Activity-driven dynamics algorithm

Yann-Edwin Keta
(Dated: 31/01/2021, 19:45)

CONTENTS

I. INTRODUCTION

Ref. [1] introduces "activity-driven dynamics" (ADD) from the observation that, for any given set of self-propulsion vectors, the time for the particles to reach a force-balanced state does not grow with the persistence time τ_p of self-propulsion. Therefore, on the time scale of τ_p and in the limit $\tau_p \to \infty$, the particle configuation instantaneously adapts to changes of the self-propulsion – the time evolution of the system is driven only by changes in the active forces, hence the name "ADD".

This separation of time scale, between (1) the evolution of the self-propulsion and (2) the movement towards a corresponding force-balanced state, is exploited in ADD by computing (1) for each time step of $\mathcal{O}(\tau_p)$ and (2) accordingly over a τ_p-independent time. It is therefore possible to reach the large-τ_p limit with a dramatic reduction in computation time.

Ref. [2] describes an "intermittent" regime at intermediate persistence time and low active driving. Would this regime be the consequence of particles reaching a force-balanced state before the diffusion of self-propulsion directions destabilises the configuration, the ADD alorithm should be relevant to simulate it – Ref. [1] applies ADD to study Eshelby-like events, which are presented in Ref. [2] as a characteristic of the intermittent regime.

We highlight some similarities with the "athermal quasi-static random displacement" (AQRD) method of Ref. [3] in which a random local strain vector is first associated to each particle, these are then moved quasi-statically in these directions, with a minimisation at each step to find the constrained local minimum of potential energy. This method is equivalent to self-propelled forcing in the limit of zero rotational noise, where the forcing is slower than any other relaxation process.

II. ADD FOR INERTIAL ABPS

A. Model

Refs. [1, 4] introduce the ADD algorithm for inertial active Brownian particles (ABPs) without thermal noise

$$m\ddot{\boldsymbol{r}}_i(t) = -\gamma\dot{\boldsymbol{r}}_i(t) - \nabla_i U(t) + \gamma v_0 \boldsymbol{u}(\theta_i(t)) \tag{1}$$

$$\dot{\theta}_i(t) = \sqrt{2/\tau_p}\,\eta_i(t) \tag{2}$$

with $\boldsymbol{r}_i$ and θ_i the position and orientation of the i-th particle, m the particle mass, γ the friction coefficent, U the interaction potential, v_0 the self-propulsion velocity, $\boldsymbol{u}(\theta_i) = (\cos\theta_i, \sin\theta_i)$, τ_p the persitence time, and η_i a zero-mean unit-variance Gaussian white noise.

Ref. [1] highlights that U can in general contain arbitrary many-body interactions.

We want to compute the dynamics on a time scaled by the persistence time

$$t' = t/\tau_p \tag{3}$$

and thus rewrite Eqs. 1, 2

$$m\frac{1}{\tau_p^2}\frac{\mathrm{d}^2\boldsymbol{r}_i}{\mathrm{d}t'^2}(t') + \gamma\frac{1}{\tau_p}\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t'}(t') = -\nabla_i U(t') + \gamma v_0 \boldsymbol{u}(\theta_i(t')) \tag{4}$$

$$\frac{\mathrm{d}\theta_i}{\mathrm{d}t'}(t') = \sqrt{2}\,\eta_i'(t') \tag{5}$$

with η_i' a zero-mean unit-variance Gaussian white noise in the scaled time variables ($\eta_i' = \sqrt{\tau_p}\eta_i$). In the $\tau_p \to \infty$ limit, the left hand side of Eq. 4 vanishes and the particle configuration thus always satisfies

$$0 = -\nabla_i \left(U - \sum_i v_0 \boldsymbol{u}(\theta_i) \cdot \boldsymbol{r}_i \right) = -\nabla_i U_{\mathrm{eff}} \tag{6}$$

hence minimising an effective potential tilted by the active forces U_{eff}.

B. Numerical implementation

Orientation dynamics (Eq. 5) is integrated first over a time step $\delta t'$

$$\theta_i(t' + \delta t') = \theta_i(t') + \sqrt{2\delta t'}\,\eta_i' \tag{7}$$

where η_i' is random number taken from a Gaussian distribution with zero-mean and unit-variance.

Position dynamics (Eq. 4) is then integrated with time step Δt to minimise U_{eff} (Eq. 6) – this is done for a time $t_{\min}$ until either (i) the total force on each particle falls below a threshold

$$\sqrt{\frac{1}{N}\sum_i \left|-\nabla_i U_{\mathrm{eff}}\right|^2} \leq F_c \tag{8}$$

or (ii) the minimisation time $t_{\min} \propto \Delta t$ reaches a threshold

$$t_{\min} \leq t_{\mathrm{step}} \tag{9}$$

and such that, in the $\tau_p \to \infty$ limit, we have $t_{\mathrm{step}} \ll \tau_p \delta t'$.

In order to perform this minimisation, authors of Ref. [1] use the exponential Euler method [5] on

$$\dot{\boldsymbol{v}}_i(t) = -\frac{\gamma}{m}\boldsymbol{v}_i(t) + \frac{1}{m}\left[-\nabla_i U(t) + \gamma v_0 \boldsymbol{u}(\theta_i(t' + \delta t'))\right] \tag{10}$$

$$\dot{\boldsymbol{r}}_i(t) = \boldsymbol{v}_i(t) \tag{11}$$

thus yielding

$$\boldsymbol{v}_i(t + \Delta t) = \Gamma \boldsymbol{v}_i(t) + \frac{1}{\gamma}(1 - \Gamma)\left[-\nabla_i U(t) + \gamma v_0 \boldsymbol{u}(\theta_i(t' + \delta t'))\right] \tag{12}$$

$$\boldsymbol{r}_i(t + \Delta t) = \boldsymbol{r}_i(t) + c_1 \boldsymbol{v}_i(t) + c_2\left[-\nabla_i U(t) + \gamma v_0 \boldsymbol{u}(\theta_i(t' + \delta t'))\right] \tag{13}$$

where

$$c_1 = \frac{m}{\gamma}\left(1-\Gamma\right) \tag{14}$$

$$c_2 = \frac{m}{\gamma^2}\left(\frac{\gamma\Delta t}{m} - 1 + \Gamma\right) \tag{15}$$

$$\Gamma = \exp\left(-\frac{\gamma\Delta t}{m}\right) \tag{16}$$

and $\boldsymbol{v}_i$ is the velocity of i-th particle.

III. ADD FOR OVERDAMPED AOUPS

Ref. [1] already mentions the applicability of ADD to overdamped active Ornstein-Uhlenbeck particles (AOUPs). We develop here the corresponding equations and numerical implementation.

We consider overdamped AOUPs without thermal noise

$$\dot{\boldsymbol{r}}_i(t) = -\nabla_i U(t) + \boldsymbol{p}_i(t) \tag{17}$$

$$\dot{\boldsymbol{p}}_i(t) = -D_r \boldsymbol{p}_i(t) + \sqrt{2DD_r^2}\,\boldsymbol{\eta}_i(t) \tag{18}$$

with $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ the position and propulsion vector of the i-th particle, U the interaction potential, $D_r = \tau_p^{-1}$ the rotational diffusivity, D the translational diffusivity, and $\boldsymbol{\eta}_i$ a zero-mean unit-variance Gaussian white noise on each component – note that we have set the mobility $\mu = 1/\gamma = 1$.

On the time scale (Eq. 3)

$$t' = D_r t \tag{19}$$

we then rewrite Eqs. 17, 18

$$D_r \frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t'}(t') = -\nabla_i U(t') + f\tilde{\boldsymbol{p}}_i(t') \tag{20}$$

$$\frac{\mathrm{d}\tilde{\boldsymbol{p}}_i}{\mathrm{d}t'}(t') = -\tilde{\boldsymbol{p}}_i(t') + \sqrt{2}\,\boldsymbol{\eta}_i'(t') \tag{21}$$

$$f = \sqrt{DD_r} \tag{22}$$

with $\boldsymbol{\eta}_i'$ a zero-mean unit-variance Gaussian white noise in the scaled time variables ($\boldsymbol{\eta}_i' = \sqrt{D_r^{-1}}\boldsymbol{\eta}_i$). In the $D_r^{-1} \to \infty$ limit, at constant $f = \sqrt{DD_r}$, the left hand side of Eq. 20 vanishes and the particle configuration thus always satisfy

$$0 = -\nabla_i\left(U - f\sum_i \tilde{\boldsymbol{p}}_i \cdot \boldsymbol{r}_i\right) = -\nabla_i U_{\text{eff}} \tag{23}$$

hence minimising an effective potential tilted by the active forces U_{eff}.

With the initial distribution, corresponding to steady state,

$$P(\tilde{\boldsymbol{p}}_i(0)) = \frac{1}{2\pi}\exp\left(-\frac{1}{2}|\tilde{\boldsymbol{p}}_i(0)|^2\right) \tag{24}$$

propulsion dynamics (Eq. 21) is integrated first on a time step $\delta t'$

$$\tilde{\boldsymbol{p}}_i(t'+\delta t') = (1-\delta t')\tilde{\boldsymbol{p}}_i' + \sqrt{2\delta t'}\,\boldsymbol{\eta}_i' \tag{25}$$

where $\boldsymbol{\eta}_i' = (\eta_{i,x}', \eta_{i,y}')$ are two random numbers taken from a Gaussian distribution with zero-mean and unit-variance.

Position dynamics (Eq. 20) is then integrated with time step Δt to minimise U_{eff} (Eq. 23), with the stopping conditions Eqs. 8, 9

$$\boldsymbol{r}_i(t+\Delta t) = \boldsymbol{r}_i(t) + \Delta t\left[-\nabla_i U(t) + f\tilde{\boldsymbol{p}}_i(t'+\delta t')\right] \tag{26}$$

where we have used Euler method, in analogy with Ref. [1], although a FIRE minimisation [6, 7] of U_{eff} may also be appropriate.

At high packing fraction ϕ and intermediate persitence time D_r^{-1}, we expect $|-\nabla_i U|^2 = \mathcal{O}(f^2)$ while $|\dot{\boldsymbol{r}}_i|^2 \ll f^2$, therefore Eq. 23 also holds. ADD might thus also be suitable for this regime.

IV. LIMITS

As we have introduced it, ADD relies on the separation of time scales between the propulsion dynamics and the relaxation to an effective potential energy minimum, hence making $\tau_p \to \infty$ a necessary but not sufficient condition for the procedure to work.

In particular, at low density (dilute limit) and intermediate density (*e.g.*, such that MIPS may be observed), we do not expect the dynamics to be dominated by the minimisation of the effective potential.

[1] Rituparno Mandal and Peter Sollich, "How to study a persistent active glassy system?" arXiv preprint arXiv:2012.01195 (2020).

[2] Rituparno Mandal, Pranab Jyoti Bhuyan, Pinaki Chaudhuri, Chandan Dasgupta, and Madan Rao, "Extreme active matter at high densities," Nature communications **11**, 1–8 (2020).

[3] Peter K Morse, Sudeshna Roy, Elisabeth Agoritsas, Ethan Stanifer, Eric I Corwin, and M Lisa Manning, "A direct link between active matter and sheared granular systems," arXiv preprint arXiv:2009.07706 (2020).

[4] Rituparno Mandal and Peter Sollich, "Multiple types of aging in active glasses," Physical Review Letters **125**, 218001 (2020).

[5] Marlis Hochbruck and Alexander Ostermann, "Exponential integrators." Acta Numer. **19**, 209–286 (2010).

[6] Erik Bitzek, Pekka Koskinen, Franz Gähler, Michael Moseler, and Peter Gumbsch, "Structural relaxation made simple," Physical review letters **97**, 170201 (2006).

[7] Julien Guénolé, Wolfram G Nöhring, Aviral Vaid, Frédéric Houllé, Zhuocheng Xie, Aruna Prakash, and Erik Bitzek, "Assessment and optimization of the fast inertial relaxation engine (fire) for energy minimization in atomistic simulations and its implementation in lammps," Computational Materials Science **175**, 109584 (2020).