Time versus temperature rescaling for coarse grain molecular dynamics simulations

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Résumé en anglais	Coarse graining procedures are intended to well reproduce the structure of a material while increasing the simulations efficiency. However, the dynamics usually accelerates with coarse graining and a scaling procedure has to be used for dynamical data calculations. Most often a simple time-scaling coefficient is used for this purpose. However, for low temperature liquids this simple scaling procedure is questionable. Because supercooled liquids in their approach to the glass transition temperature do not follow a simple dynamics. In order to test if this scaling procedure is still pertinent at low temperature, we use molecular dynamics simulations of a coarse grain model of the methylmethacrylate molecule compared to simulations with the All atom model. We compare two different rescaling procedures, a time rescale and a temperature rescale procedure. Using these two procedures we compare the behaviors of the mean square displacements, the incoherent scattering functions, the self and distinct part of the Van Hove correlation functions and the non-Gaussian parameters. Results show that the temperature rescaling procedure reproduces well the All atom dynamical data at low temperatures, while the time rescaling procedure is correct only in the Brownian regime. We also find that the melting and the glass-transition temperatures are relatively well reproduced with the temperature rescaling procedure.
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