168<sup>th</sup> MSS Seminar Wednesday, July 5, 15:30 hrs, Room 00.156, Cauerstraße 3, Erlangen.



## Current challenges in particle scale modelling in geomechanics

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This presentation will introduce some current challenges in particle scale modelling from a geomechanical perspective. Recent developments on simulating both granular materials and clay will be introduced. The talk will firstly focus on coupled thermal-hydro-mechanical behaviour of granular materials. The potential to use thermal DEM to develop new experimental protocols and to advance understanding of material response to thermal cycles will firstly be outlined. Then challenges associated with developing effective frameworks for coupled fluid-particle simulations will be considered, focusing both on accuracy and computational efficiency. The second half of the presentation will introduce the challenges associated with simulating assemblies of clay particles. The focus will be on kaolinite. Key concepts that will be introduced include the need to simulate large system sizes, the importance of considering the non-monotonic nature of the force-separation relationship and the challenges associated with considering particles that have a heterogeneous surface charge distribution.



Image of fully resolved simulation of fluid flow in pore space (top) used to develop conductance models for pore network model (bottom)



Coarse grained molecular dynamics model of kaolinite (top) and SEM image of kaolinite (bottom, from Mineralogical Society of Great Britain and Ireland)