Artificial Intelligence to Advance Modeling and Understanding of Soil Organic Carbon

Haodi Xu[1], Joshua Fan[2], Feng Tao[3], Md Nasim[2], Carla P. Gomes[2], Yiqi Luo[1]

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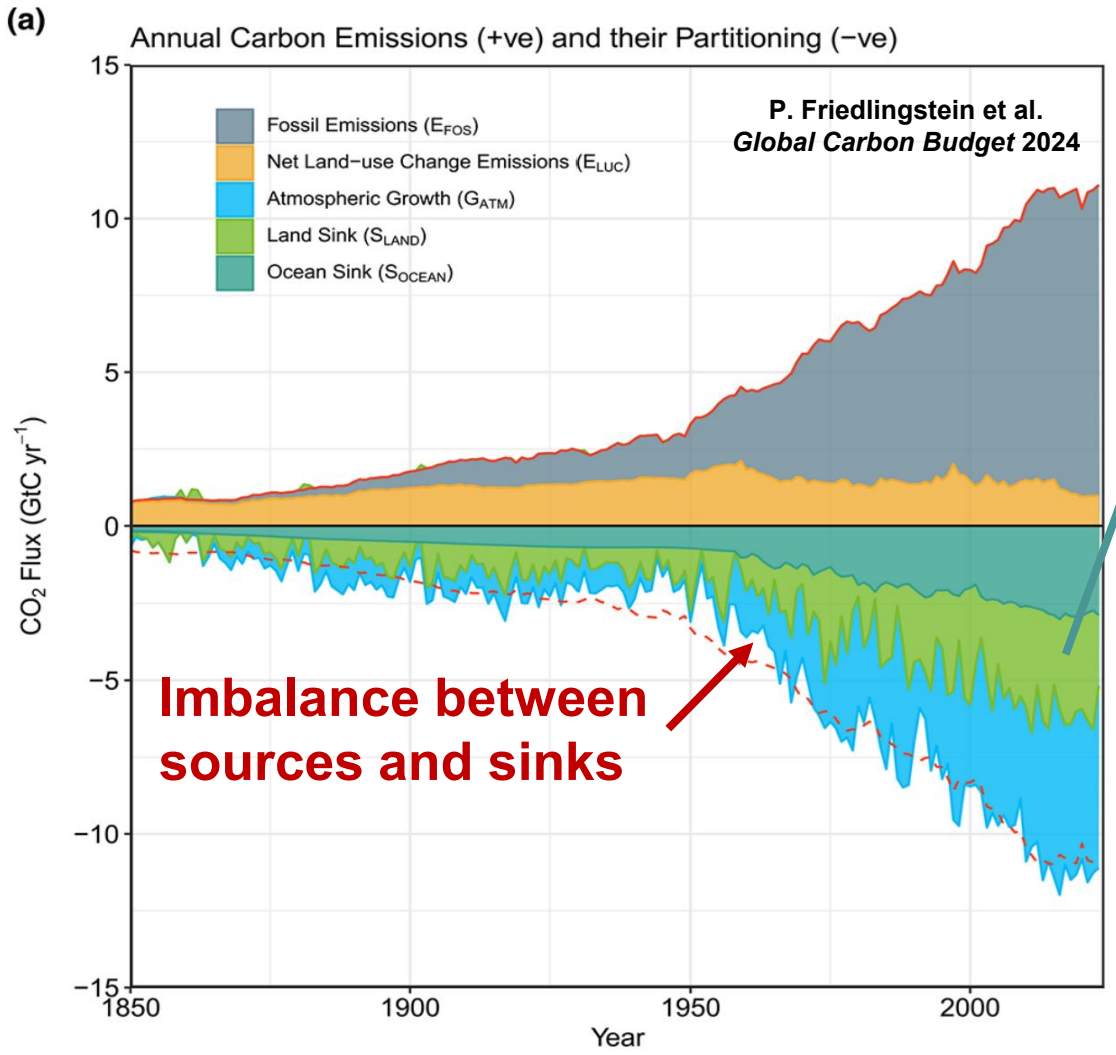
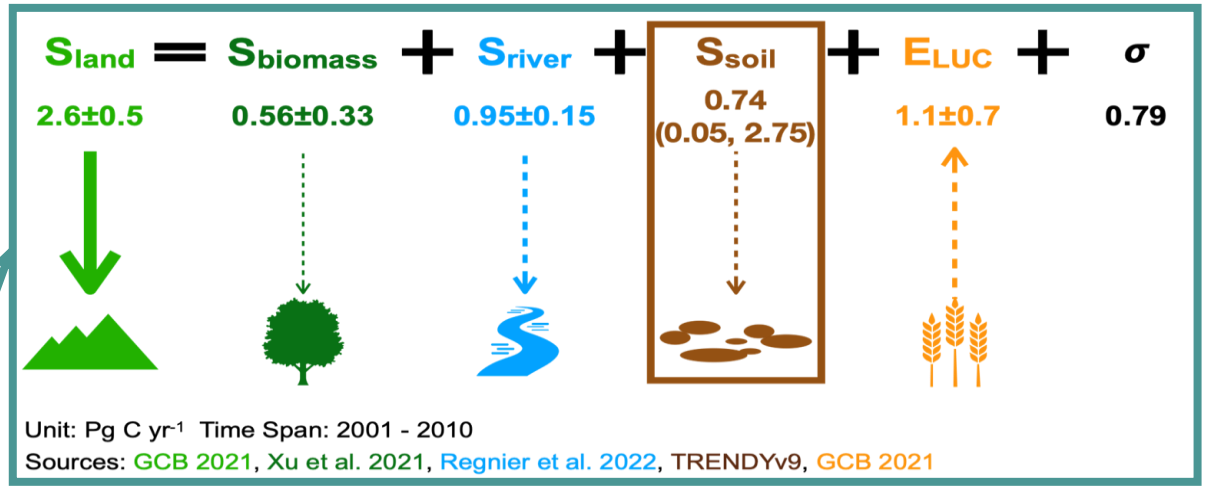
Soil is Critical in Understanding Global Carbon Cycle





- Imbalance within global carbon cycle can partially explained by the uncertainties in land carbon sinks
- Soils hold a large part of uncertainties in land carbon sinks

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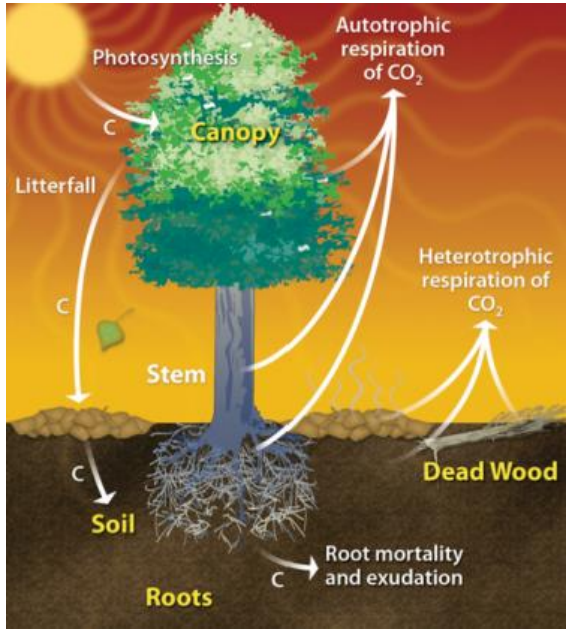
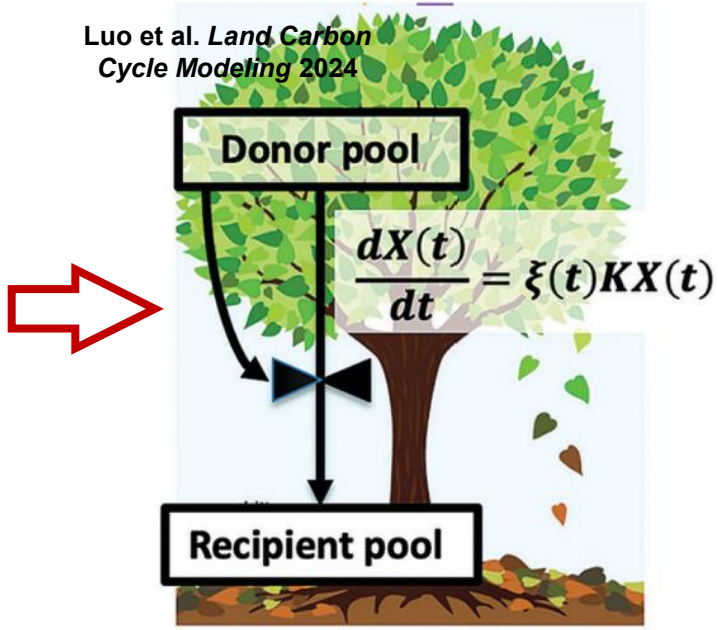
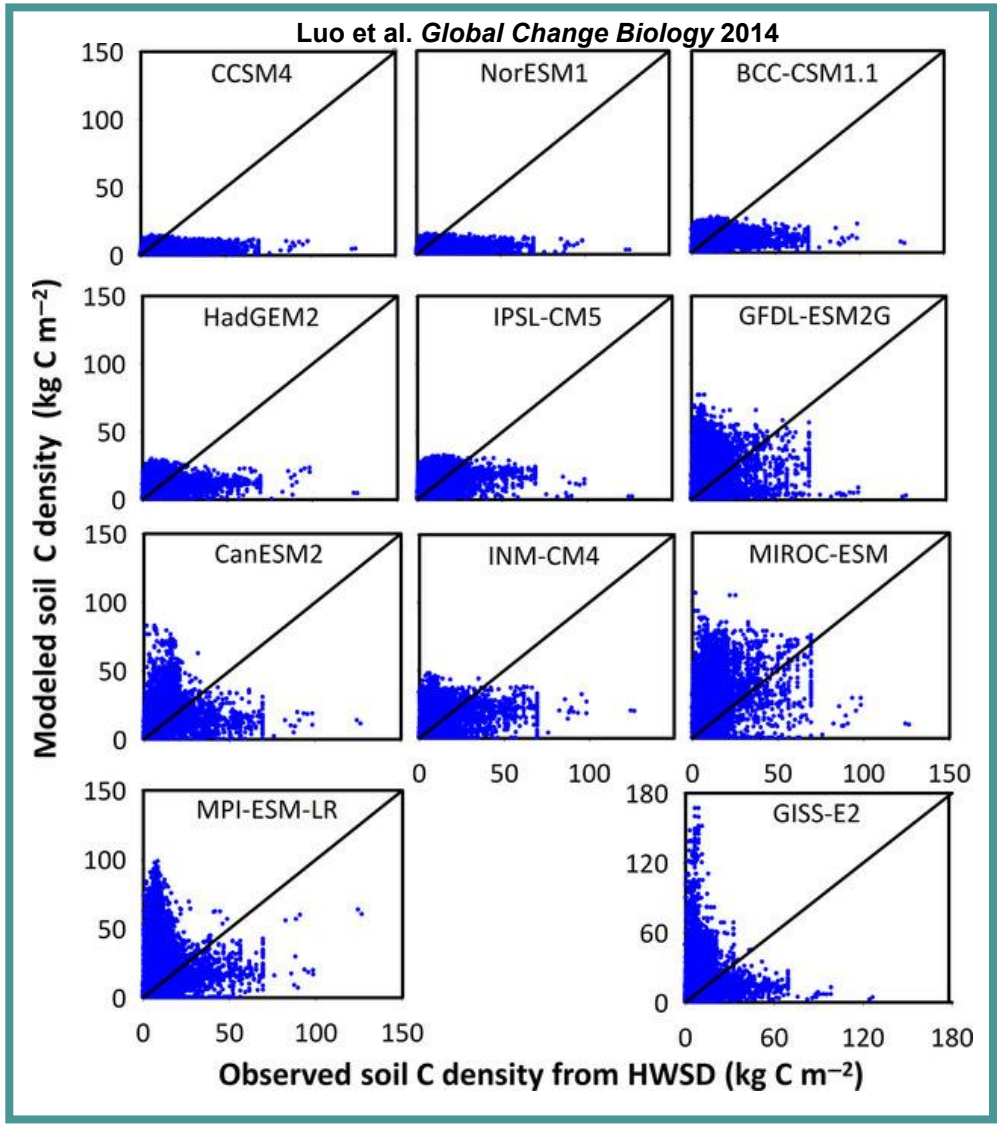
Modeling SOC Dynamics







- Our knowledge of SOC processes can be incorporated into process-based models
- Yet high uncertainties remain in capturing the global SOC cycle

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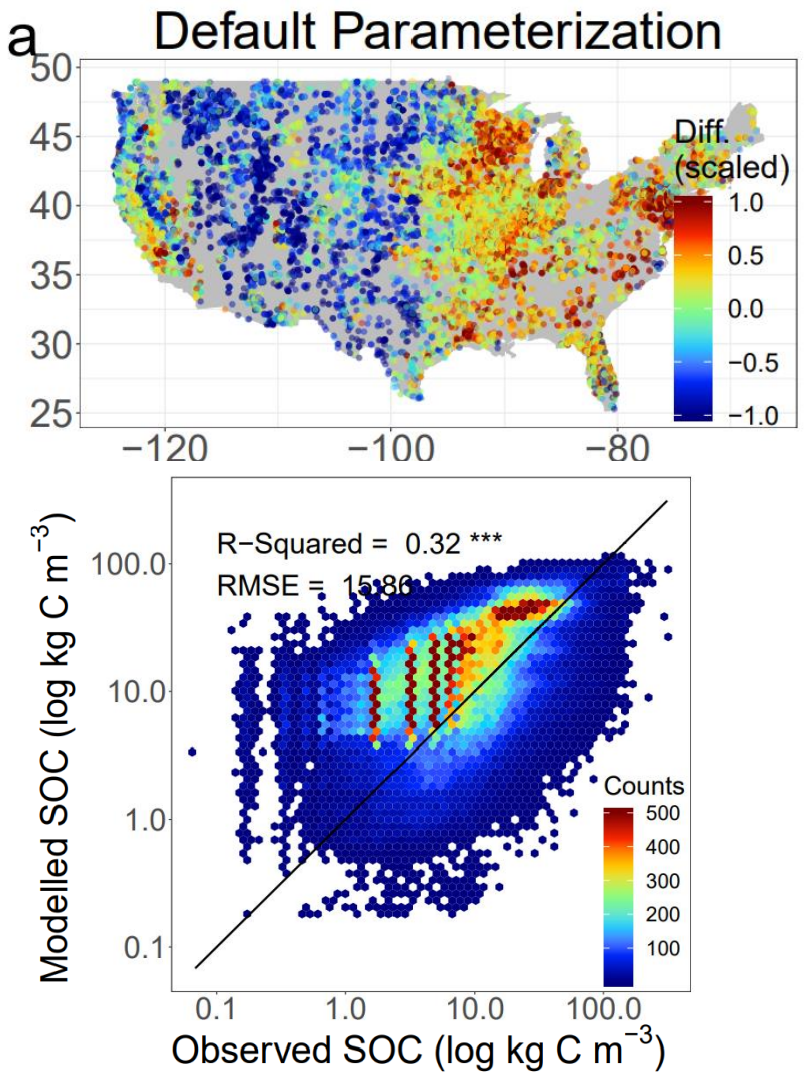
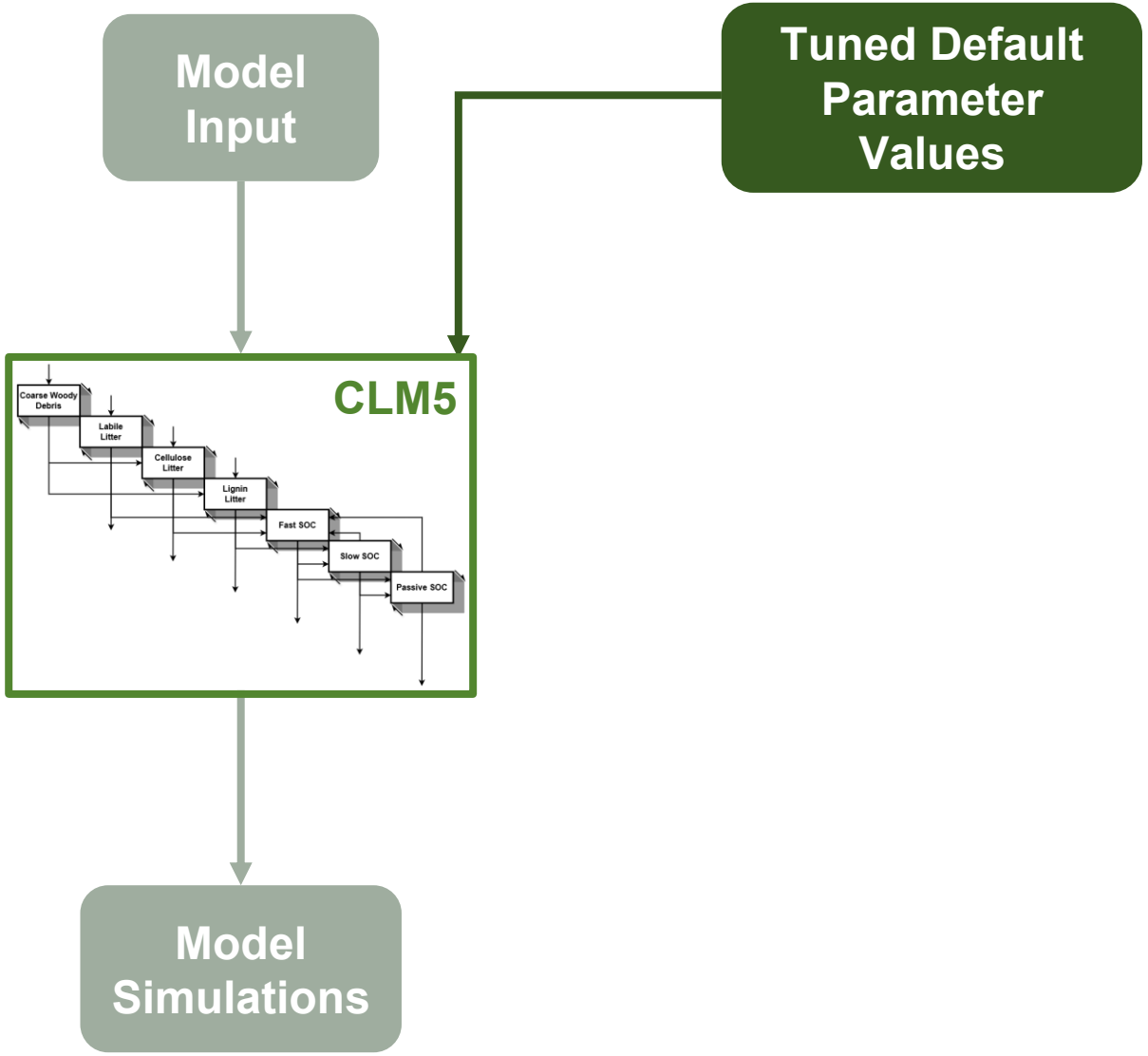
Modeled SOC across Conterminous US





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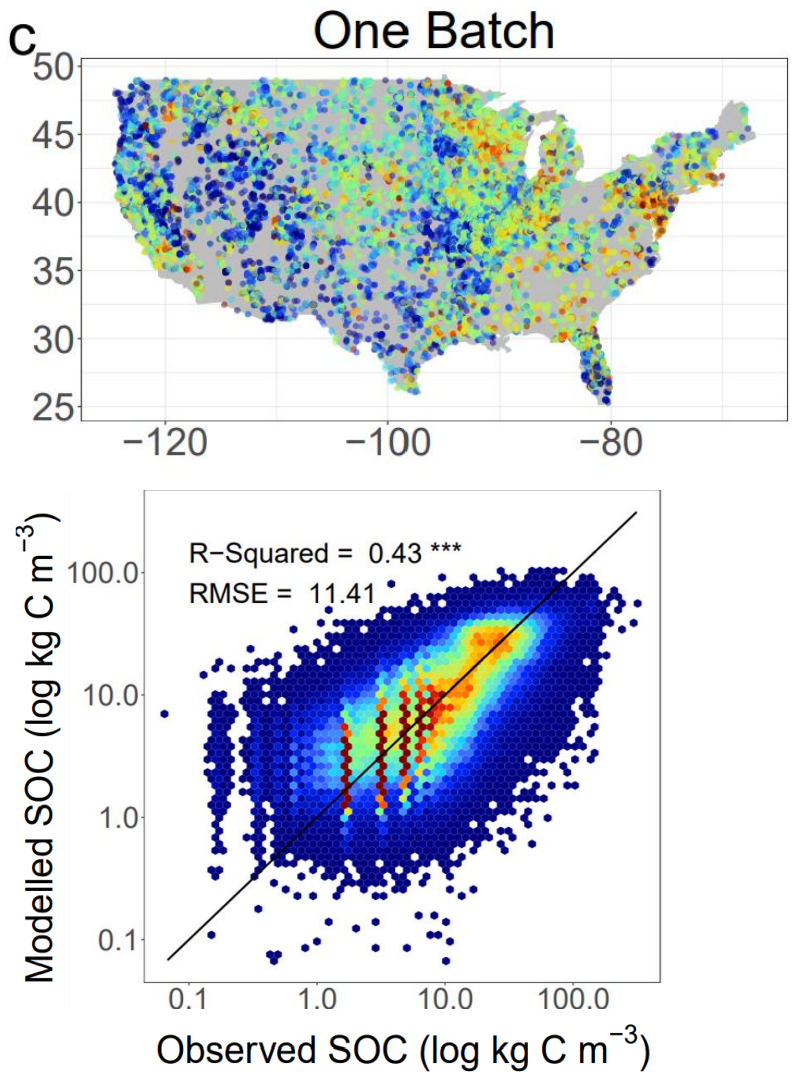
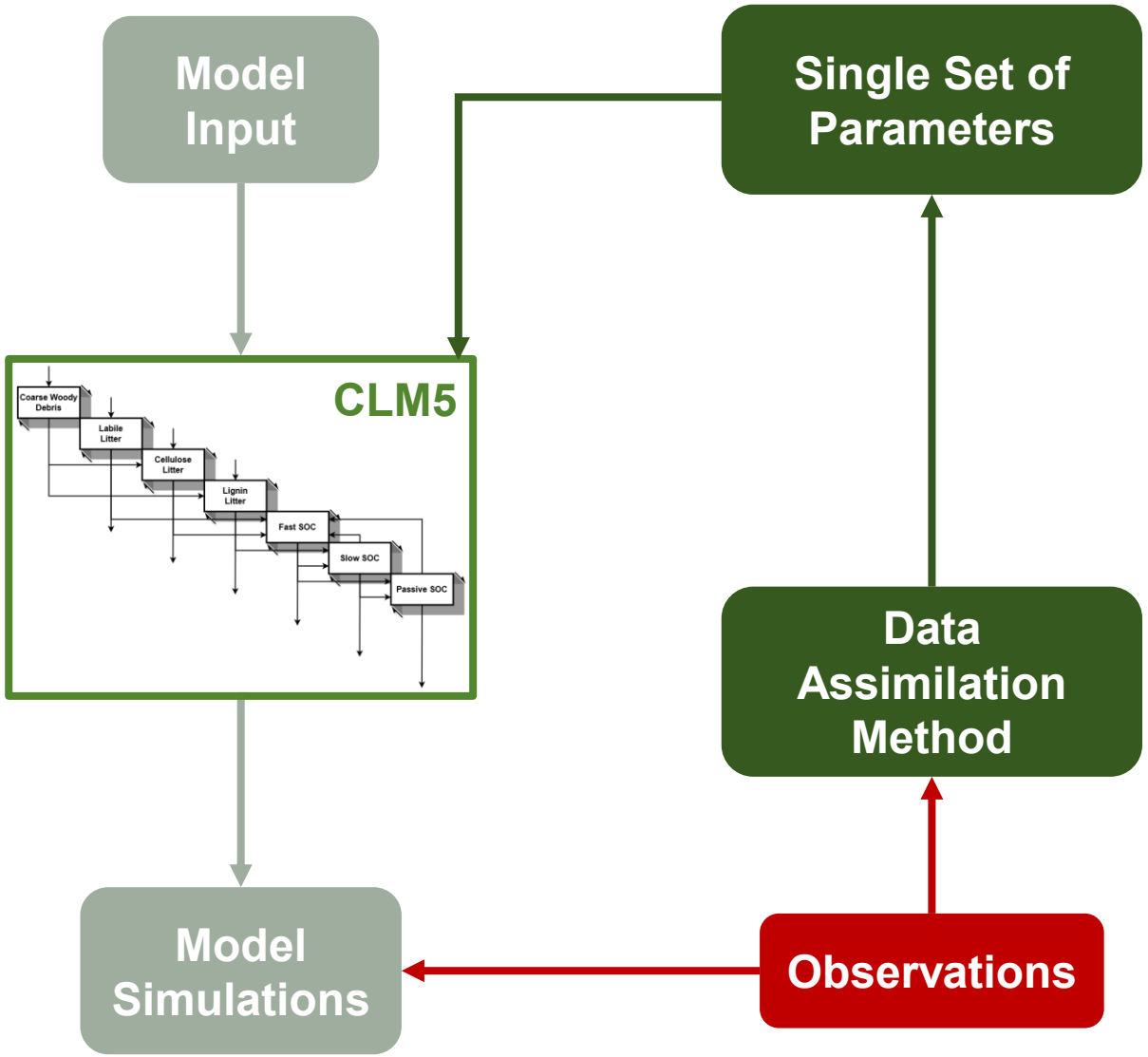
Data Assimilation with One Set of Parameters





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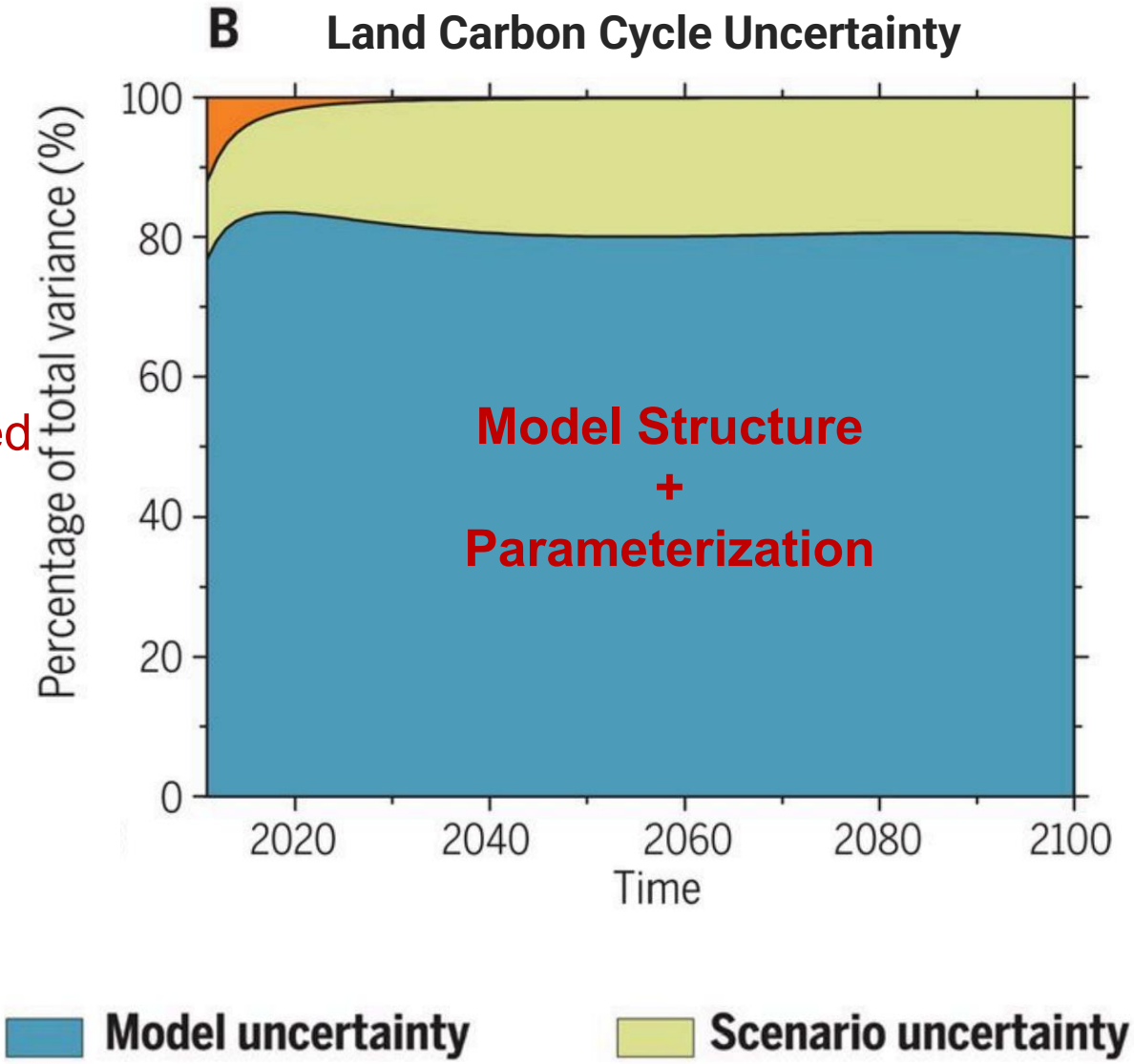
Model Structure: processes relatively well defined
Parameterization: quantify the processes not explicitly represented



Bonan et al., *Science*, 2018

Heterogeneity of soils is one of the major sources of uncertainty, can hardly be represented by a single set of parameters

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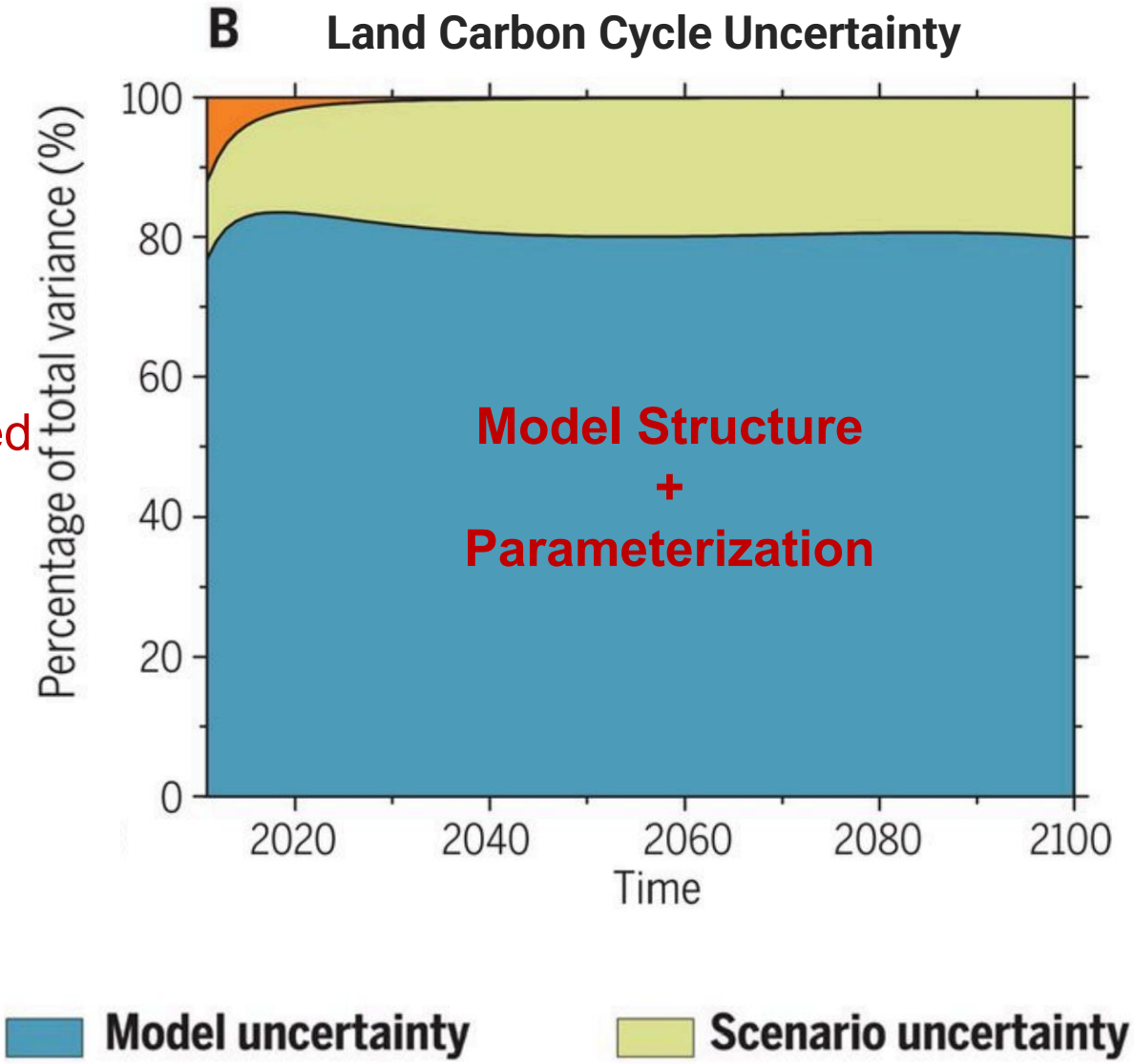

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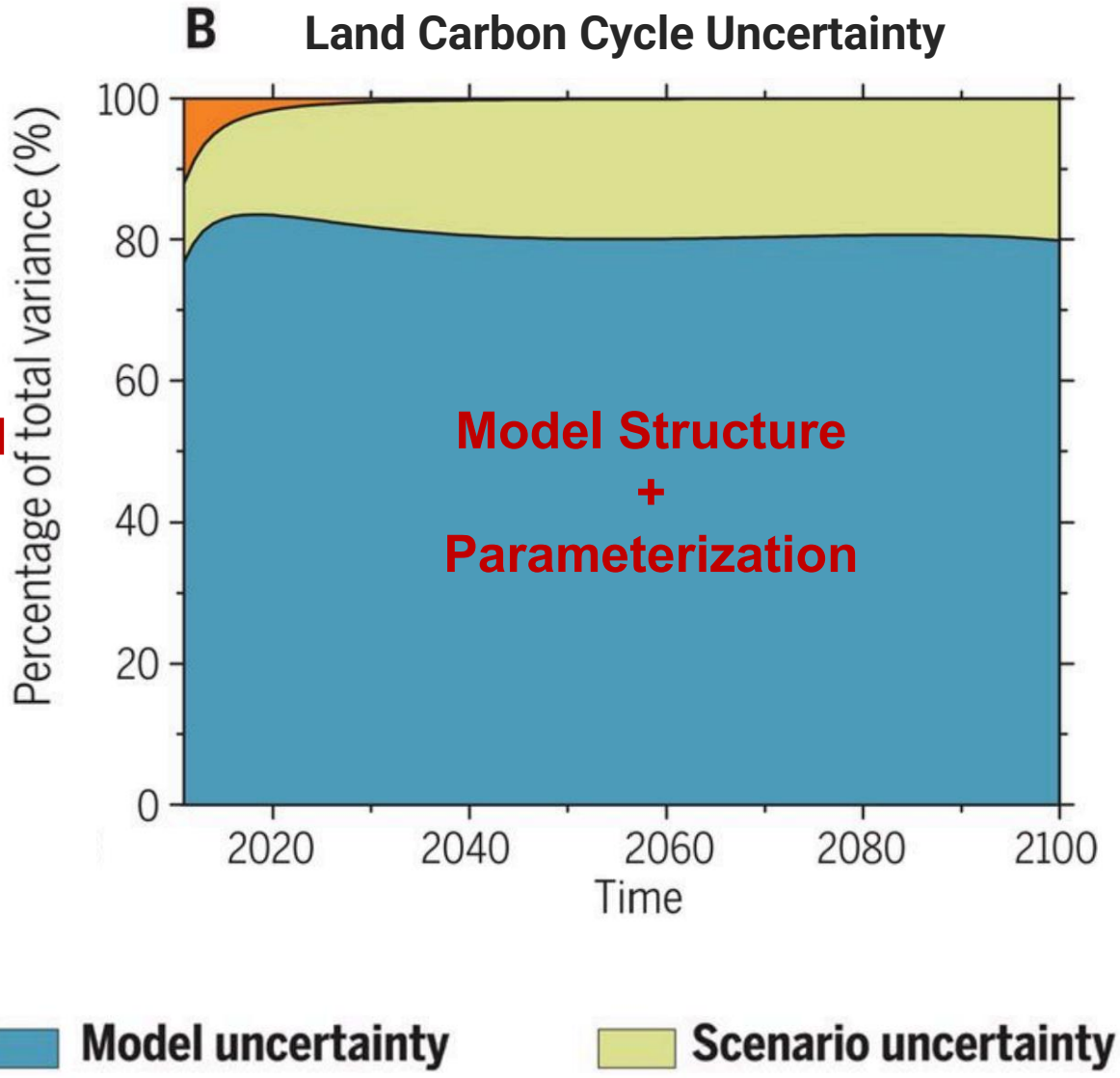
Heterogeneity of soils is one of the major sources of uncertainty, can hardly be represented by a single set of parameters

Model Structure: processes relatively well defined
Parameterization: quantify the processes not explicitly represented

Identify parameter sets that accurately simulate SOC storage, allowing the model to more effectively represent the complexity of real soil systems.



Bonan et al., *Science*, 2018

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Environmental Information

Climate

Soil pH

Lon, Lat, Elevation

Soil Texture

Bulk Density

Land Cover

⋮

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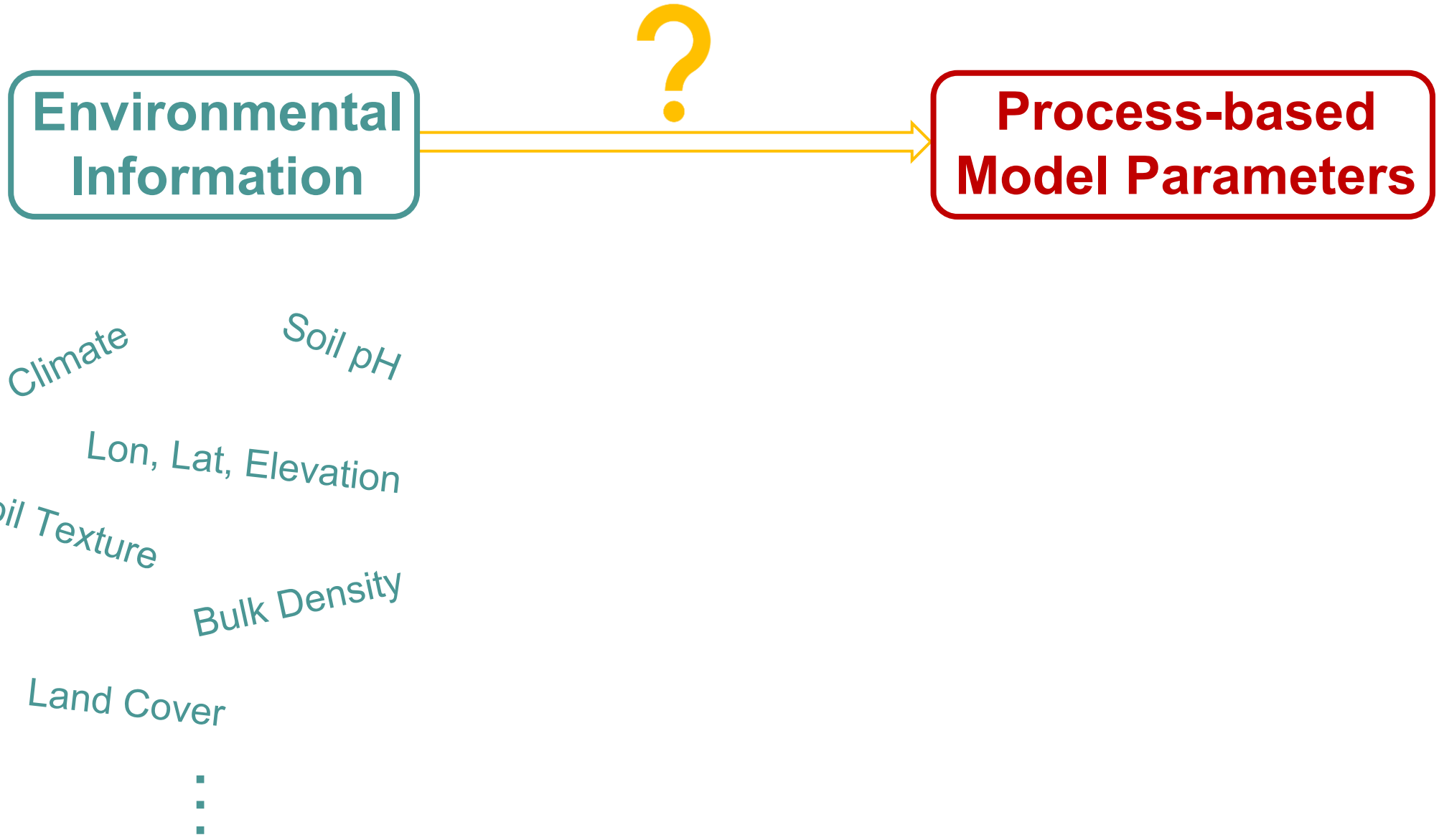

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Artificial Intelligence (Deep Learning)

Environmental Information

Process-based Model Parameters

Climate

Soil pH

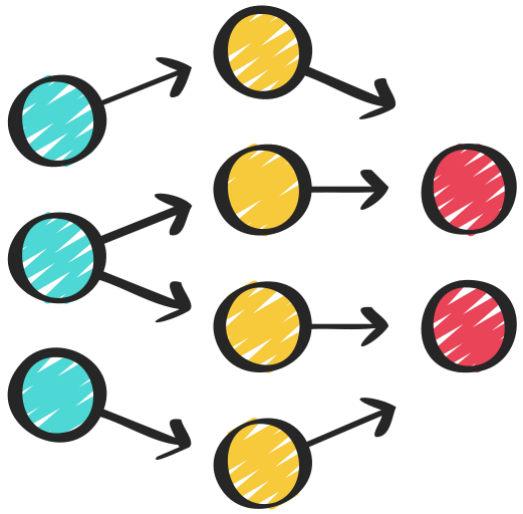
Lon, Lat, Elevation

Soil Texture

Bulk Density

Land Cover

⋮



Microbial Carbon Use Efficiency

Substrate Decomposability

Temperature Sensitivity

⋮

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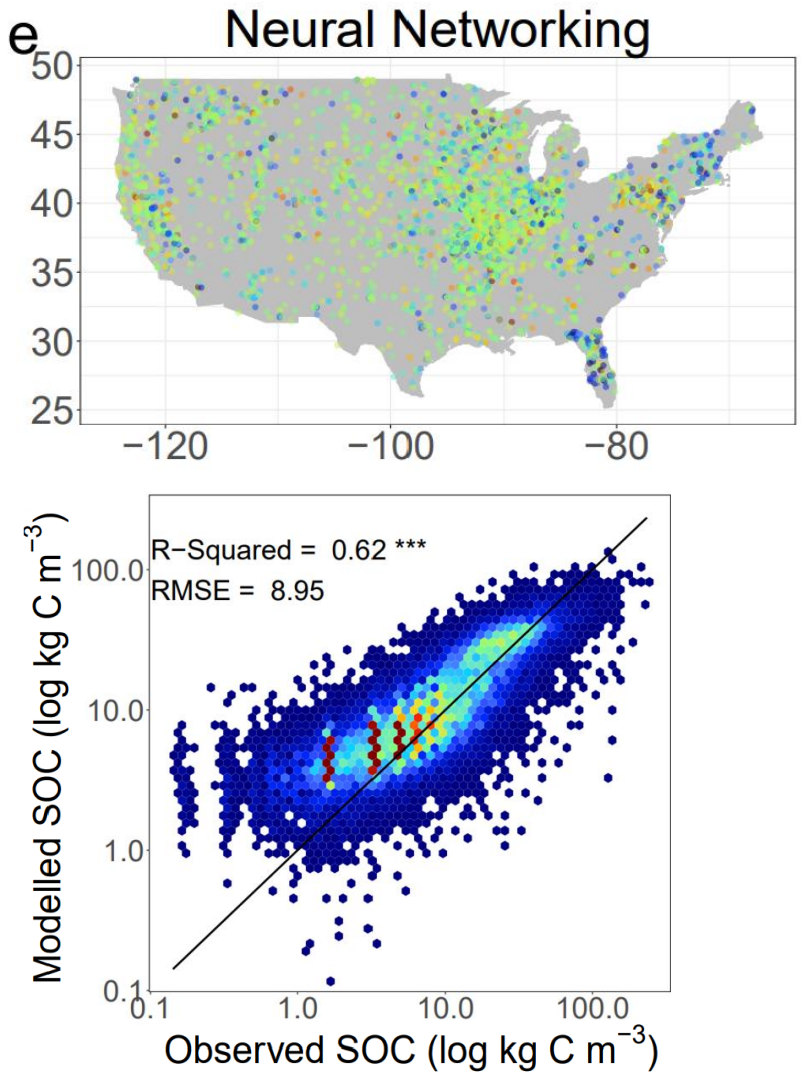
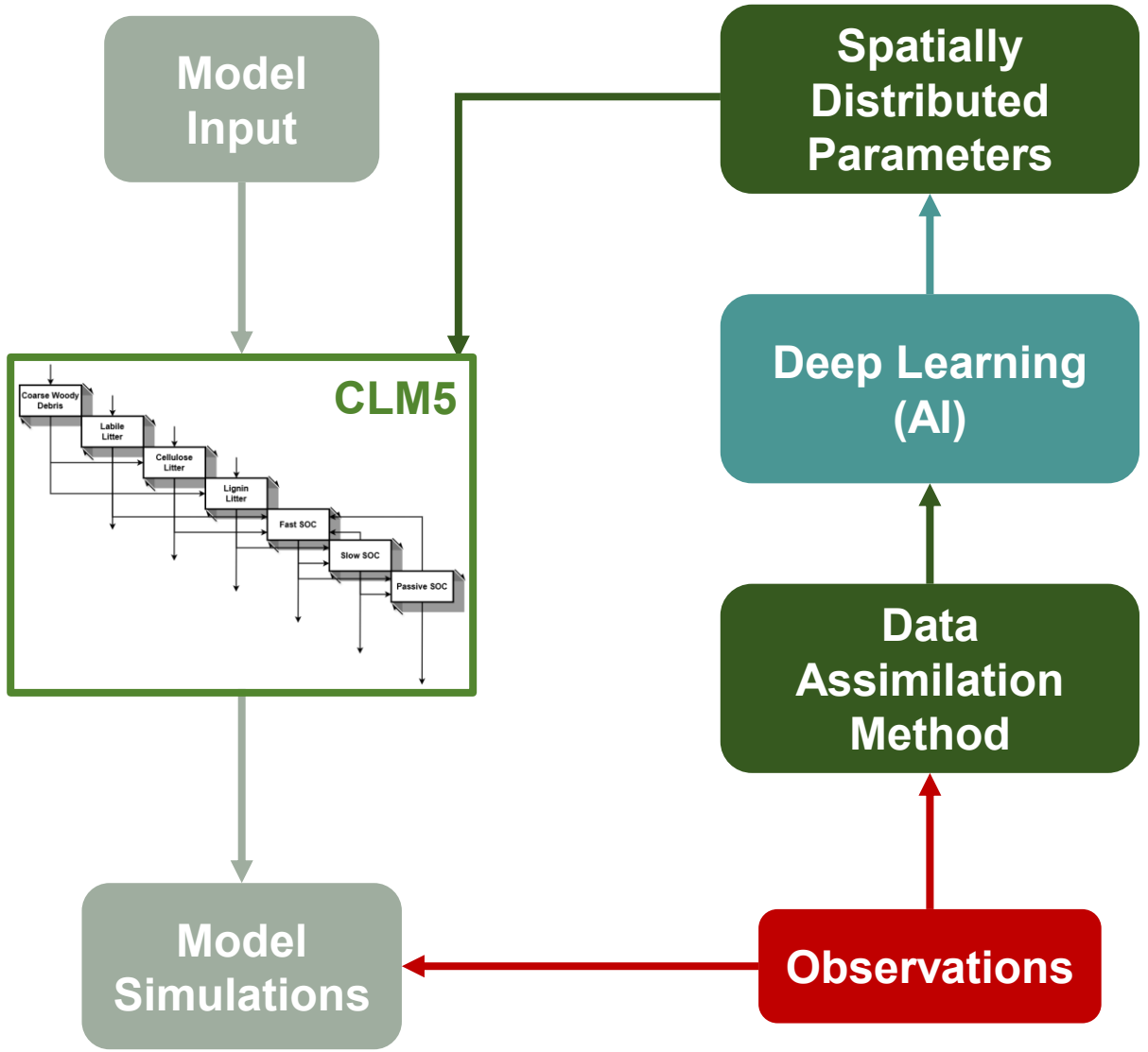
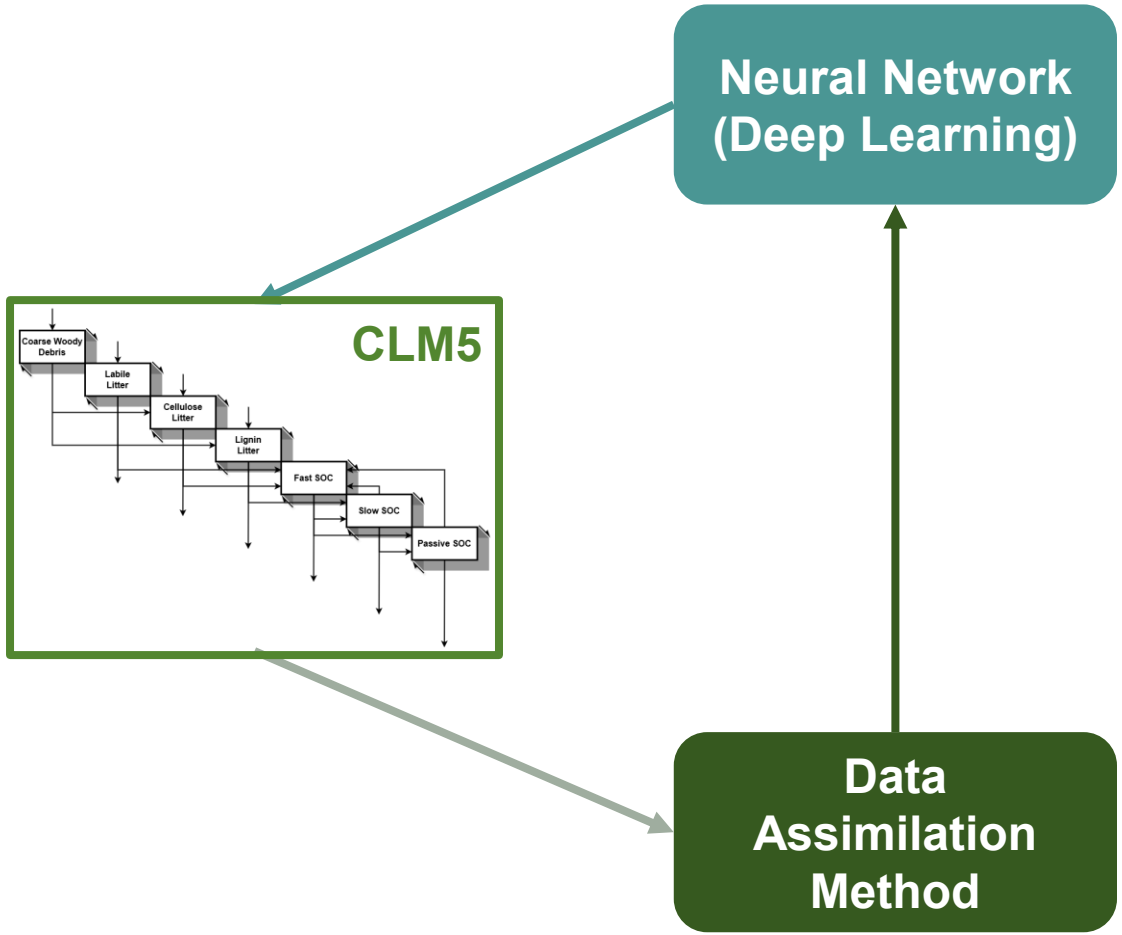
PROcess guided deep learning and DAta driven modeling (PRODA)





The need to further improve PRODA



PRODA includes three components:

- High computational cost due to **Bayesian-based** data assimilation method (e.g. MCMC)
- Limited flexibility with observed data
- Hard to understand and use

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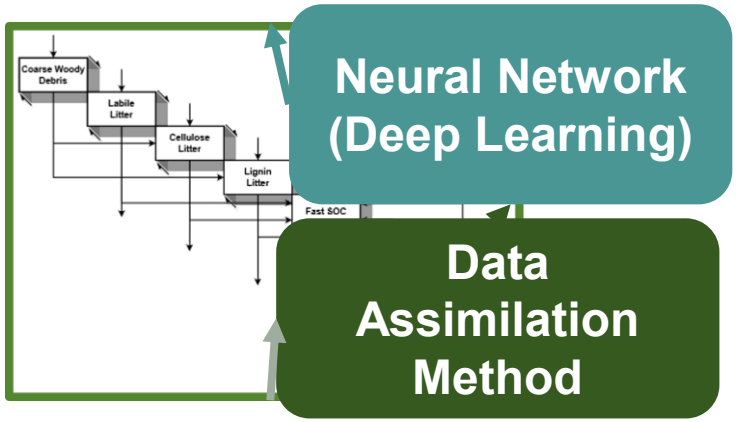
The need to further improve PRODA



PRODA includes three components:

- High computational cost due to **Bayesian-based** data assimilation method (e.g. MCMC)
- Limited flexibility with observed data
- Hard to understand and use

Combine these altogether?

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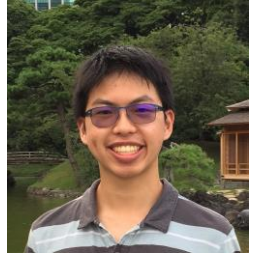

A Biogeochemistry-Informed Neural Network (BINN)

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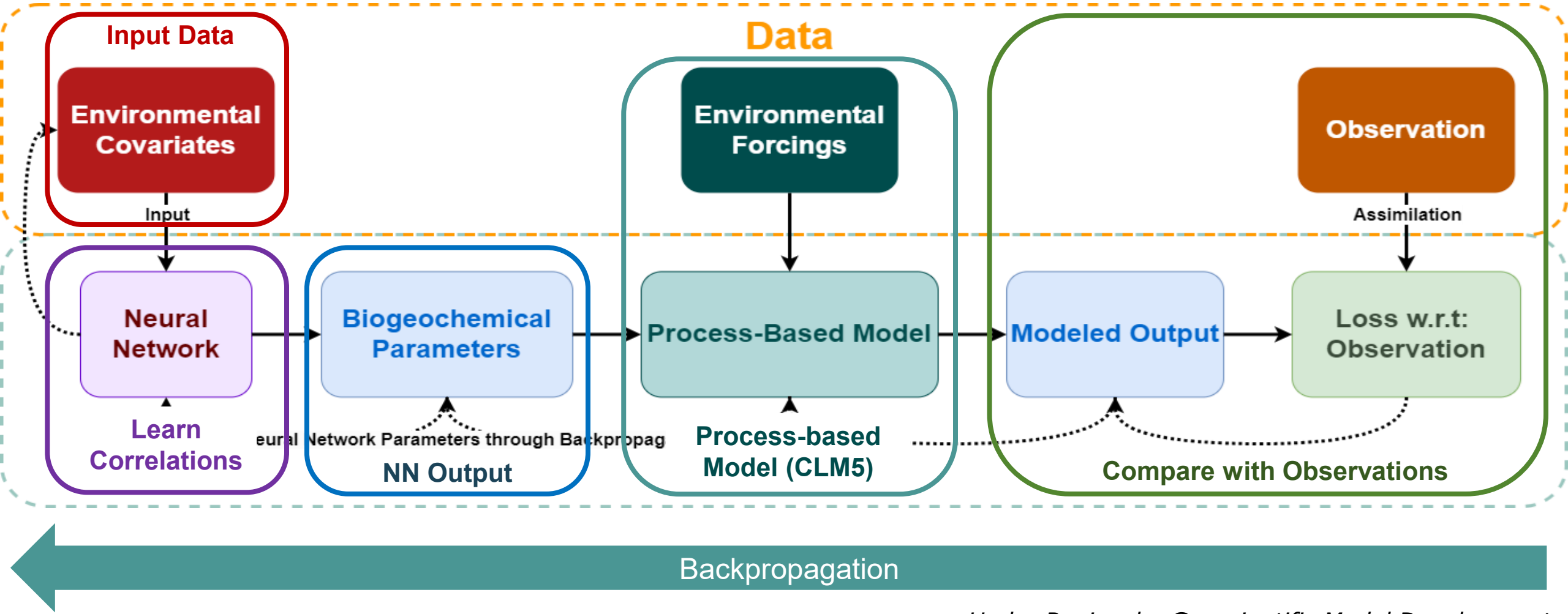
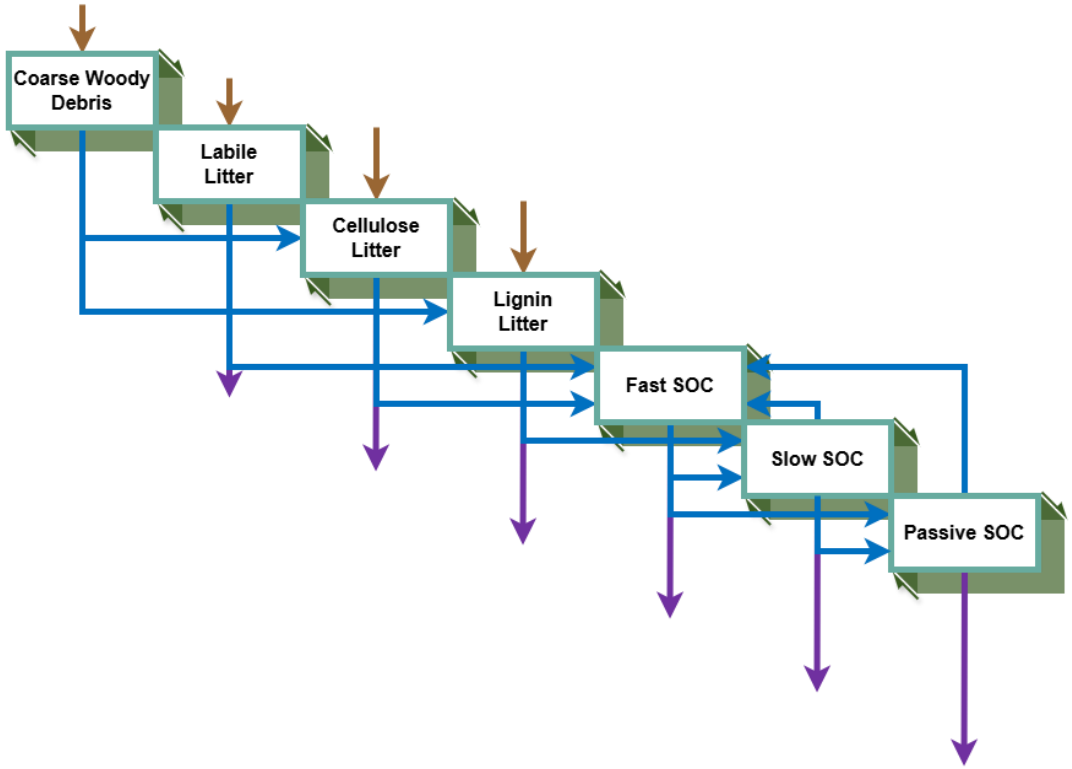
Workflow of BINN



Under Review by Geoscientific Model Development

Matrix Representation of CLM5



Changes in Carbon in each pool through out the time

C movement among different pools

Carbon Dynamics through Diffusion

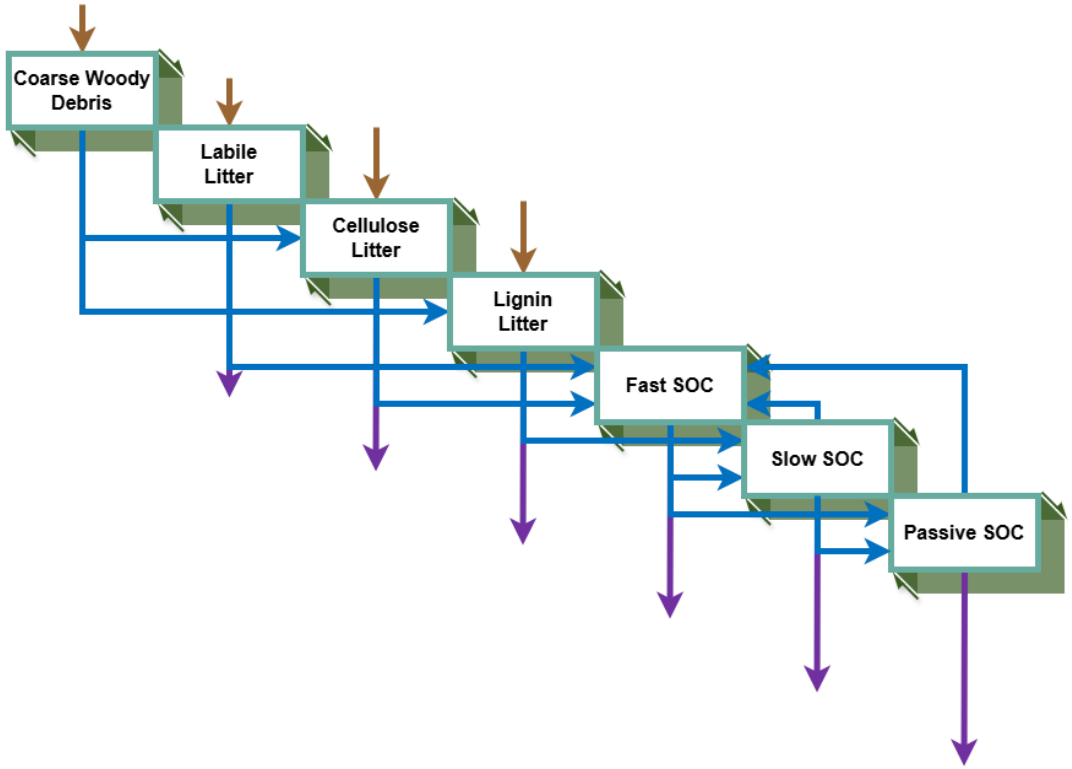
$$\frac{dX(t)}{dt} = B(t)I(t) - A\,\xi(t)KX(t) - V(t)X(t)$$

Carbon Input

The intrinsic decomposition rate of each C pool, modified by the environmental scalar

Each matrix is constructed from one or more unique parameters (21 parameters in total)

Matrix Representation of CLM5



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: Model Components, quantified by 21 model parameters

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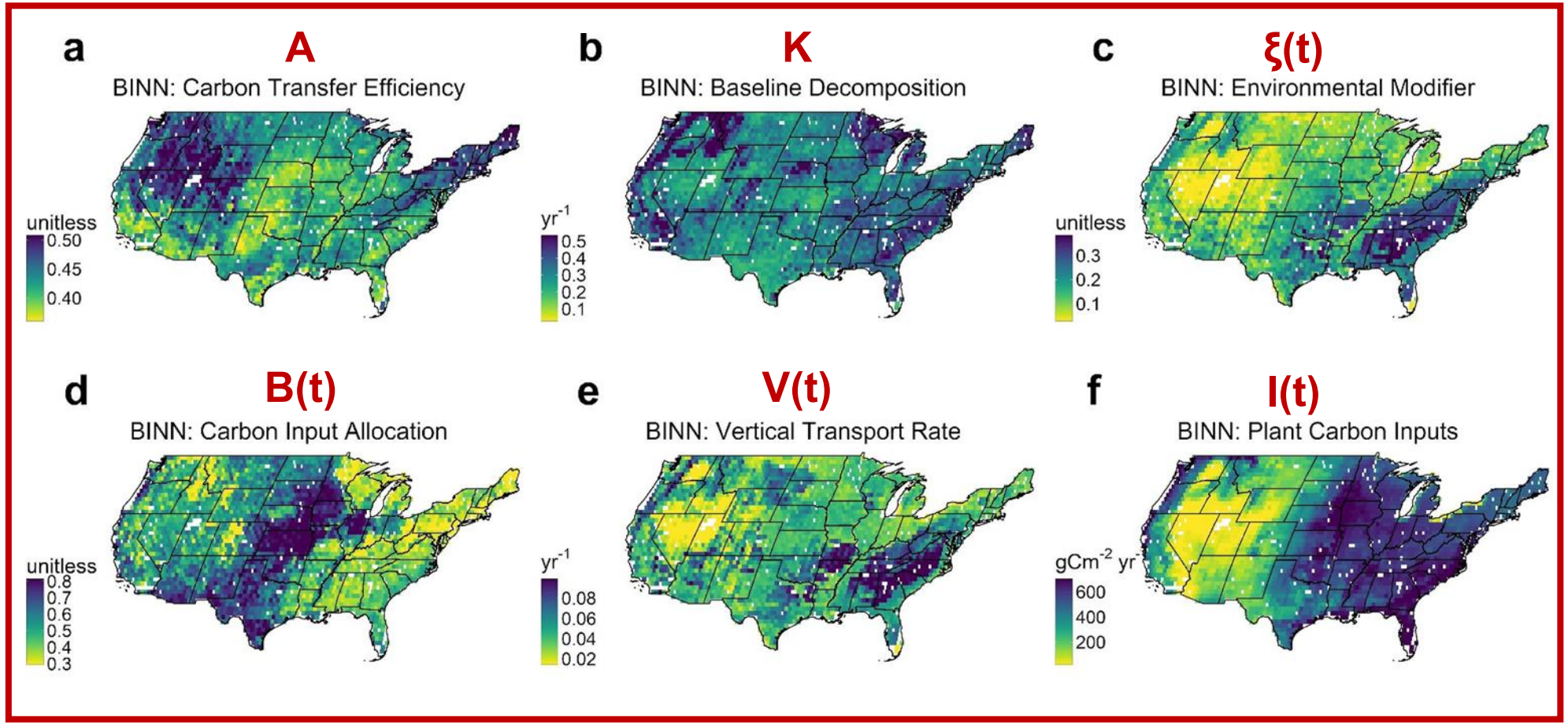
BINN discovers the spatial distribution of underlying mechanisms from SOC observations and environmental covariates (without any data for these mechanisms)



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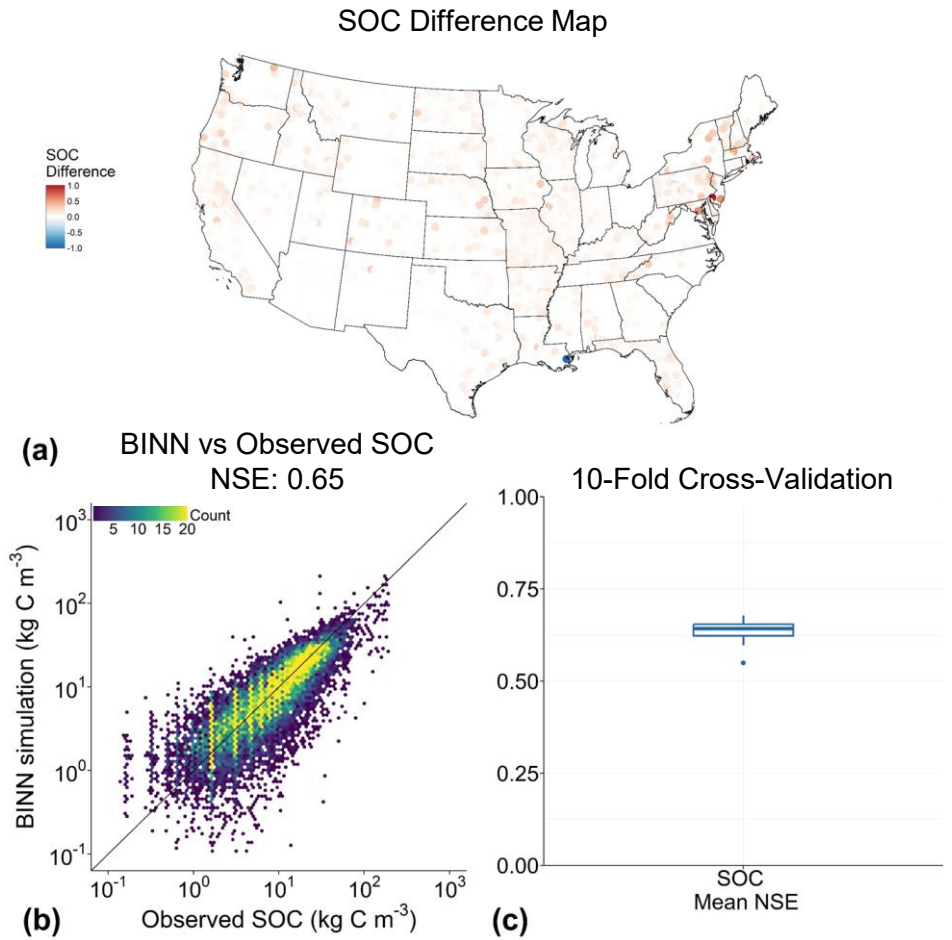
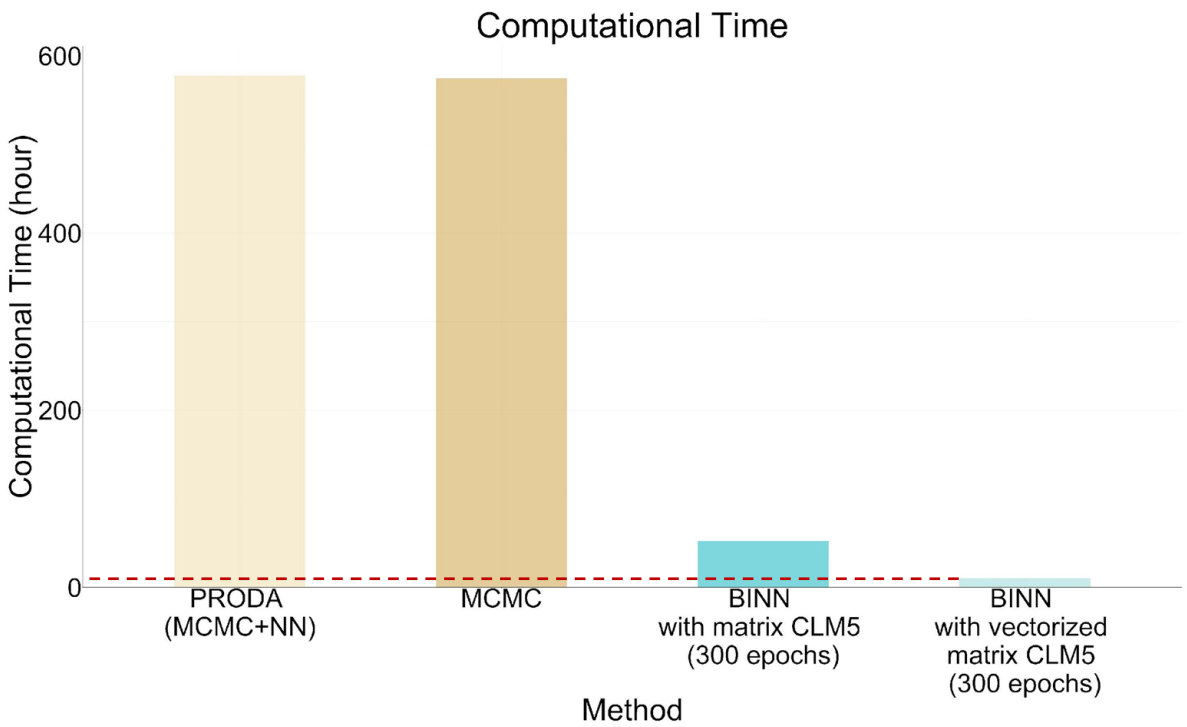
More Realistic Representations of SOC Distribution



Way Less Computational Requirements (More than 50 times)



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Data

Environmental Covariates

Environmental Forcings

Observation

Input

Assimilation

Neural Network

Biogeochemical Parameters

Process-Based Model

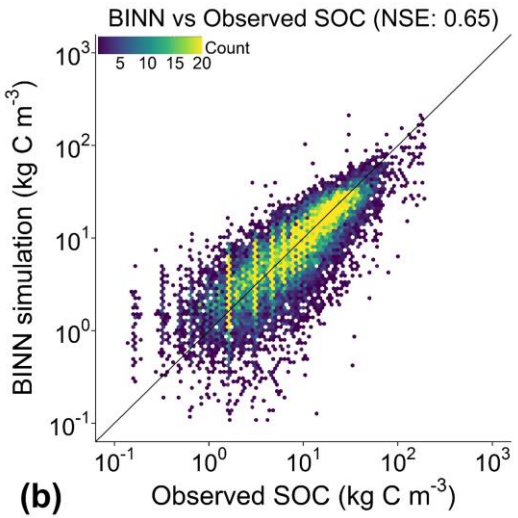
Modeled Output

Loss w.r.t: Observation

Update Neural Network Parameters through Backpropagation

BINN

SOC Model



(b)

Data

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Environmental Forcings

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Assimilation

Neural Network

Biogeochemical Parameters

Process-Based Model

Modeled Output

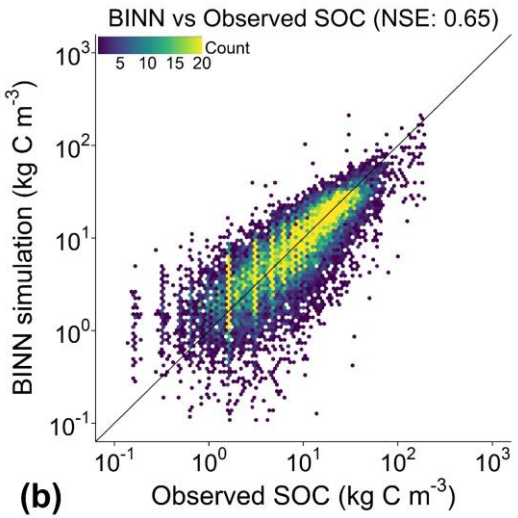
Loss w.r.t: Observation

Update Neural Network Parameters through Backpropagation

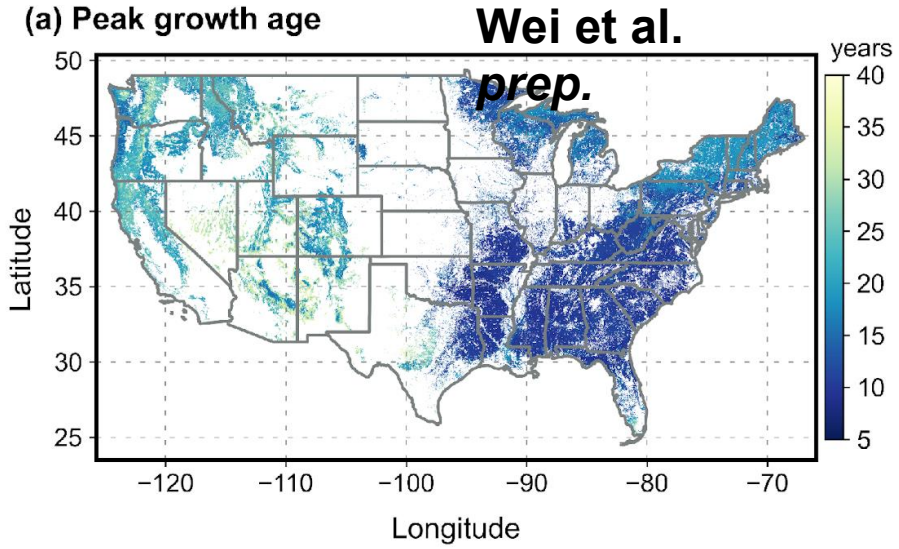
BINN

SOC Model

Forest Growth Model



(b)



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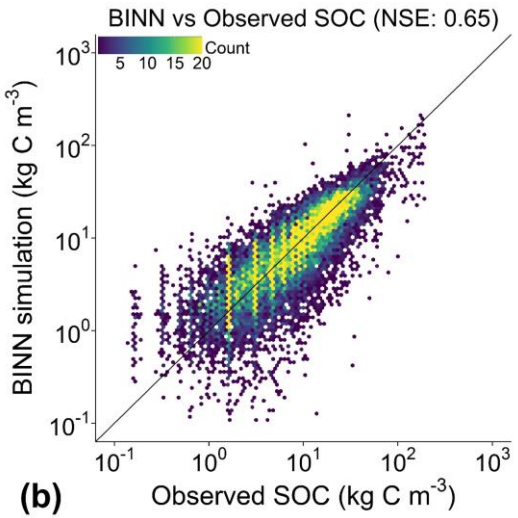
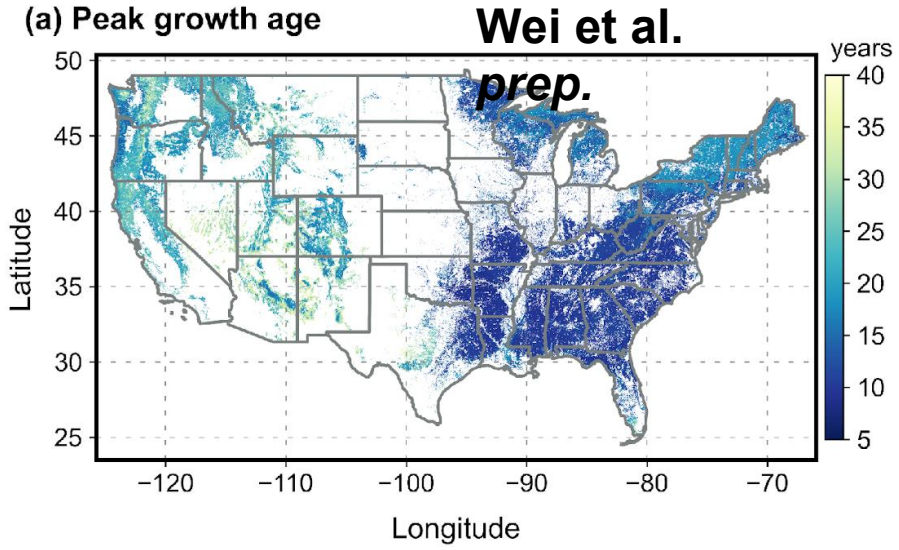
SOC Model

Forest Growth Model





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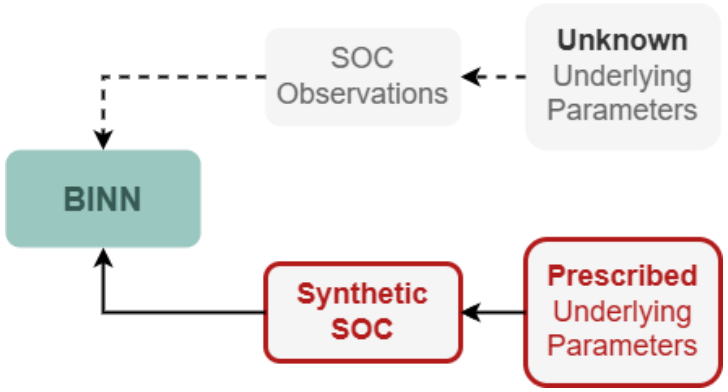
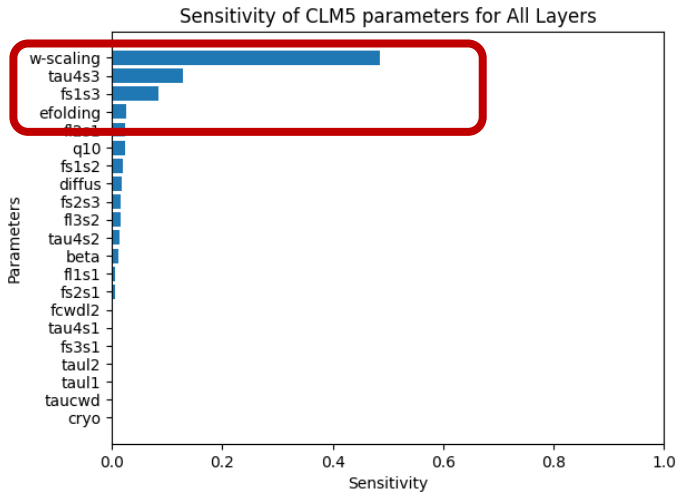
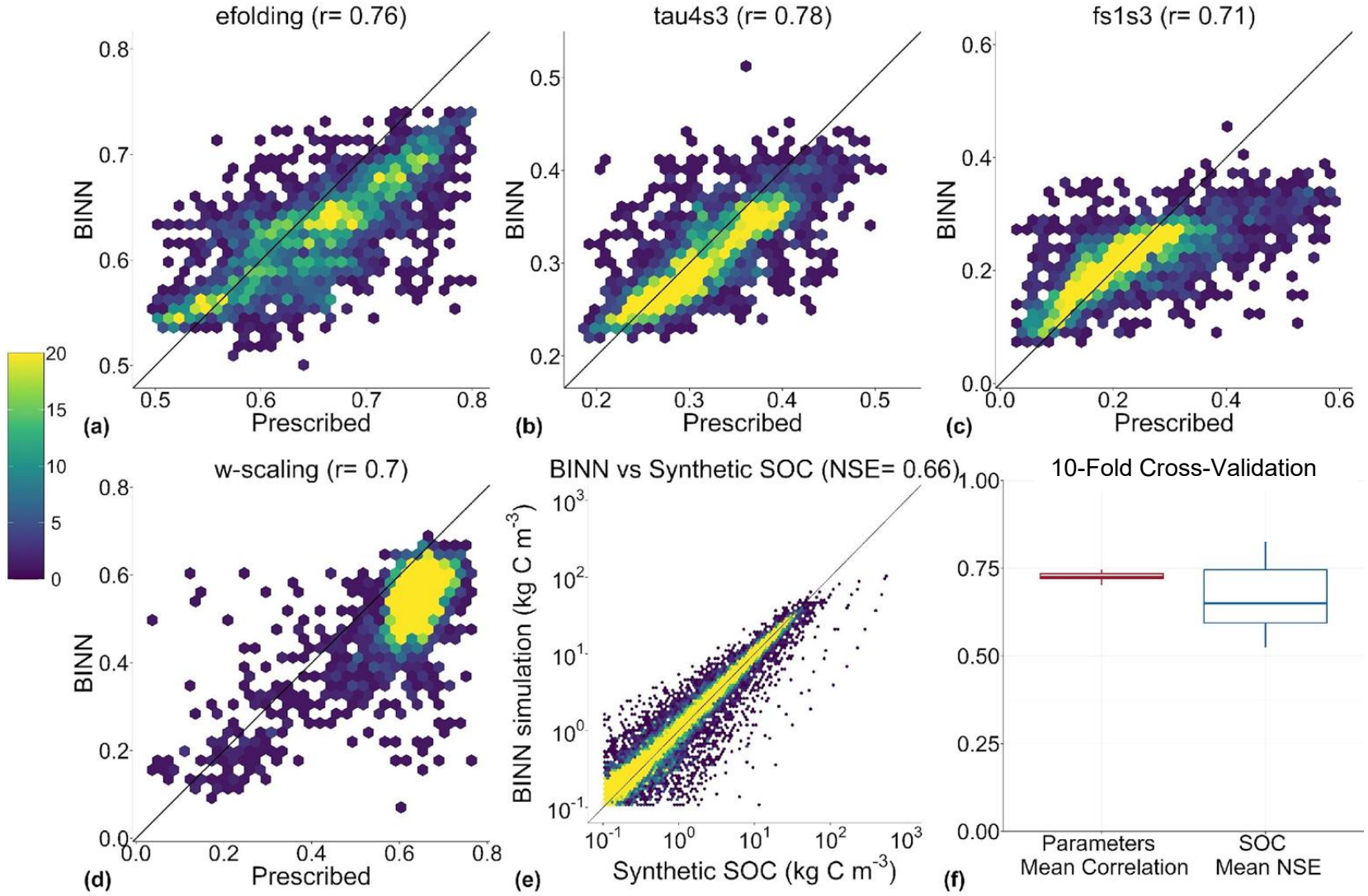
Recovery Experiment with 4 Most Influential Parameters







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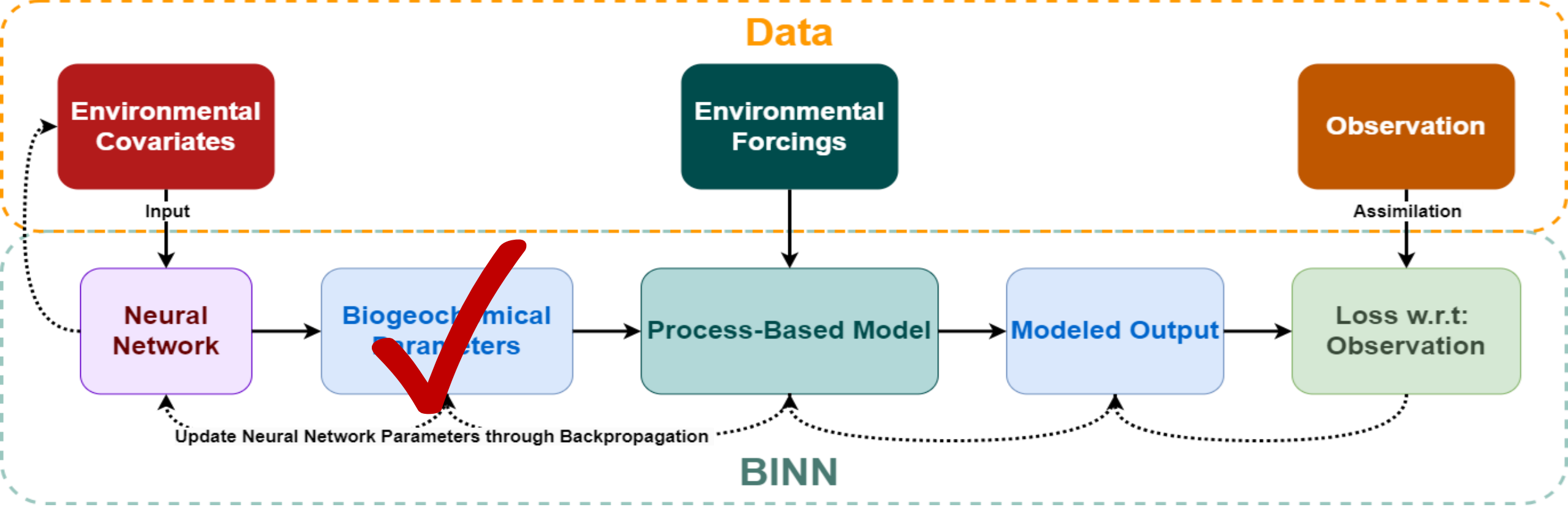
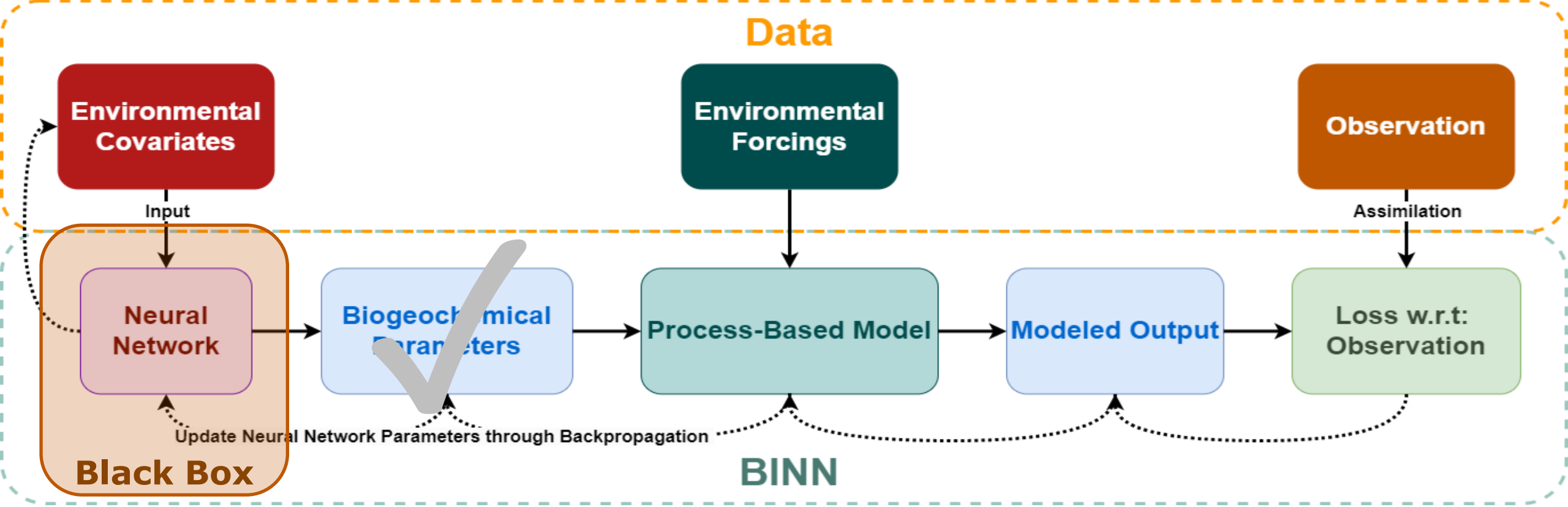


Recover causes from data (biogeochemical parameters)

Discover emerging mechanisms governing SOC from big data (observations)



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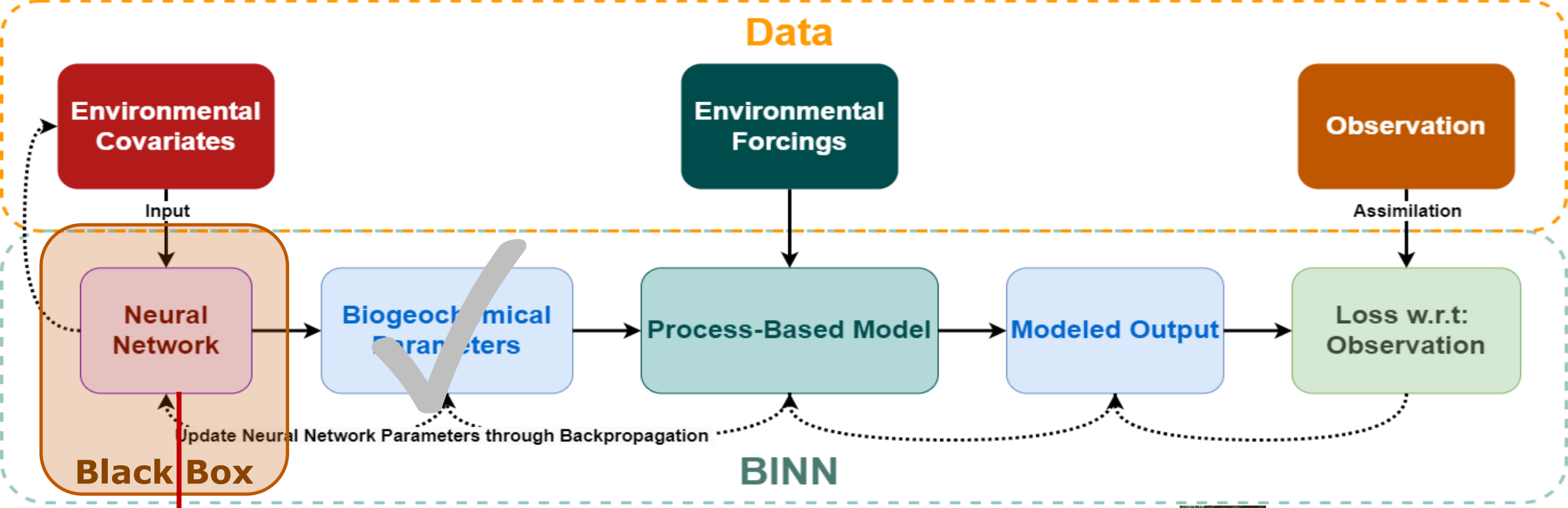

Kolmogorov Arnold Network (KAN)

An alternative to neural networks that is easier to interpret

Scientifically-Interpretable Reasoning Network(ScIReN)

Submitted to NeurIPS 2025

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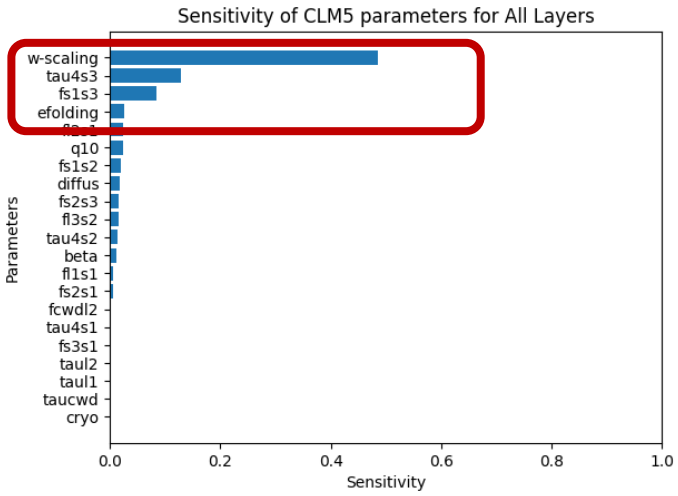
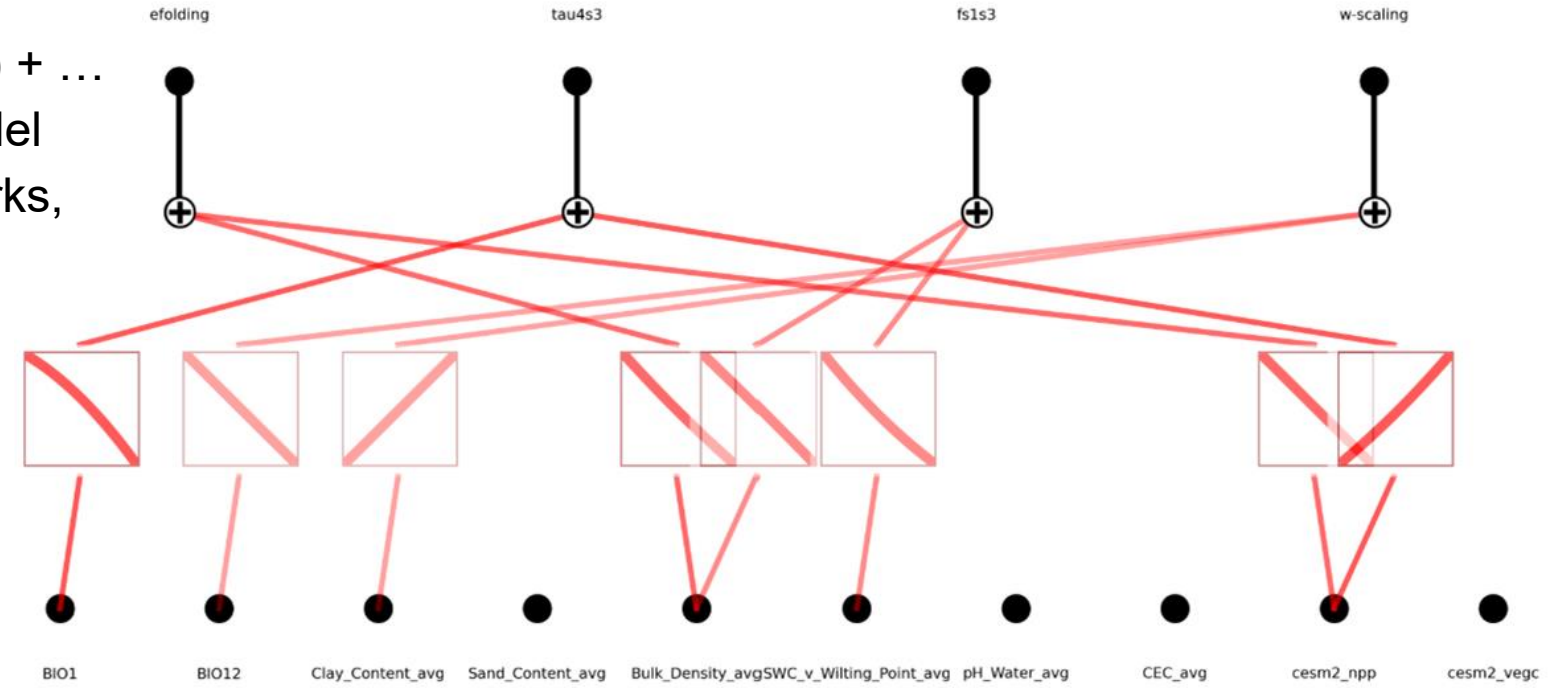
Structure of KAN

- Curves show how changing one environmental variable will affect a biogeochemical parameter
- Each output = sum of interpretable contributions from each input, e.g.
  - parameter = $(input1)^2$ + exp(input6) + …
- 1-layer KAN = generalized additive model
  - Not as expressive as neural networks, but similar accuracy in our case
  - Can add more layers



Outputs (Biogeochemical Parameters) - not observed



Inputs (Environmental Covariates) - observed

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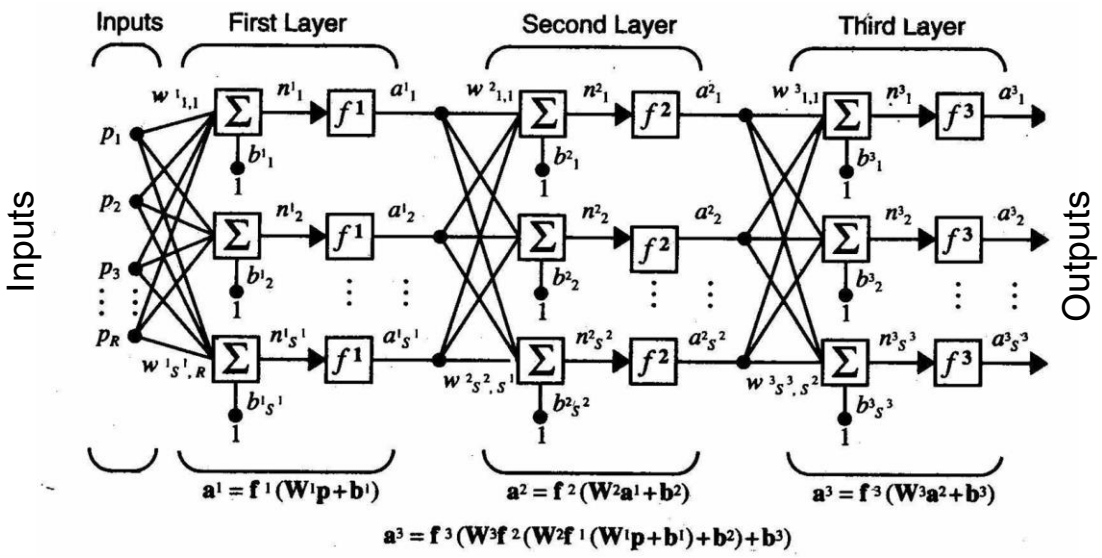
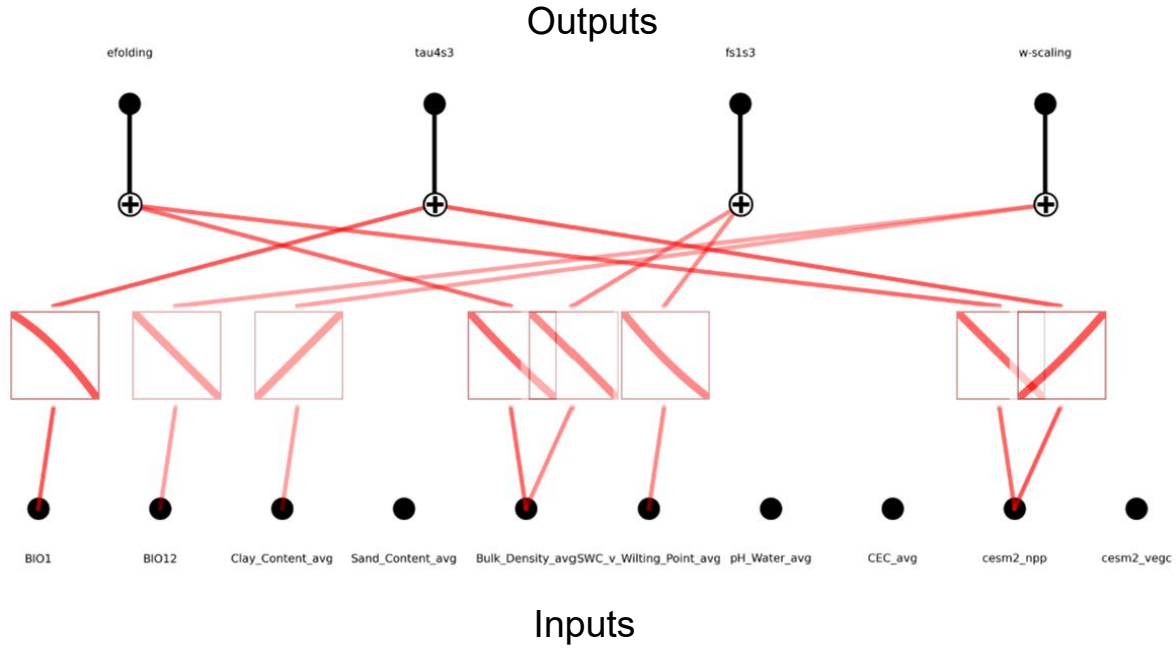
Difference between NN and KAN

- **Standard neural networks:** every input variable affects every output
  - Inputs are mixed together and passed through nonlinearities - hard to understand
  - Unclear how each input (environmental variable) influences each output (biogeochemical parameters)



- **Kolmogorov-Arnold Networks:** learn **interpretable** functional relationships between inputs and outputs
  - Apply a 1D function on each edge (link), then add contributions from each input
  - **Sparsity:** focus on a few crucial relationships; remove unnecessary connections



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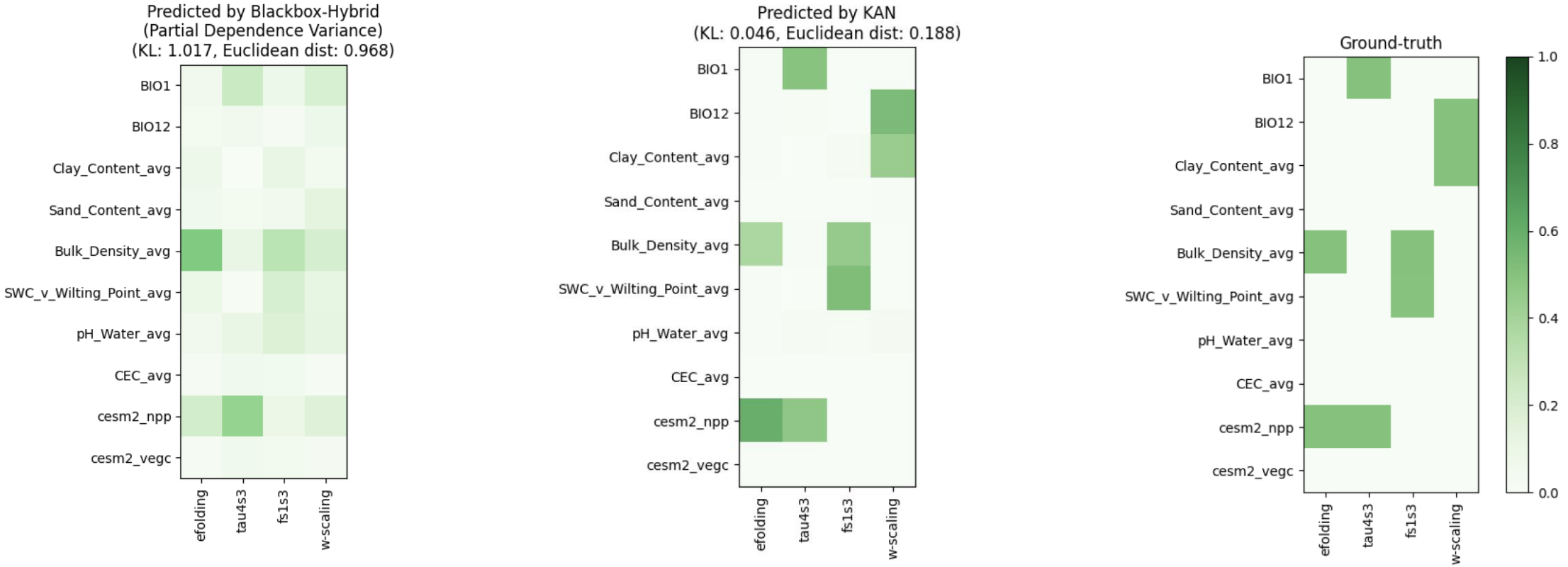
Functional Relationship Retrieval Test

- Prescribed functional relationships between 10 environmental inputs and 4 most sensitive biogeochemical parameters in CLM5
- BINN does not reveal functional relationships. Even after applying a post-hoc interpretation method (Partial Dependence Variance), we find it did not even implicitly learn the correct relationships.
- ScIReN (center) revealed the relationships very accurately.



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In Conclusion, BINN/SciReN can …

Recover causes from data (biogeochemical parameters)

Discover emerging mechanisms governing SOC from big data (observations)

Uncover novel relationships between environmental conditions and underlying mechanisms

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Thanks for Listening

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