Journal of Computational Physics 257 (2014) 57–82

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Numerical methods for computing effective transport properties of flashing Brownian motors ☆

Juan C. Latorre [a], Peter R. Kramer [b,c,*], Grigorios A. Pavliotis [d]

[a] Institute of Mathematics, Freie Universität Berlin, Arnimallee 6, 14195 Berlin, Germany
[b] Department of Mathematical Sciences, Rensselaer Polytechnic Institute, 110 8th St., Troy, NY 12180, United States
[c] Zentrum für Interdisziplinäre Forschung, Wellenberg 1, 33615 Bielefeld, Germany
[d] Department of Mathematics, Imperial College London, London SW7 2AZ, United Kingdom

ARTICLE INFO

Article history:
Received 18 January 2013
Received in revised form 3 September 2013
Accepted 5 September 2013
Available online 13 September 2013

Keywords:
Flashing ratchet
Homogenization
Continued fraction method
Hermite polynomials

ABSTRACT

We develop a numerical algorithm for computing the effective drift and diffusivity of the steady-state behavior of an overdamped particle driven by a periodic potential whose amplitude is modulated in time by multiplicative noise and forced by additive Gaussian noise (the mathematical structure of a flashing Brownian motor). The numerical algorithm is based on a spectral decomposition of the solutions to two equations arising from homogenization theory: the stationary Fokker–Planck equation with periodic boundary conditions and a cell problem taking the form of a generalized Poisson equation. We also show that the numerical method of Wang, Peskin, Elston (WPE, 2003) for computing said quantities is equivalent to that resulting from homogenization theory. We show how to adapt the WPE numerical method to this problem by means of discretizing the multiplicative noise via a finite-volume method into a discrete-state Markov jump process which preserves many important properties of the original continuous-state process, such as its invariant distribution and detailed balance. Our numerical experiments show the effectiveness of both methods, and that the spectral method can have some efficiency advantages when treating multiplicative random noise, particularly with strong volatility.

1. Introduction

We will develop and discuss numerical approaches to computing the long-time effective dynamics of a particle undergoing overdamped dynamics in a periodic potential, randomly modulated as a function of time, and driven additionally by thermal fluctuations. In order to reduce the number of parameters under consideration, we rescale the spatial variable with respect to the period L of the potential and the temporal variable with respect to the time which the particle takes to fall from a maximum near to the minimum of the potential under the zero temperature dynamics. The resulting rescaled equation of motion for the particle in one dimension can then be written in the form [1]:

$$\mathrm{d}X(t) = -\phi'\big(X(t)\big)F(t)\,\mathrm{d}t + \sqrt{2\theta}\,\mathrm{d}W(t), \tag{1}$$

☆ The research of JCL was supported by the DFG Research Center Matheon "Mathematics for Key Technologies" (FZT86) in Berlin and partially supported by NSF CAREER grant DMS-0449717. The work of PRK was partially supported by NSF CAREER grant DMS-0449717. PRK wishes to thank the Zentrum für Interdisziplinäre Forschung (ZiF) for its hospitality and support during its "Stochastic Dynamics: Mathematical Theory and Applications" program, at which part of this work was completed. The research of GP is partially supported by the EPSRC, Grant Nos. EP/H034587 and EP/J009636/1. GP wishes to thank the Biocomputing group at the Institute of Mathematics, FU Berlin for its hospitality and support during a visit at which part of this work was completed.

* Corresponding author at: Department of Mathematical Sciences, Rensselaer Polytechnic Institute, 110 8th St., Troy, NY 12180, United States. Tel.: +1 (518) 276 6896; fax: +1 (518) 276 4824.
E-mail addresses: jlatorre@zedat.fu-berlin.de (J.C. Latorre), kramep@rpi.edu (P.R. Kramer), g.pavliotis@imperial.ac.uk (G.A. Pavliotis).

0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.09.006

where $X(t)$ denotes the particle position as a function of time, $\theta = k_B T/\bar{\phi}$ is the ratio of the thermal energy $k_B T$ to the amplitude of potential variations $\bar{\phi}$, $\phi(x)$ is the periodic potential structure rescaled to have an order unity scale of variation, $W(t)$ is a standard Brownian motion with $\langle \mathrm{d}W(t)\rangle = 0$ and $\langle \mathrm{d}W(t)\,\mathrm{d}W(t')\rangle = \delta(t-t')\,\mathrm{d}t\,\mathrm{d}t'$, and $F(t)$ describes the random temporal modulations of the potential, which may be assumed without loss of generality to have its amplitude (in mean and/or variance) normalized as desired. For simplicity, we will restrict attention to the situation in which $F(t)$ is an autonomously prescribed stochastic process, i.e., its dynamics are determined independently of $X(t)$.

Eq. (1) is an example of a Brownian motor [2], a class of stochastic systems which are used to characterize and analyze the mechanisms behind the functioning of biological molecular motors [3] as well as to design artificial microscale and nanoscale machines [4,5]. An overdamped dynamical description (without inertia) is appropriate because of the small length scales and physical values of the other parameters. The periodic environment reflects the ordered assembly of an extended microtubule, actin fiber, or artificial substrate. Thermal fluctuations play an important but not entirely dominant role so that θ in practice tends to be somewhat but not much less than 1. Temporal modulations in the potential are induced by some external means, which typically does work on the particle. In biological settings, the potential in question is the binding potential between the molecular motor and the microtubule or actin fibers, and is modulated by chemical processes such as the binding of ATP or release of phosphate, as well as physical processes such as an unbound "head" of the motor "searching" for and landing on a binding site [6]. These physical and chemical processes proceed with effectively random delays because they typically rely on some component fluctuating under thermal effects until it manages to achieve a certain state so that the process goes forward. Consequently, continuous-time Markov chains (or sometimes renewal processes with more general waiting distributions [7]) are often used to describe the modulations $F(t)$ [8–11], with each state corresponding to a possible geometric conformation of the motor (except for its center of mass position, encoded by $X(t)$). In synthetic motors, the modulation $F(t)$ may often be periodic by design [4,5]. We will here particularly focus on the special case of a continuous modulation by an Ornstein–Uhlenbeck process. Such continuous stochastic modulations of the potential could, for example, represent interference of the motion of the molecular motor due to other organelles and structures in the cellular environment.

Eq. (1) is a simplified "amplitude-modulated flashing ratchet" model which integrates all these physical features in an essentially minimalist way, and its study has played a key role in the development of the theoretical understanding of molecular motors [2]. That said, the equations describing actual molecular motors, taking into account more detail regarding their mechanochemical dynamics and relevant spatial degrees of freedom, are generally more complex than the flashing ratchet model (1) [12–15]. We nonetheless choose to use the simple model (1) to most clearly explain the foundational issues regarding a new simulation approach for molecular motors models governed at least in part by continuous-state stochastic processes. The efforts needed to extend the methodology developed here to more general molecular motor models will be briefly considered in Section 6.

A central practical question in the theory of Brownian motors is the overall long-time behavior of the particle. The periodicity of the potential and statistical stationarity, or time-periodicity, of its modulations imply, through a central limit theorem argument [16], that the statistics of $X(t)$ at long time are Gaussian and characterized completely by the mean drift

$$\mathrm{U} \equiv \lim_{t\to\infty} \frac{\langle X(t)\rangle}{t} \tag{2}$$

and diffusivity

$$\mathrm{D} \equiv \lim_{t\to\infty} \frac{\langle (X(t)-\mathrm{U}t)^2\rangle}{2t}, \tag{3}$$

where $\langle\cdot\rangle$ denotes a statistical average over all randomness. Of particular interest is how these transport parameters, characterizing the large-scale, long-time behavior of the motor, are related to the microscopic design parameters (such as θ, the structure of the potential ϕ, and parameters characterizing the fluctuation $F(t)$) in the detailed stochastic differential equation model (1). Analytical approaches are generally only possible in asymptotic limits, such as adiabatically slow or rapidly fluctuating modulations $F(t)$ [2,17]. Some work has pursued such questions through direct Monte Carlo simulations [10,18] of the stochastic differential equation (1). This approach is, however, rather expensive because the trajectories must be followed through many spatial periods and typically also several realizations. Moreover, the nature of the Brownian motor, in particular the relevant parameter regime $\theta \lesssim 1$, is such that the particle takes a substantial amount of time to hop from one spatial period to another [19,20]. Accurate computations are further hampered by the slow convergence of a Monte Carlo simulation with respect to computational effort (square root accuracy gains with respect to simulation time and/or number of realizations).

Deterministic numerical approaches can be alternatively developed based on the equivalence of the stochastic differential equation (1) for trajectories and the Fokker–Planck partial differential equation

$$\partial_t \rho(x,f,t) = -\partial_x\big(-\phi'(x) f \rho(x,f,t)\big) + \theta\,\partial_{xx}\rho(x,f,t) + \mathcal{L}_f^*\rho(x,f,t), \tag{4}$$

for the probability density $\rho(x,f,t)$ of the particle position x at time t. In Eq. (4), $\mathcal{L}_f$ is the infinitesimal generator operator associated to the Markov process $F(t)$, and $\mathcal{L}_f^*$ its adjoint. Kostur [19] developed finite element simulations of this equation with adaptive time stepping to achieve and estimate the long-time behavior for several canonical Brownian motor models,