UNIL | Université de Lausanne

Ensemble Project

Universities of Basel, Bern, Lausanne & Neuchâtel (Switzerland)
Swiss Federal Institute of Technology, Zürich (Switzerland)
Stanford University (USA)

Functional error modeling for Bayesian inference in hydrogeology

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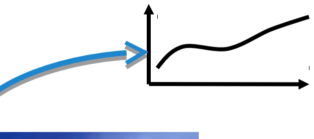
PhD supervisor Prof. Ivan Lunati

Institute of Earth Sciences
University of Lausanne

| le savoir vivant |

Challenges in groundwater problems

Motivation



Typical question:
What is the concentration of contaminant in the drinking water?

Problem:
Many uncertainties in the aquifer properties

Solution: Monte Carlo approaches

Uncertainty quantification, inversion, history matching, …

Challenges in groundwater problems
Monte Carlo approaches

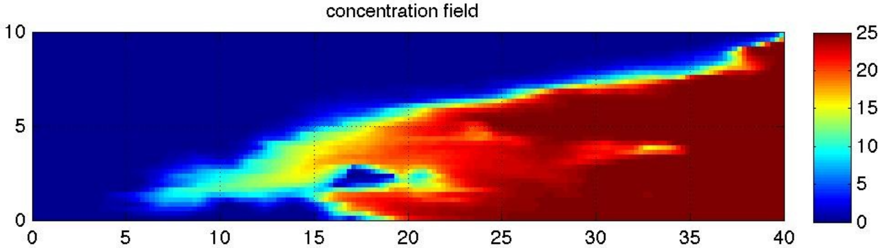
Description of the uncertainty on the permeability field

- Generate multiple geostatistical realizations
  - Based on prior knowledge
  - Methods: object-based, multipoint statistics, process-based, …

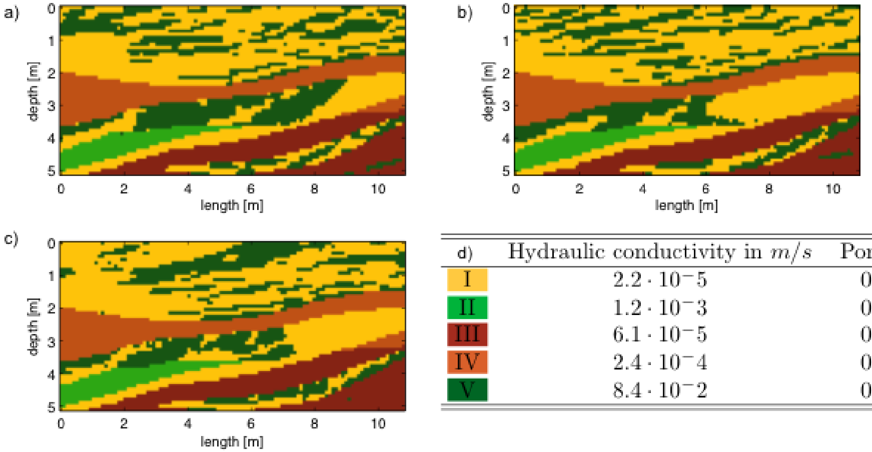
“Truth” inspired from the Herten test case (Bayer et al. 2011)

Issue

- Not the quantity of interest!
- Flow simulation for each of the realizations
  - Typical order: 10^3-10^5 simulations
  - > Untractable computational cost



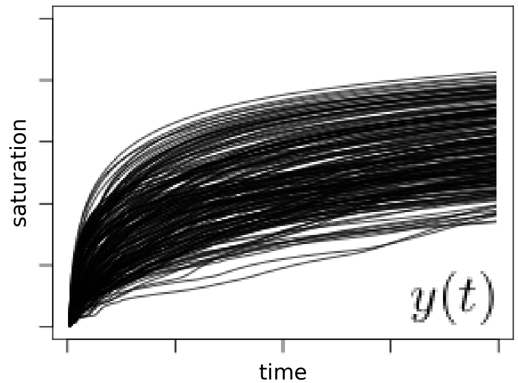
Simulation of saline intrusion



d)	Hydraulic conductivity in m/s	Porosity
I	$2.2 \cdot 10^{-5}$	0.21
II	$1.2 \cdot 10^{-3}$	0.32
III	$6.1 \cdot 10^{-5}$	0.13
IV	$2.4 \cdot 10^{-4}$	0.16
V	$8.4 \cdot 10^{-2}$	0.25

3 examples of geostatistical realizations generated using Direct Sampling (Mariethoz et al. 2010)

How to simulate flow?



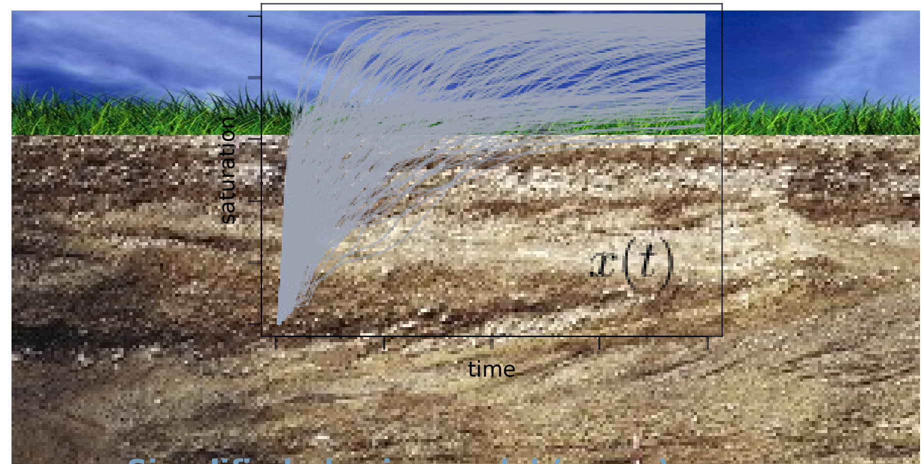
Exact model

- Full physics flow simulation
- Too costly
- Impossible to solve systematically for all geostatistical realizations
- Only for a few of them

Example: two-phase problem

$$\nabla \cdot \left[\left(\frac{k_n(S)}{\mu_n} + \frac{k_w(1-S)}{\mu_w} \right) k \nabla p \right] = 0$$

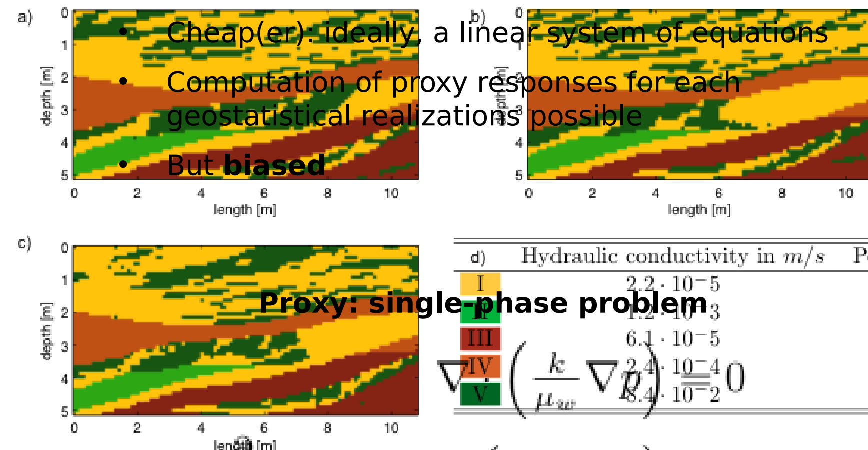
$$\frac{\partial}{\partial t}(\phi S) - \nabla \cdot \left(\frac{k_n(S)}{\mu_n} k \nabla p \right) = 0$$



“Truth” inspired from the Herten test case (Bayer et al. 2011)

Simplified physics model (proxy)

- Approximation of the physical processes
- Cheap(er): ideally, a linear system of equations
- Computation of proxy responses for each geostatistical realizations possible
- But **biased**



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V	$8.4 \cdot 10^{-2}$	0.25

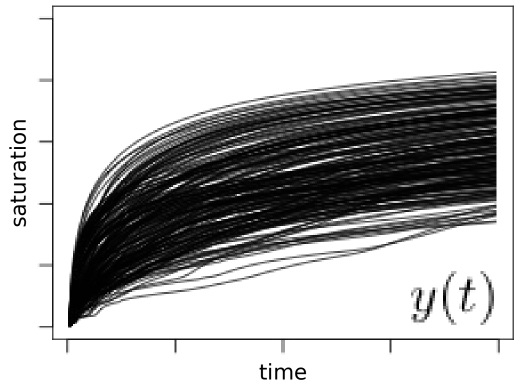
Proxy: single-phase problem

$$\nabla \cdot \left(\frac{k}{\mu_w} \nabla p \right) = 0$$

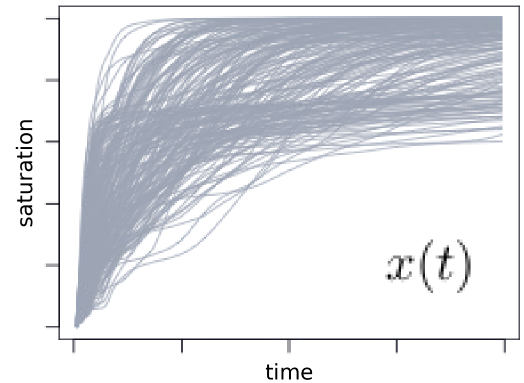
$$\frac{\partial}{\partial t}(\phi S) - \nabla \cdot \left(S \frac{k}{\mu_w} \nabla p \right) = 0$$

3 examples of geostatistical realizations generated using Direct Sampling (Mariethoz et al. 2010)

How to simulate flow?



Mapping between the two models



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- But **biased**

Error model

- To “recover” the missing physics
- Mapping between curves = regression model

How? Existing solutions:

→ On a learning set of realizations

→ Using Functional PCA

(Ramsay et al. 2006, 2009)

- Concurrent linear model

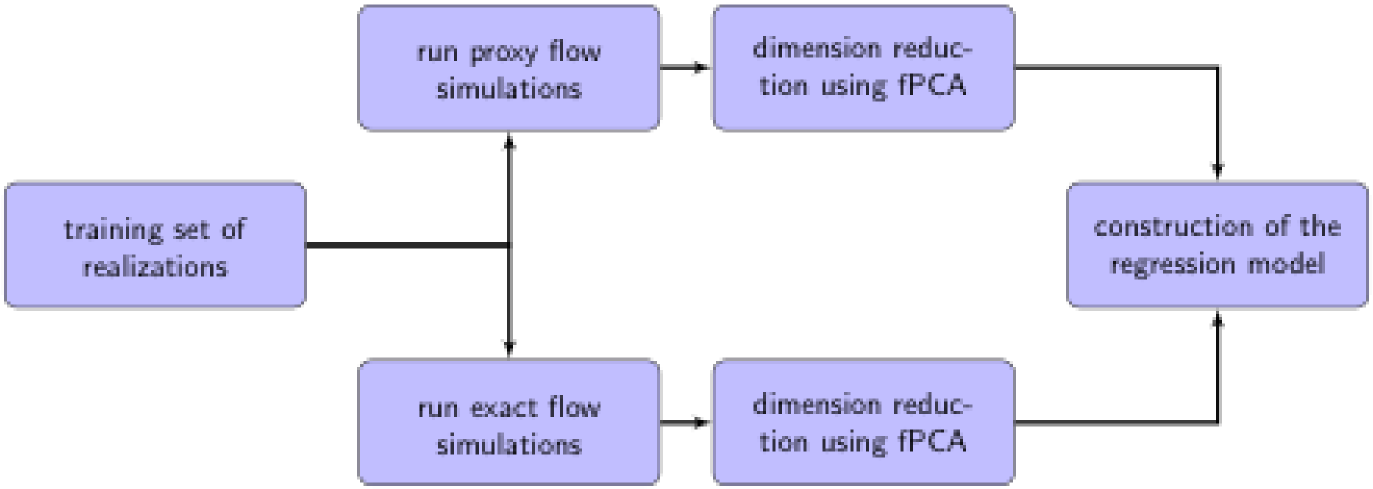
$$y_i(t) = \beta_0(t) + \beta_1(t)x_i(t) + \epsilon_i(t)$$

- Fully functional linear model

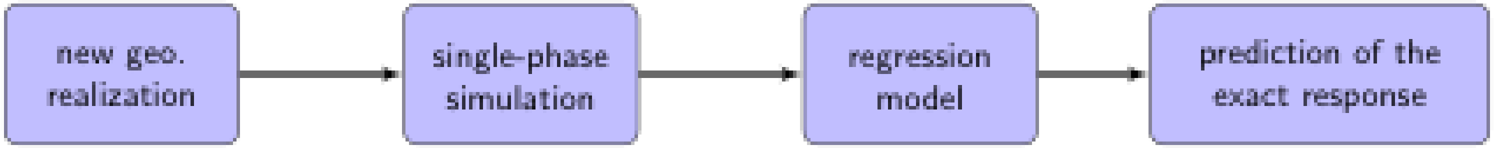
$$y_i(t) = \beta_0(t) + \int \beta_1(s,t)x_i(s)ds + \epsilon_i(t)$$

Workflow

Training phase of the error model



Prediction of the of the error model



Leak of oily pollutant

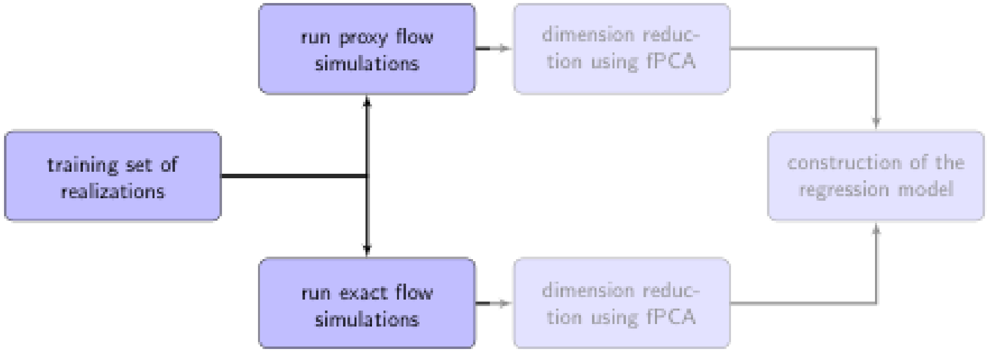
Drinking well

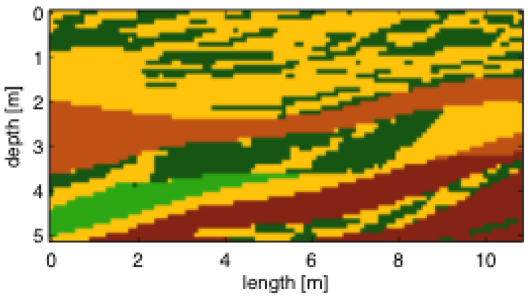
Description of the uncertainty:
1000 geostatistical realizations

ILLUSTRATION 1

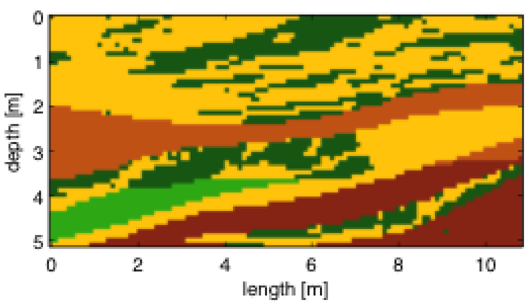
UNCERTAINTY QUANTIFICATION

Workflow





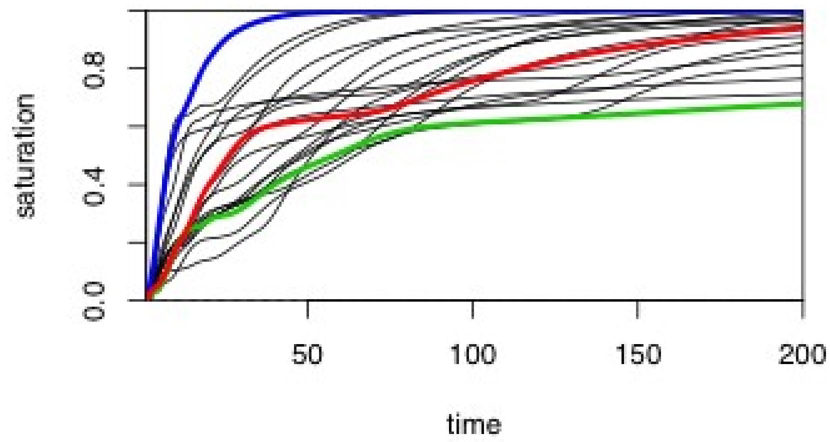
Blue curves



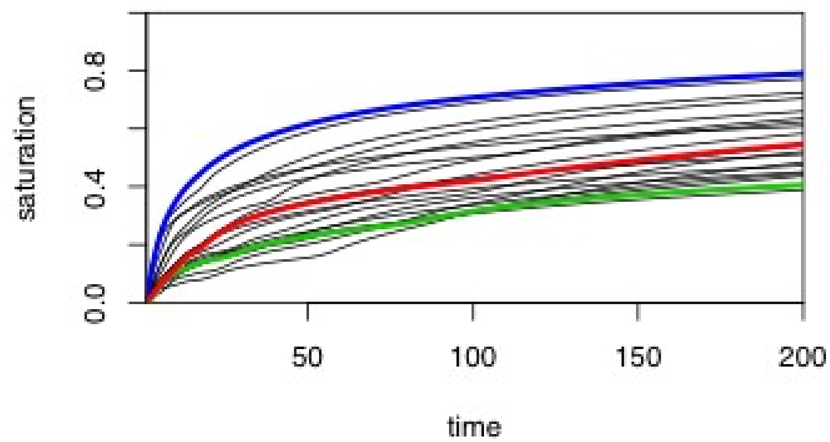
Green curves

Training set of 20 realizations

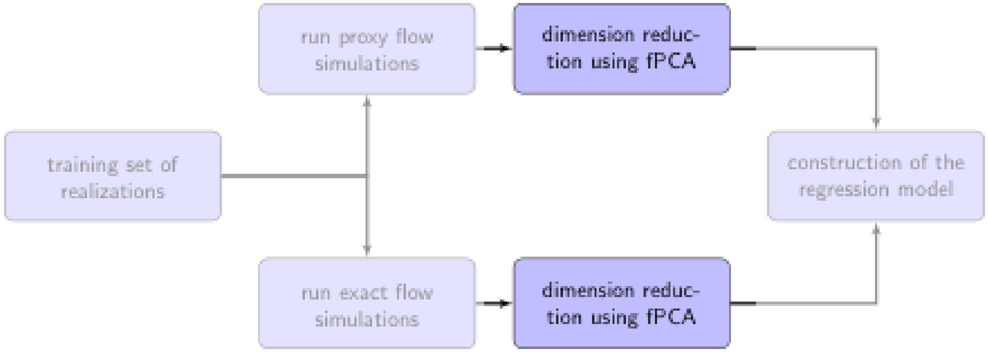
a) proxy breakthrough curves

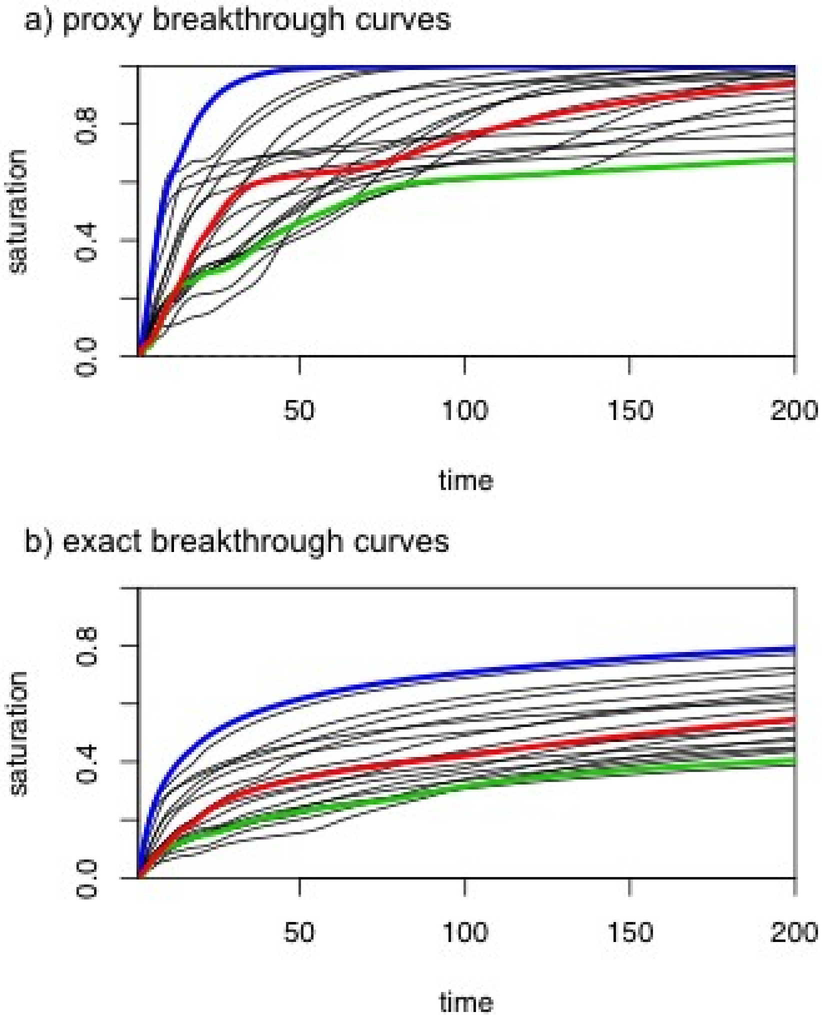


b) exact breakthrough curves



Workflow





FPCA $$x_i(t) \approx \bar{x}(t) + \sum_{j=1}^{N} s_{ij}\zeta_j(t)$$

Principal components (or harmonics) $\zeta_j(t)$ that maximises

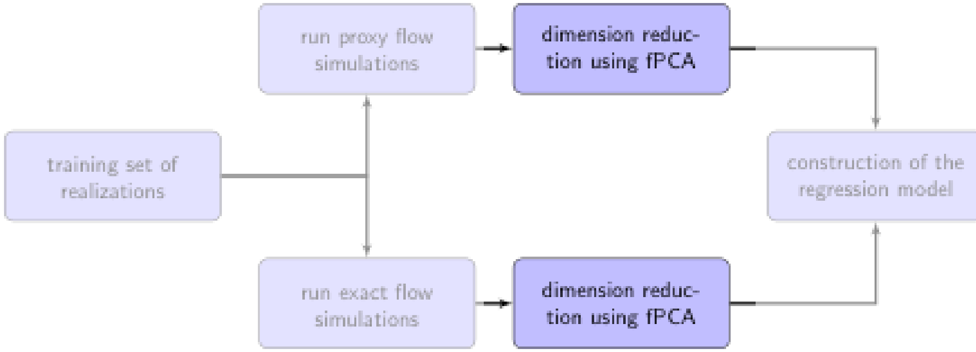
$$d_i = \mathrm{var}\Big(\int \zeta_i(t)[x_j(t) - \bar{x}(t)]dt \Big)$$

Principal components scores

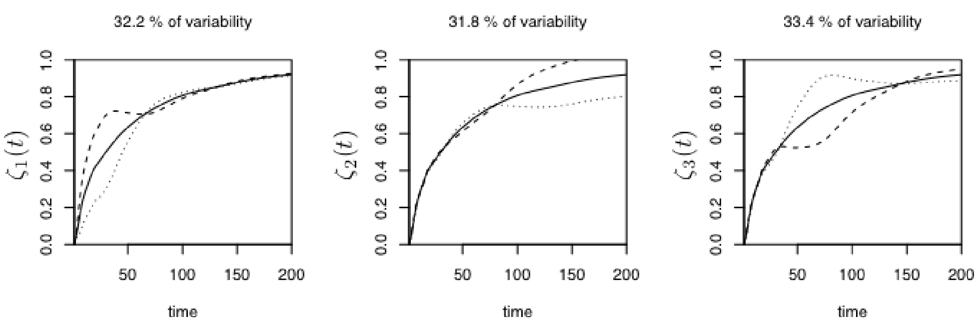
$$s_{ij} = \int [x_i(t) - \bar{x}(t)]\zeta_j(t)dt$$

Proportion of data explained by the i^{th} harmonics $$\frac{d_i}{\sum d_j}$$

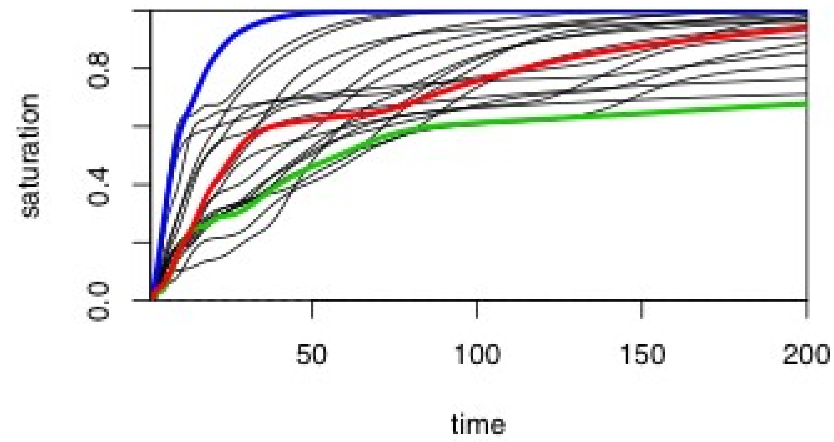
Workflow



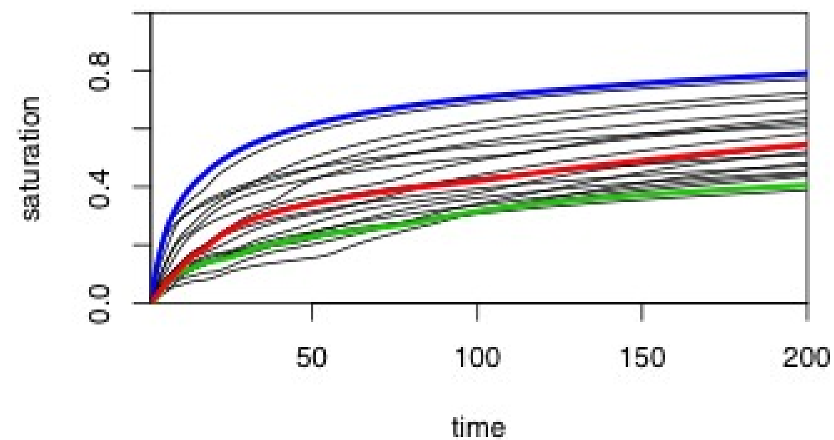
a) proxy harmonics



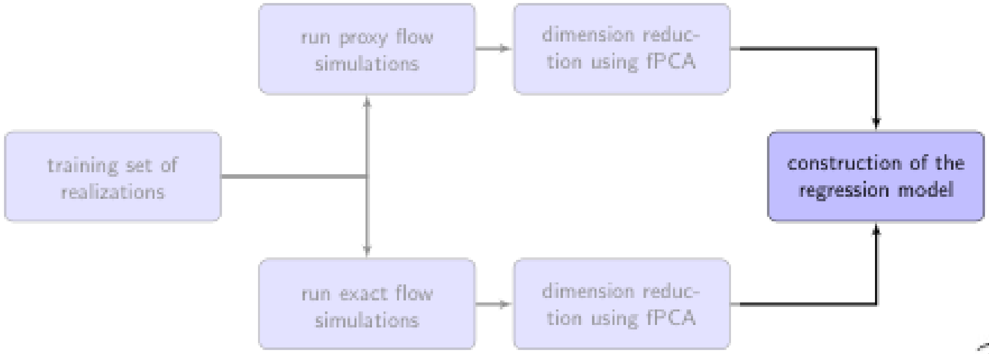
a) proxy breakthrough curves



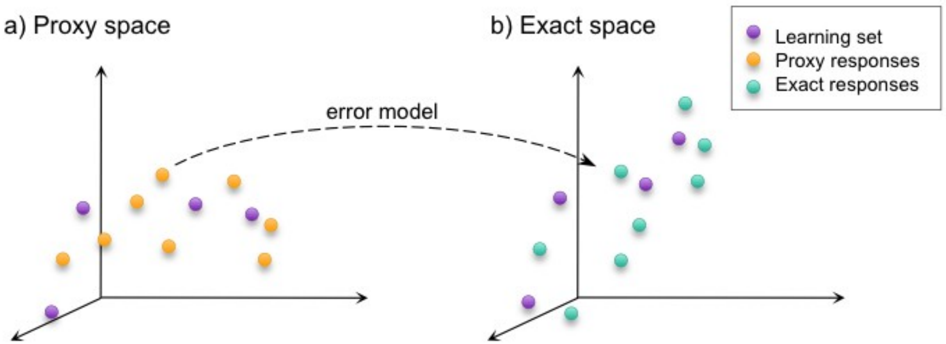
b) exact breakthrough curves

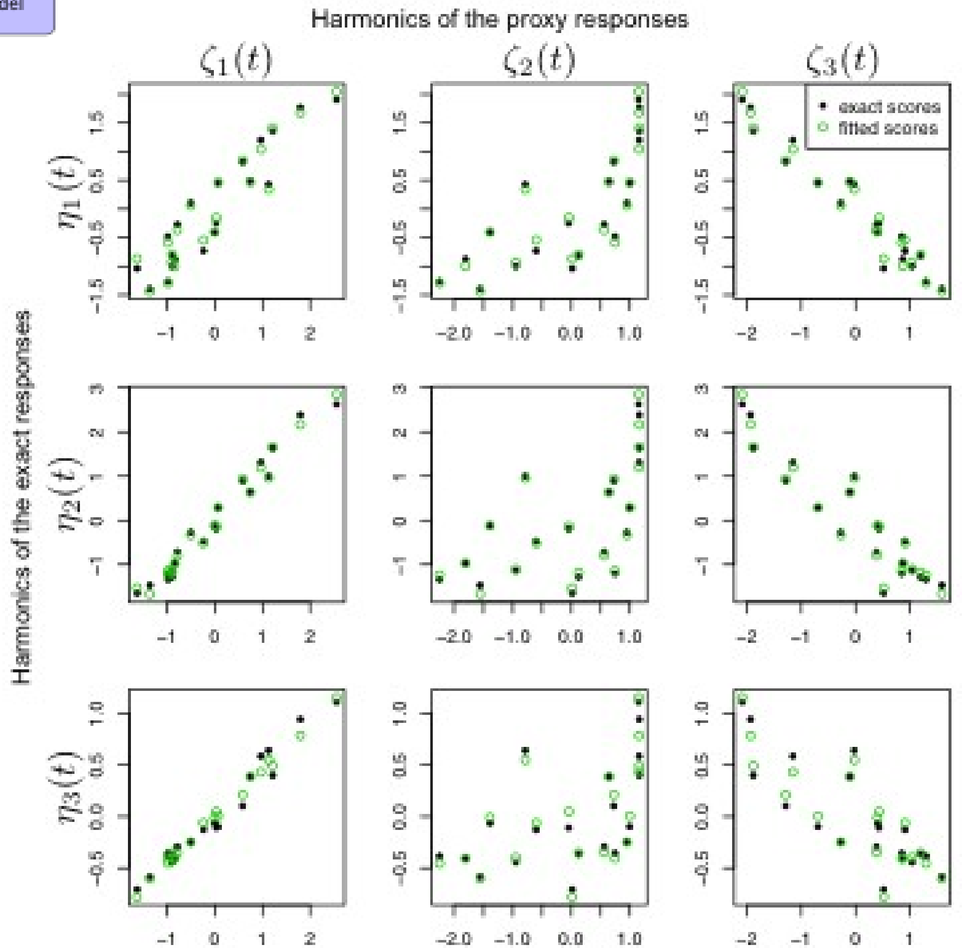


Workflow



$$x_i(t) \approx \bar{x}(t) + \sum_{j=1}^{3} s_{ij}\zeta_j(t)$$





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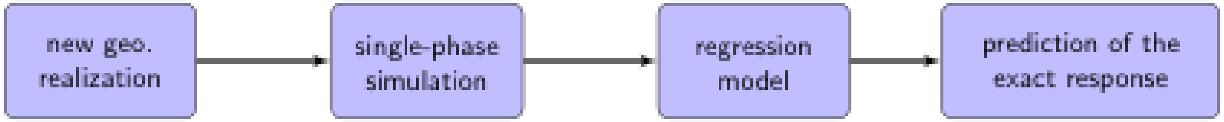
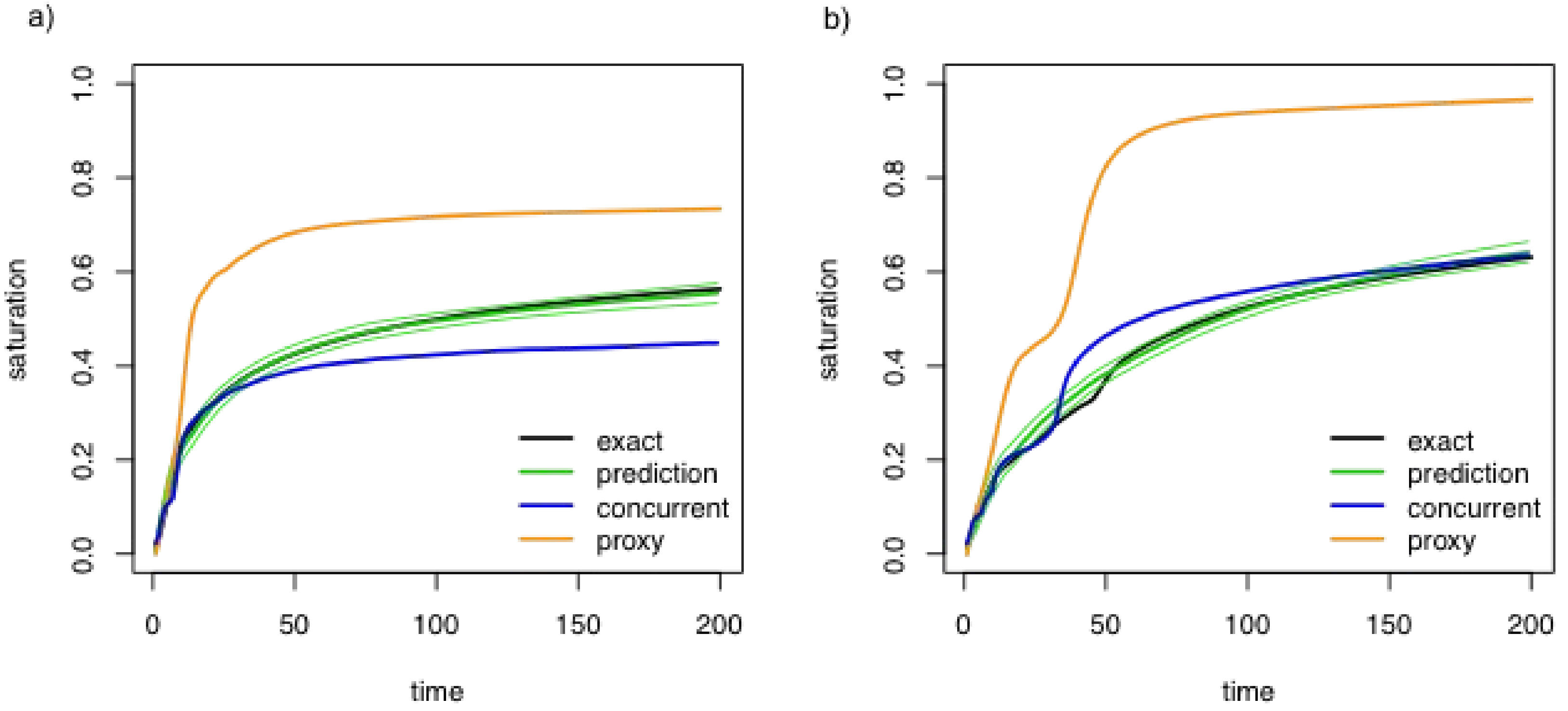
Two examples of predictions

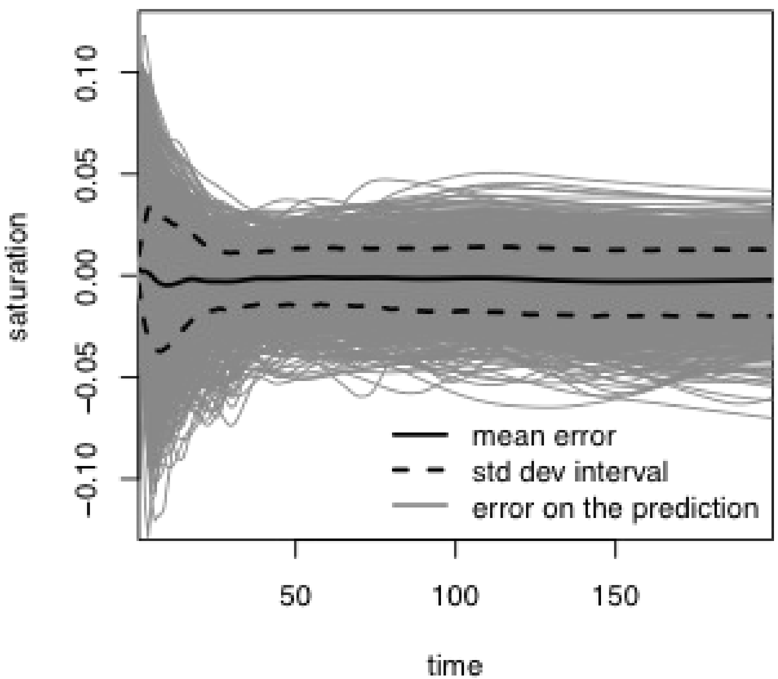




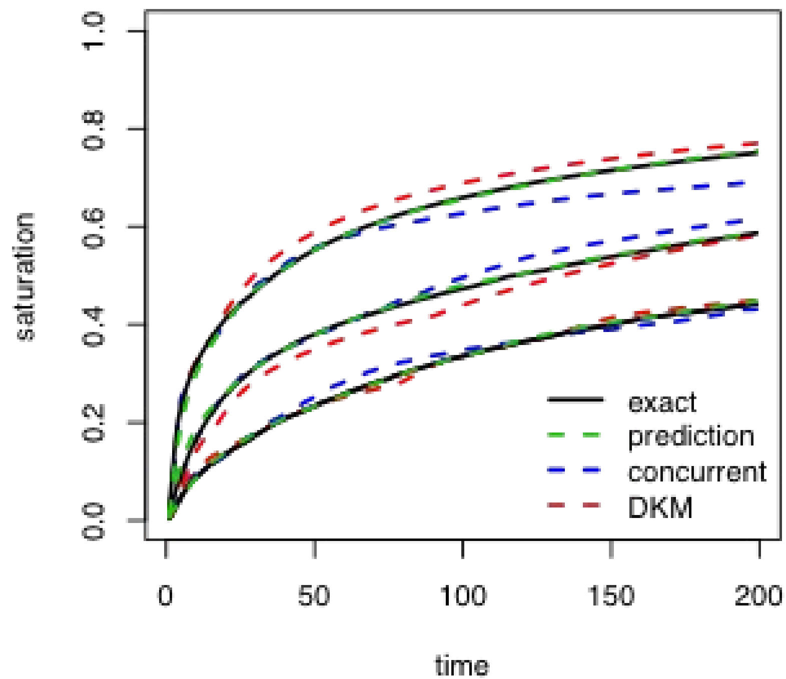
Prediction of the ensemble
1000 realizations

new geo. realization → single-phase simulation → regression model → prediction of the exact response

c) *Error curves: predicted – exact*



d) *Point-wise quantiles P10-50-90*



Good prediction of the point-wise quantiles

Prediction for each of the curves ✉ useful beyond UQ

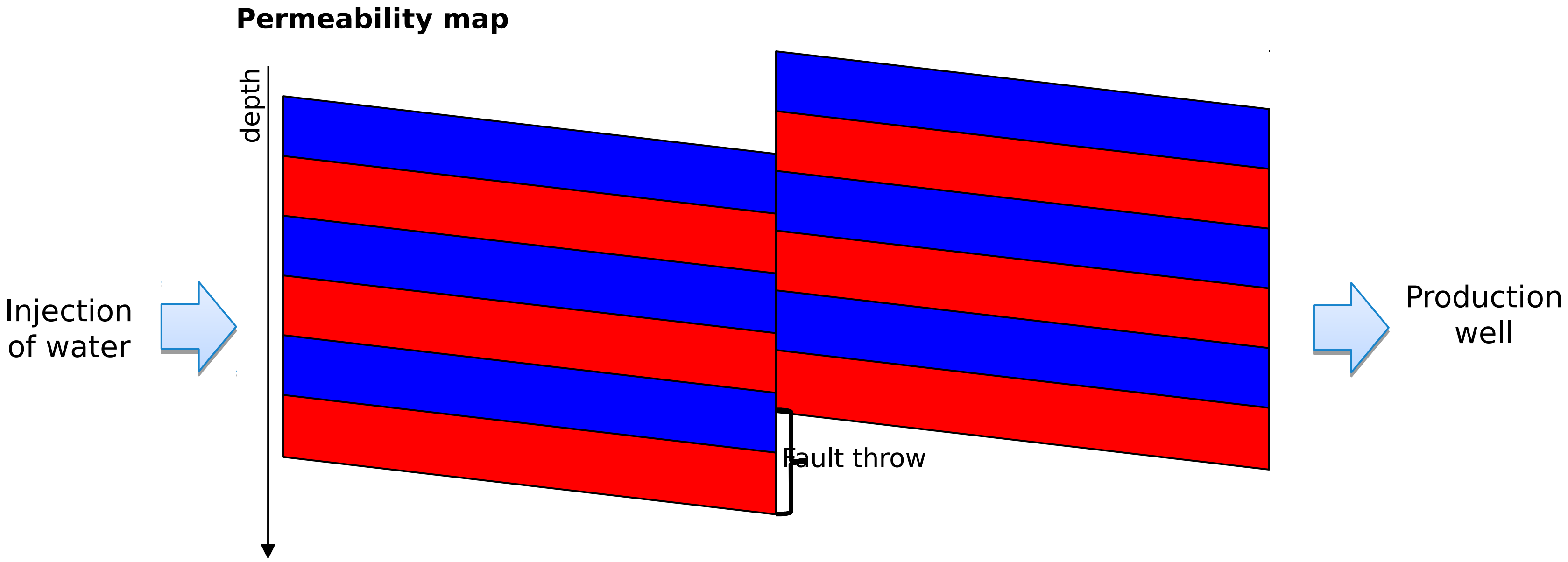
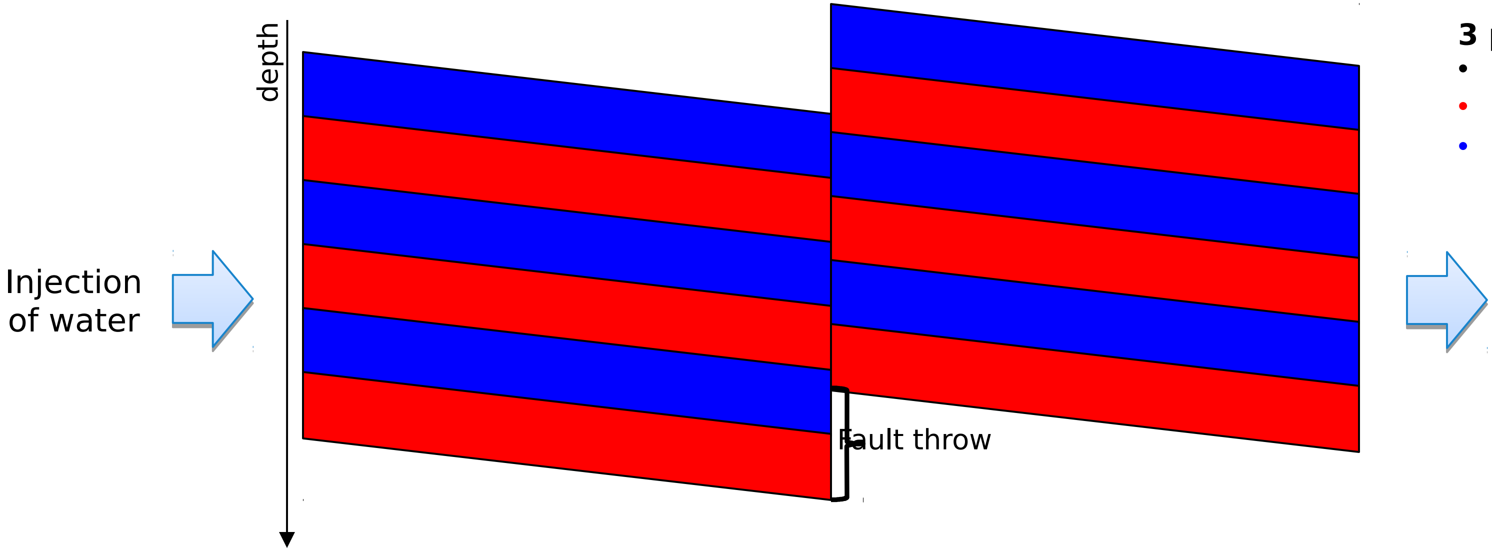


ILLUSTRATION 2

HISTORY MATCHING

IC Fault test case

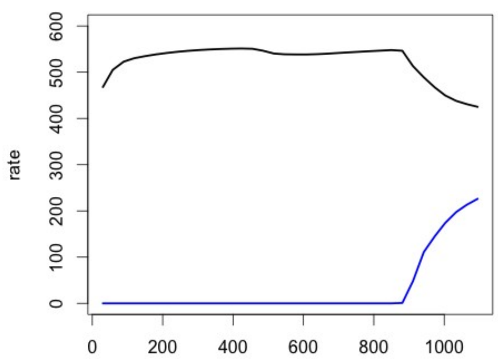
Permeability map



Imperial College Fault problem
Z Tavassoli, JN Carter, PR King (2004)

3 parameters:
- Fault throw = ?
- K_{high} = ?
- K_{low} = ?

Observed data:
- Oil production rate
- Water production rate



Goal:
Sample the parameters given the observed data

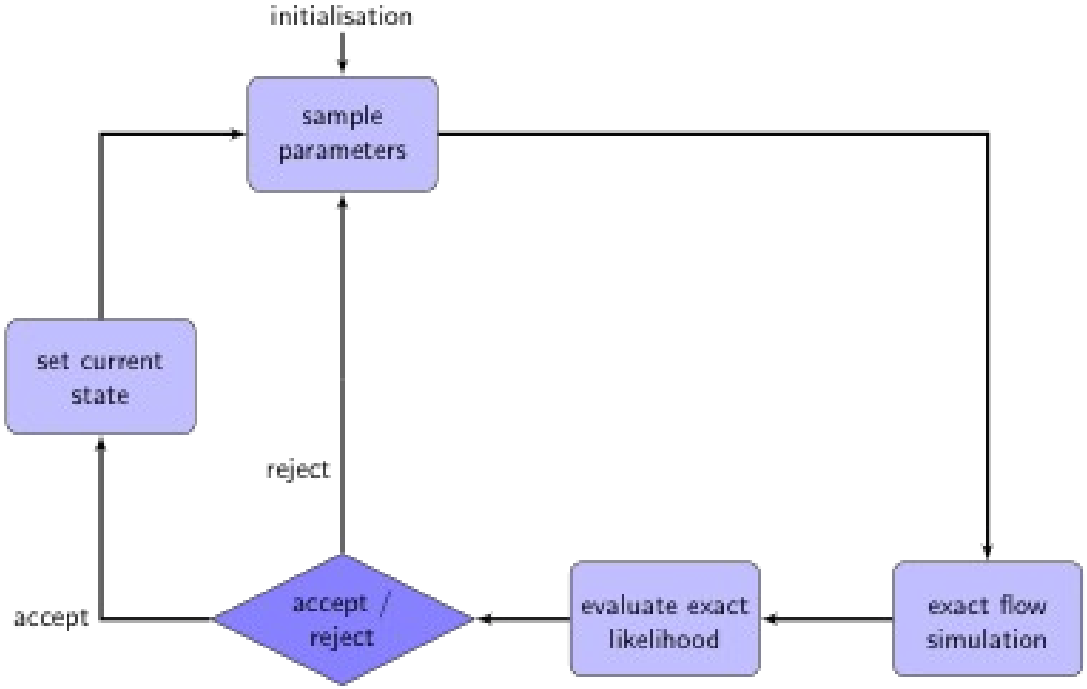
$$p(\theta|y) \propto \mathcal{L}(\theta; y)p(\theta)$$

Choice of simplified physics model: single-phase simulation

→ Provides information on the connectivity of the realizations

→ Cheap: pressure problem is solved only once

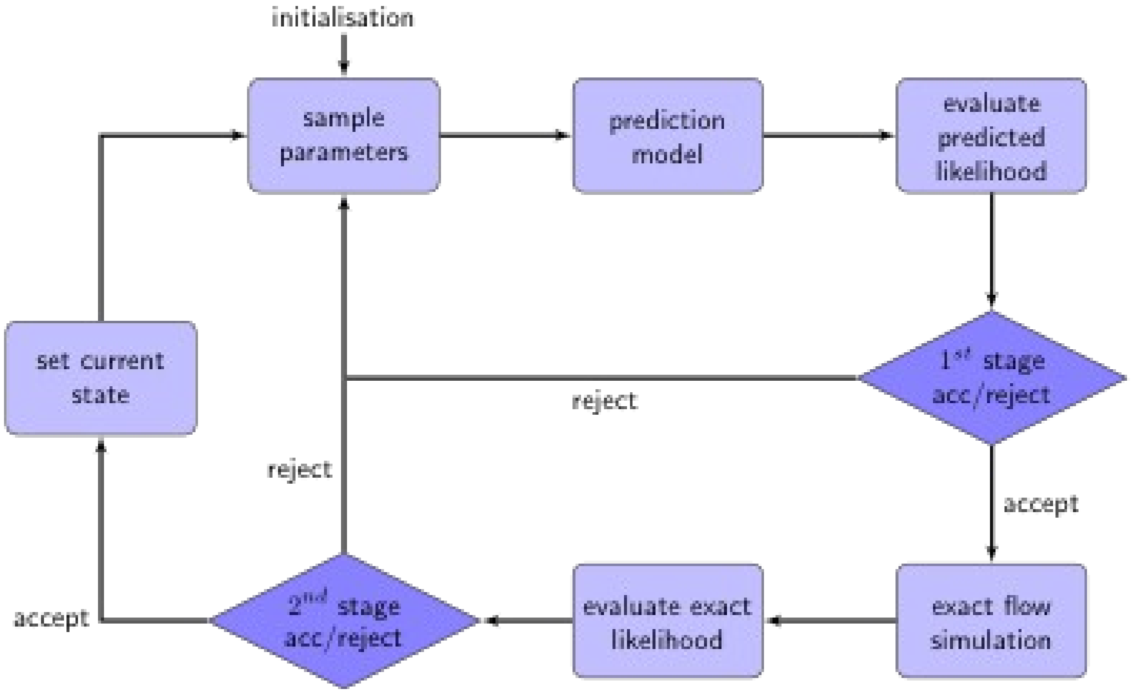
2-stage MCMC



Metropolis-Hastings

- To sample the posterior probability density function
- Typical application 10^5 iterations
- finite length chains should be able to explore all areas of the prior space
- Increase the step length of the chains?
  - Drastic reduction of the acceptance rate
  - High number of wasted simulations

2-stage MCMC



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- Increase the step length of the chains?
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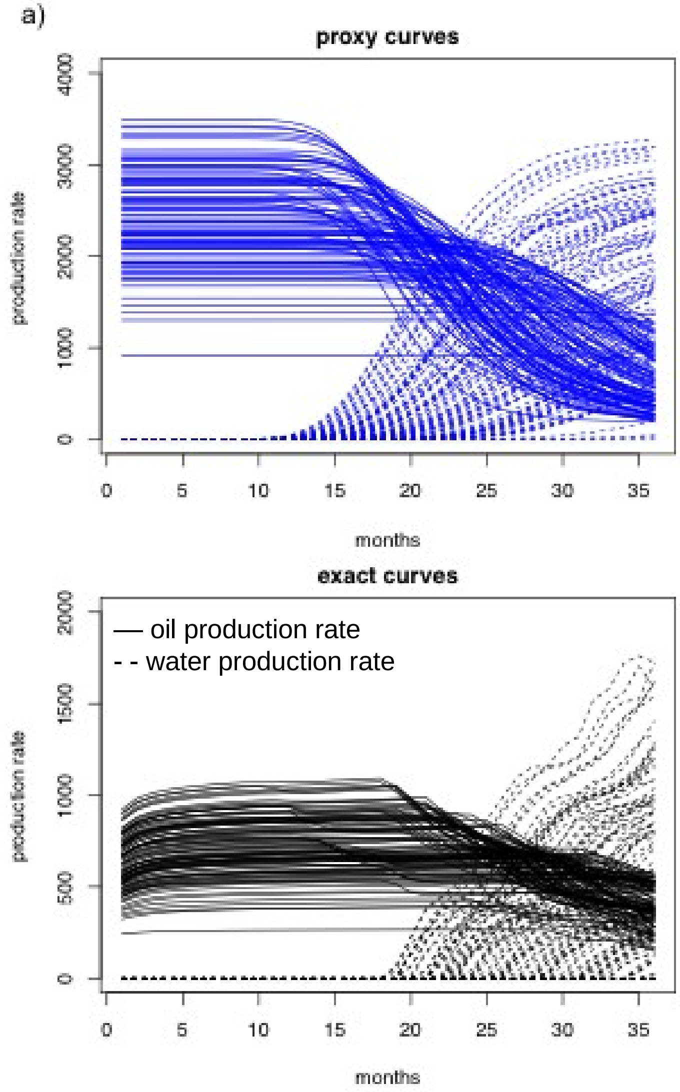
  - High number of wasted simulations

2-stage MCMC*

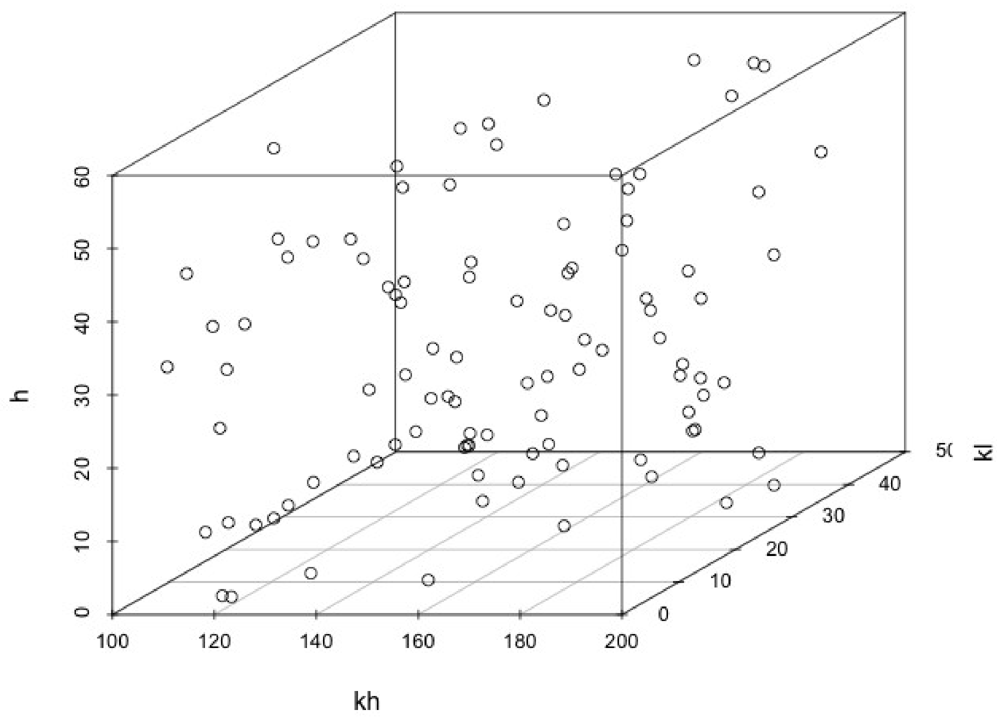
- Avoid unnecessary run of the exact solver
- Reject samples based on the predicted response

**Christen and Fox (2005), Efendiev et al. (2005, 2006)*

Training set and dimension reduction



Training set: 100 curves sampled from the parameters space



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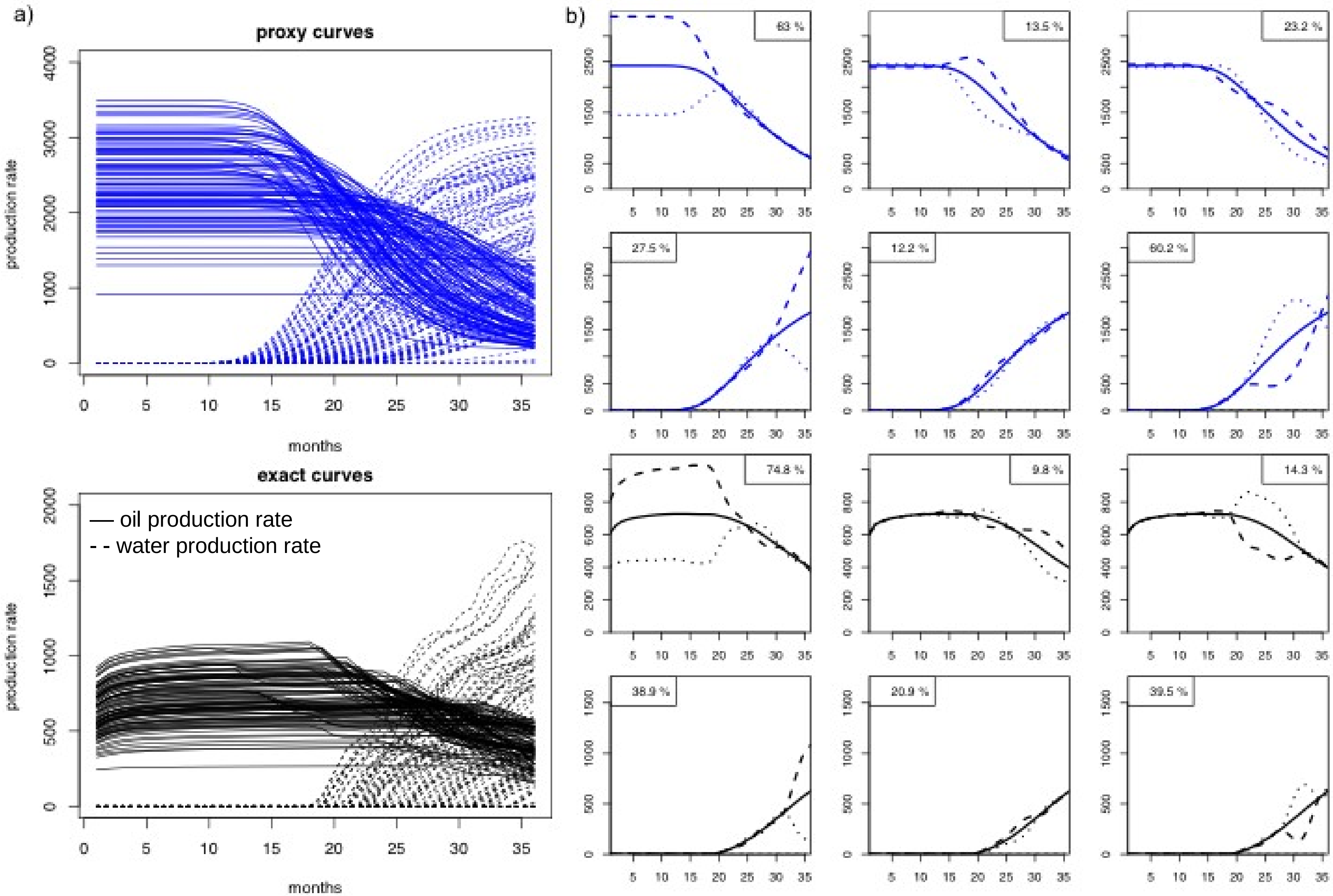
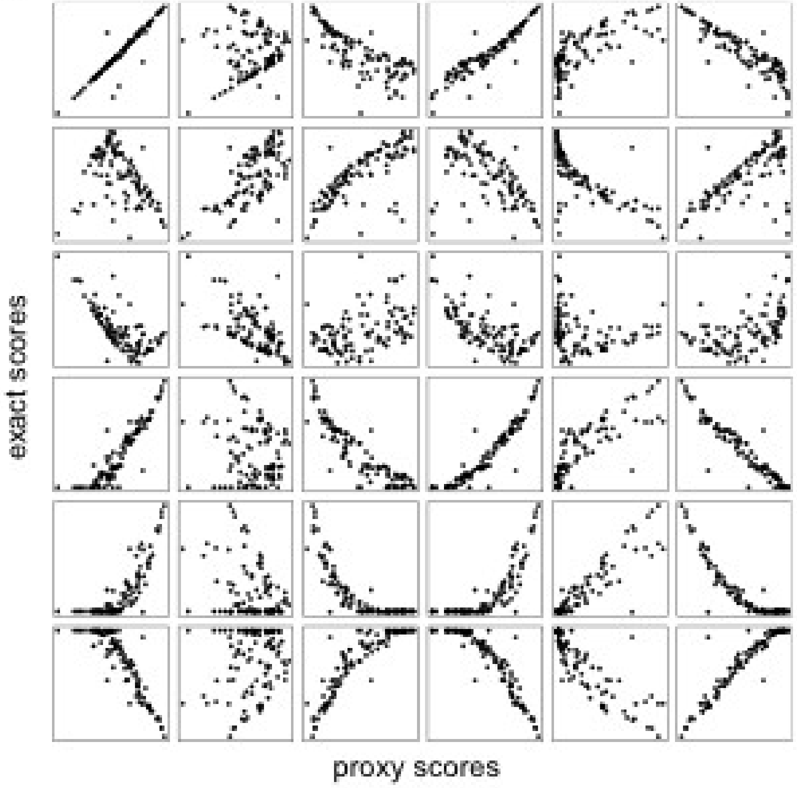
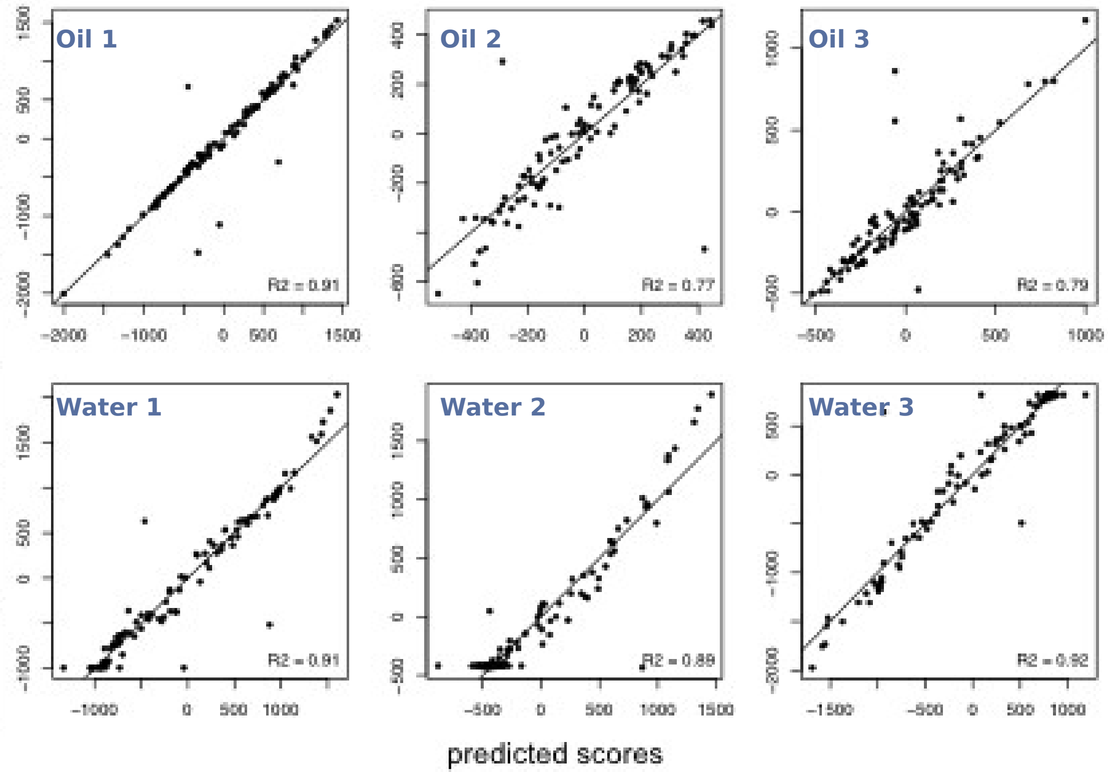


Construction of the regression model

a) **Scatterplot of the exact and proxy scores**

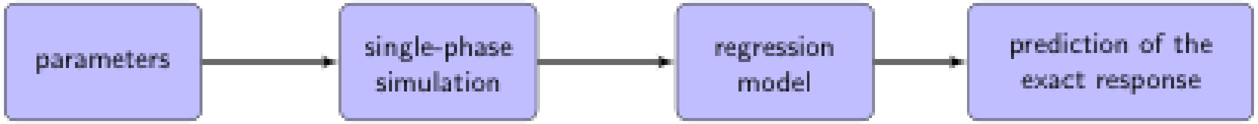


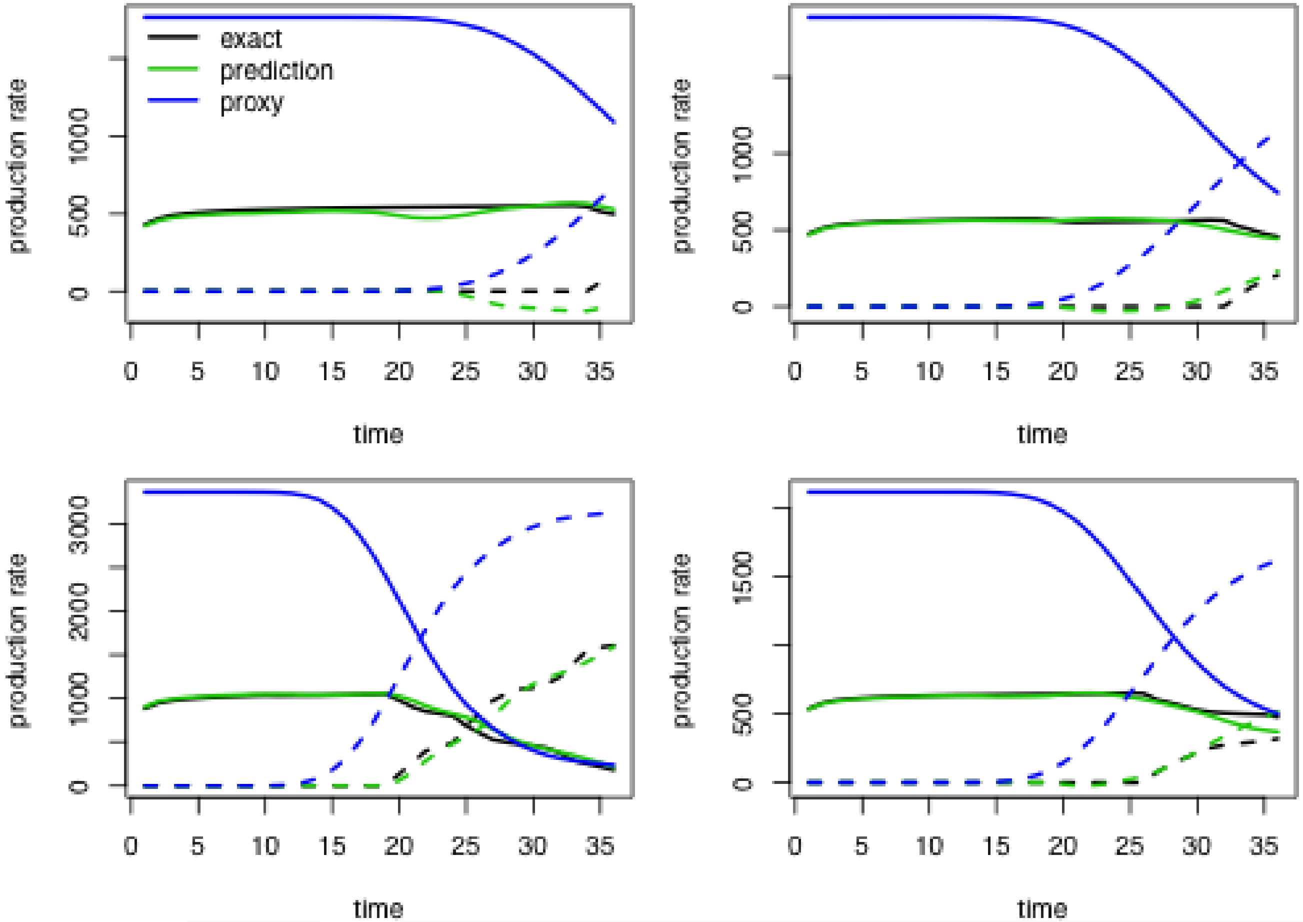
b) **Plot of the exact VS predicted scores**



The proxy is useful to predict the exact response

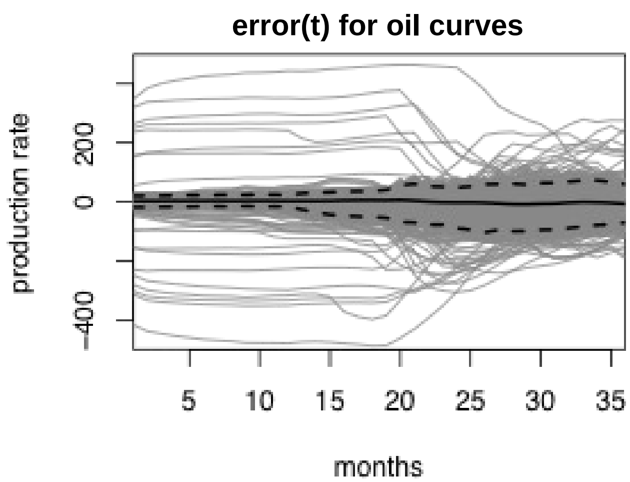
Four examples of predictions

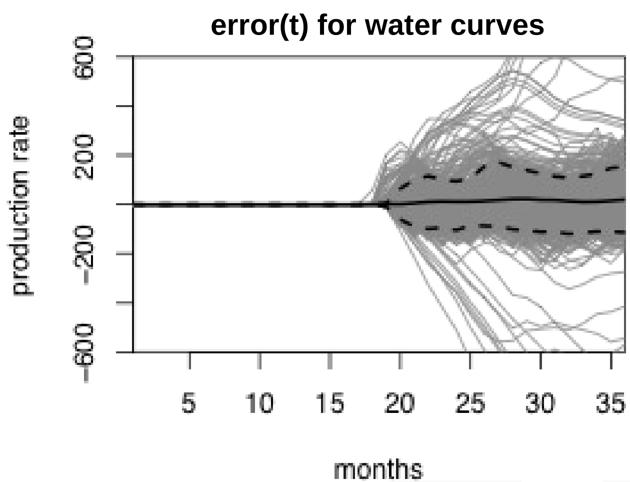




Evaluation of the performance of the error model

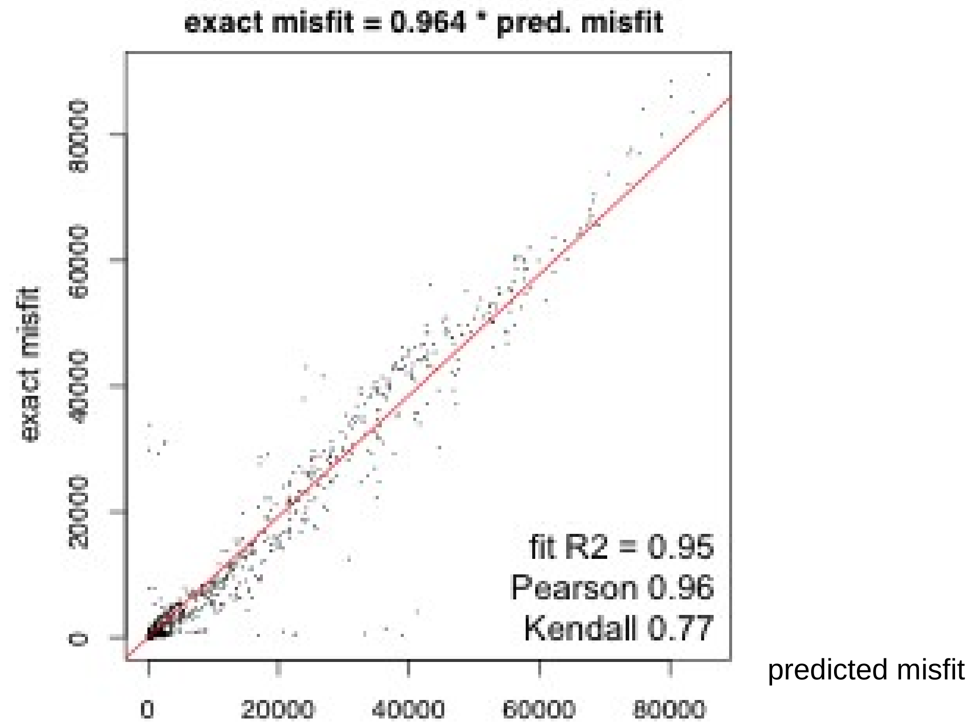
Test set of 1000 realizations



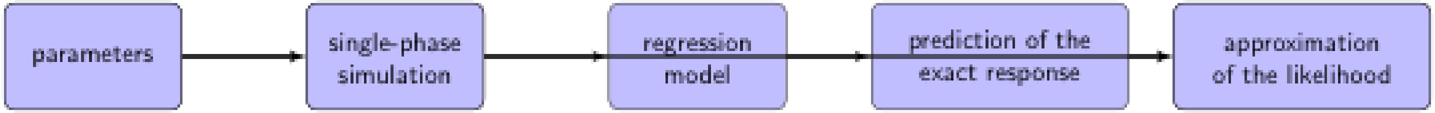


Predicted curves → predict the misfit:

$$M = \frac{1}{36}\sum_{t=1}^{36}\frac{(C_{ref}^{oil}(t) - C^{oil}(t))^2}{2\sigma^2} + \frac{1}{7}\sum_{t=30}^{36}\frac{(C_{ref}^{water}(t) - C^{water}(t))^2}{2\sigma^2}$$

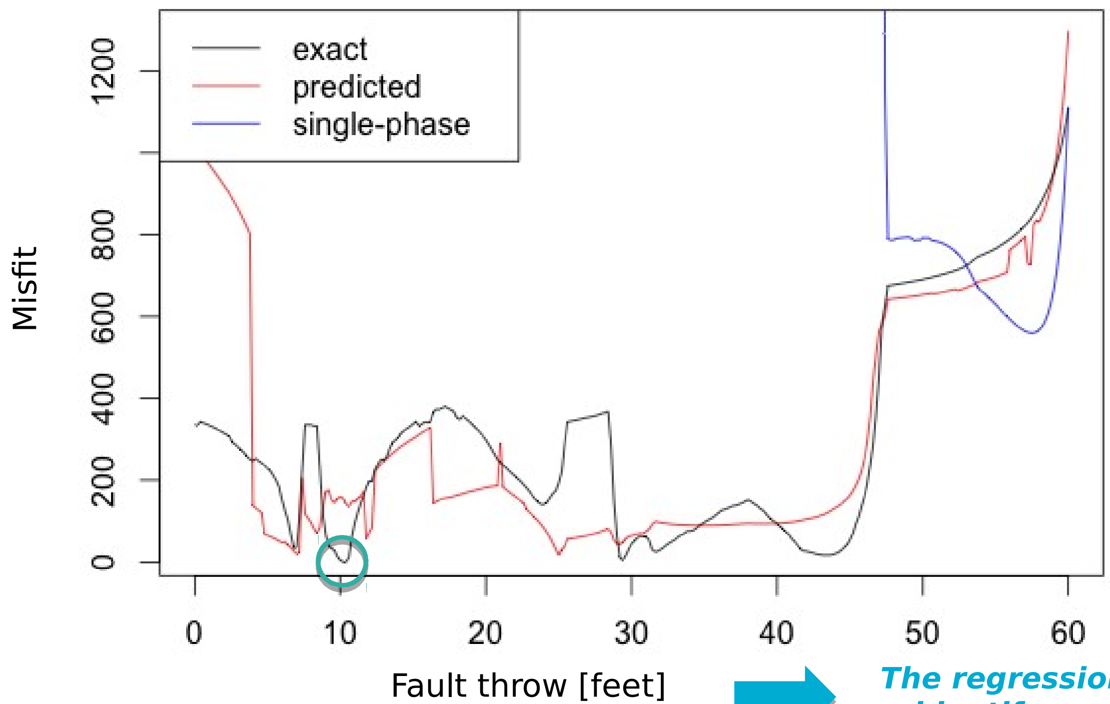


Is the error model necessary?



$$\mathcal{L} = e^{-M} \qquad M = \frac{1}{36}\sum_{t=1}^{36}\frac{(C_{ref}^{oil}(t) - C^{oil}(t))^2}{2\sigma^2} + \frac{1}{7}\sum_{t=30}^{36}\frac{(C_{ref}^{water}(t) - C^{water}(t))^2}{2\sigma^2}$$

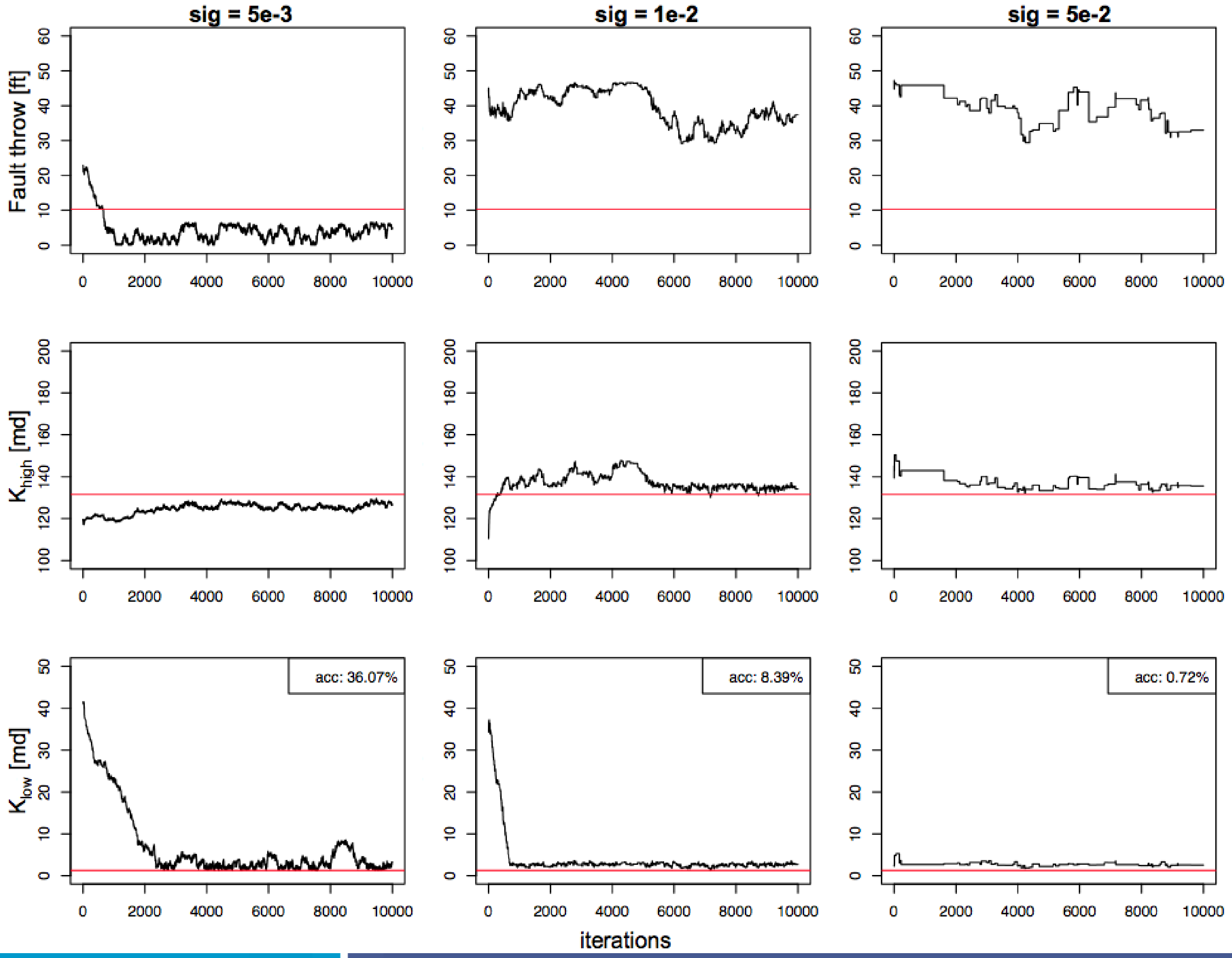
K_{high} = 131.6
K_{low} = 1.3
true parameter



The regression model is necessary to identify regions in the parameter space

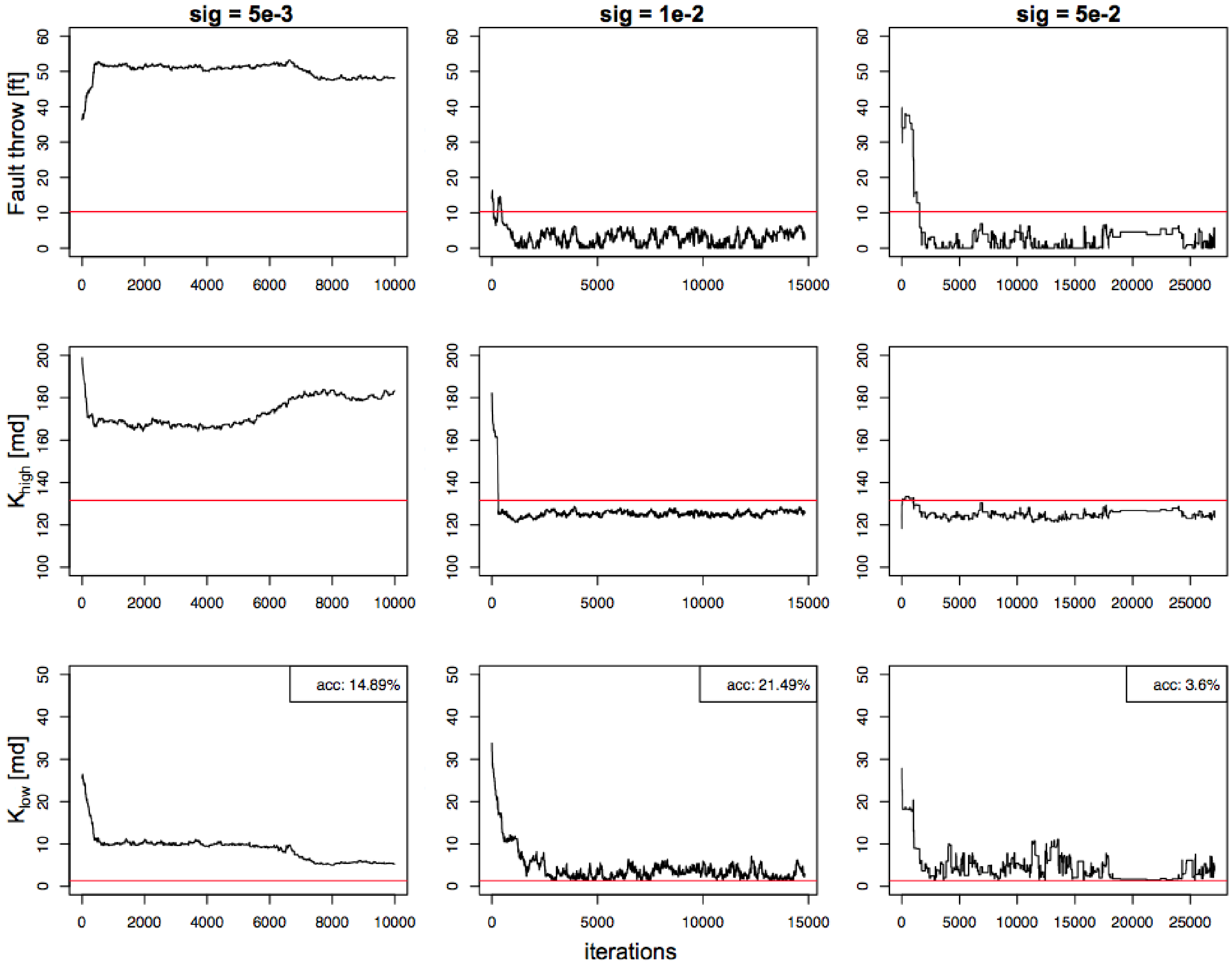
Metropolis-Hastings results

3 chains for different step size
Length: 10'000 evaluations



2-stage MCMC results

3 chains for different step size
Length: equivalent MH



Comparison of the results

random walk	nb of it.			nb of acc. 1stage sim			nb of acc. 2stage sim			acc. rate			
σ	C1	C2	C3	C1	C2	C3	C1	C2	C3	C1	C2	C3	mean
	Metropolis-Hasting												
$5 \cdot 10^{-3}$	10'000	10'000	10'000				1'631	3'247	1'291	18.1%	36.1%	14.3%	22.8%
$1 \cdot 10^{-2}$	10'000	10'000	10'000				1'683	755	628	18.7%	8.4%	7.0%	11.4%
$5 \cdot 10^{-2}$	10'000	10'000	10'000				179	65	48	2.0%	0.7%	0.5%	1.1%
	Two-stage MCMC												
$5 \cdot 10^{-3}$	10'000	10'000	10'000	4'760	5'299	176	367	789	41	7.7%	14.9%	23.3%	15.3%
$1 \cdot 10^{-2}$	14'372	14'815	31'738	9'666	9'656	7'820	2'060	2'075	331	23.3%	21.5%	4.2%	16.3%
$5 \cdot 10^{-2}$	28'337	31'777	27'108	9'341	9'261	9'370	393	518	337	4.2%	5.6%	3.6%	4.5%

2-stage MCMC with the error model

- Higher acceptance rate
- Longer chains can be run for the same computational cost

However

- Nowhere near convergence
- ICF still a very challenging problem
- As the Swiss say: “ça va pas mieux mais plus longtemps !”

Conclusion
Key ideas

Prediction model

= proxy + error model

= single-phase + FPCA regression

- Why single-phase flow simulations:
  - Connectivity is what varies between realisations
  - Cheap: pressure is solved only once
- Why error modelling:
  - Missing physics has to be taken in account

Advantages

- Strong reduction of computational costs
- Allows the evaluation of the relevance of the proxy for the specific problem

Outlook

- On going work: sensitivity analysis
- Application to seawater intrusion in coastal aquifer
- Evolve to more complex regression model -> Kernel methods

Acknowledgements

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References

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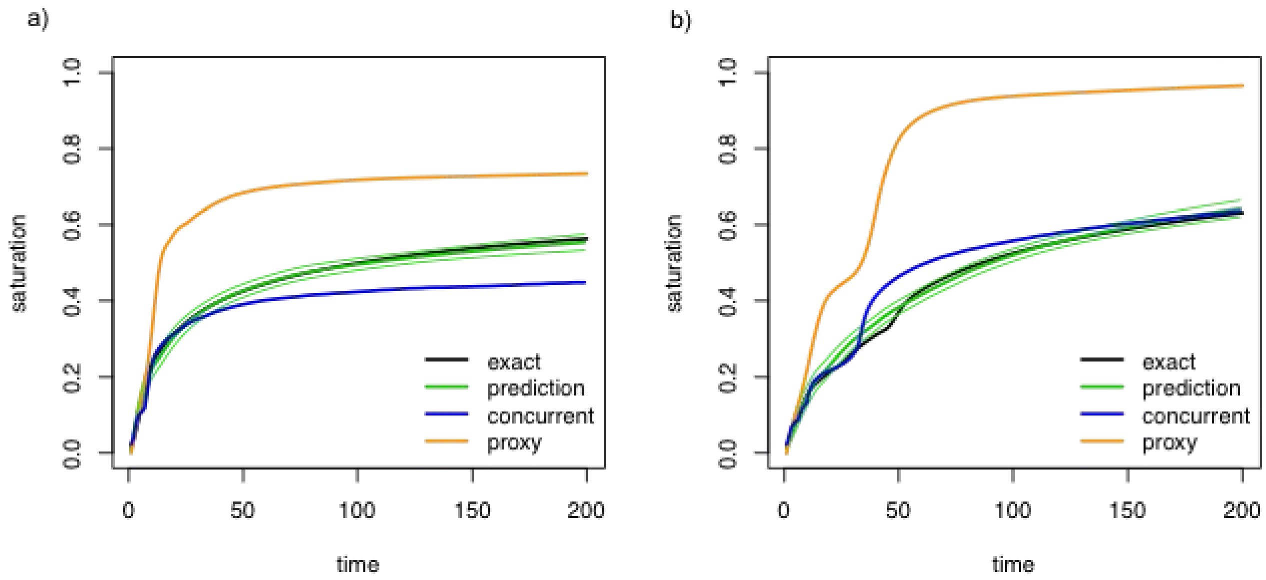
THANK YOU FOR YOUR ATTENTION

Simultaneous confidence bands



$$Pr\Big(\tilde{y}(t) \in [\hat{y}(t) - w_\alpha(t), \hat{y}(t) + w_\alpha(t)] \text{ for all } t\Big) = 1 - \alpha$$

$$w_\alpha(t) = \sqrt{\left(\frac{D_{ex}(N_l - D_{app} - 1)}{N_l - D_{ex} - D_{app}}\right) F_{D_{ex}, N_l - D_{ex} - D_{app}}(\alpha)} \times \sqrt{(1 + \mathbf{b}'(\mathbf{B}'\mathbf{B})^{-1}\mathbf{b})\left(\frac{N_l}{N_l - D_{app} - 1}\right)\boldsymbol{\eta}'(t)\hat{\boldsymbol{\Sigma}}\boldsymbol{\eta}(\boldsymbol{t})},$$

with $\boldsymbol{\eta}(t)$ the values of the exact harmonics

$\hat{\boldsymbol{\Sigma}}$ the covariance matrix of errors

$F(\alpha)$ Fisher's α quantile