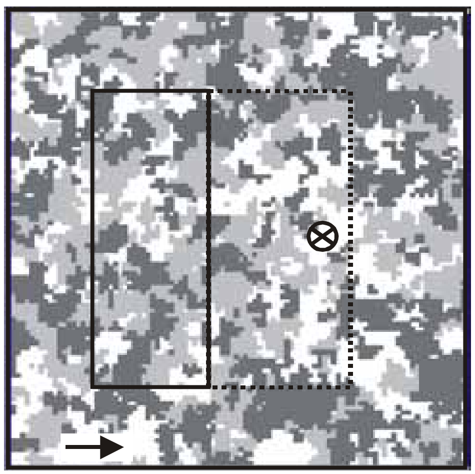
Application to example site DES vs. SGA



evolutionary search is stochastic:

50 randomly initialized equal optimization runs with predefined number of model calls

setting of decision variable limits:

pumping rate maximum is set case-specific or automatically (*boundary update*)

objective values:

pre-selected optimal values of pumping rate are set as objective values ***fov***

some configurations are called more than once

for the SGA *bookkeeping* is conducted

(Bayer & Finkel, Water Resour. Res. 2004)

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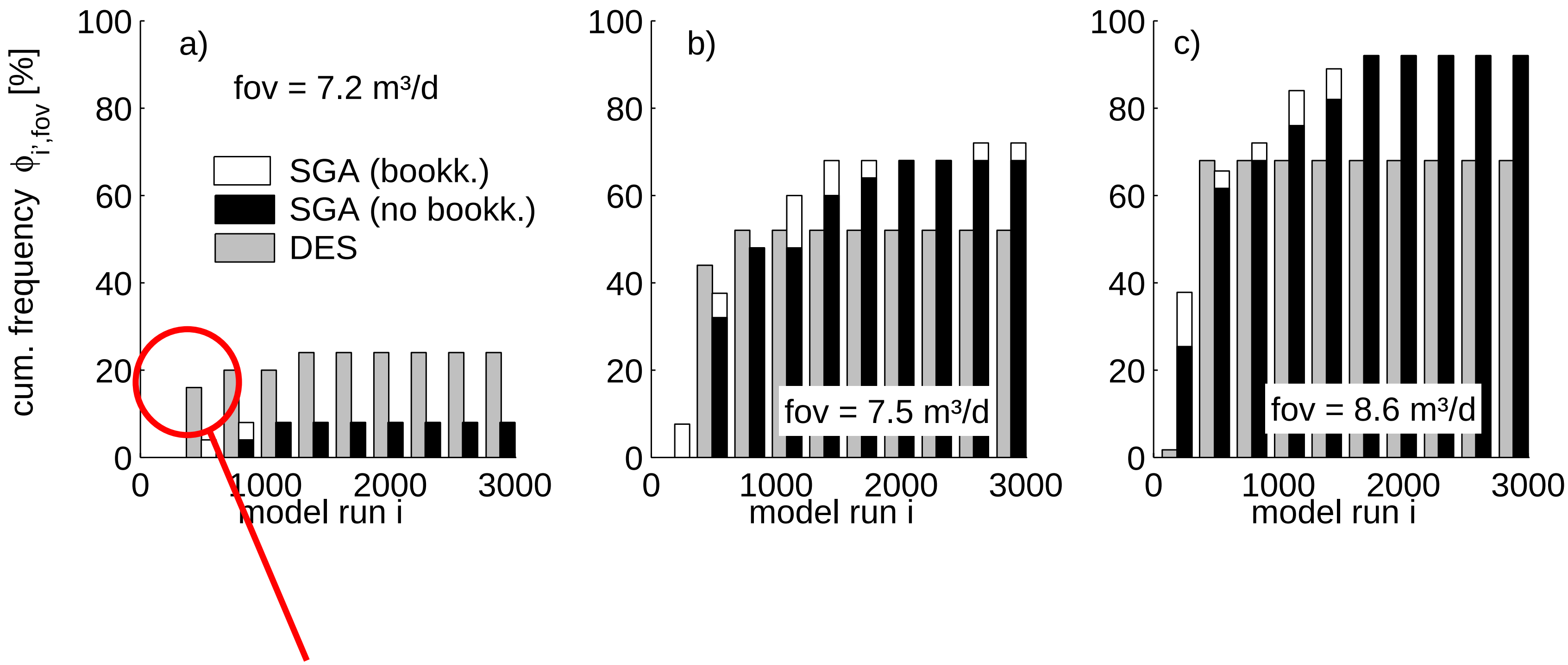
1-well case

"MR_{fov}" : calculated average model runs required to find a solution for a selected objective value *fov*.



5 optimization runs
á 350 model calls
→ MR_{fov} = 1750 model calls

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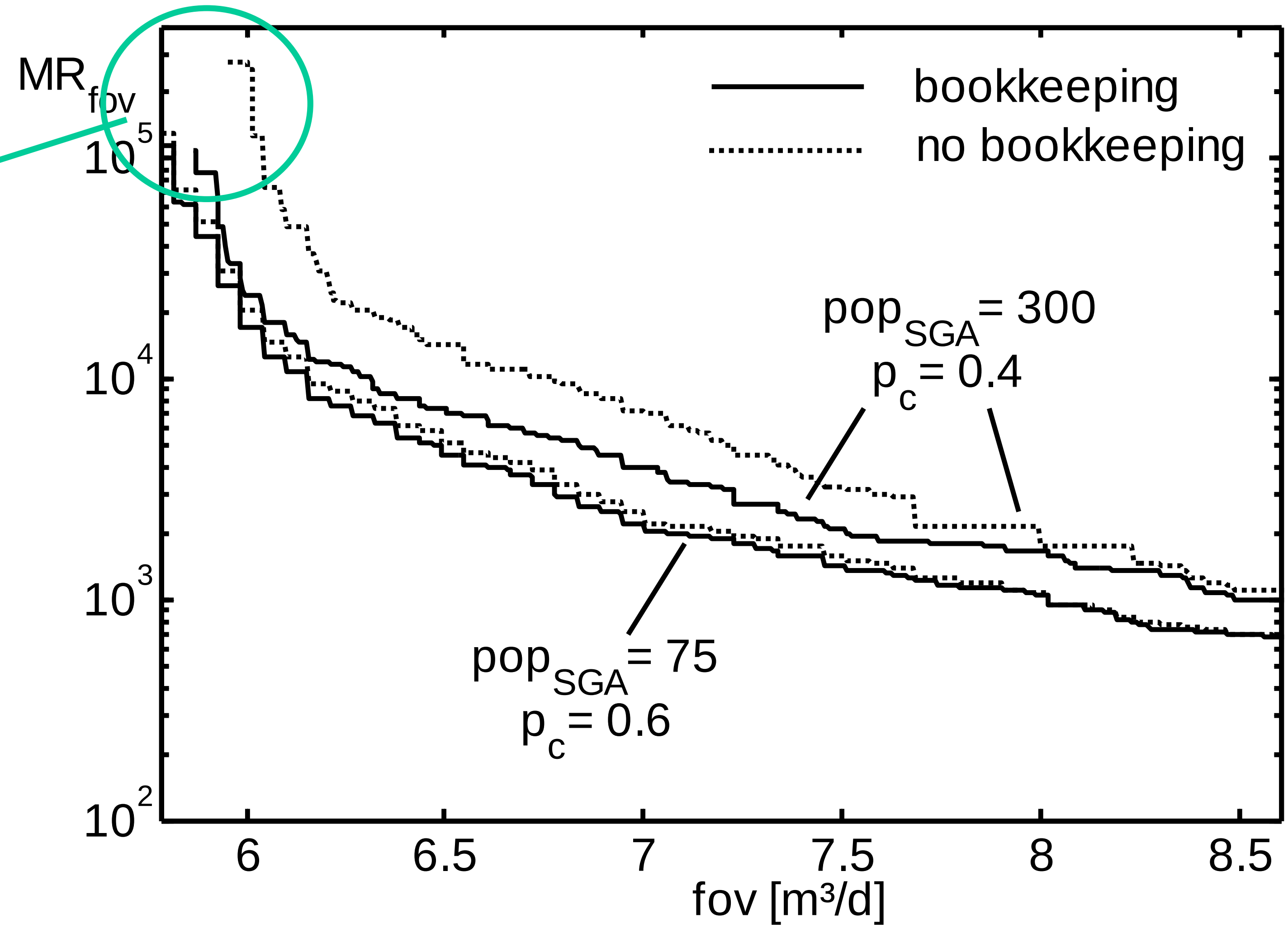
4-well case: SGA

No solution found!
(+ boundary update)



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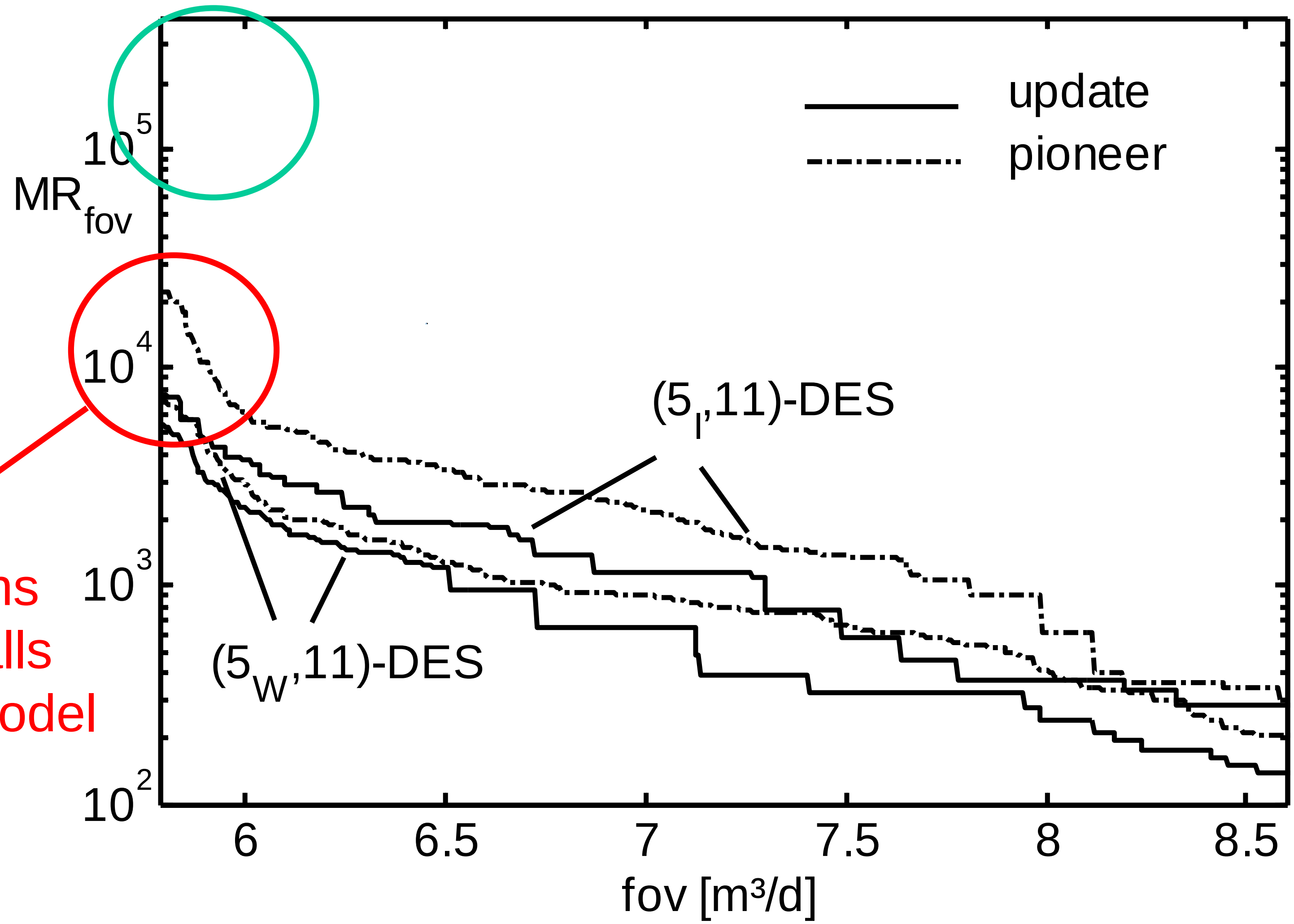
4-well case: DES



4 optimization runs
á 1,400 model calls
→ MR_{fov} = <u>5,600</u> model calls

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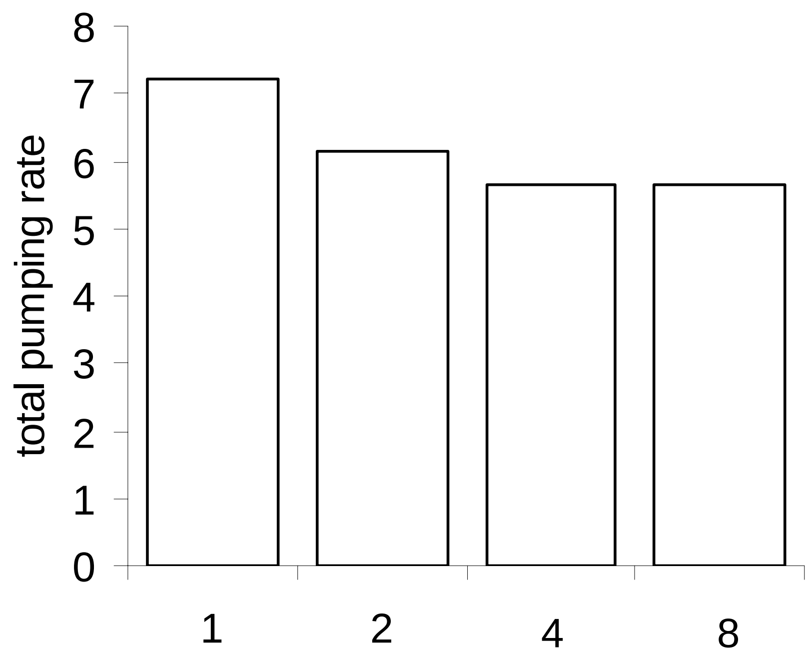
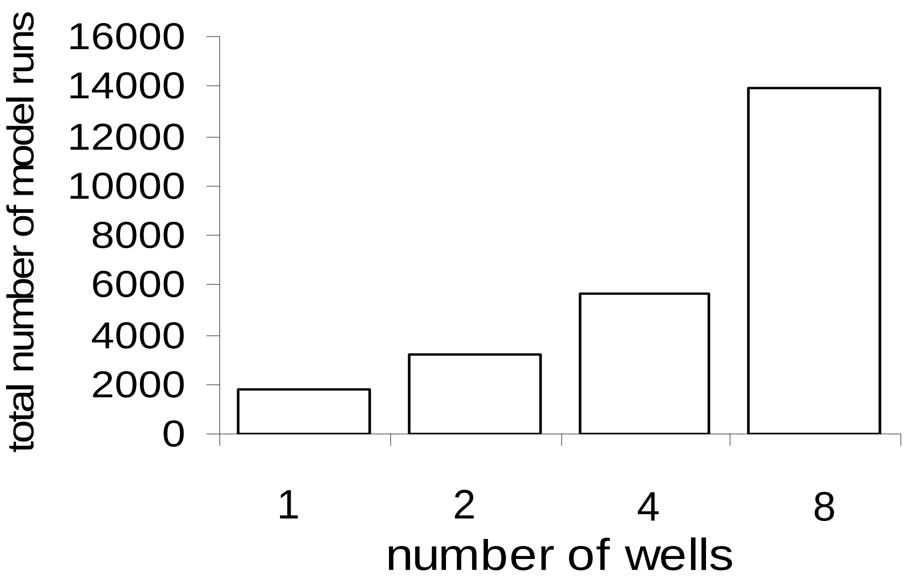
Conclusions: DES

→ Increasing the number of wells reduces the minimum total pumping rate



→ Increasing the complexity leads to a ~ linear increase of required model runs



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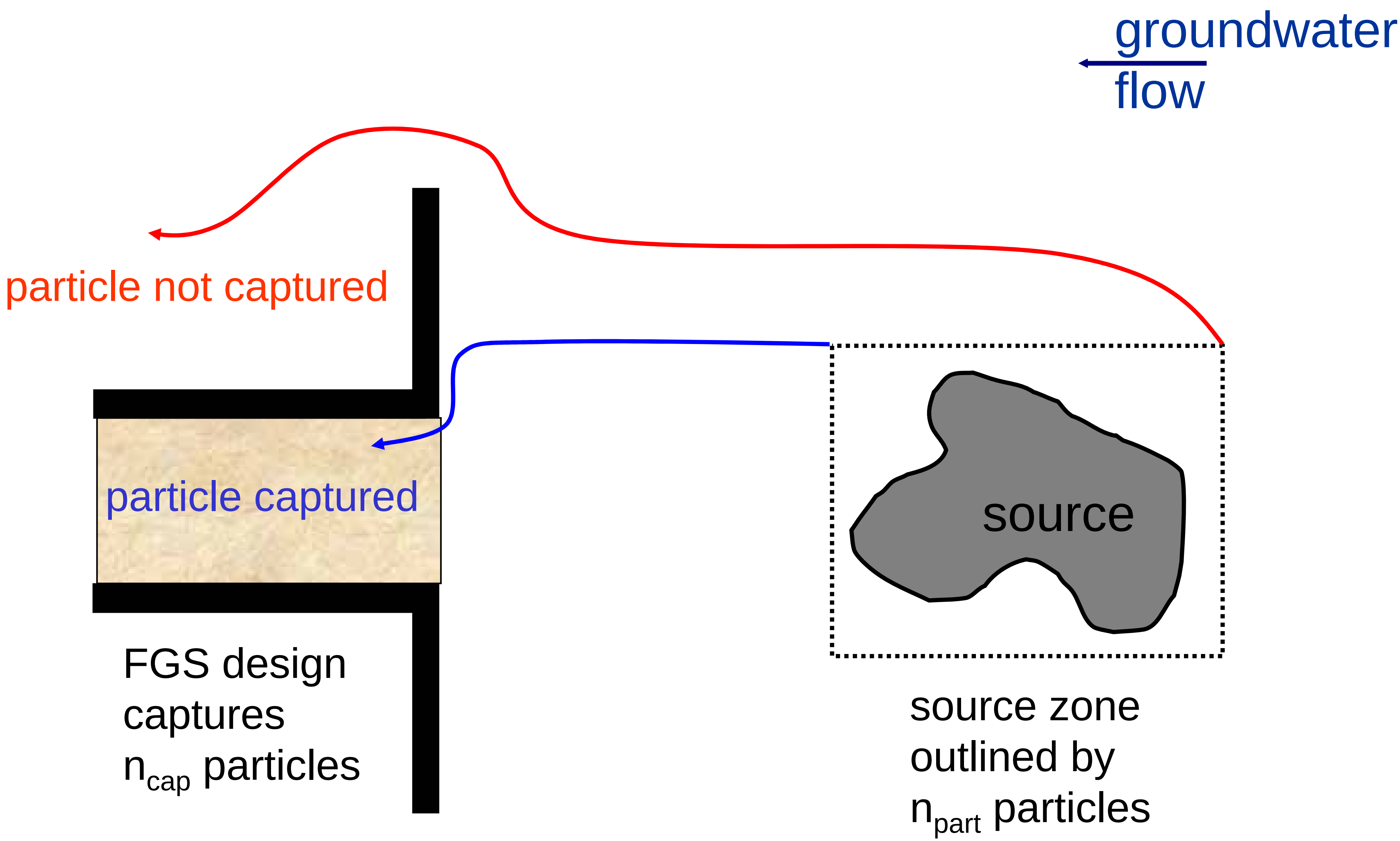

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$$Cost = (2\times\Sigma l_g + \Sigma w_f)\times C_f + 2\times\Sigma w_g \times C_g + \Sigma(w_g \times l_g)\times C_{reac}$$

where

C_f : unit funnel costs

C_g : unit gate costs

C_{reac} : unit reactive material cost

plume capture constraint honoured by exponential penalty term:

$$fit = \begin{cases} Cost \times a\text{^}((b\times((n_{part}/n_{cap})-1))\text{^}c), \text{ if } n_{cap} \neq 0 \\ \text{inf, otherwise} \end{cases}$$

where

$a,b,c > 0$: to be selected according to the range of the unit costs

n_{part} : number of tracked particles

n_{cap} : number of particles captured

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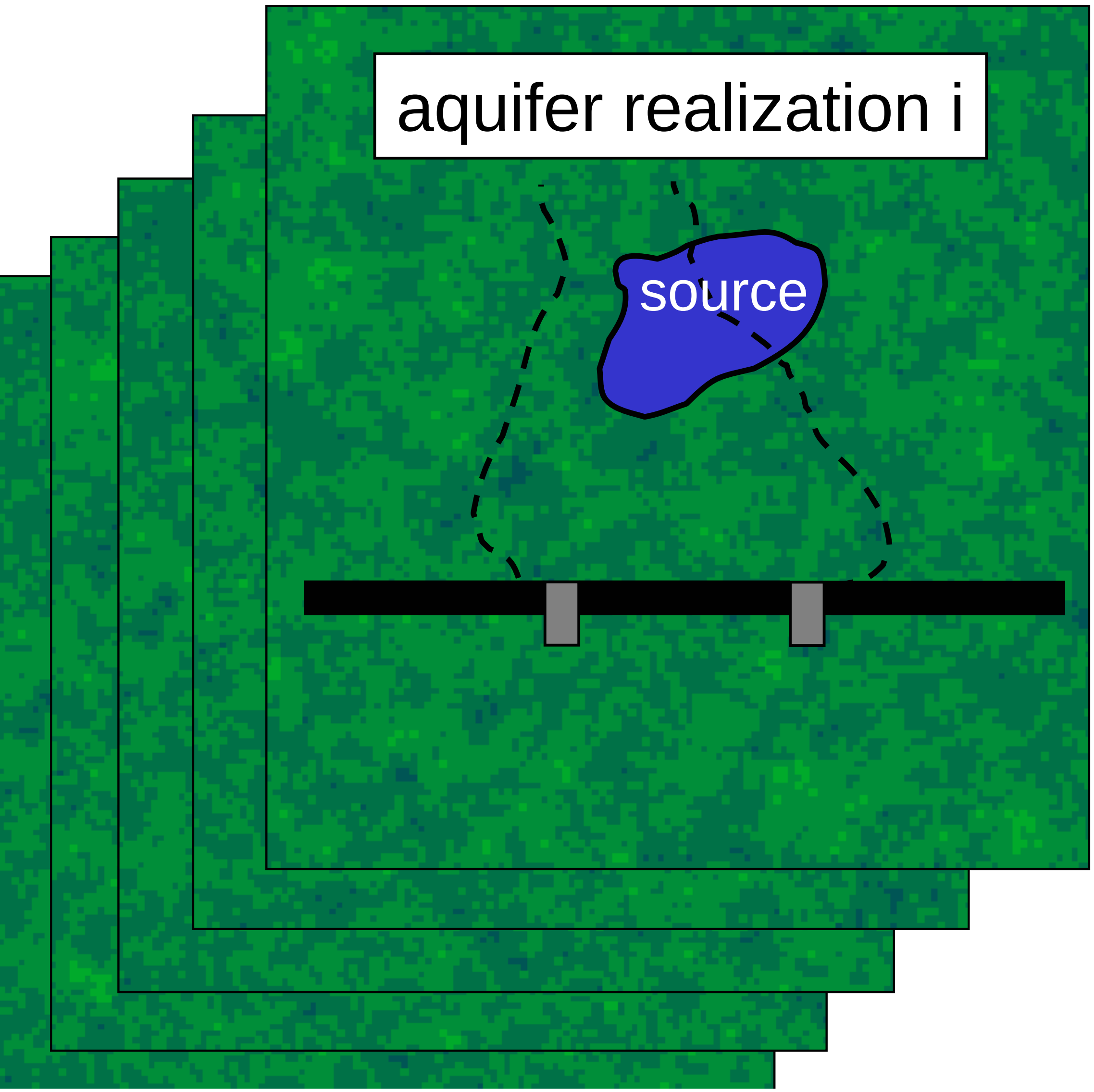
Additional constraint: One design fits all?



- natural aquifer heterogeneity creates uncertain description of flow field

- multiple equiprobable aquifer realizations as part of the objective function

- fit = max (fit_i,i = 1,..,5)

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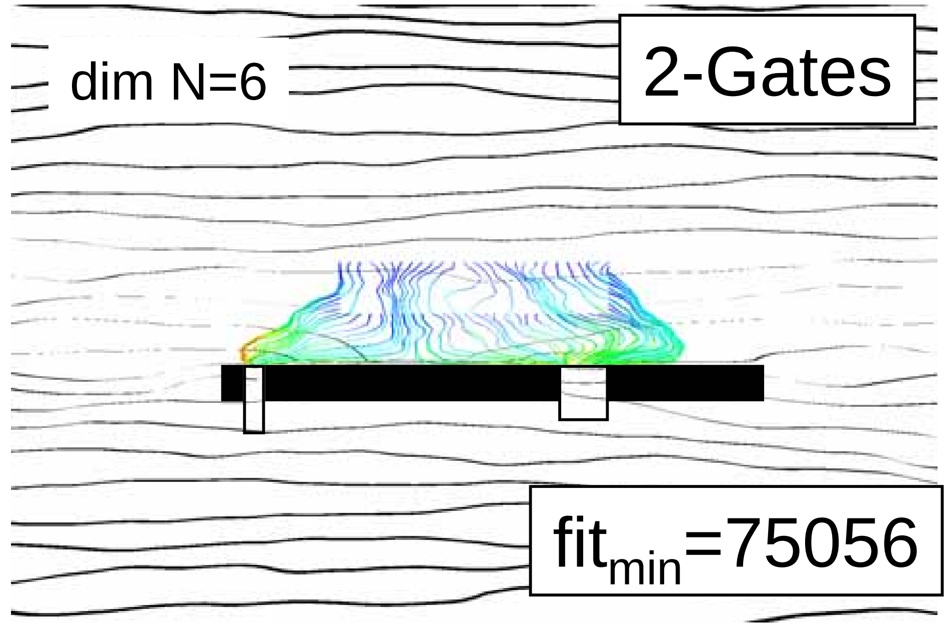
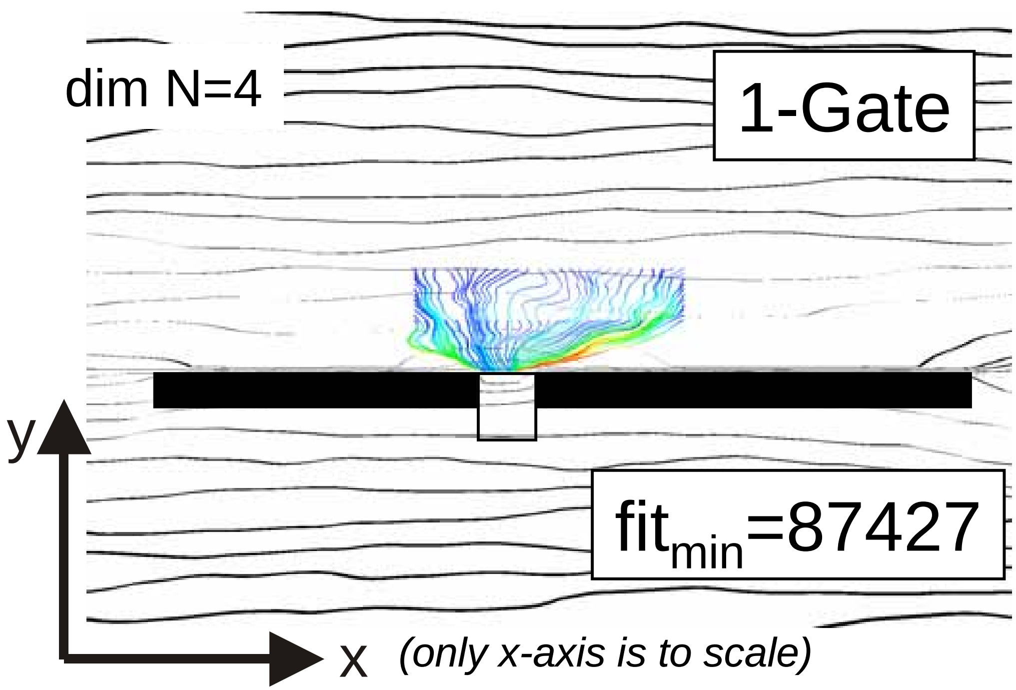
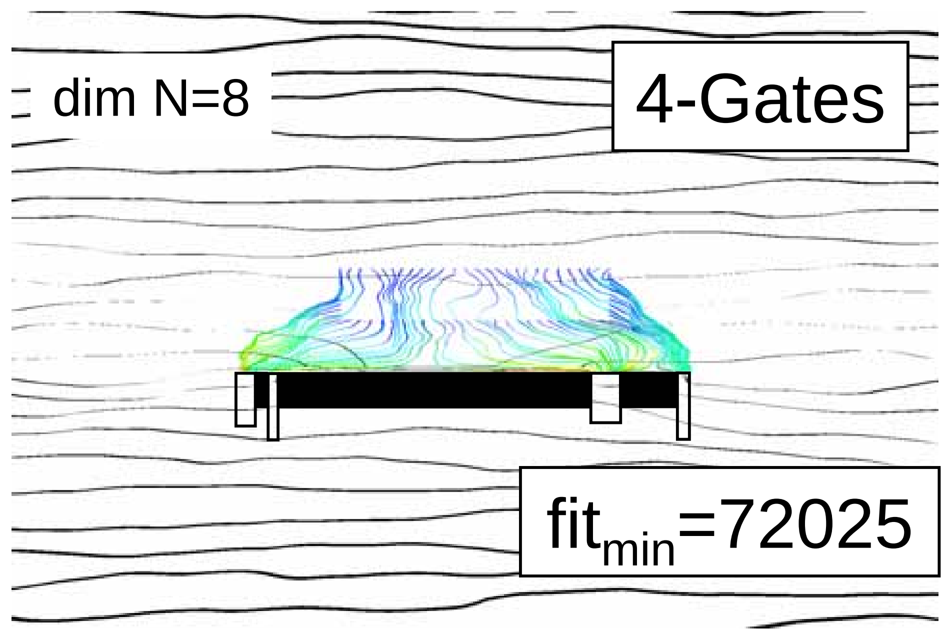
DES results:







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Conclusions

Advantages of DES

- More robust & efficient, less stochastic & less model runs than SGA
- More suitable for in case of real valued object parameters, applicability in case of discrete object parameters
- Relevance of object parameter limits reduced by self adaptation

Lessons learnt + Outlook

- Number of model runs scales ~linear with problem dimension for DES
- Efficiency of boundary update: additional use of available information
- Limitations for DES in case of „hard“ discretisized problem formulations?
  →Further inspection of applicability for Funnel&Gates Systems
- Missing: Requirement of stop criterion for practical use