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Sequential scale-up scheme to describe graphene-flow-interaction: from atomistic to sub-continuum

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Summary

No proper simulation method exists in between the molecular simulation method at nanometer scale using the first principles or empirical inter-molecular interaction and the continuum simulation method at micrometer-plus scale. The nanotechnology deals principally with those systems whose characteristic scales reside in such a scale-gap. Considering this, we develop a sequential scale-up scheme starting from the atomistic up to micrometer-plus scales. In the present paper we take, as an example, the system of graphenes that may or may not be fluttering in airflow, and apply to it our sequential scale-up scheme to see its capability.

The graphene is unique in that it has both nanometer (i.e., the single atomic layer depth) and micrometer-plus (i.e., the width) scales. Therefore, present application of our scale-up scheme to the graphenes in airflow may be one of the most critical tests to check its capability. Our scheme consists of the following three steps: Firstly we perform the molecular dynamics simulation in a realistic setting to find the inelastic reflection of the fluid atoms from the graphene [1]. Secondary the graphenes are coarse-grained to the collection of interacting virtual-particles using the recursive coarse-grained particles method [2]. Thirdly the coarse-grained graphenes are placed in the airflow described with the lattice Boltzmann method, in which the fluid-solid interaction is modeled by the immersed boundary method with the inelastic reflection coefficient [3-5]. Details of the simulation results will be presented.

Keywords: molecular dynamics, coarse graining, lattice Boltzmann, graphene, inelastic reflection

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