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Computing solvent-induced forces in the solvation approach called Semi Explicit Assembly EMILIANO BRINI, Laufer Center for Physical and Quantitative Biology, 5252 Stony Brook University, Stony Brook, NY 11794-0001, USA, MICHELLE H. HUMMEL, Department of Mathematics and Statistics, University of New Mexico, Albuquerque, New Mexico 87131, USA, EVANGELOS A. COUTSIAS, Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY 11794-3600, USA, CHRISTOPHER J. FENNELL, Department of Chemistry, Oklahoma State University, Stillwater, OK 74078, USA, KEN A. DILL, Laufer Center for Physical and Quantitative Biology, 5252 Stony Brook University, Stony Brook, NY 11794-0001, USA — Many biologically relevant processes (e.g. protein folding) are often too big and slow to be simulated by computer methods that model atomically detailed water. Faster physical models of water are needed. We have developed an approach called *Semi Explicit Assembly* (SEA) [C.J. Fennell, C.W. Kehoe, K.A. Dill, PNAS, 108, 3234 (2011)]. It is physical because it uses pre-simulations of explicit-solvent models, and it is fast because at runtime, we just combine the pre-simulated results in rapid computations. SEA has also now been proven physically accurate in two blind tests called SAMPL. Here, we describe the computation of solvation forces in SEA, so that this solvation procedure can be incorporated into standard molecular dynamics codes. We describe experimental tests.

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