26th MSS-Seminar

Wednesday, Jan. 11th, 15:30, Nägelsbachstr. 49b

From micro-structure to macro-properties in granular/porous materials

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a statistical mechanical approach

Dr Rafi Blumenfeld
Earth Science and Engineering, Imperial College London, UK
& Cavendish Laboratory, Cambridge University, UK

This talk describes work in progress, aiming to derive systematically macro-scale physical properties from the grain-scale structure. The micro-scale structure of porous materials is the most significant factor impacting their macro-scale transport and mechanical properties. I describe our first steps towards implementing a systematic method and testing it on numerically produced systems. The method consists of the following steps.

(i) Description of the local structure quantitatively by a tensor, with locality achieved by tessellating the space into specialized volume elements, called quadrons.

(ii) Feeding the mathematical description into a statistical mechanical formalism and deriving meso-scale structural properties as expectation values over a certain partition function.

(iii) Derivation of meso-scale distributions from relations between structural and physical properties, such as permeability and heat transfer.

(iv) Upscaling of the physical properties, either via equivalent network analysis or by effective medium modelling, depending on the required length-scale.

Initial tests of aspects of the method on numerically generated two-dimensional and three-dimensional structures are presented.