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On control of transport in Brownian ratchet mechanisms

Subhrajit Roychowdhury[a,*], Govind Saraswat[a], Srinivasa Salapaka[b], Murti Salapaka[a]

[a] Department of Electrical and Computer Engineering, University of Minnesota-Twin Cities, 2-270 Keller Hall, Minneapolis, MN 55455, USA
[b] Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, 1206 West Green Street, Urbana, IL 61801, USA

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ABSTRACT

Engineered transport of material at the nano/micro scale is essential for the manufacturing platforms of the future. Unlike conventional transport systems, at the nano/micro scale, transport has to be achieved in the presence of fundamental sources of uncertainty such as thermal noise. Remarkably, it is possible to extract useful work by rectifying noise using an asymmetric potential; a principle used by Brownian ratchets. In this article a systematic methodology for designing open-loop Brownian ratchet mechanisms that optimize velocity and efficiency is developed. In the case where the particle position is available as a measured variable, closed loop methodologies are studied. Here, it is shown that methods that strive to optimize velocity of transport may compromise efficiency. A dynamic programming based approach is presented which yields up to three times improvement in efficiency over optimized open loop designs and 35% better efficiency over reported closed loop strategies that focus on optimizing velocities.

1. Introduction

Engineered nanoscale systems are posed to enable high efficiency and unparalleled precision in specificity in fabrication and manufacturing of materials and structures. Such a capability can result in new materials and devices with a vast range of applications in diverse areas such as medicine, electronics, and bio-materials [2,16,17,19,25]. The success of such a paradigm critically rests on the quality of transport of micro/nanoscale components from sources to destinations. An associated goal is the differentiation of components into separate groups based on different properties. Key insights on engineering transport mechanisms can be obtained from how biology utilizes micro/nano scale objects to achieve macro scale functionality. For example, in eukaryotic cells, material is transported on microtubular networks by motor proteins (kinesin and dynein) [11,26]; a detailed understanding of the underlying transport mechanisms can play a significant role in realizing productive engineered transport systems at the molecular scale. Use of biological constructs to realize such systems has found recent focus [7,23,27]. However, considerable challenges remain on both the fundamental understanding of transport mechanisms at the molecular scale and related engineering tasks.

A significant challenge for realizing efficient transport at the nano/molecular scale is posed by noise. Unlike in macroscale systems, *thermal noise* that causes Brownian motion often determines the limits of performance of molecular scale systems. For example, a kinesin motor protein (which together with dynein carry cargo inside a cell) moves on microtubules (MTs) with a characteristic step length of 8 nm; the motion caused by thermal noise has similar magnitude of standard deviations and thus a kinesin molecule has to achieve robust transport under a significant source of noise.

Remarkably, there are mechanisms that take advantage of Brownian motion to achieve directed motion. In the presence of Brownian motion, *Brownian ratchet* mechanisms use spatially periodic potential that are alternately turned on and off, to realize transport in preferred directions. For achieving the preferential bias in the motion, it is essential that the potential be asymmetric within the period; similar to the potential in a ratchet-and-pawl mechanism [10]. Moreover, in *Brownian ratchet* mechanisms, without the Brownian motion, no mean movement of particles is possible [2,18]; thus here Brownian motion is indeed an enabling factor. In many naturally occurring systems the potential is realized only at the vicinity of the moving entity, thus being more efficient [1].

In many engineered realizations where noise is marshaled for enabling motion in a desired direction, a spatially periodic potential is realized over the whole extent of the transport regime. The resulting mechanisms are also used to separate different constituents of a mixture by exploiting the dependence of diffusion constants on

* Corresponding author. Tel.: +1 6125985316.
E-mail address: subhra@umn.edu (S. Roychowdhury).

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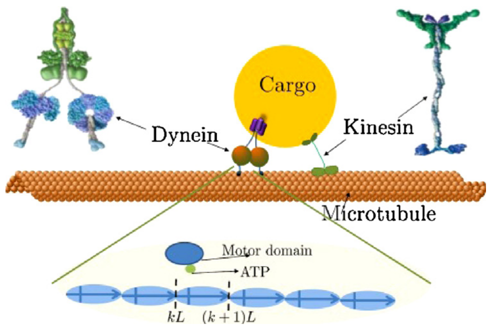

Fig. 1. The top schematic shows the transport of a cargo by motor proteins Kinesin and Dynein that *walk* on linear lattice provided by microtubules (MT). A simple model of MT is a linear arrangement of dipole moments (which is shown in the bottom figure). When an ATP/ADP molecule (which has a charge) is attached to the motor domain, the motor protein will feel the electrostatic force due to the dipole moments which depends on whether an ATP or an ADP is attached. The string of dipole moments provides the periodic asymmetric potential and the acquisition and loss of ATP/ADP switches the ratchet potential. It is possible that the rate of switching between the ADP and ATP molecules is dependent on where the motor domain is with respect to the MT unit that is modeled as a dipole. It is postulated that due to conformational changes in the motor protein structure, ATP/ADP exchange rate is different in the first α fraction of the dipole length in comparison to the case when the motor domain is anywhere in the rest of the $1-\alpha$ fraction.

physical properties (such as size) which results in different transport velocities. A flashing ratchet potential can also be realized, for example, using periodically asymmetric and transversely interleaved geometric patterns etched on surfaces and using electric fields in the transverse direction of motion (see geometric ratchets in [16,25]). In many applications only open-loop strategies are viable; for example, in geometric ratchets, the patterns are fixed and cannot be altered in real-time. Also, open-loop strategies have significant relevance when transport of many dispersed particles is involved. In open loop strategies a key design issue is to determine the on-and-off time schedule for the potential which optimizes transport efficiency and time to destination. Results in this article enable determination of optimal open-loop schedules that yield maximum efficiency/velocity for a given physical system without resorting to exhaustive Monte Carlo methods. In particular, the *stalling force* that prohibits appreciable forward transport, schedules that severely limit forward transport and schedules that result in non-negligible forward transport are determined. The viable range of on–off schedules are used to obtain bounds on forward and backward transport that can occur in a single on–off cycle, which are used to obtain an analytical estimate of the probability density function of the particle position. Error bounds on the estimated pdf of the position from the true pdf are obtained. The analysis and results above provide critical guidance in the design of ratchet mechanisms, which will lead to better transport mechanisms in applications, for example, in colloidal self-assembly [16,25] and separation of mixtures [2].

Closed-loop strategies hold significant promise of increasing transport efficiency in Brownian ratchet based mechansms. As alluded to earlier, motor-proteins, such as kinesin and dynein carry cargo inside a cell over MT networks (see Fig. 1). Each MT is formed by dimer units, which can be modeled as dipoles. Motor-proteins acquire ATP and ADP molecules that have different charge densities and thus by conversion between these molecules (via hydrolysis) the effective interaction potential between the motor complex and the microtubule is changed. The electrostatic force felt by the motor depends on where the ATP/ADP molecule is in relation to the dimer unit, providing a natural feedback mechanism; and thermal forcing provides the noise component. Thus all the ingredients that constitute a Brownian ratchet, with feedback, are present in the molecular motor based transport [4,22]. Engineered systems can be synthesized and used to study the effect of feedback mechanisms that govern changes in the potential. These studies can be used to develop *efficient* feedback strategies in the transport of a single particle. Although closed-loop strategies are considered in the literature, most focus on maximizing velocity of transport (for example, [9]) and do not consider efficiency ([5] does emphasize importance of transport efficiency). In this article, the trade-off between the average velocity of the particle and the energy required are obtained by solving a multiobjective stochastic optimization problem. It is shown that optimal feedback control strategies can be obtained using a dynamic programming formulation in a tractable manner. Similar approach have been adopted for a flashing ratchet system in [21], although the objective there was limited to maximization of velocity under certain conditions. A key insight obtained is that optimizing average velocity may compromise efficiency. For a given set of physical parameters the study provides guidelines on the choice of velocities to target maximum efficiency. Apart from providing guidance on engineered systems, the study of feedback mechanisms will enable the study of molecular motors, where analytical results can be used to decipher experimental data to assess whether feedback is essential (or the extent to which feedback is needed) to explain the data. Since often for many particle systems, the objectives are cast in terms of the center of mass of the particle positions [5,6], efficient single-particle feedback strategies can prove helpful when applied to a virtual particle at the center of mass of the particle ensemble. The closed-loop performance also provides bound on the limits-of-performance of many particle systems.

The paper is organized as follows: In Section 2, the basic operating principle of flashing ratchets is discussed and a mathematical model is provided. In Section 3, a systematic framework to maximize velocity and efficiency for open-loop operation is developed. In Section 4, the problem of maximizing efficiency is cast as a multi-objective optimization problem, which is converted into a dynamic programming problem. A solution together with an analysis of the computational cost is derived. Simulation results accompany the analysis throughout the article. Finally, the findings of the present work are summarized in Section 5.

2. Principle of operation and modeling

Brownian rectifiers constitute a class of mechanisms that realize transport in a preferential direction via 'rectification' of thermal noise. To understand how a Brownian ratchet rectifies noise to obtain preferential movement of particles, consider a simple version of a ratchet shaped potential (see Fig. 2(a)) that remains on and off in an alternating manner for time intervals t_{on} and t_{off}, respectively.[1] Here the potential is periodic with a period L and has positive slope (the corresponding force, $-(\partial V/\partial x)$, is negative) in the interval $(kL, (k+\alpha)L)$ and a negative slope (the corresponding force is positive) in the interval $((k-1+\alpha)L, kL)$ of the kth spatial period. Consider a particle located at the kth valley at time $t=0$. We represent the dynamics of the particle in terms of the time evolution of the probability density function $p(x, t|x_0 = kL, 0)$, which is the probability of the particle being at position x at time t given that it was at $x=kL$ at time $t=0$. Thus, $p(x, 0|kL, 0) = \delta(x-kL)$, where $\delta(x)$ is the Dirac-delta function. Suppose the potential is off in the time interval $[0, t_{off}]$; then the motion of the particle is governed by Brownian motion and the pdf is given by (see Fig. 2(b))

$$p(x, t|kL, 0) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-kL)^2}{4Dt}\right). \qquad (1)$$

[1] And hence the name 'flashing ratchet'