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DPD with effective pair potential from integral equation theory of molecular liquids ALEXANDER KOBRYN, DRAGAN NIKOLIĆ, OLGA LYUBIMOVA, SERGEY GUSAROV, ANDRIY KOVALENKO¹, National Institute for Nanotechnology, National Research Council of Canada, 11421 Saskatchewan Drive, Edmonton, Alberta T6G2M9, Canada — A coarsening method of soft matter systems in solution is presented, in which the coarse grained (CG) force field is determined based on the statistical mechanical, integral equation theory of molecular liquids in interaction site representation, also known as reference interaction site model (RISM). Coarse graining is accomplished by a structure-matching procedure for solute CG beads without solvent that reproduces the corresponding distribution of all-atom solute in solvent obtained from RISM. Termed as an effective pair potential, the introduced potential of interaction between CG beads includes the effect of solvent and is used in dissipative particle dynamics (DPD) instead of the conservative force potential defined heuristically. It enables high flexibility in specifying the composition of solute CG beads and allows excluding solvent from explicit consideration in DPD. The suggested CG molecular model has been tested computationally and is shown to be a useful tool in investigating both structural and dynamic properties of polymer solutions and a promising platform for studies of macromolecular, supramolecular, and biomolecular systems in solution that require thermodynamic consistency, high accuracy, and computational efficiency.

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