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Consistent Hybrid Simulation of MD and CFD SHUGO YASUDA, RYOICHI YAMAMOTO, Department of Chemical Engineering, Kyoto University; CREST, Japan Science and Technology Agency — The idea of multi-scale hybrid simulation is expected to be very useful for overcoming several difficult problems remain unsolved in frontiers of computational science in general. A striking example is the case of hydrodynamics of complex fluids or soft matters, for most of which no reliable constitutive relation is known explicitly. Our strategy to overcome this problem is very straightforward. We are developing a multi-scale hybrid method which combines computational fluid dynamics (CFD) as a fluid solver and molecular dynamics (MD) as a direct generator of constitutive relations in a consistent way. The numerical algorithm is rather simple. We perform usual lattice-mesh based simulations for CFD level, but each lattice is associated with a small MD cell which generates a "local stress" according to a "local flow field" given from CFD instead of using any constitutive functions at CFD level. Some algorithms to smooth out noses arising from MD simulations in a consistent way are being developed. Comparisons of the numerical results obtained by our hybrid-simulations and those by normal CFDs with a Newtonian constitutive relation are made in order to show the validity of our hybrid simulation method.

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