

Coupling Scales in process-based soil organic carbon modelling including dynamic aggregation

Alexander Prechtel¹, Simon Zech¹ and Nadja Ray²

¹Modelling and Numerics, Department of Mathematics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

²Mathematical Institute for Machine Learning and Data Science, Catholic University of Eichstätt-Ingolstadt, Germany

EGU 17.4.2024, SSS5.2: Carbon sequestration in soils



- Soils harbor twice as much carbon as the atmosphere
⇒ high public relevance to **quantify the fate of organic matter (OM) and carbon in soils**
- **Soil structure** is directly related to **particulate organic matter (POM) dynamics**: the break-up of **soil aggregates** and their formation influences the persistence of organic carbon (OC) in soils

The dilemma: microscale processes drive questions of global relevance

⇒ process-based mechanistic, temporally and spatially explicit model describing the interaction of

- dynamic (re-)arrangement of soil aggregates
- turnover of OM by microbes
- simultaneous soil surface interactions

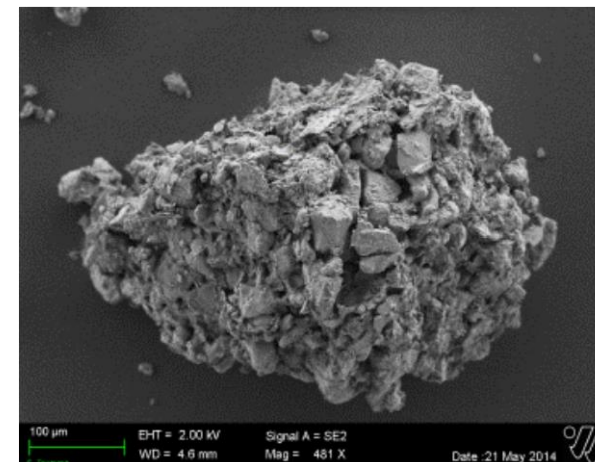


Figure: Picture by courtesy of DFG RU 2179 „MAD Soil - Microaggregates: Formation and turnover of the structural building blocks of soils“.

Why use pore scale models? We want to think **BIG!**



Plant Sc
DOI 10.
MAR

Cha
of rl

T. Roo
W. Ott

Receive
© The.

Abstra
Backgr
food p
essenti
predict
assess
affect t
Scope
in etnu

Global Change Biology

RESEARCH RE

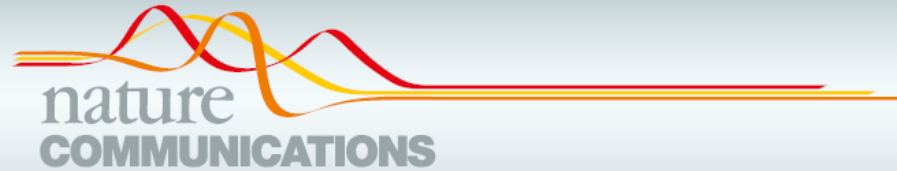
Soil organic

SHARON M. O'RO
MCBRATNEY²

¹UCD School of Biosystem
Environment, The Univers
Sydney, NSW 2015, Aust
Hochelaga Blvd, Québec, C

Abstract

Mechanistic understand
cycle. Greater attention
icity to protect/enhance
require consideration o
landscape scale, with c
standing of SOC across
emphasis on stabilizing SOC.
well each is represented in th
soil security is examined. We
Instead, SOC has come to be viewed as a stable pool subject to carbon flux. Better understanding exists for SOC



ARTICLE

<https://doi.org/10.1038/s41467-020-14411-z>

OPEN

Soil structure is an important omission in Earth System Models

Simone Fatichi ^{1*}, Dani Or ^{2,3}, Robert Walko⁴, Harry Vereecken⁵, Michael H. Young ⁶,
Teamrat A. Ghezzehei ⁷, Tomislav Hengl ⁸, Stefan Kollet⁵, Nurit Agam ⁹ & Roni Avissar⁴

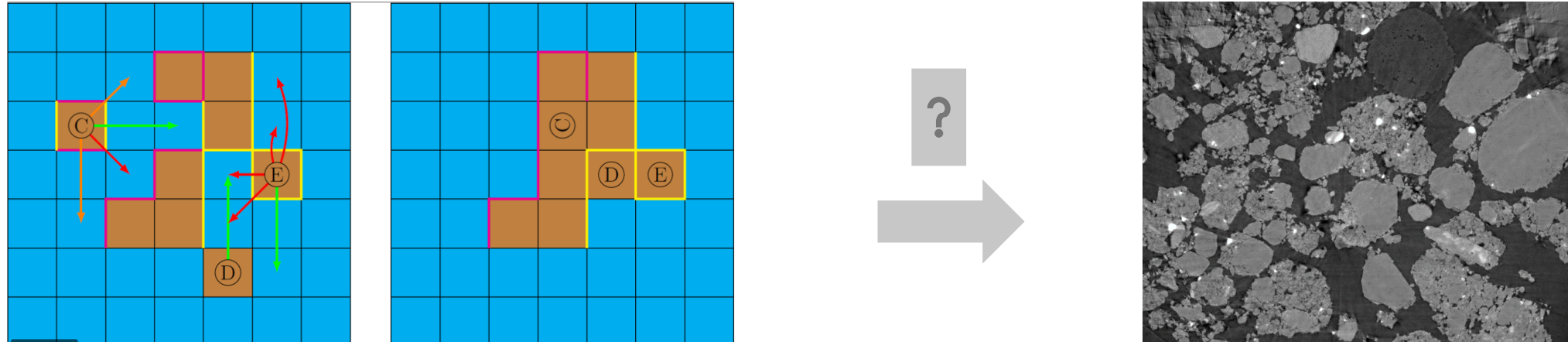
AgroParisTech, UMR ECOSYS,
Thiverval-Grignon, France

²School of Water, Energy and
Environment, Cranfield University,

Macroscopic models of soil organic matter (SOM) turnover have faced difficulties in reproducing SOM dynamics or in predicting the spatial distribution of carbon stocks. These models are based on a largely inadequate linear response

The idea for the pore scale...

Can we use cellular automata to study the interaction of soil structures, organic matter and biofilms?



- complexity of soils vs. simplicity of models
- in contrast to lab scenarios: easy variation of a manifold of conditions and isolation of mechanisms / effects possible
- direct access to all parameters of resulting structures - at every time step
- can the reduced perspective help understanding reality?

The numerical output of a particular calculation is not much help [...]; one needs to know how the various features of the problem interact to produce the outcome

Fowkes & Mahony (1994): An Introduction to Mathematical Modelling

Concepts

Schematic overview

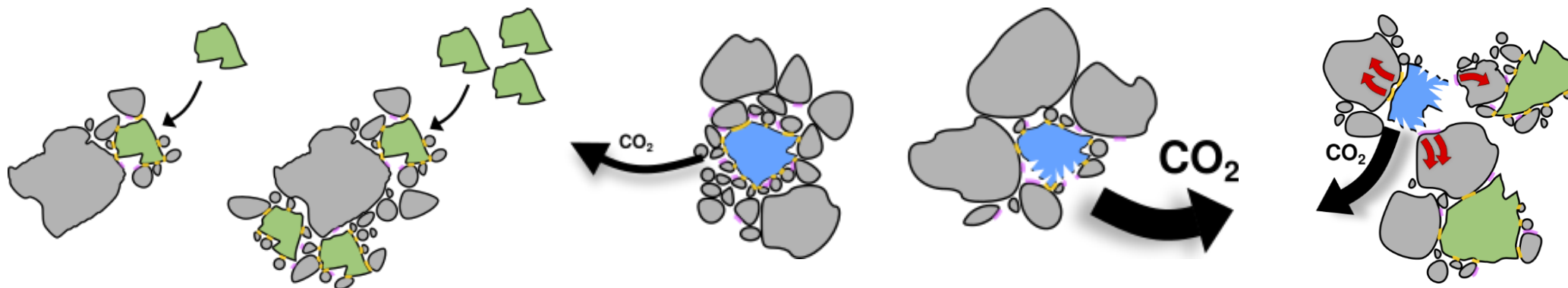
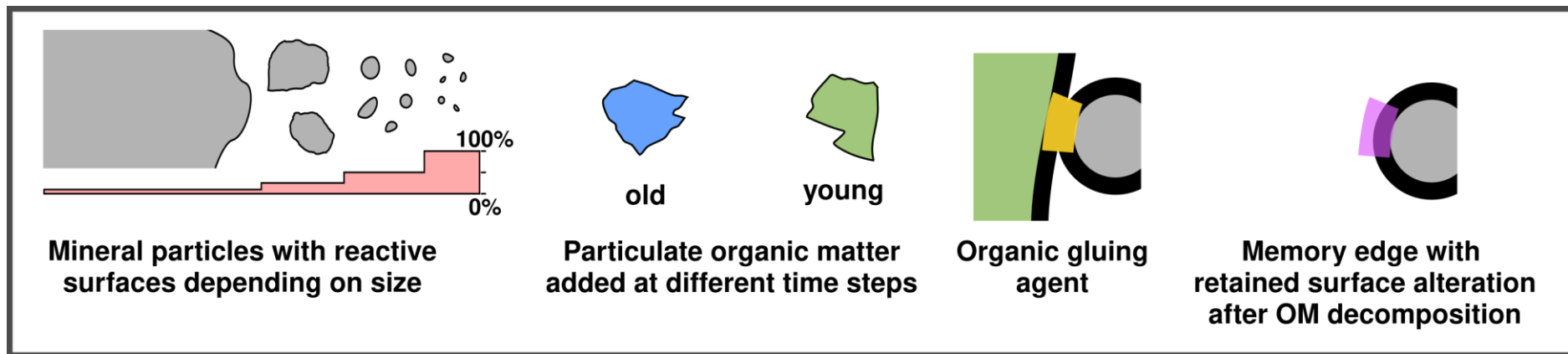


Figure: Schematic overview of model components, processes and resulting observations.

Drivers: POM input POM decomposition rate Soil texture Surface sites with different reactivity

Processes and Mechanisms

Realized in a Cellular Automaton Setting



RHIZOSPHERE
SPATIOTEMPORAL
ORGANISATION
SPP 2089



- Size-dependent movement of water-stable particles (Brownian motion, Stokes-Einstein relation)
- Attraction by electric forces
- Attraction of reactive surface contacts (organo-mineral etc..)
- Biomass growth (Michaelis-Menten Kinetics with organic carbon and oxygen, nitrogen...)
- Evolution of gluing agents
- Bio-perturbation, tillage, drying-wetting: random brake-up
- Cellular Root growth
- Root Exudation and spreading

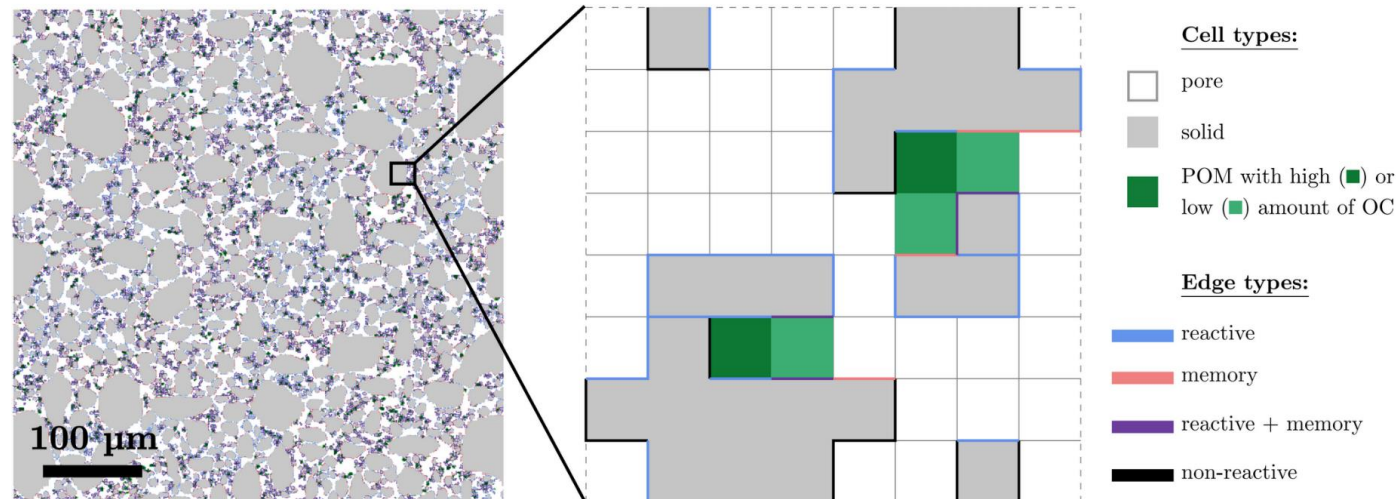
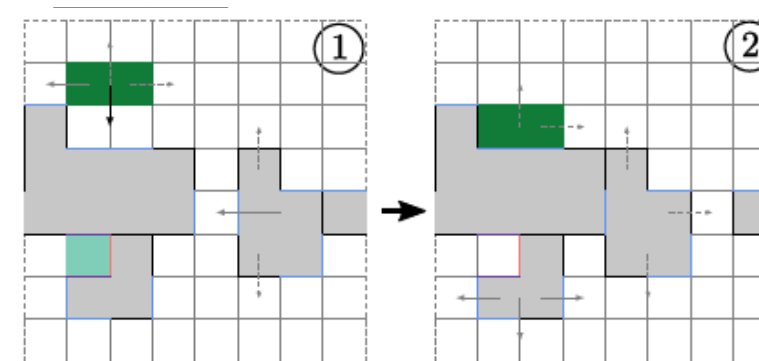


Figure 1: Schematic representation (*right*) of the computational domain (*left*) with pixels of type solid (■), pore (□) or POM with different amounts of OC (high (■) or low (■)) and edges of type reactive (—), non-reactive (—), memory (—) or both reactive and memory (—).



Disentangling the interplay of soil organic carbon storage and structure dynamics

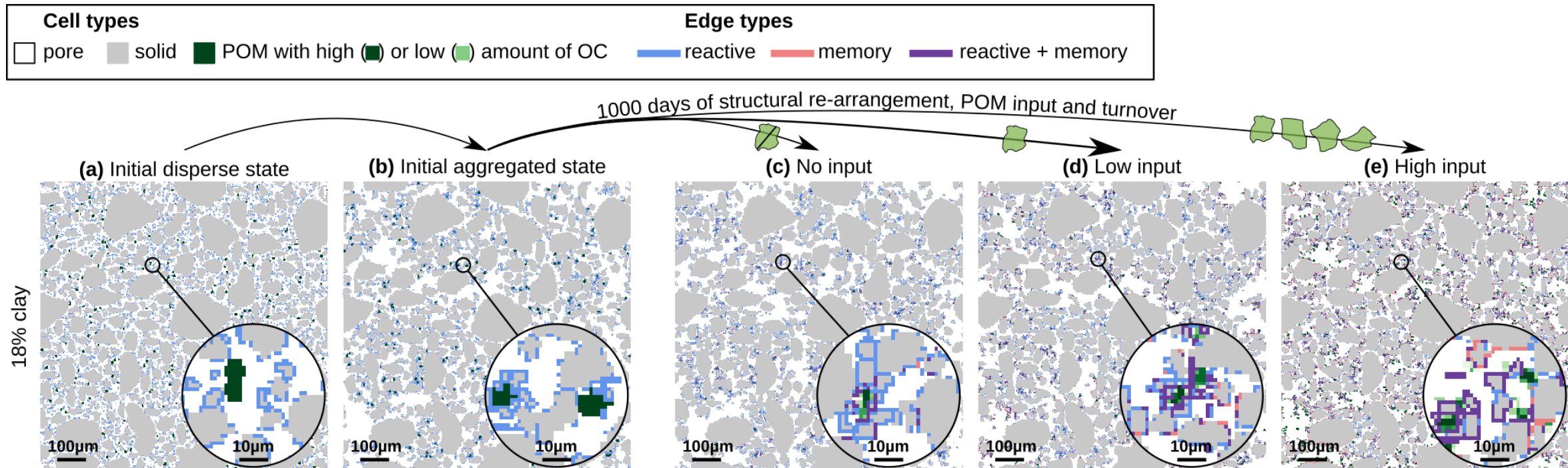


Figure: Conceptual overview over modelled scenarios and exemplary states (i.e. one repetition each) for different steps of the model, soil texture with 18% clay content and varying input scenarios: Random initial disperse state with shapes from dynamic image analysis (a), aggregated initial state after application of CAM (b), final state after no input (c), low input (d) and high input (e) scenario.

Zech et al. (2022), *Global Change Biology*.

Results

POM dynamics

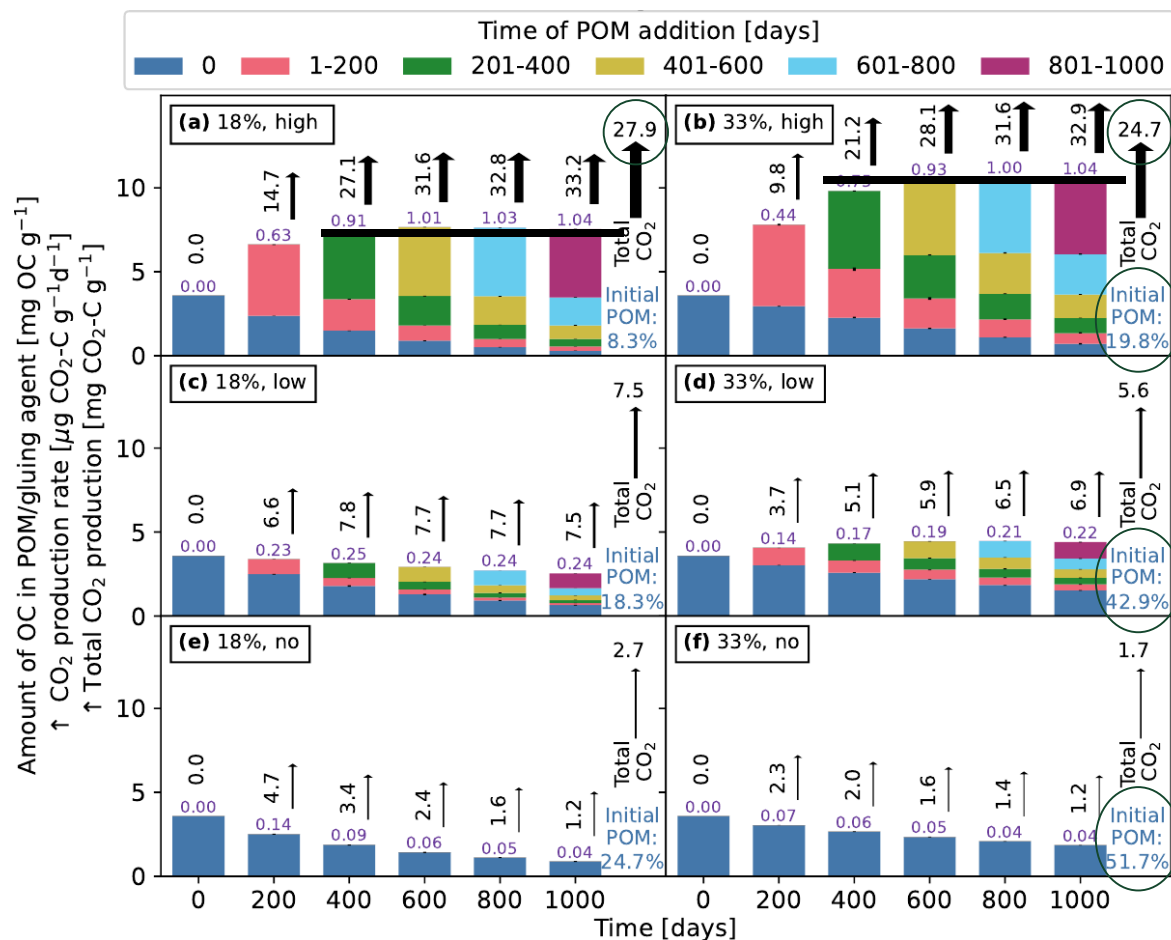


Figure: Amount of OC in different fractions of POM by age and gluings agent, CO₂ production rate, total CO₂ production and remaining share of initial POM in different input scenarios and for both soil textures and different input scenarios with low decomposition rate.

- Stationary states for POM concentrations through balance of POM input and degradation, even in high input setting
- **Effect of soil structure:** Higher clay content leads to higher POM content and lower total CO₂
- **Effect of structural re-arrangement:** Increased POM input leads to higher decomposition of initial, occluded POM => **structural priming effect**

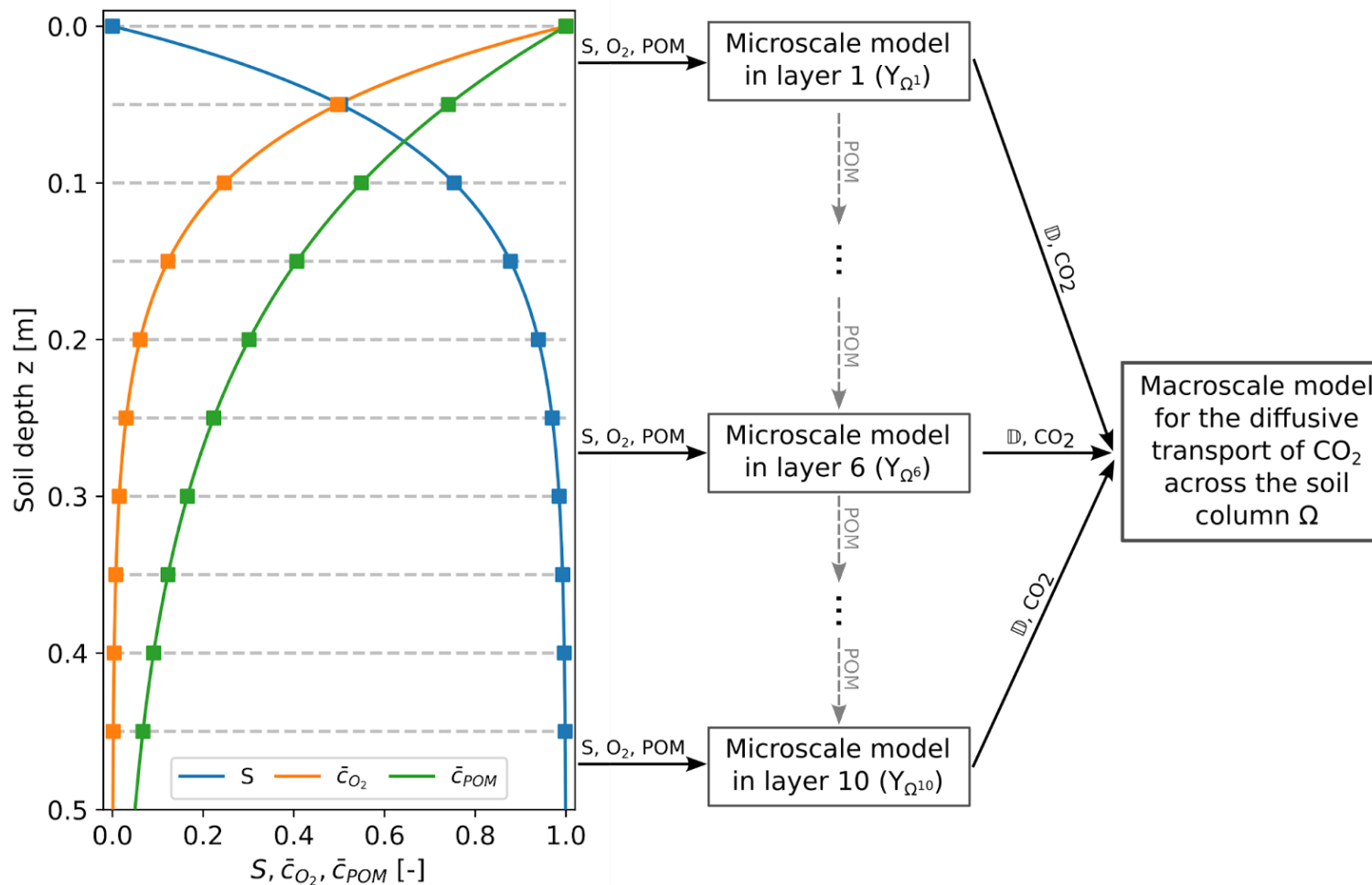
Zech et al. (2022), Global Change Biology.

Coupling the scales

Combine micro- and macroscales problems



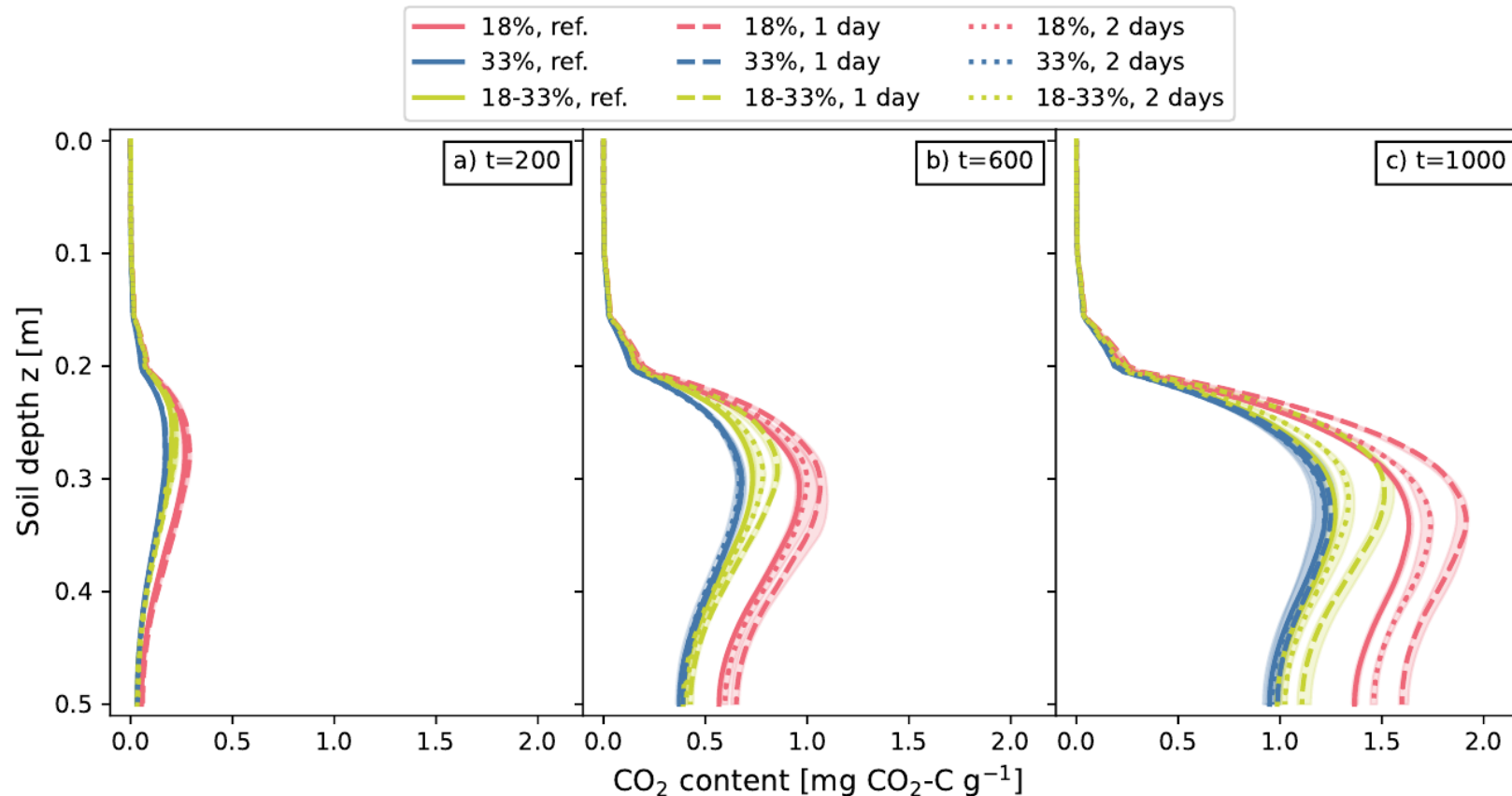
RHIZOSPHERE
SPATIOTEMPORAL
ORGANISATION
SPP 2089



- CO_2 transport across soil profile (macroscale) is informed by a pore-scale (microscale) model for C turnover
- The macroscopic environmental conditions water **saturation**, **POM** content, and **oxygen** concentration influence the microscale problem

Zech et al. (2024), J. Plant Nutr. Soil Sci.

Coupling scales in process-based soil organic carbon modeling including dynamic aggregation



Macroscopic profile of remaining CO₂ content after 200 (a), 600 (b) and 1000 (c) days. Median of 10 repetitions with error band representing lower and upper quartile.

Zech et al. (2024), J. Plant Nutr. Soil Sci.

- The coupled simulations of macroscopic transport and pore scale carbon and aggregate turnover reveal **the complex, nonlinear interplay** of the underlying processes.
- Limitations by diffusive transport, oxygen availability, texture dependent occlusion and turnover of OM drive CO₂ production and carbon storage.

Image and process-based micro-macro models for carbon turnover allow the

- **Discrimination**
Study the detailed processes acting at the pore scale – and decide *then* if or when which lumped parameter (function)s are reasonable
- **Variation**
Ability to simulate and evaluate scenarios systematically
- **Access**
Visualisation, access to parameters and temporal evolutions not assessible in wet lab
- **Scaling**
Bridge the scales on the basis of large data sets and mathematical techniques
- **Reduction**
Investigate „What if...?“ *under the given configuration*

- Zech, Prechtel, Ray (2024). **Coupling scales in process-based soil organic carbon modeling including dynamic aggregation.** J Plant Nutr. Soil Sci. 187 (1), 130-142, <https://doi.org/10.1002/jpln.202300080>.
- Rötzer, Prechtel, Ray (2023). **Pore scale modeling of the mutual influence of roots and soil aggregation in the rhizosphere.** Front. Soil Sci. 3, 155889.
- Zech, Schweizer, Bucka, Ray, Kögel-Knabner, Prechtel (2022). **Explicit spatial modeling at the pore scale unravels the interplay of soil organic carbon storage and structure dynamics.** Glob. Change Biol. 28:4589–4604.
- Zech, Ritschel, Ray, Totsche, Prechtel (2022). **How water connectivity and substrate supply shape the turnover of organic matter—Insights from simulations at the scale of microaggregates.** Geoderma 405, 115394.
- Zech, Dultz, Guggenberger, Prechtel, Ray (2020). **Microaggregation of goethite and illite evaluated by mechanistic modeling.** Appl. Clay Sci. 198, 105845.
- Rupp, Guhra, Meier, Prechtel, Ritschel, Ray, Totsche (2019). **Application of a cellular automaton method to model the structure formation in soils under saturated conditions: A mechanistic approach.** Front. Environ. Sci. 7, 170.
- Rupp, Totsche, Prechtel, Ray (2018). **Discrete-continuum multiphase model for structure formation in soils including electrostatic effects.** Front. Environ. Sci. 6, 96.
- Ray, Rupp, Prechtel (2017). **Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media.** Adv. Water Resour. 107, 393-404.

Thank you for
your attention!



This research was kindly supported by DFG
“MAD Soil - Microaggregates: Formation and turnover of the structural building blocks of soils” (Research Unit 2179) and Priority Program 2089
“Rhizosphere spatiotemporal organisation - a key to rhizosphere functions”