2P140 アクチンフィラメント上のミオシン頭部のバイアス運動への疎水および静電相互作用の寄与
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Contribution of hydrophobic and electrostatic interactions in the biased motion of myosin head along actin filament
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Myosin head moves in a stepwise manner while it keeps attached to the actin filament (Kitamura et al., Nature 397, 129 (1999)). This movement is mostly directed forward but with 10% backward stepping. Such biased stochastic motion is not accounted for by the conventional lever-arm or ratchet model. We have proposed that myosin motion can be biased if the motion is coupled to the conformational change of myosin head (Terada et al., PNAS 99, 9202 (2002)).

In previous reports, we have simulated the motion of myosin head along the actin filament with coarse-grained molecular dynamics where polypeptide structures are represented as connected beads. The probability of the forward motion is sensitive to strength and functional form of interactions between actin and myosin at their interface, which originate from subtle combinations of hydrophobic and electrostatic interactions. To better describe such complexity, we modify interaction potentials at the actin-myosin interface by introducing the sequence-dependent water-mediated potential (Papoian et al. JACS 125, 9170 (2003)), which was derived from the database analysis of protein-protein interaction. This potential have three variants depending on the degree of unfolding of each protein prior to binding. The simulation with this potential elucidates the contribution of hydrophobic and electrostatic interactions in the biased motion as well as the importance of coupled folding and binding.

2P142 結合型ラチェットモデルにおいて双安定性が輸送性を与える影響
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The effect of the bistability on the transport properties in the elastically coupled Brownian ratchet model
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Brownian ratchet is one of the theoretical models which describe the stochastic motility of molecular motors. Recently, Wang and Bao have provided the transport coherence in the elastically coupled classical ratchet model. They have shown that the Peclet number, which indicates the transport coherence, increases as increasing the elastic constant. However, in contrast with the coupled classical ratchet, Julicher and Prost's coupled ratchet model has the bistability of the velocity. Their coupled ratchet is widely recognized, and the bistability has been verified experimentally. In this paper, we have numerically investigated the transport properties, such as the velocity, energetic efficiency, Peclet number, and so on, in the elastically coupled Brownian ratchet, provided by Julicher and Prost. Furthermore, we have analyzed the dynamical stability of the coupled ratchet and discussed the effect of the bistability on the transport properties, based on the stochastic dynamical systems theory.

2P141 アクトミオシン滑り運動のゆらぎ解析によるエネルギー変換機構について
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Fluctuation analysis of actomyosin sliding movement and mechanochemical coupling
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Recent single molecule experiments have very well described the dynamics of individual myosin molecules but that in muscle has not been well known. In order to examine that, we analyzed the fluctuations of sliding velocities of actin filaments in myosin-coated surface assay (analog of muscle) at various ATP concentrations. We found that the mean of sliding velocity was proportional to the standard deviation (σ) at the wide range of ATP concentrations. This result indicates that the fluctuations of velocity is larger than that expected from fluctuation of the ATP turnover times. On the other hand, we also performed the same fluctuation analysis of Myosin-V which is known to move along actin filament in a tight coupling manner with a regular step-size. We found that the mean velocity of single myosin-V was proportional to the variance (σ^2) in this case. This means that the fluctuation of velocity is tightly coupled to the fluctuation of ATP turnover time and hence the step-size of myosin-V per ATP is constant. Since the result is consistent with the tight coupling dynamics of myosin-V, here we propose that the fluctuation analysis is a promising tool to investigate the sliding mechanism, and the step-size of myosin is not constant or multiple steps occur during a single ATP turnover in muscle, i. e., loose coupling.

2P143 Flashing Ratchet Model を用いた分子モーターのエネルギー効率における粒子数依存性の解析
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Effect of the Number of Molecules on the Energetic Efficiency in Molecular Motors using the Flashing Ratchet Model
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The components of motors are protein molecules that can exchange the chemical energy of adenosine triphosphate (ATP) for mechanical work. In recent experimental studies, it is suggested that the motion of a single motor arises by means of thermal fluctuations. The Flashing Ratchet Model can explain these experimental results. This model assumes that the motor molecule is a brownian particle and it moves on an asymmetric and periodic potential function. However, many motor molecules operate in the situation that they are connected with each other. Thus we construct the molecular motor models which have N motors. We develop the method for calculating the efficiency of the N -motor model. Many researches of molecular motor models have focused only on the energetic efficiency. However, we apply the method of calculating the dissipation rate to our N -motor model. Using this method, we can study how the energy of motors dissipates with motion. Specifically, we analyze a single, 2-particle, and infinitely coupled molecular motor model. We show that the efficiency increases when the number of motors increases. We can find the reasons why the efficiency among those models increases. Our study can also predict some experimental results for molecular motors such as myosin, kinesin and sarcomere, which have one or several numbers of motors.