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Equilibrium configurations of self-assembling polymers: An extended parallel tempering approach CHAKRAVARTHY AYYAGARI, DMITRY BEDROV, GRANT SMITH, University of Utah — We present a novel algorithm based on tempering a fraction of relaxation limiting interactions to accelerate the process of obtaining uncorrelated equilibrium configurations. A chain of canonically independent replicas with overlapping distributions in energy space can be simulated in parallel and occasionally attempt to exchange the configurations between adjacent replicas. Each replica is simulated in the same ensemble (canonical) but has a different tempering fraction and corresponding relaxation time associated with it. We implemented this algorithm to enhance the equilibration process in self-assembling polymers by tempering the interactions responsible for self-association. Depending on the strength of the relaxation limiting interactions, the efficiency of the algorithm is orders of magnitude higher than that of conventional canonical simulation.

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