Effective transport properties for flashing ratchets using homogenization theory

Juan C. Latorre*[1], **Peter R. Kramer** [1], and **Grigorios A. Pavliotis** [2]

[1] Rensselaer Polytechnic Institute. Troy, NY, 12180, U.S.A.
[2] Imperial College London. London, SW7 2AZ, U.K.

We study effective transport properties of Brownian motor models of molecular motors. The effective drift and diffusivity can be calculated by solving cell problems, given explicitly by homogenization theory. We briefly describe how this approach is equivalent to the Wang-Peskin-Elston (WPE) [3] numerical algorithm for calculating effective transport properties of flashing ratchets. For an on-off flashing ratchet we examine the optimization of the Peclet number as a function of the free parameters of the system. We also present a numerical method for solving the cell equations for a flashing ratchet with Gaussian multiplicative noise.

1 Effective transport properties of Brownian motors.

Brownian motor models for molecular motors have acquired a lot of interest in recent years [1]. We mainly focus our attention on models of *walking motors*, such as kinesin. The position in space (restrict attention here to one spatial dimension) of the enzyme is denoted by $X(t)$, and its equation in the overdamped (low Reynolds number regime) is

$$\mathrm{d}X(t) = -\gamma^{-1}V'(X, F(t))\mathrm{d}t + \sqrt{2K_BT\gamma^{-1}}\mathrm{d}W(t). \tag{1}$$

The particle is driven by a periodic potential $V(x,\cdot)$. The interaction of the thermal environment with the motor is taken into account by the white noise term $\mathrm{d}W(t)$ with strength given by the fluctuation-dissipation theorem, where γ is the friction coefficient. The stochastic terms $F(t)$ accounts for chemical reactions which effectively change the potential landscape. This term is essential in order to keep the system away from equilibrium and thus be capable of transforming thermal energy into useful mechanical work. Equation (1) will be our working equation.

We now present briefly the results found in [2] for calculating the effective transport properties of Brownian motors given by equation (1). By performing a homogenization analysis (a singular perturbation analysis) on the Kolmogorov-backward equation associated with the process (1), one finds that the long-time mean velocity or *effective drift* of the process is given by (we may rescale time and space such that $\gamma = 1$ and the period of the potential $L = 1$),

$$U_{\text{eff}} = \int_{[0,1]}\int_{\mathrm{E}_f} -V'(z,f)\rho(z,f)\,\mathrm{d}f\,\mathrm{d}z, \qquad \mathcal{L}_0^*\rho(z,f) = -\partial_z\left((-V'(z,f))\rho\right) + D\partial_{zz}\rho + \mathcal{L}_f^*\rho = 0, \tag{2}$$

where $\mathcal{L}_f^*$ is the adjoint of the generator of F with state space E_f. $\rho(\cdot)$ is then the solution to the stationary Fokker-Planck equation (FPE) in the periodic domain. The long-time or *effective diffusivity* is given by

$$D_{\text{eff}} = D + \langle([-V'(z,f)]\,\chi)\rangle_\rho + 2D\langle\frac{\partial\chi}{\partial z}\rangle_\rho, \quad -V'(z,f)\partial_z\chi + D\partial_{zz}\chi + \mathcal{L}_f\chi = V'(z,f) + U_{\text{eff}}. \tag{3}$$

The auxiliary field $\chi(z,f)$ is the solution to the cell problem in the periodic domain, which is unique up to an additive constant (which can be set arbitrarily) in $\mathrm{L}^1_\rho([0,1])$.

2 Discrete-state flashing ratchets.

We consider the case in which $V(X,F) = V(X)F(t)$, where $F(t)$ is a discrete-state Markov chain. This particular Brownian motor model is referred to as the flashing ratchet. The WPE numerical algorithm to calculate effective transport properties of flashing ratchet models is derived in [3]. The resulting algebraic equation for U_{eff} is an appropriate finite volume approximation of the stationary FPE (equation (2)). The equivalence of the WPE approach for D_{eff} and the homogenized equation (3) is found by performing a homogenization analysis on the Kolmogorov-forward equation (FPE) and the WPE finite volume approximation of the resulting equation. We turn our attention now to a simple Brownian motor model, in which $F(t)$ is a two-state Markov chain taking values $F(t) = \{1,0\}$ (*on-off* flashing ratchet). The Peclet number, $Pe = U_{\text{eff}}/2D_{\text{eff}}$, is a quantitative measure of coherent transport in the system. We notice that the optimization of effective drift does not necessarily lead to coherent transport of the motor, for diffusivity may dominate over drift. We rather wish to optimize the Peclet

* latorj@rpi.edu, Phone: +01 518 276 6345

number respect to the free parameters in the system (D, k_{12}, k_{21} and α, a measure of the asymmetry of the potential, setting $\max|V(x)| = 1$). In the small temperature regime we find that the optimal values of the switching rates for fixed D scale like $k_{12}^* \sim O(1)$ and $k_{21}^* \sim O(D)$. A physical interpretation of this result can be made in terms of optimal waiting times between transitions of the Markov chain in order to create a resonance with the time the particle takes to jump to consecutive periods of the potential.

3 Flashing ratchet with multiplicative Gaussian noise.

We consider now the following flashing ratchet model,

$$\mathrm{d}X = -V'(X(t))F(t)\mathrm{d}t + \sqrt{2D}\mathrm{d}W_1(t), \qquad \mathrm{d}F = -\tau^{-1}F(t)\mathrm{d}t + \sqrt{2\sigma\tau^{-1}}\mathrm{d}W_2(t).$$

Here $F(t)$ is an OU-process with correlation time τ and stationary variance σ.

We propose the following numerical method to solve the cell problems and find the effective transport properties. We write the solution to the FPE (respectively the auxiliary field χ) in terms of orthonormal Hermite polynomials, which are the eigenfunctions of the generator of the OU process. This decomposition transforms the stationary FPE (the cell problem respectively) into a tridiagonal system of ordinary differential equations, which again are solved by a spectral method. The resulting algebraic equations are solved recursively (see, for instance, [4]). The effective drift and diffusivity are recovered easily from the solution of the equations. In Figure 1 we show some numerical results.

4 Conclusions.

We have presented an argument showing the equivalence between the WPE numerical algorithm and the homogenization analysis for calculating effective drift and diffusivity of flashing ratchet models. The WPE equations can be derived by homogenizing the Kolmogorov-forward equation. We then turned our attention to the problem of maximizing the Peclet number of the motor as a function of the free parameters in the system. For a flashing ratchet with multiplicative Gaussian noise (OU process) we have presented a numerical method based on spectral decomposition for solving numerically the cell problems. Our results have excellent agreement compared to Monte Carlo simulations. We also compare our results against a discrete version of the OU process in the form of a discrete state Markov chain and find the effective diffusivity using the WPE algorithm. We find that for large values of σ the WPE algorithm fails to give accurate results. In this case one must include more states in the discrete approximation of the noise, thus significantly increasing the cost of solving the equations involved in the WPE algorithm.

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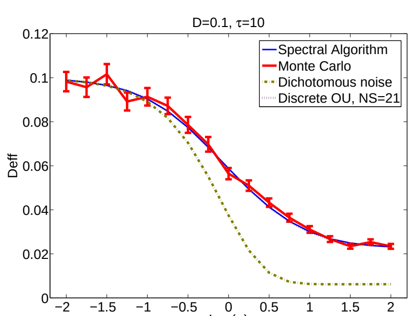
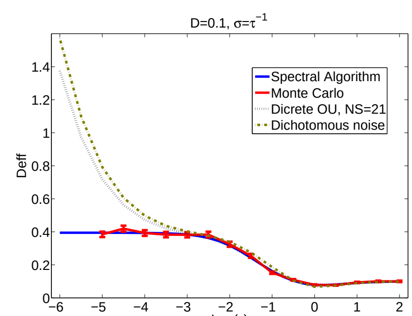


a)



b)

Fig. 1 Numerical calculation of D_{eff} for $V(x) = \sin 2\pi x$ ($U_{\mathrm{eff}} = 0$). We compare the spectral method for solving the homogenized equations against Monte Carlo simulations, WPE algorithm with a discretization of the OU process as a Markov chain (with 21 states), and a dichotomous flashing ratchet with same variance and correlation time as a comparison of the importance of the continuous noise with respect to a discrete one. a) τ is fixed, b) $\sigma\tau = 1$ to keep the effective strength of the Gaussian noise fixed.