Patterns in time-dependent parameters reveal deficits of a catchment-scale herbicide transport model

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Background and Motivation

- Pesticides in catchments dominated by agricultural land use
  - Small headwater catchments are at risk of high pesticide concentrations caused by fast transport processes
  - These processes show a high spatial and temporal heterogeneity, i.e. the system is of large complexity
  - The system behaves in a ***stochastic*** way at the resolution we observe it; e.g., the same precipitation and pesticide application, observed at an aggregated level, lead to different streamflow and in-stream concentrations
- Models and uncertainty
  - Model structural uncertainty is an important source of uncertainty for strongly simplified dynamic pesticide transport models
  - Many current approaches rely on a deterministic formulation of the processes, even though the system behaves stochastically

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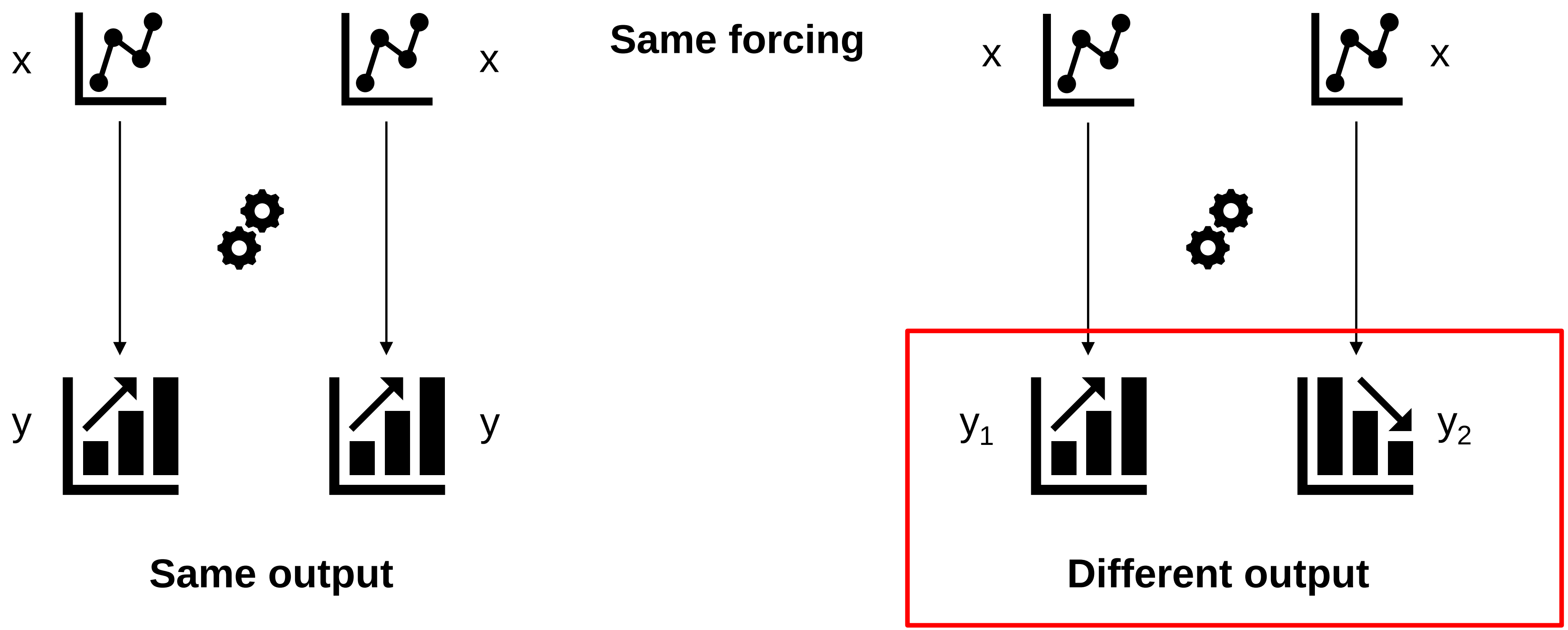
Idea (1/2)

Deterministic process model (DPM)

Stochastic process model (SPM)



Idea (2/2)

- Stochastic process models …
  - … are less susceptible to structural errors, since they allow for multiple model trajectories for the same set of forcing and parameters
  - … allow to better account for the intrinsic stochasticity present in many complex environmental systems (at the resolution at which they are observed)

- Therefore, we investigate the following:
  - Can stochastic process models based on time-dependent parameters reveal deficits in the process formulation of a conceptual herbicide transport model[1)]?
  - Can we improve the uncertainty quantification of such a model by acknowledging the inherent stochasticity of the system?

[1)] The model is described in detail in Ammann et al., 2020

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Methods

Notation

upper case: random variables

lower case: real numbers

bold: vectors

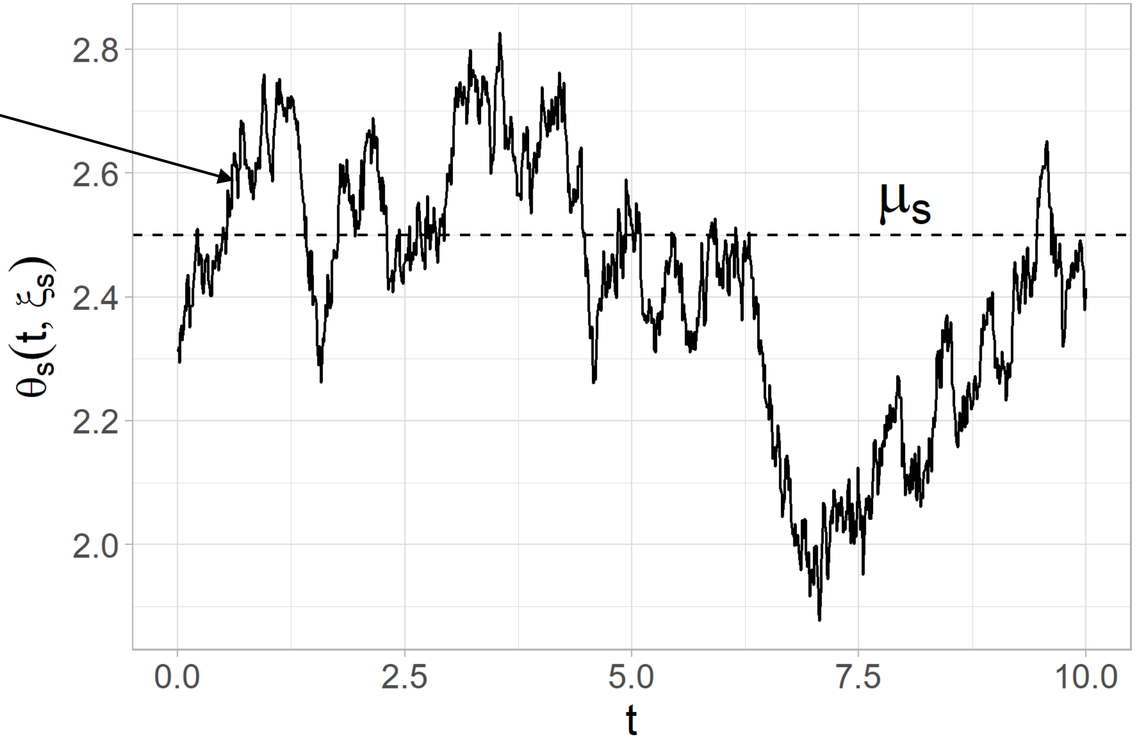
Constant & stochastic model parameters

$$\boldsymbol{Y}_{\text{obs}}(t) = \boldsymbol{Y}\left(t, \boldsymbol{\theta}_{-s}, \boldsymbol{\Theta}_s(t, \boldsymbol{\xi})\right) + \boldsymbol{Z}_{\text{obs}}(t, \boldsymbol{Y}, \boldsymbol{\psi})$$

Observations | Model output | Residual stochasticity: random measurement error

$\boldsymbol{\Theta}_s$: Ornstein-Uhlenbeck process with parameters:

$$\boldsymbol{\xi}_s = \{\mu_s, \sigma_s\, \tau_s\}$$



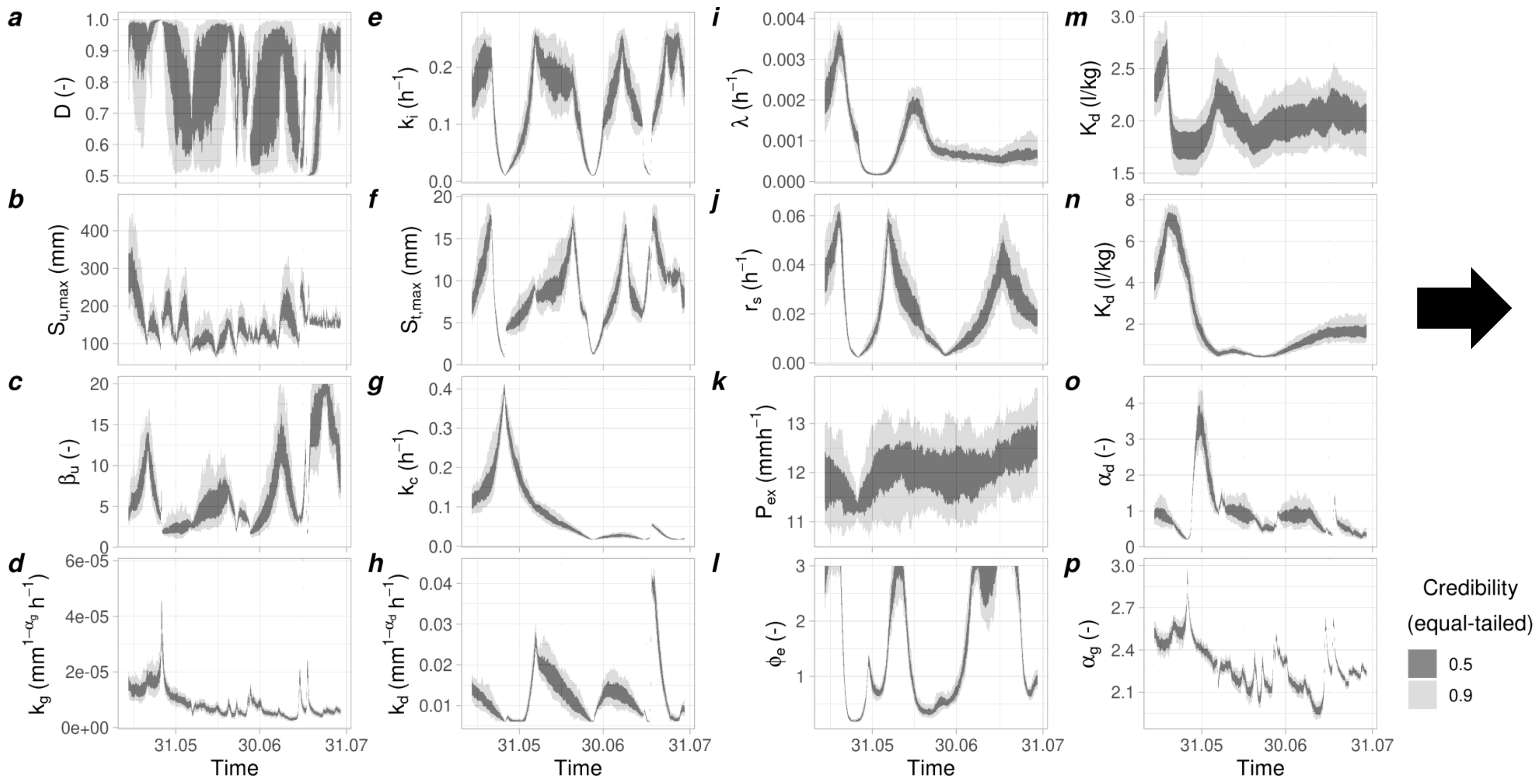
We infer the joint posterior of

$$\{\boldsymbol{\theta}_{-s}, \theta_s(t), \sigma_s, \mu_s, \boldsymbol{\psi}\}$$

relying on the Bayesian paradigm

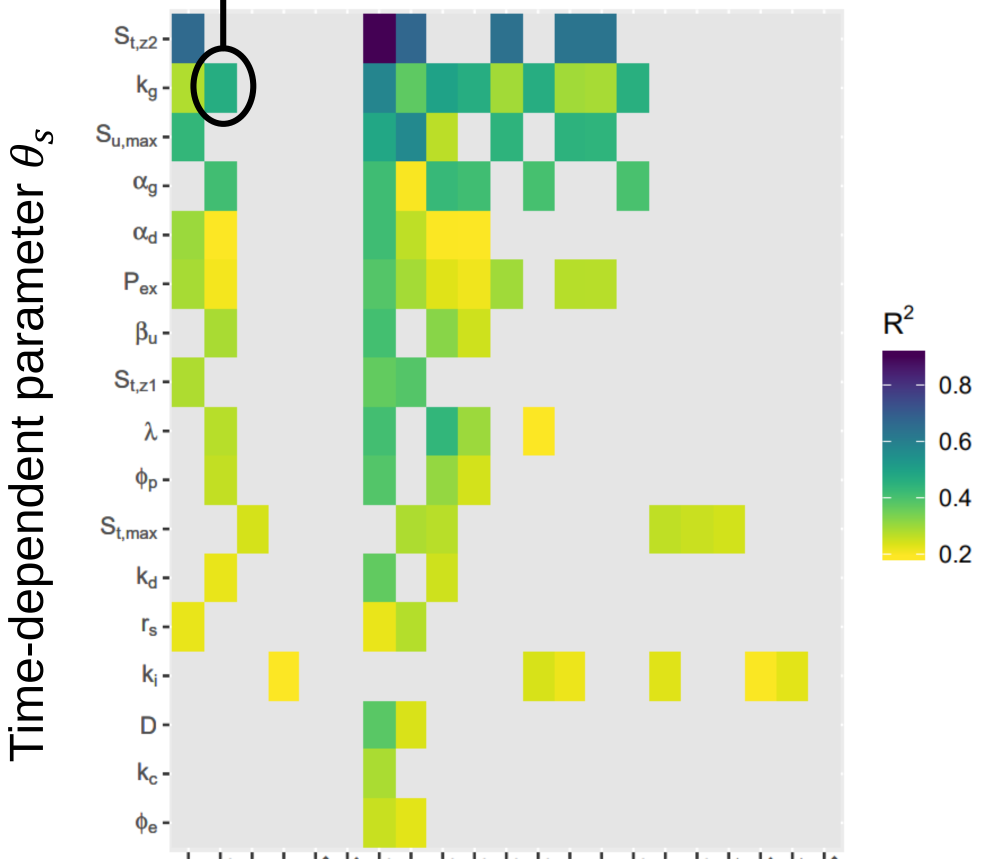
Preliminary results: estimated temporal dynamics of parameters

Time-dependent parameter, $\theta_s(t)$

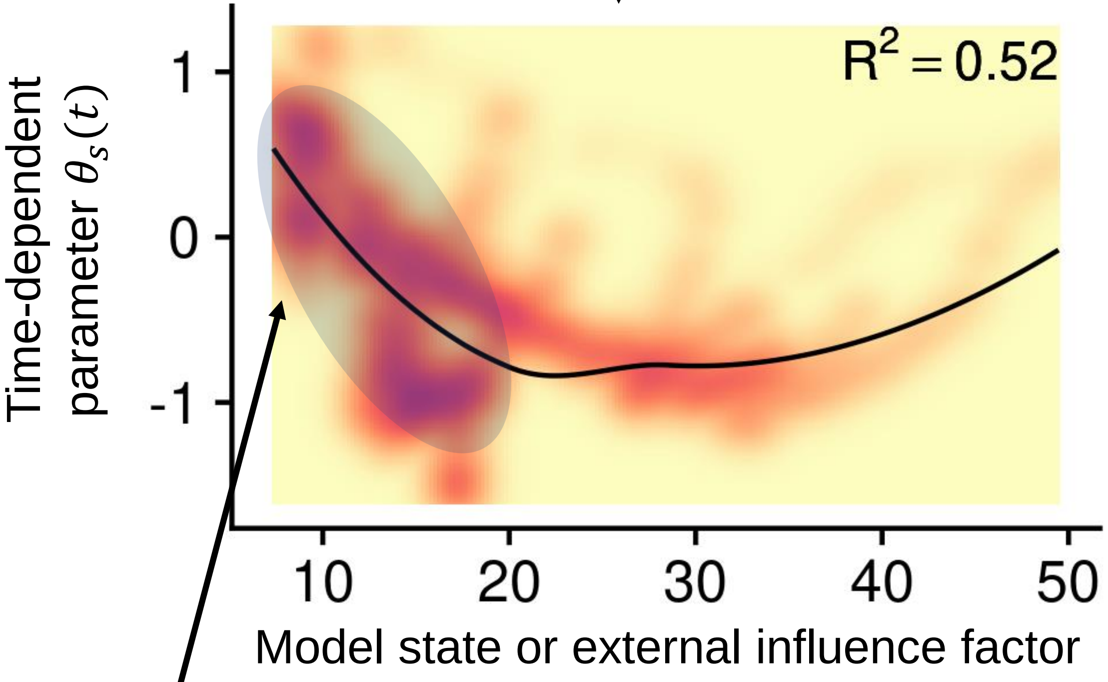


Is there a pattern?

Preliminary results: patterns in time-dependent parameters



Model states and external influence factors



Sustained baseflow in dry periods that cannot be fully captured with the present model structure

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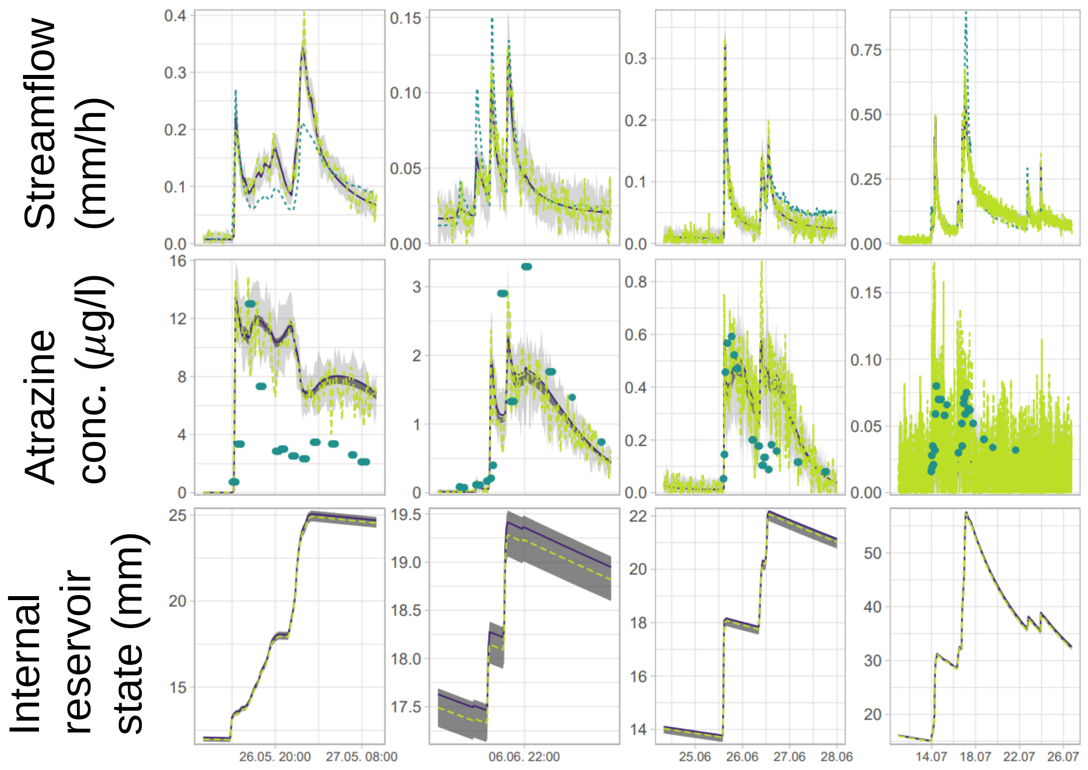
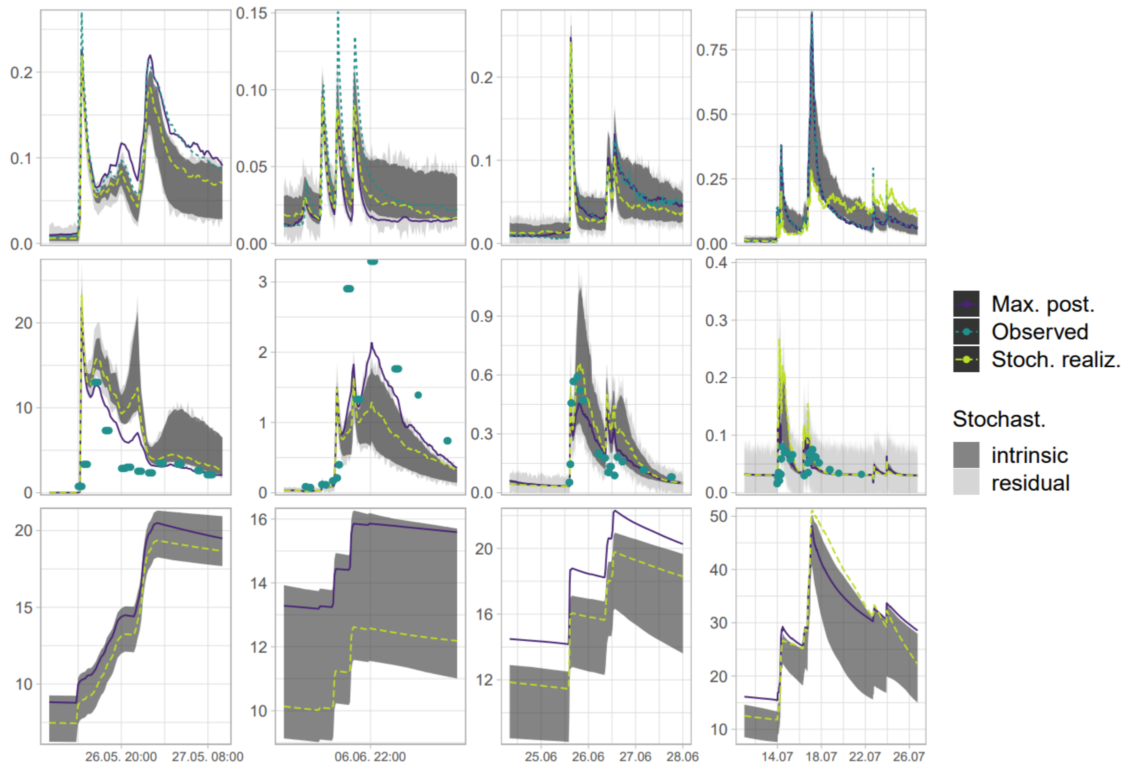
Preliminary results: prediction with DPM and with SPM

Deterministic process model (DPM)



Stochastic process model (DPM)



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Preliminary results: prediction with DPM and with SPM

Deterministic process model (DPM)

Residual stochasticity is dominating

Obtaining reasonable realizations of (autocorrelated) true model output is difficult: short-term variability of model output is too large

Uncertainty of interal states is generally underestimated (due to small parametric uncertainty caused by large number of data points)

Stochastic process model (SPM)

Realistic partitioning between intrinsic stochasticity and residual random observation error

Naturally correlated model output with reasonable uncertainty bands, originating from the propagation of the intrinsic stochasticity

Larger (and more realistic) estimate of the uncertainty of internal states is obtained naturally from the intrinsic stochasticity

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Preliminary conclusions

- Stochastic process models …
  a. … account for the obviously stochastic behaviour of catchments at the resolution we observe them and are less susceptible to structural errors thanks to added flexibility
  b. … can reveal interesting systematic model deficiencies, e.g., underestimation of baseflow
  c. … lead to a more realistic distinction between intrinsic stochasticity and random output observation uncertainty
  d. … allow for a more realistic estimate of the uncertainty of internal model states compared to deterministic process models

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How to proceed?

- Stochastic process models are very promising tools and their use in water quality applications should be explored in more detail. How well can we capture model structural uncertainty with time-dependent parameters?
- Key challenges that remains to be addressed are:
  - Inference is numerically challenging: better algorithms are needed
  - How do we decide which part of a model's process formulation should be stochastic? Which parts of the process model are most susceptible to structural errors that need to be accounted for through additional stochasticity?
  - How can we formulate good priors that constrain the parameters in light of a potentially large amount of data? Can we avoid "hard" boundaries of the prior?

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