Mathematical Analysis of a Modified Langevin Dynamics

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Mots-clés : Langevin dynamics, Molecular dynamics, Variance, Perturbation theory, Talay-Tubaro expansions

Adaptively Restrained Particles Simulations (ARPS) were recently proposed in [**?**] with the purpose of speeding up molecular simulations. The main idea is to modify the Hamiltonian such that the kinetic energy is set to zero for small velocities, which allows to save computational time since particles do not move and forces need not be updated. ARPS can be combined with Langevin dynamics in order to speed up the computation of macroscopic quantities.

The aim of this work is to understand how simulation errors depend on the parameters of the method. We distinguish the statistical error and the systematic error related to the finiteness of the time step Δt. The statistical error is controlled by variance, that is given by

$$\sigma^2 = -2 \left\langle A - \mu(A), \mathcal{L}^{-1} \left(A - \mu(A) \right) \right\rangle_{L^2(\mu)} \tag{1}$$

where μ is the invariant measure, $\mathcal{L}$ is the generator of the stochastic process and A an observable. First we demonstrate by use of weighted L^∞ estimations that the ARPS-Langevin dynamics are well defined. In the main part of this work, we quantify the increase of variance of the ARPS-Langevin process as a function of the ARPS parameters. For small parameters, we express the generator of the ARPS-Langevin dynamics as a perturbed generator of the Langevin dynamics, and study the asymptotic expansions of the variance (**??**) in the restrained dynamics parameter ε.

$$\sigma_\varepsilon^2 = \sigma^2 + \mathcal{O}(\varepsilon)$$

For large values of ε, we perform numerical simulations. For a simple 1D system we approximate $\mathcal{L}^{-1}$ by Galerkin approach and for higher-dimensional systems we discretize the stochastic differential equations by the symplectic Euler method and analyze a model of a dimer surrounded by solvent particles.

Finally, we analyze the systematic error via Talay-Tubaro expansions. We make explicit the dependence of the leading-order error term on the ARPS parameters.

Références

[1] Artemova, S., Redon, S., *Adaptively restrained particle simulations*, Physical review letters, 109(19), 190201, (2012).

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