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Constraint-based parameter sampling to leverage expert knowledge for conditioning soil biogeochemical models

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Process-based models support the understanding of complex biogeochemical interactions and process chains

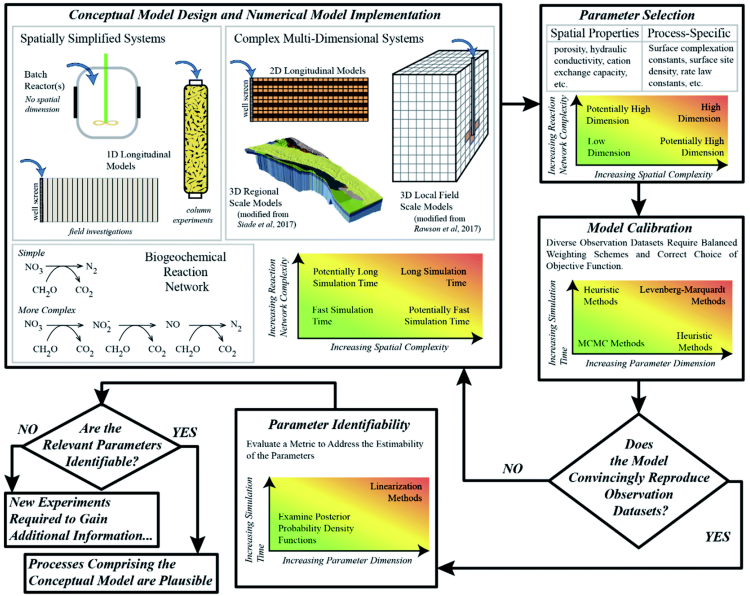
Challenge

Complex models have weakly constrained high-dimensional parameter spaces

Core idea

Leverage expert knowledge to improve iterative model development

- reduce parameter uncertainties
- increase parameter identifiability
- restrict simulations to plausible predictions



Siade et al. (2021)
https://doi.org/10.1039/D1EM00303H

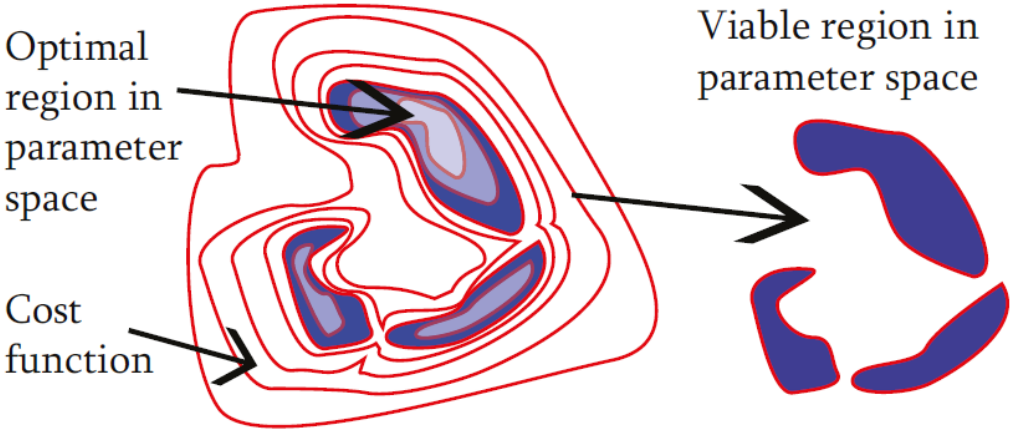
General approach

Expert knowledge = evidence-based expectations

Express expert knowledge as constraints at two levels

- Parameter constraints
- Process constraints

Viable parameter regions => plausible predictions



Efficient sampling of the viable parameter region

Zamora-Sillero et al. (2011)
https://doi.org/10.1186/1752-0509-5-142

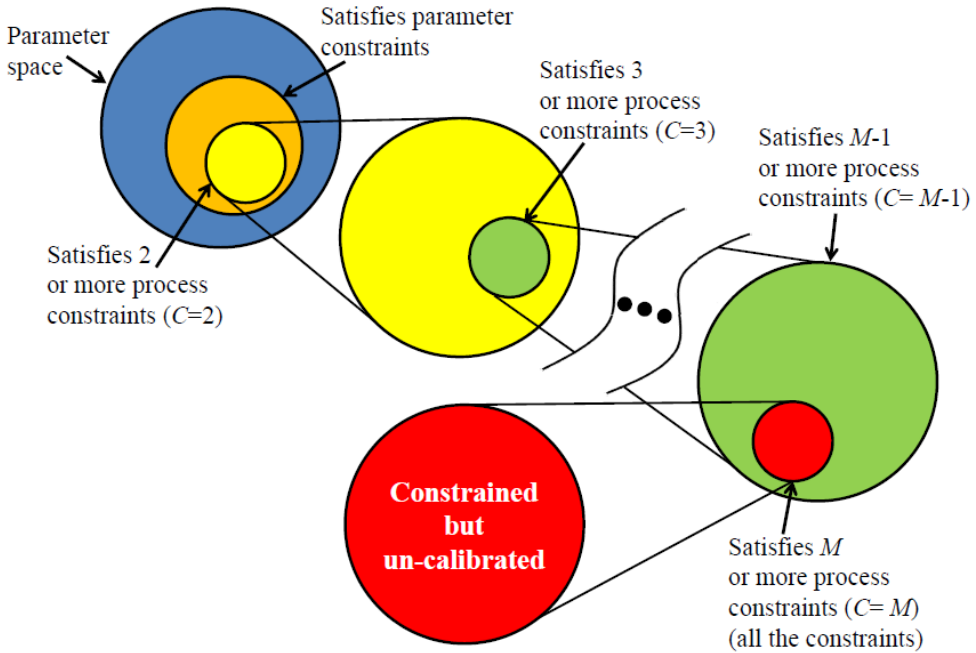
Algorithm

Constraint-based search

Step-wise identification of the viable parameter region

Limitation

Sampling scheme provides non-representative samples of the viable parameter region



Gharari et al. (2014)
https://doi.org/10.5194/hess-18-4861-2014

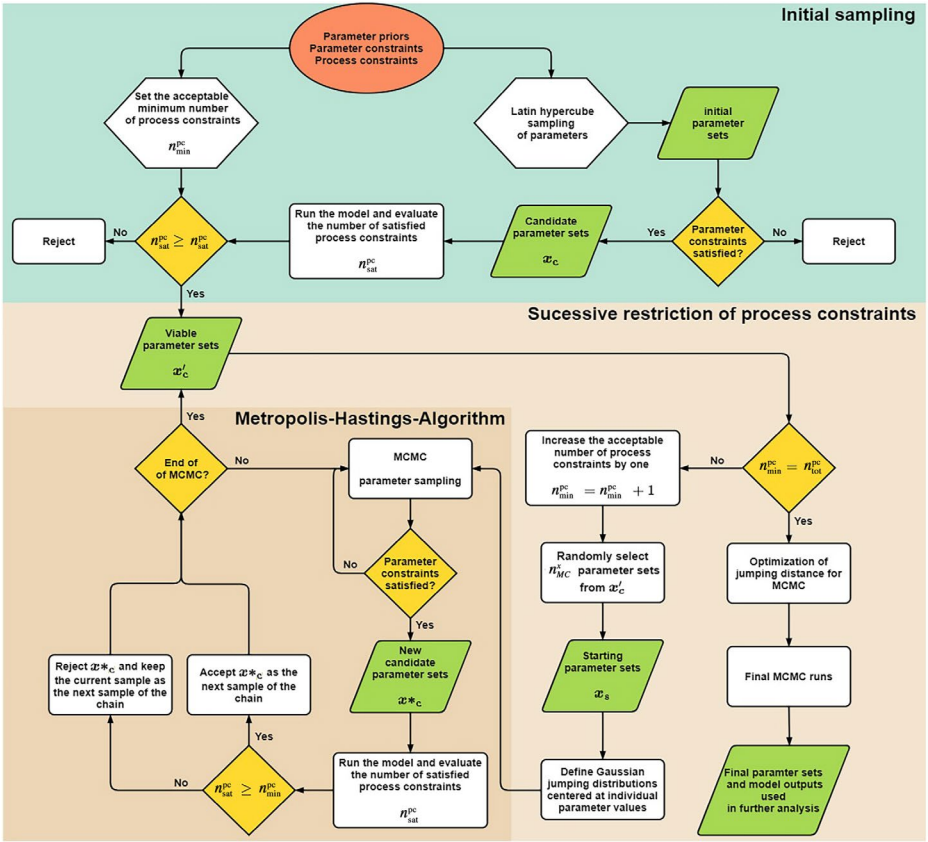
Algorithm

Constraint-based search

Markov Chain Monte Carlo

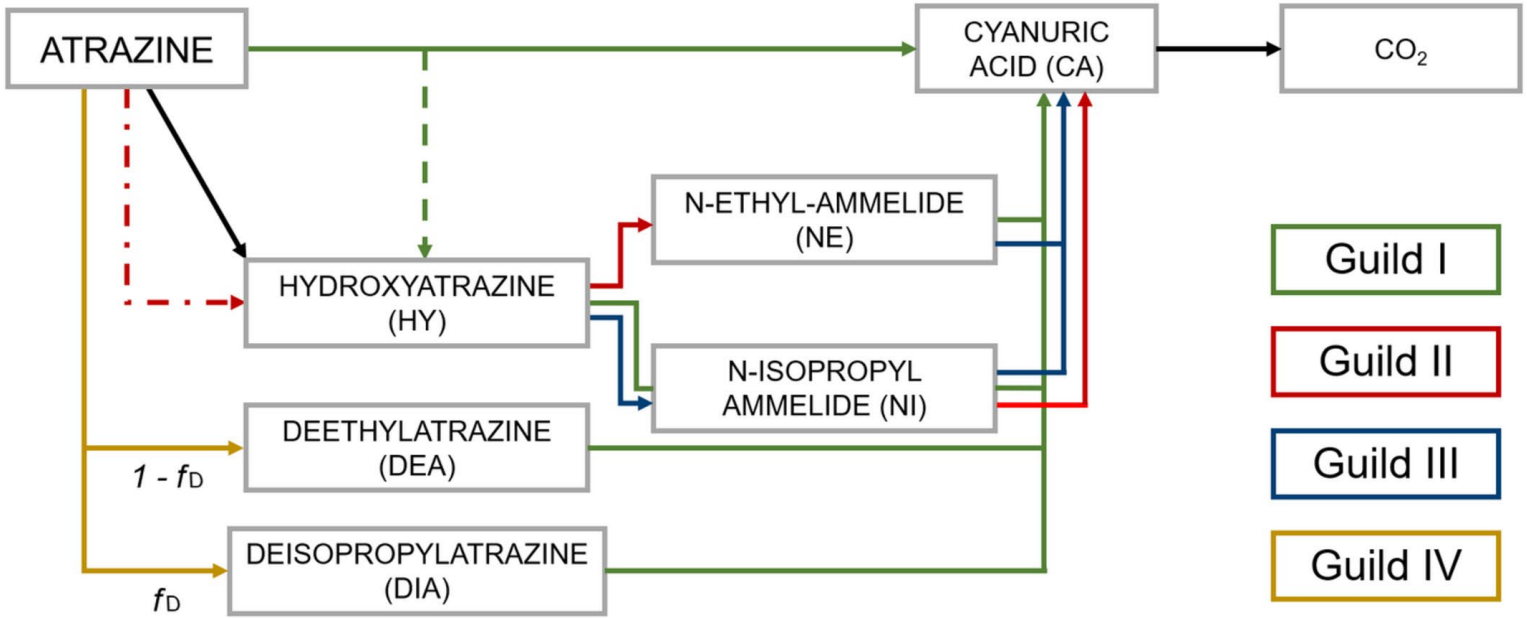
Step-wise identification of the viable parameter region

Representative posterior estimates of viable parameter regions



Chavez Rodriguez et al. (2022)
https://doi.org/10.1111/ejss.13211

Biodegradation of the herbicide atrazine in soil



Chavez Rodriguez et al. (2022)
https://doi.org/10.1111/ejss.13211

Application

Parameter constraints

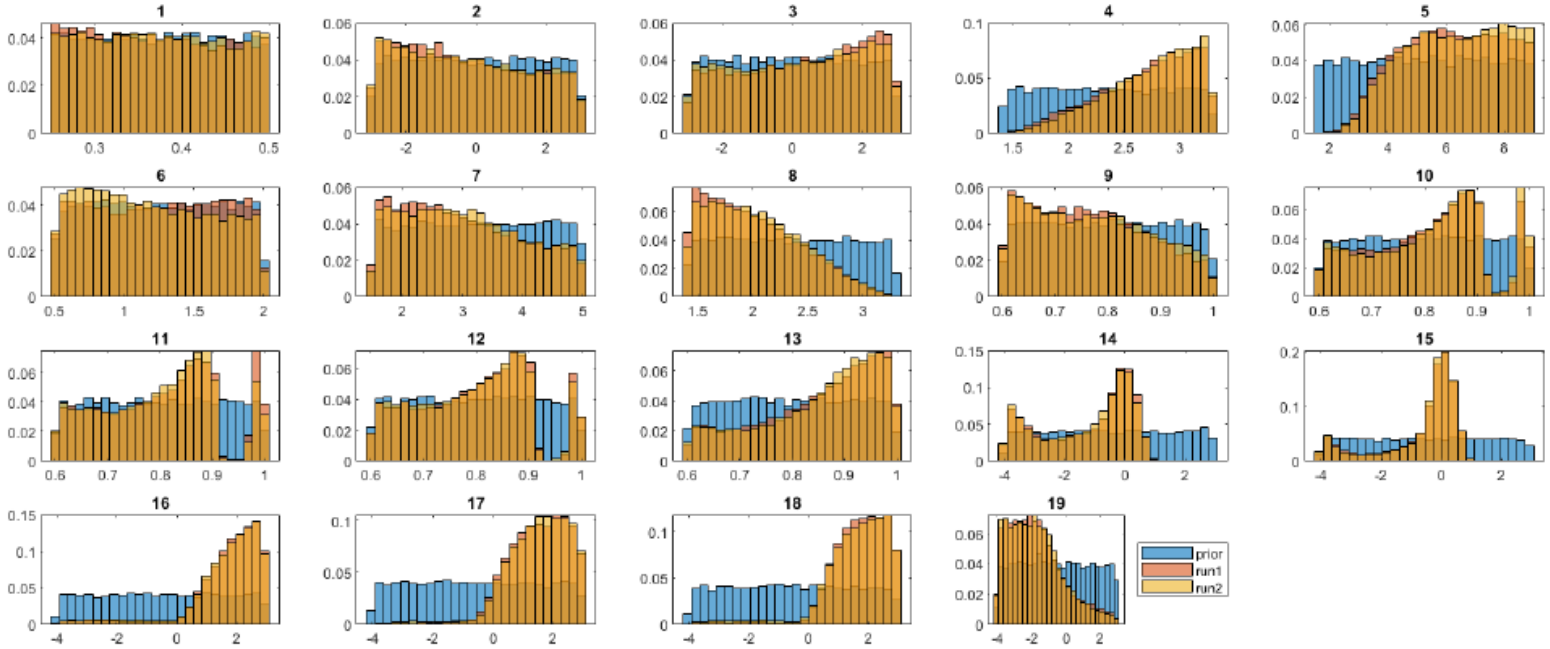
- Defined parameter ranges
- Relationships between kinetic or physicochemical parameters

Process constraints

- Ranges of DT_{50} values for biodegradation of atrazine and metabolites
- Minimum residual atrazine concentration in soil
- Plausible ranges of mineralized atrazine

Chavez Rodriguez et al. (2022)
https://doi.org/10.1111/ejss.13211

Viable parameter regions (model „M6“, first-order decay)



Chavez Rodriguez et al. (2022)
https://doi.org/10.1111/ejss.13211

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Take home

Constraint-based model conditioning

- is widely applicable to biogeochemical models (also beyond soil systems)
- allows to systematically leverage expert knowledge for constructing robust prior parameter distributions
- supports sensitivity analysis, calibration and the process of data-informed iterative model development

Check the code! (MATLAB)

https://doi.org/10.5281/zenodo.5501948