Simulating wet active polymers by multiparticle collision dynamics

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The conformational and dynamical properties of active Brownian polymers embedded in a fluid depend on the nature of the driving mechanism, e.g., self-propulsion or external actuation of the monomers. Implementations of self-propelled and actuated active Brownian polymers in a multiparticle collision (MPC) dynamics fluid are presented, which capture the distinct differences between the two driving mechanisms. The active force-free nature of self-propelled monomers requires adaptations of the MPC simulation scheme, with its streaming and collision steps, where the monomer self-propulsion velocity has to be omitted in the collision step. Comparison of MPC simulation results for active polymers in dilute solution with results of Brownian dynamics simulations accounting for hydrodynamics via the Rotne-Prager-Yamakawa tensor confirm the suitability of the implementation. The polymer conformational and dynamical properties are analyzed by the static and dynamic structure factor, and the scaling behavior of the latter with respect to the wave number and time dependence are discussed. The dynamic structure factor displays various activity-induced temporal regimes, depending on the considered wave number, which reflect the persistent diffusive motion of the whole polymer at small wave numbers, and the activity-enhanced internal dynamics at large wave numbers. The obtained simulation results are compared with theoretical predictions.

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I. INTRODUCTION

A wide class of active-matter agents exploits viscous drag with the surrounding fluid for propulsion [1–3]. Biological microswimmers, e.g., bacteria, algae, ciliates, and phytoplankton, are propelled by flagella or cilia, where the frictional anisotropic of the rotating or beating flagella or cilia provides directed motion [1,2,4]. Synthetic microswimmers have been designed, which mimic biological microswimmer propulsion mechanisms or are powered by phoretic processes, e.g., thermophoresis or diffusiophoresis [2–5]. Moreover, fluid-mediated interactions determine the collective behavior of microswimmers. An example is the motility-induced phase separation of dry active Brownian particles in two dimensions [6–9], which is suppressed by fluid-mediated interactions [10–12]. The provided examples underline the fundamental importance of hydrodynamic interactions by the embedding fluid for self-propelled objects and its elementary nature for locomotion, with far-reaching consequences for the structural and dynamical aspects of active matter assemblies.

A particular kind of active matter is filaments or polymer-like structures. As is well known, the dynamics of passive polymers in solution is determined by fluid-mediated interactions [13–15]. By now, various studies reveal the relevance of hydrodynamics [16,17] and hydrodynamic interactions on the dynamics of active polymers, with a major impact even on the polymer conformations [18–20].

So far, active polymers in dilute bulk solution have been considered mainly by employing the Rotne-Prager-Yamakawa (RPY) hydrodynamic tensor [21,22] to account for hydrodynamic interactions [18,19,23]. However, this approach poses severe challenges for polymers confined in complex geometries, where the hydrodynamic tensor needs to fulfill, e.g., no-slip boundary conditions on walls, and can often not be determined analytically. Here, other simulation approaches, which describe the fluid explicitly, are advantageous. An example is the multiparticle collision (MPC) dynamics method [24–26]. MPC is a coarse-grained, particle-based mesoscale simulation approach for fluids with inherent thermal fluctuations. It has been shown that MPC obeys the Navier-Stokes equations with an ideal gas equation of state [24,27], and that it correctly captures hydrodynamic correlations [28,29]. MPC has been utilized in a broad range of equilibrium, nonequilibrium, and active system simulations, in particular, in combination with a mechanoelastic elastic model of a microswimmer [30–32], as well as the more generic squirmer model [11,33–40]. The versatility of the MPC method facilitates a straightforward coupling with other simulation techniques, e.g., molecular dynamics simulations for embedded objects [11,26,36,41,42]. Moreover, the MPC algorithm is highly parallel, and is suitable for GPU implementation with a high performance gain [43].

In this article, we present an implementation of an active Brownian polymer in MPC, where a polymer is comprised of linearly linked monomers. Two types of active polymers are considered, with self-propelled monomers (S-ABPO), and with monomers, which experience an external active force (E-ABPO). In both cases, the pointlike monomers are considered as active particles, which are propelled by an active force in a direction, which changes diffusively. The two types of monomers differ in the coupling between the active force

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and the fluid. A self-propelled monomer is active-force free and torque free. Hence, no Stokeslet flow emerges directly by the active motion. In contrast, the external forces of E-ABPOs give rise to such a flow field. The implementation of E-ABPOs in MPC is straightforward and very similar to passive polymers exposed to an external gravitational or electric field [44–46]. Certain aspects for E-ABPOs have already been presented before [19,20]. However, in the case of S-ABPOs the equations of motion and their interaction with the MPC fluid have to be adjusted to properly account for their active-force-free character. In MPC, with its sequence of streaming and collision steps, the active contribution to the monomer velocity has to be omitted in the collision step, and only thermal contributions have to be included to prevent the generation of a Stokeslet by active forces.

The polymer conformational and dynamical properties are analyzed in terms of the static and dynamic structure factors for the two types of polymers for various activities and persistence lengths, which illustrates the impact of activity on the polymer conformations at different intramolecular lengthscales. Specifically, for small wave numbers, the time dependence of the dynamic structure factor is given by the center-of-mass mean-square displacement of the active polymer. The internal polymer dynamics is visible for large wave numbers and a stretched exponential decay of the dynamic structure factor is obtained, with an exponent close to 2, the value for the active ballistic motion, as predicted by the provided analytical approximations.

The flow field of self-propelled particles typically includes higher-order multipole contributions, e.g., force dipoles, source dipoles, etc. [40,47–53]. In combination with polymer conformational changes, the interference of such monomer flow fields leads to autonomous filament or polymer motion even when individual monomers are nonmotile [16,49,54]. In the current approach, we consider point particles and neglect the force field by active stresses, thus the monomers correspond to neutral swimmers [40]. Already the flow fields created by intramolecular (and external) forces yield complex flow patterns, from the level of single monomers to the full polymer, which lead to particular conformational and dynamical features, such as hydrodynamically induced shrinkage of S-ABPOs [18]. Yet, simulations of dumbbells comprised of squirmers reveal an influence of the squirmer active stress on the dumbbell motility [40]. Here, further studies on polymers are desirable to resolve the influence of swimmer-specific multipoles on the polymer properties.

The paper is organized as follows. Section II outlines the MPC approach. The active polymer model and its implementation in the MPC fluid are described in Sec. III for self-propelled as well as externally driven monomers. Section IV presents results for the conformational properties of the polymers, and Sec. V discusses their dynamical aspects, in particular, the dynamic structure factor. Finally, Sec. VI summarizes our findings and presents conclusions.

II. MULTIPARTICLE COLLISION DYNAMICS FLUID

The MPC fluid consists of N point particles of mass m with the positions $\boldsymbol{r}_i$ and velocities $\boldsymbol{v}_i$ $(i = 1, \ldots, N)$. Their dynamics proceeds in two steps: streaming and collision. During the streaming step, particles move ballistically over a time interval h, which is denoted as collision time, in absence of external forces and fields. Hence, the positions and velocities are updated as [25,26]

$$\boldsymbol{r}_i(t+h) = \boldsymbol{r}_i(t) + h\boldsymbol{v}_i(t), \tag{1}$$

$$\boldsymbol{v}_i(t+h) = \boldsymbol{v}_i(t). \tag{2}$$

The presence of external fields modifies the dynamics and the equations of motion may have to be solved by, e.g., the velocity Verlet algorithm [19,45,46]. In the collision step, the system is partitioned into a lattice of cubic cells of length a, which define the local interaction environment. Coupling and linear momentum exchange between the N_c particles of a collision cell is achieved by a rotation of the relative velocities $\Delta\boldsymbol{v}_i(t) = \boldsymbol{v}_i(t) - \boldsymbol{v}_{\mathrm{c.m.}}(t)$, with respect to the center-of-mass velocity $\boldsymbol{v}_{\mathrm{c.m.}}(t) = \sum_i \boldsymbol{v}_i(t)/N_c$ of the cell, around a randomly oriented axis by an angle α [26]. The orientation of the rotation axis is chosen randomly and independently for every cell and collision step. This yields the final velocities

$$\boldsymbol{v}_i(t+h) = \boldsymbol{v}_{\mathrm{c.m.}}(t+h) + \mathbf{R}(\alpha)\Delta\boldsymbol{v}_i(t+h), \tag{3}$$

with $\mathbf{R}(\alpha)$ the rotation matrix [55]. This scheme conserves momentum on the collision cell level. However, angular momentum is not conserved, which does not affect the polymer dynamics, because the monomers are treated as point particles and, hence, possess no rotational degrees of freedom. Angular momentum conserving algorithms are provided in Refs. [11,56,57]. A constant local temperature is maintained by a collision cell-based, Maxwellian thermostat, where the relative velocities of the particles in a collision cell are scaled according to the Maxwell-Boltzmann scaling method [55]. By the construction of the algorithm for S-ABPOs, the thermostat only affects the thermal velocities of the monomers and the MPC particles, and not the active velocity. In the case of E-ABPOs the relative velocities, including contributions by activity velocities, are scaled, as for any other external force. Discretization in collision cells implies violation of Galilean invariance, which is reestablished by a random shift of the collision-cell lattice after every streaming step [26,58].

III. ACTIVE BROWNIAN POLYMERS

A. Polymer model

We consider linear semiflexible polymers composed of N_m active pointlike monomers of mass M, positions $\boldsymbol{r}_k$, and velocities $\boldsymbol{v}_k$ $(k = 1, \ldots, N_m)$, which are connected by harmonic bonds with the potential U_l. Bending stiffness is taken into account by restrictions of bond orientations via the bending potential U_b, and excluded-volume interactions by a truncated purely repulsive Lennard-Jones potential, where [19]

$$U_l = \frac{\kappa_l}{2}\sum_{k=2}^{N_m}(|\boldsymbol{R}_k| - l)^2, \tag{4}$$

$$U_b = \frac{\tilde{\kappa}_b}{2}\sum_{k=2}^{N_m-1}(\boldsymbol{R}_{k+1} - \boldsymbol{R}_k)^2, \tag{5}$$