

# OVERCOMING THE SPACE AND TIME SCALE CHALLENGES IN ATOMISTIC SIMULATIONS: NUMERICAL METHODS AND APPLICATIONS TRACK NUMBER 1100

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## ABSTRACT

The role of atomistic simulations in mechanics and material sciences is constantly growing, with applications to many processes: defect motions, propagation of fractures, dislocations, epitaxy, mechanics of nanomaterials, etc... The objective of this minisymposium is to gather scientists both interested in methodological aspects related to some applications and in the theoretical development of efficient numerical methods.

The simulation of materials at the atomistic scale raises two major difficulties, namely bridging space scales and time scales between the microscopic description, and the macroscopic phenomena of interest. To obtain meaningful results, one needs to consider systems with a huge number of atoms, integrated over very long times. Naive simulations are thus useless in many cases, and many numerical techniques have been proposed to deal with these difficulties. We will focus in particular on coarse-graining techniques which consist in replacing a dynamics on the positions of the atoms by a jump Markov model between states (kinetic Monte Carlo models or Markov state models), and numerical methods to accelerate dynamics (such as accelerated dynamics algorithms *à la* A.F. Voter).

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