

# Polycrystalline precipitation of calcite

First steps towards a dynamical description of geological vein sealing

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➔ **Talk:**

**Friday, April 19th 2013**

**13:30, R408, Haus A**

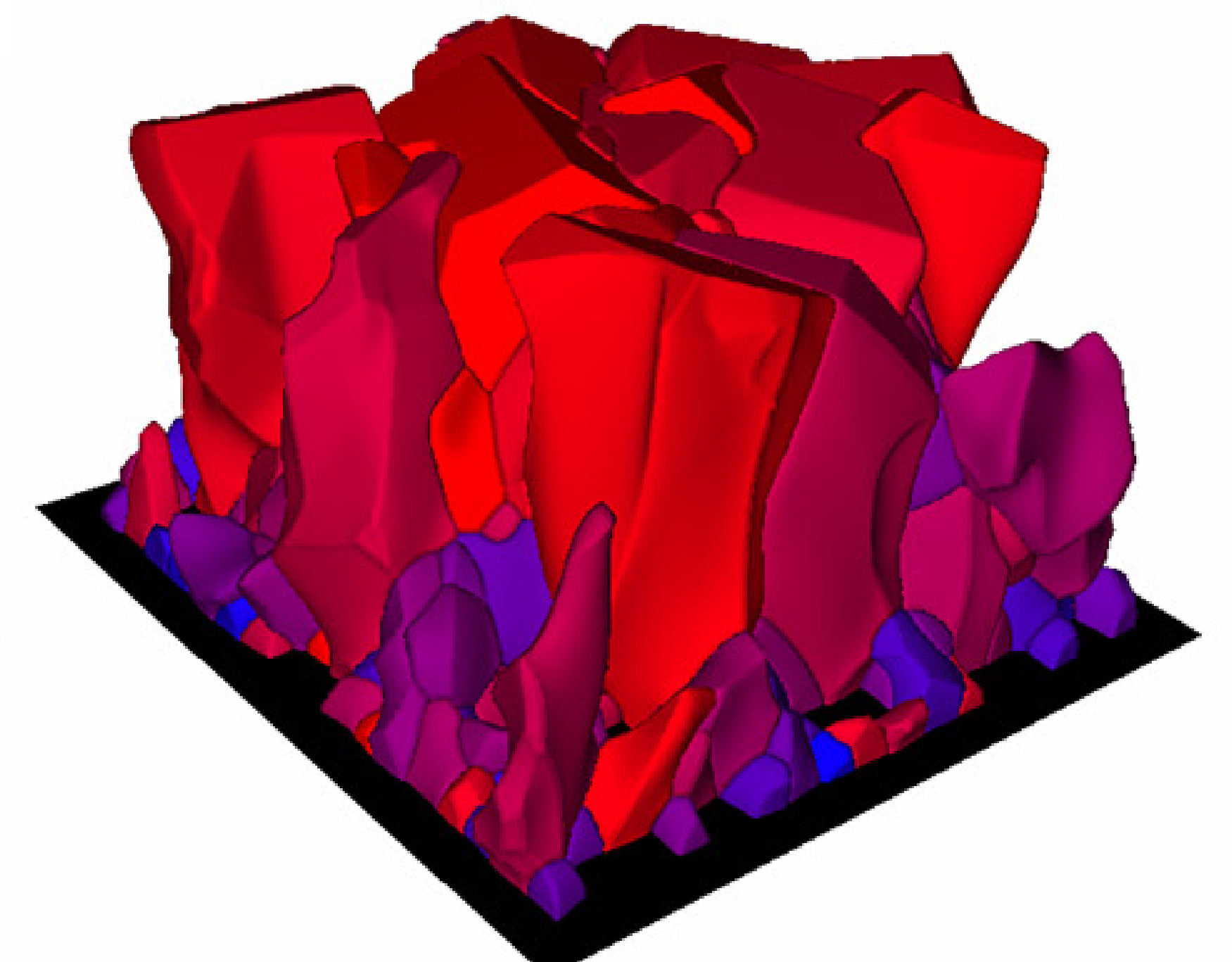
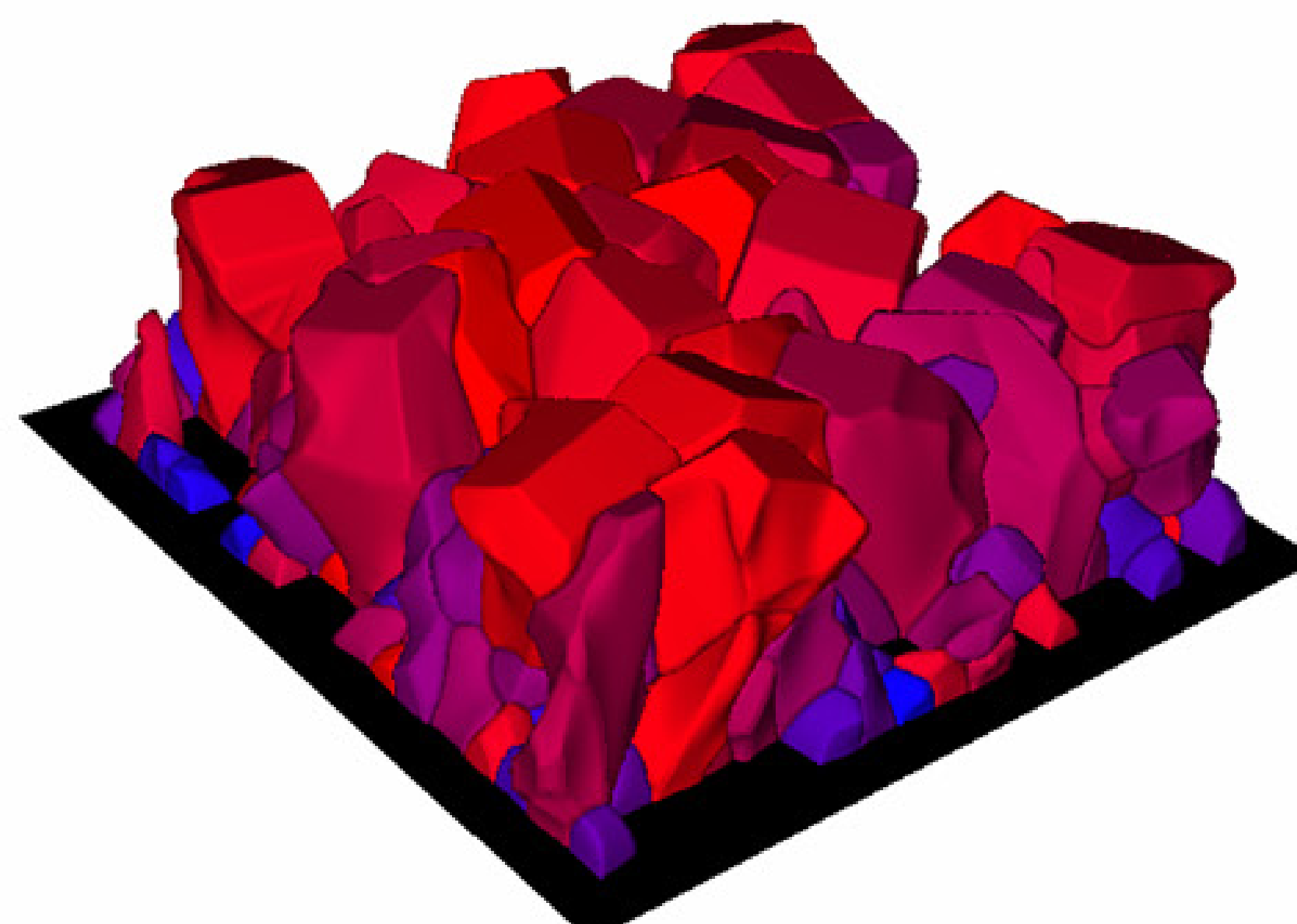
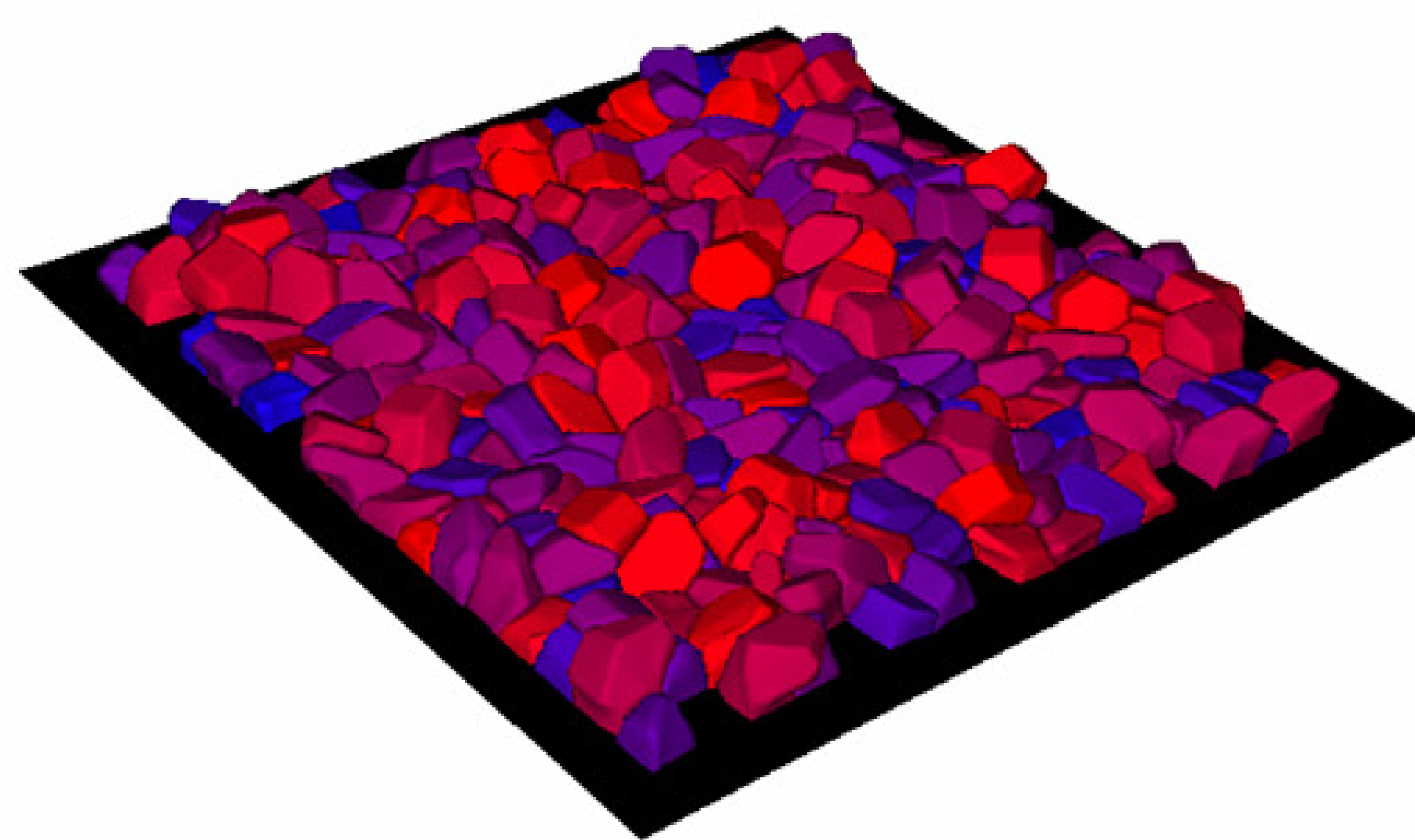
**Lochnerstraße 4-20**

FREE Participation for

- Master Students

- PhD Students

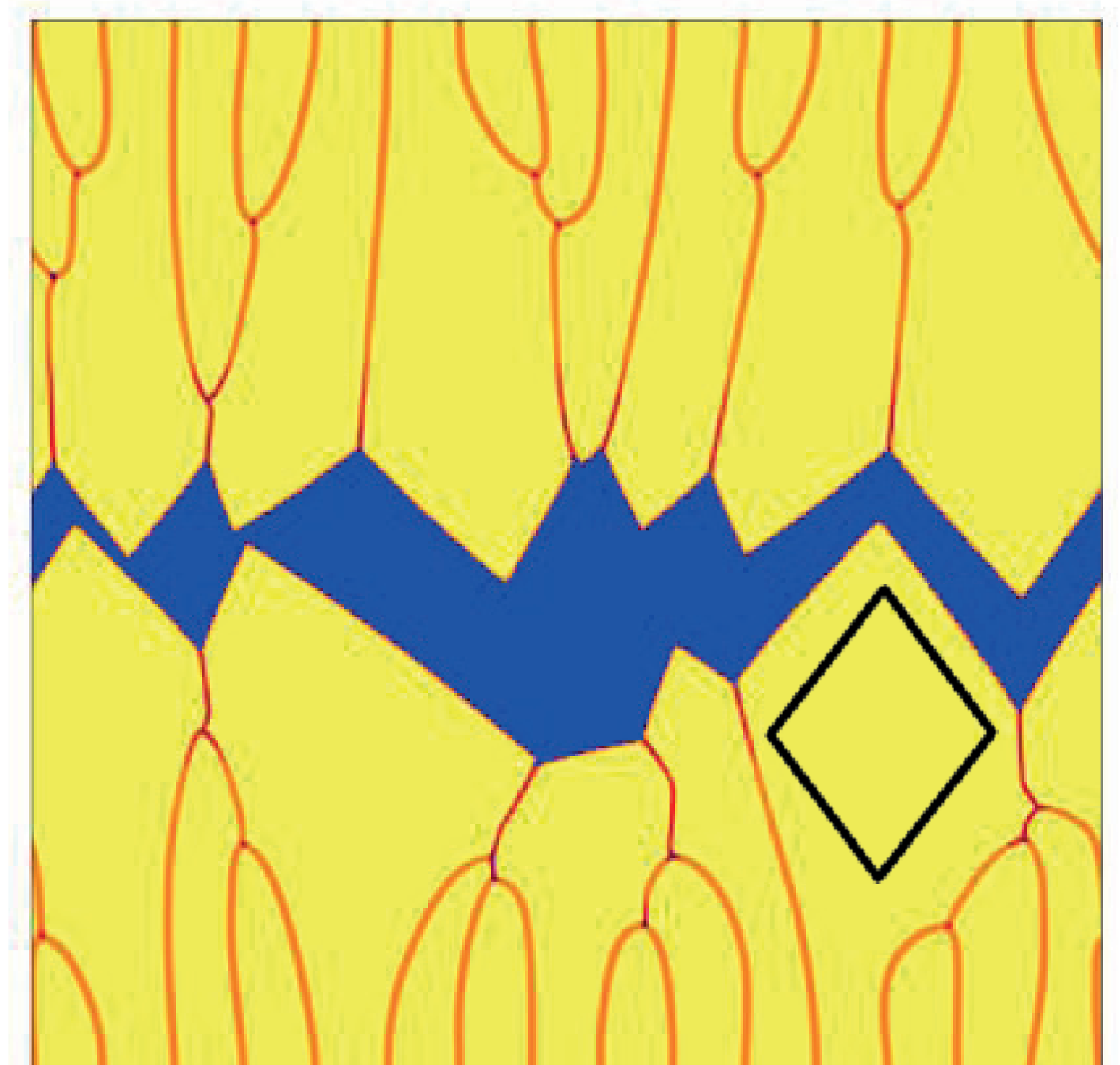
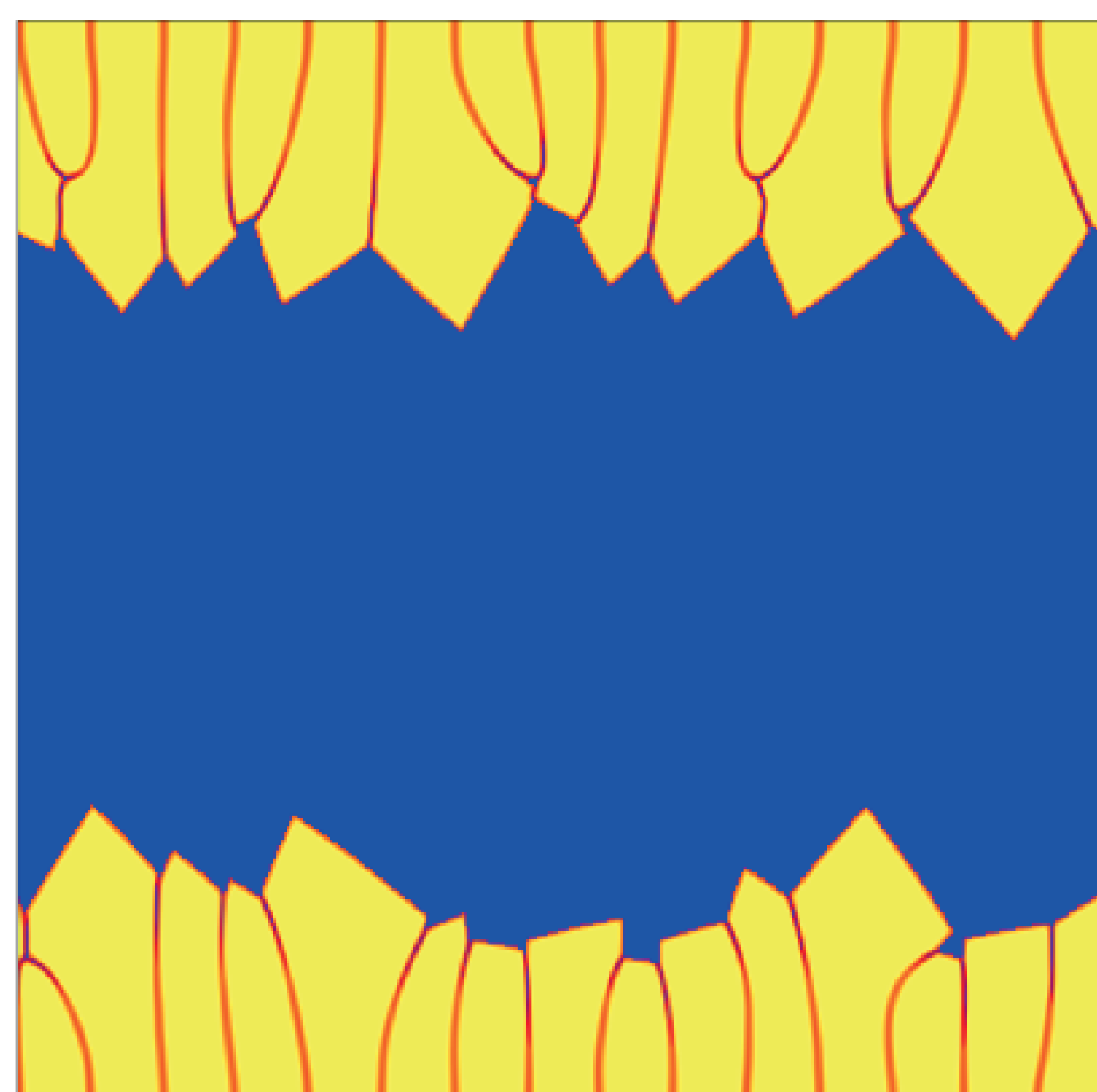
- Post docs



➔ To study changes of macroscopic hydraulic properties of open rock fractures with time and the resulting microstructures on the grain scale, a physical model capable of treating the precipitation kinetics of calcite is necessary. We adopt a multi phase-field model for this purpose, which offers the parametric flexibility to include all specific details as well as the computational efficiency to get simulation results in a reasonable amount of time [1,2]. It is based on the non-equilibrium thermodynamics of bulk phases and interfaces, and has been coupled to mass and heat diffusion and advective transport. First we introduce the geological problem and give a brief overview on the complex crystallization kinetics of calcite, which shows a multitude of shape variations and forms solid solutions with various elements like Mn and Mg. Then the attempt of a short introduction into the spirit of the model is undertaken, illustrated by former results including zeolite growth and freezing of water. For calcite competitive growth, first simulation results in 2D and 3D using a strongly simplified scenario are shown. Finally, the necessary steps to adapt the model to data from the examined geological vein systems studied in the project are discussed.

[1] F. Wendler, C. Mennerich, M. Jainta and B. Nestler, *J. Cryst. Growth* 327 (2011) 189 – 201.

[2] A. Choudhury and B. Nestler, *Phys. Rev. E* 85 (2012) 021602.



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