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Concurrent triple-scale simulation of molecular liquids MATEJ PRAPROTNIK, Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany & National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia, KURT KREMER, Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, RAFAEL DELGADO-BUSCALIONI, Depto. Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Campus de Cantoblanco, Madrid, Spain — We present a triple-scale simulation of a molecular liquid, in which the atomistic, coarse-grained and continuum descriptions of the liquid are concurrently coupled. The presented approach successfully sorts out the problem of large molecules insertion in the hybrid particle-continuum simulations and thus opens up the possibility to perform efficient grand-canonical molecular dynamics simulations of open molecular liquid systems.

Matej Praprotnik
Max Planck Inst. for Polymer Research, Ackermannweg 10, Mainz, Germany &
National Inst. of Chemistry, Hajdrihova 19, Ljubljana, Slovenia

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