2P302 混雑環境下での分子機械の動作と反応拡散経路
Formation of Reaction-Diffusion Pathways by Molecular Machines in the Crowded Intracellular Environment

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Biological cells utilize a variety of molecular machines. Interactions between machines are usually mediated by other molecules. In a system crowded with macromolecules, in cells typically, it is not always simple how such intermediate molecules reach their target. Communication and thus operations of machines are affected by the transportation of these intermediates. On the other hand, molecular machines show mechanical motion, driven or affected by ligands. Such motion may drive neighboring molecules and alter the spatial structure around, which may facilitate or hinder the above-mentioned communication. Hence, the molecular distribution may be coupled with the machine dynamics.

In this work, we study such interplay, using a simple particle model. We model each molecule as a semi-hard sphere (circular disk). Operation of each machine is represented by a phase oscillator [1]. The conformational motion is taken into account in such a way that the diameter (exclusion volume) varies, as a function of the phase variable. Allosteric activation by the product molecule is assumed.

At high density, once a cluster of inactive machines is formed, activator products only occasionally penetrate and reactivate it. Paths of the product flow are formed and maintained by machine motion. This model does not depend on any details of chemistry and may be applicable to a cluster of other kinds of active agents, such as collective motion of cells.

[1] V. Casagrande, Y. Togashi, A. S. Mikhailov, Phys. Rev. Lett. 99, 048301 (2007).

2P303 メトリック・トポロジカル近傍がつくる群れのモデルとその機能
The Emergent Property in a Flock from the Metric-Topological Interaction

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Almost all flock models are constructed using a self-propelled particle system (SPPs). In an SPP method, each individual will interact with neighbors found within a certain radius. Recent investigations are forcing us to reconsider the notion of the neighborhood in flocks. Cavagna et al. found a scale-free correlation in which the sub-flocks use the same information and where their size is proportional to the flock size. This finding indicates that the flock neighborhood dynamically changes the shape and formation of the flock. They defined this state of the flock as the "noise critical phenomenon". However, is it a sufficient interpretation of the scale-free correlation? The agent of the type-token model, which we proposed, changes its neighborhood by adjusting between the type and token cognitions. These differences in the neighborhood of each agent enables their flock to rapidly change direction without external noise and shows a scale-free correlation that is supported with empirical research. The typetoken model suggests that the flock emerges as a scale-free correlation without considering noise critical phenomena.

2P304 バイズ推定を用いた運命決定を行う反応の可逆性と情報抽出の効率
Relation between Reversibility and Efficiency of Bayesian Decision Making

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Cells are generally subject to noisy environments. Still, they should precisely detect changes of environment for their responses and actually they do. This suggests that some structures of intracellular reactions can be equipped to efficiently extract relevant information from the noisy environment. Recently, one of the authors revealed that intracellular kinetics with dual positive feedbacks could implement a dynamic Bayesian decision making [1]. It was further demonstrated that the kinetics could detect the changes of environment with relatively high precision from noisy input. However, the kinetics is physically unrealistic because it assumes irreversibility in reactions. In general, reactions progress in both directions with respect to the free energy changes between reactants and products. In this study, we consider backward reactions in addition to forward reactions of the structure, and assume the amount of energy resources (e.g. ATP) drive the forward reaction. Following biochemical kinetic theory [2], we investigate how the efficiency of Bayesian decision making is related to the extend of the irreversibility. We found that the irreversibility is indeed essential to identify the changes by the kinetics, and there exists an optimum ratio because of the trade-off between the accuracy and necessary energy resources. [1] T. J. Kobayashi, to be published in Phys. Rev. Lett. (2010) [2] D. A. Beard and H. Qian, Chemical Biophysics, Cambridge Univ. Press (2008)

2P305 細胞の自発運動は走性情報処理の効率にどのように寄与するか?

How does spontaneous cell migration contribute to the efficiency of tactic response?

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Directional cell migration is a fundamental process associated with many physiological phenomena such as embryogenesis, immune response, wound healing, and cancer metastasis. Recently, cellular spontaneous activity and its fluctuation become to be a focus of interest for providing a basis for directional cell migration in response to environmental stimuli. We focused on the relationship between spontaneous and directional cell migration, and investigated it quantitatively in Dictyostelium discoideum. Based on a series of statistical analysis of hundreds of cellular trajectories under spontaneous migration and electrotaxis, a generalized Langevin model for directional cell migration was proposed, and numerically confirmed to reproduce corresponding cellular behaviors successfully. This suggested that electrotaxis is realized by biasing spontaneous cell migration properly, and velocity memory is relevant to cellular effective response for uncertain environment. On the other hand, recently several groups proposed different types of model for cell migration, and it is required to evaluate which type of model is more plausible and descriptive for cell migration dynamics and how general our findings are. In this presentation, we indeed evaluate a series of models for cell migration quantitatively, especially focusing on the role the velocity memory. Then, we discuss whether our results for electrotaxis are general and applicable for chemotaxis or not, in search for the dynamical relationship between cellular sensing and migration.

2P306 3次元樹状構造形成と信号伝播
Pattern formation in 3-dimensional branching paths and signal propagation

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The branching structures can be widely observed in open systems such as bacterial colonies, blood vessels, slime molds and so forth. There are several models for describing 2-dimensional (2D) branching pattern. In the recent study, I also proposed a simple 2D cellular automation (CA) model based on a reaction-diffusion kind model. However, large part of observed branching patterns is in 3D and only few general pattern formation models for 3D are proposed.

Signal propagation in 3D branching structure is interesting topic to understand fundamental mechanism of the structure. In order to understand such geometry in signal processing mechanism, the 3D branching patterns formed by extended CA model and verification of 2D image input to 3D branching paths are showed in this study. Extended 2D CA model is adopted by 2D patterns stack of each time step in 2D branching path formation. As for signal dynamics, excitation pulses described by general reaction-diffusion model in branching paths are regarded as signal. Also, input signal was regarded as a digital 2D image at the ends of branching paths. The direction of signal propagation was limited to uni-direction (afferent direction) for the purpose of simplification. Output was taken at root of branching paths as time-series signal. In this presentation I will show the qualitative relationship between branching pattern and condition of pattern formation, and the quantitative relationship between features of images and branching patterns.

2P307 細胞動態シミュレーションのための粗視化膜モデルの構築
Simplified coarse-grained model of cellular membranes to simulate dynamic features of cells

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Living cells have dynamic and characteristic shapes relating to their functions. To understand cells as molecular systems, it is dispensable to develop numerical modeling and to simulate cellular membranes. However, it takes a huge amount of time to simulate the membrane dynamics in an entire cell.

To eliminate this very high cost of computation time, we constructed a simple coarse-grained model of cell membrane instead of dealing with individual lipid molecules. The coarse-grained modeling has proved appropriate for protein folding studies, explaining some features of folding rate and mechanism. A simplifying feature of these coarse-grained protein models has treated implicitly the aqueous solvent environment, solvent frictional forces, and random collisions, which were described by Langevin dynamics. Here we further simplified the coarse-grained model. In our model, a membrane element was substituted for some lipid molecules. Simulation of a spherically arranged