

## Structure-induced mesoscopic approach to complex media

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The lack of universal connections between the different levels of description is the main obstacle for an efficient application of present computational methods to complex physical systems [1,2]. In any system, among all the possible levels of description, the micro- and macrolevel are particularly important due to their extremes of the structural hierarchy. When the length-scale cannot be accessed by either continuum methods because it is too small for averaging, or the atomistic methods because it is too large for simulations, these two approaches become inadequate. At meso-scales, continuum modelling paradigms start to break down, and atomistic methods begin to reach their inherent time and length-scale limitations. From this reason mesoscopic simulation methods are being currently developed to bridge this critical gap in between the extremes of length scales.

Even though some aspects of the time and length scale problems have been overcome, there remains the challenging problem of structural complexity at meso-scales [2]. Without knowing energy distribution values of local (sub-)microstructure configurations of the material system of interest, it is very difficult to prepare their initial configurations which are most relevant to the real system. This problem of configuration multiplicity is closely related to a problem of the intrinsic time scale of non-equilibrium microstructure evolution mechanisms. Both of these problems seriously influence the reliability of mesoscopic simulations.

The structure-induced manifold approach based on the higher-order contact geometry [3] is presented to deal with the two-level description of non-equilibrium transport processes in complex media such as complex fluids, porous or granular materials. If the time scale of the fast degrees of freedom is negligible in comparison with the time scale of the remaining variables of the system, the two-level description reduces to the mesoscopic one. Transport carriers are described by space-time distributions within a combined thermodynamic and microstructure-dependent kinetic approach. Knowledge of these distributions enables us to evaluate thermodynamical quantities, and define fundamental transport equations. A comparison with other models, and numerical examples are presented.

### References

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