Aggregation formation dynamics driven by 3D fluid flow in natural porous media

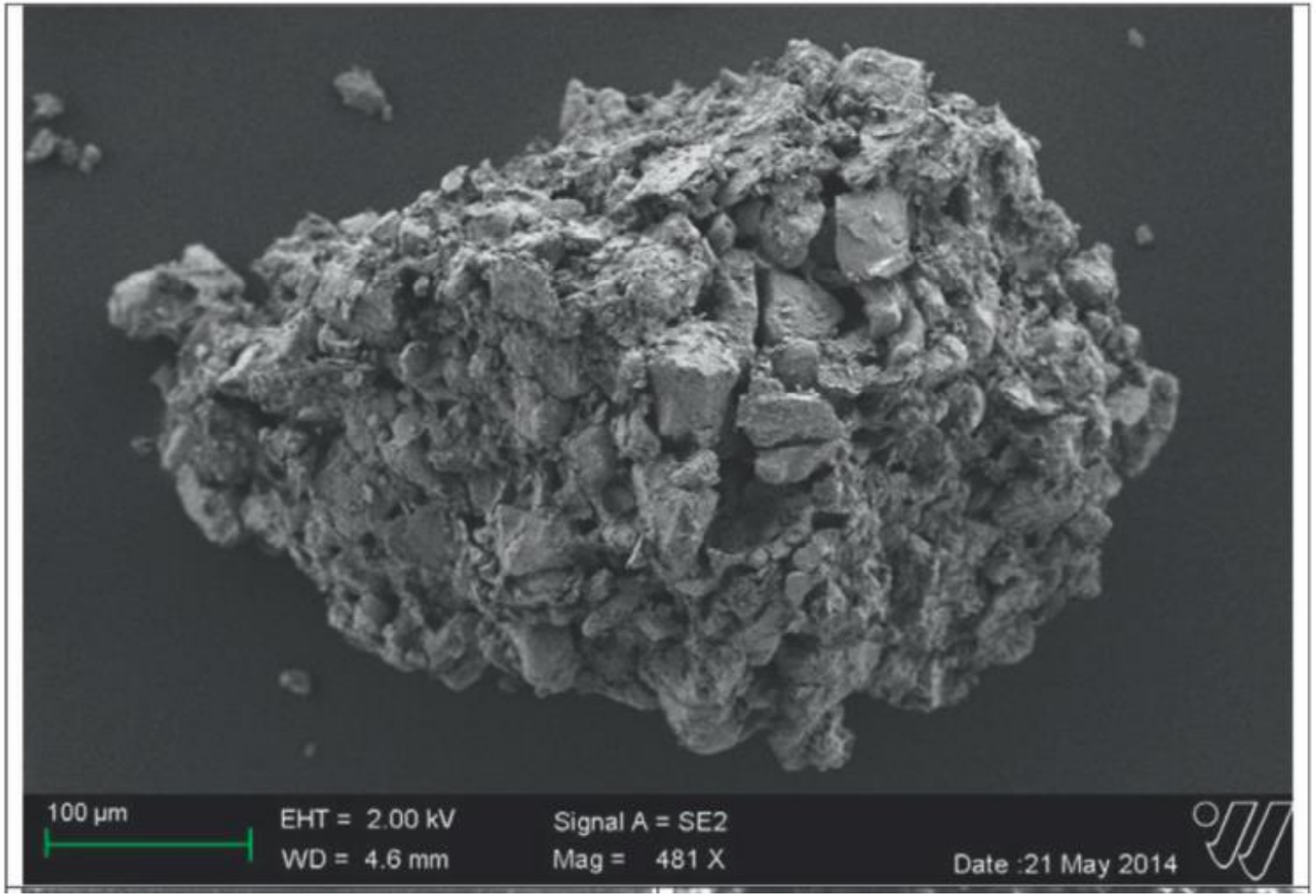
Thomas Ritschel and Kai U. Totsche
LS Hydrogeologie, FSU Jena

Micro**a**ggregate **d**evelopment in **Soil**

DFG Deutsche Forschungsgemeinschaft

EGU2020: Sharing Geoscience Online

Particle Movement and Attachment: Research question

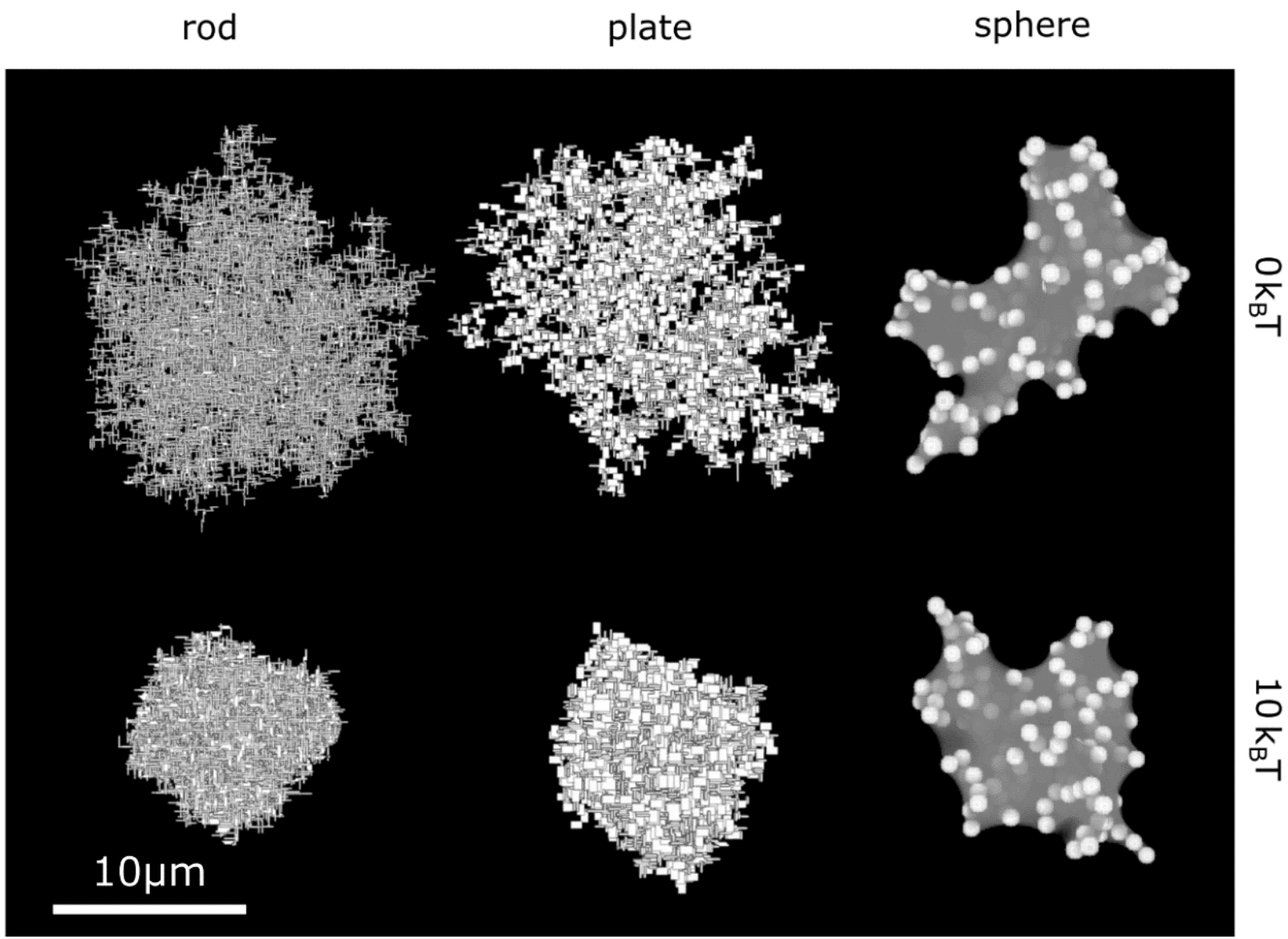


mineral-mineral interactions

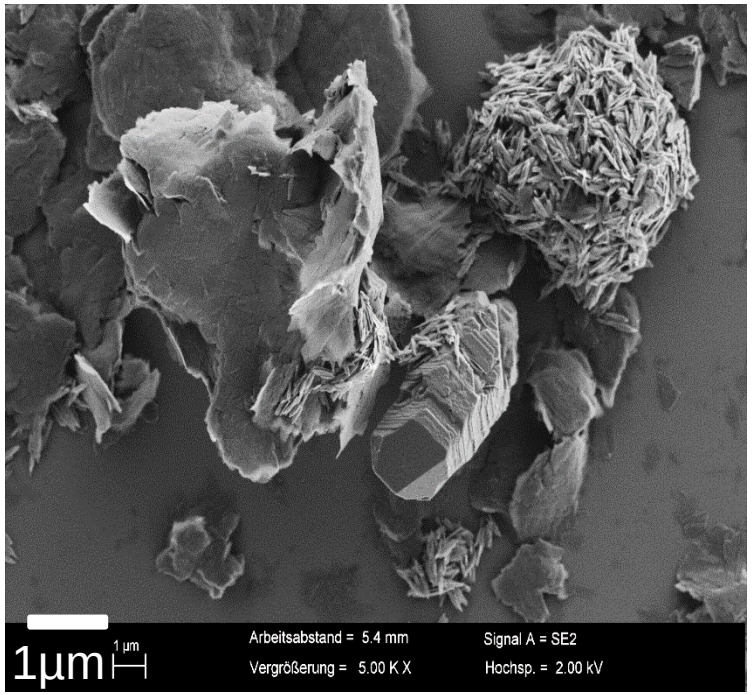
- release of colloids from surfaces
- coating of surfaces (collectors)
- aggregation of suspensions
- ...

Totsche et al. (2018)

Diffusion/Reaction-Limited Aggregation



Ritschel & Totsche (2019)



goethite needles attached into an aggregate visualized by scanning electron microscopy

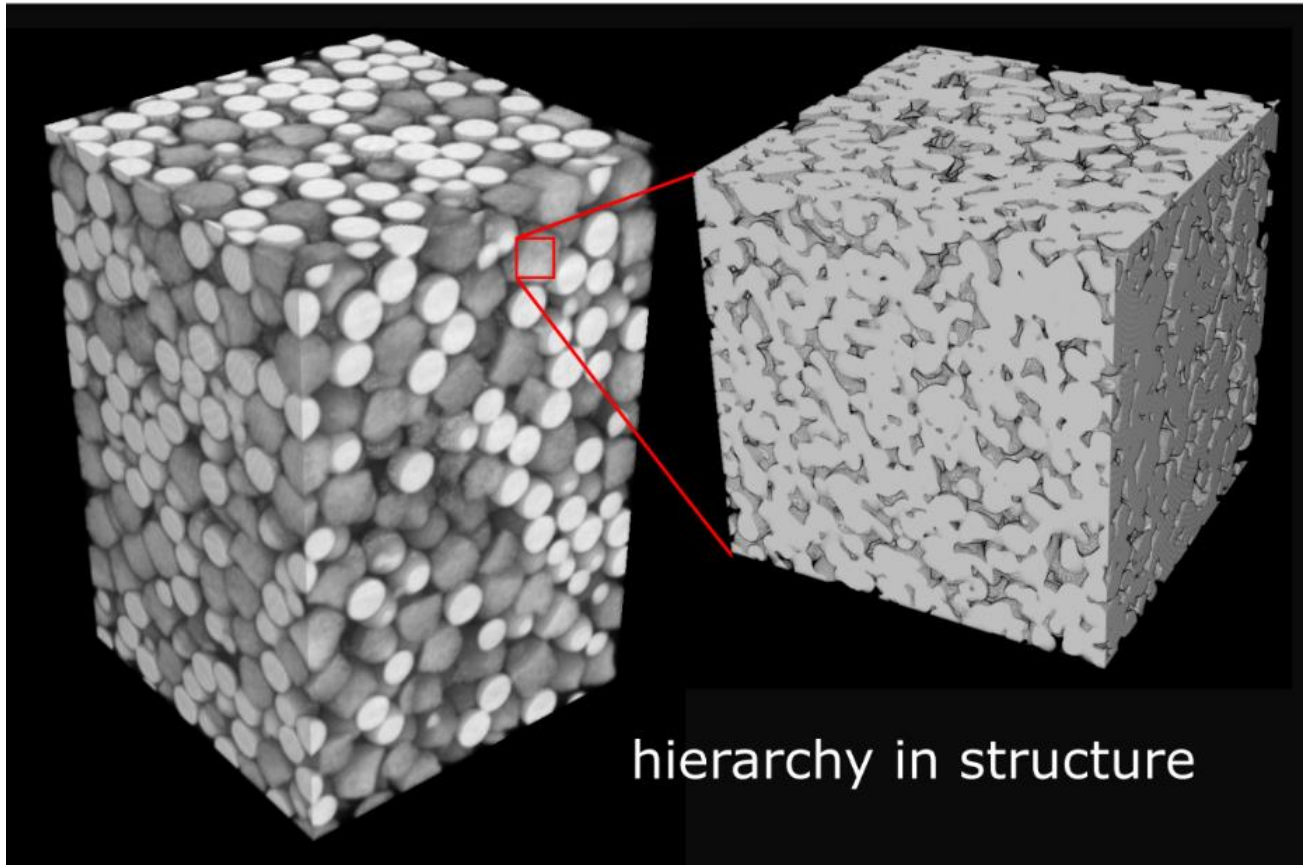
relation of DLA/RLA to observations

DLA/RLA scenario

- colloidal suspensions at rest without spatial constraints
- e.g. batch experiments, soil science in a vial

What about natural soil and rock?

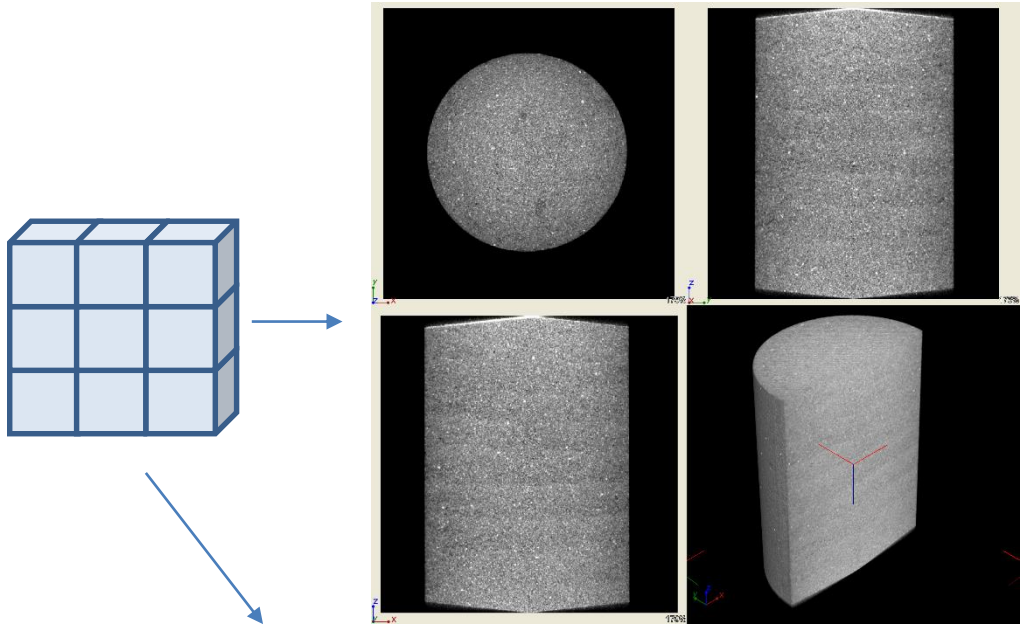
- **hierarchically structured network of pores (Ritschel et al., 2018)**
- **transient conditions**

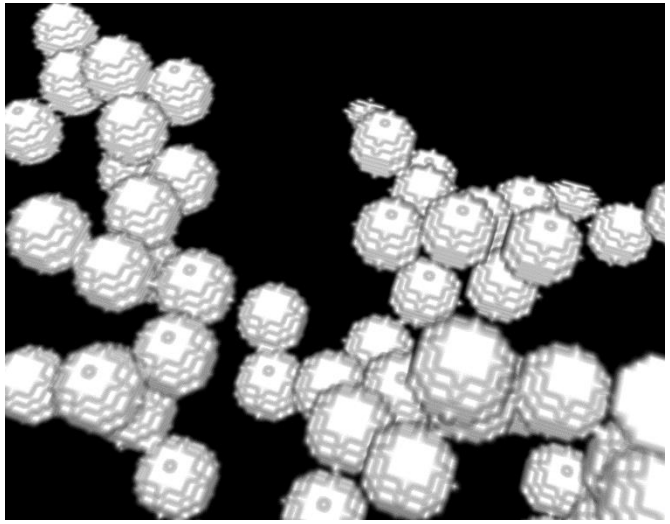


Modeling of 3D Fluid Flow

Lattice-Boltzmann Methods (vs. (Navier-)Stokes)

1. cubic lattice
   - directly translates to Xray-µCT voxel-based data (Ritschel et al., 2018)
   - compatible with our recent DLA/RLA models (Ritschel & Totsche, 2019)
2. local time-stepping
   - permits exploitation of parallel computing (GPU) for flow and movement of colloids

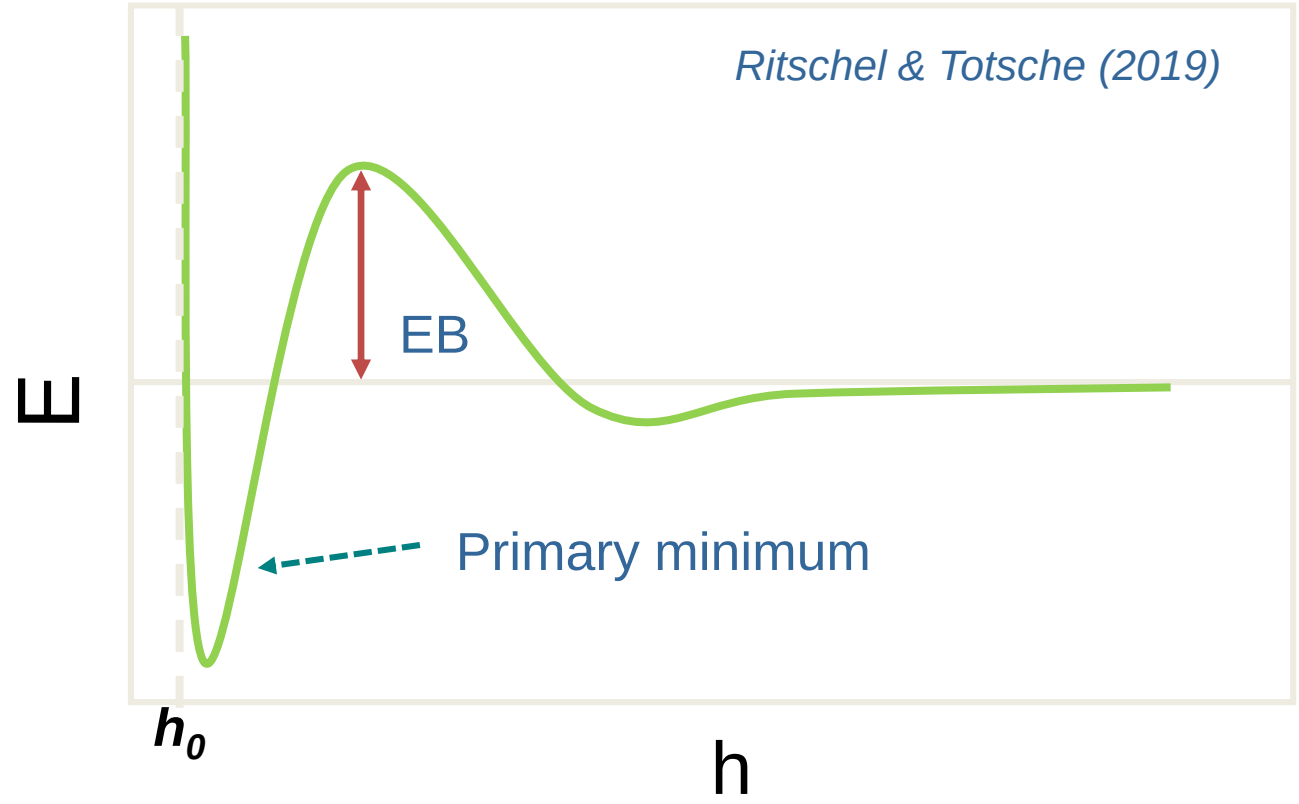




Lattice-Boltzmann Method + Aggregate Model

particle/colloid attachment

1. probabilistic attachment depending on energy barrier
2. interaction energy estimated from DLVO theory



$$P = \min\left(1, e^{-\frac{\Delta E}{k_B T}}\right)$$

energy barrier according to DLVO

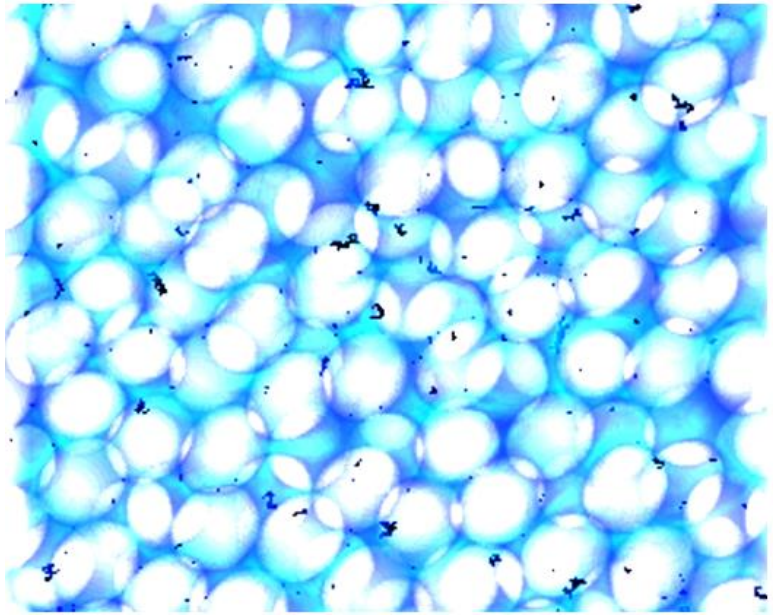
„attachment efficiency" probability of overcoming the energy barrier

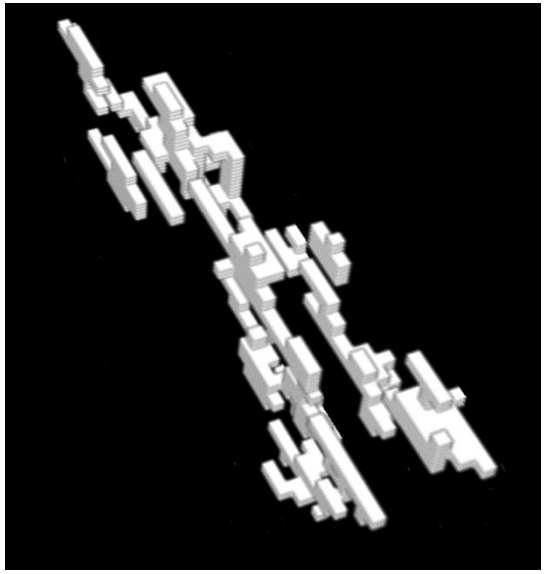
Some Highlights

Pore clogging after several passages of particles

aggregates shaped by environment
preferential flow invokes clogging

→ development of alternative flow paths





local pore size

Structures fundamentally different

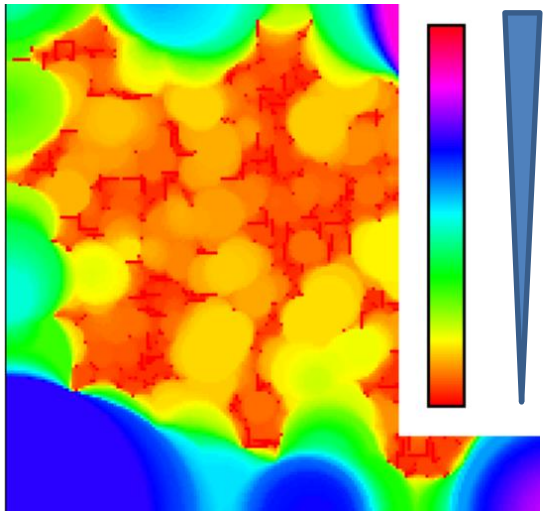
DLA/RLA clusters
fractal branches & low density

clusters in flow field
void filling due to flow possible
increased density

How to evaluate those structures quantitatively?

$$\psi_{\mathrm{m}} = \frac{2\gamma_{\mathrm{w}} \cos\theta}{\rho g r}$$

Ritschel & Totsche (2019)



Thank you very much for your attention

- **Ritschel, T., Totsche, K.U. (2019). Modeling the formation of soil microaggregates. Comput. Geosci. 127, 36-43.**
- Ritschel, T., Schlüter, S., Köhne, J.M., Vogel, H.-J., Totsche, K.U. (2018). Efficient prediction of multidomain flow and transport in hierarchically structured porous media. Water Resour. Res. 54 (11), 9033 - 9044.
- Totsche K.U., Amelung W., Gerzabek M.H., Guggenberger G., Klumpp E., Knief C., Lehndorff E., Mikutta R., Peth S., Prechtel A., Ray N., Kögel-Knabner I. (2018) Microaggregates in soils. Journal of Plant Nutrition and Soil Science *181*(1), 104-136.
- Guhra, T., Ritschel, T. Totsche, K.U. (2019). Formation of mineral – mineral and organo – mineral composite building units from microaggregate-forming materials including microbially produced extracellular polymeric substances Eur J Soil Sci. 70, 604 – 615.