composed of multiple polar groups, in which all the internal sites are included. All the sites having an average number of hydration waters, n_w , larger than one consist of a cluster of polar groups, many of which are internal sites. The largest internal site A with $n_w = 4.90$ is located in the hinge region between the α and β domains of lysozyme. The largest site A is composed of the three sub-sites, A₁, A₂ and A₃, consisting of 3, 5 and 4 polar groups respectively.

2P146 高静水圧によるタンパク質部分モル体積減少の分子動力学描像: 時間分解カークウッド-バフ法による考察
Molecular Dynamics Picture of Protein Partial Molar Volume Reduction under High Hydrostatic Pressure: Time-Resolved Kirkwood-Buff Approach

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Partial molar volume (PMV) is the contribution that the solute makes to the overall volume of the solution. It is known that the PMV of protein is decreased by the increment of hydrostatic pressure. The mechanism is, however, not fully elucidated at the molecular level.

In this study, we investigated the influence of the high hydrostatic pressure (3000 bar) on the PMV of protein apomyoglobin (AMb) by all-atom molecular dynamics simulation [1]. Using the time-resolved Kirkwood-Buff (KB) integral method [2], dynamic behavior of PMV was reproduced from the instantaneous atomic coordination of water molecules. It provides time dependency of PMV which reflects not only the protein structural fluctuation but also the dynamics of hydration water. As a result, the PMV reduction by 3000 bar pressurization, and the estimated isothermal compressibility of AMb were reasonably compared to those of experiments.

Furthermore, with the aid of the surficial KB integral method [2], we obtained the spatial distributions of PMV. New R-dependent PMV profiles enabled us to recognize the regions that increase or decrease the PMV under the high pressure condition. The results indicate that not only the change in hydration in the vicinity of protein surface but also that in the outer space of the first hydration layer does influence significantly the total PMV change.

[1] Yu, I; Nakada, K.; Tasaki, T.; Nagaoka, M. *J. Phys. Chem. B* submitted.

[2] Yu, I; Takayanagi, M.; Nagaoka, M. *J. Phys. Chem. B* 2009, 113, 3543-3547.

2P147 cAMP waves and oscillations during kin-discrimination in Dictyostelium discoideum

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It was recently discovered that when strains of wildtype *Dictyostelium discoideum* isolated from independent locations are allowed to aggregate together, cells sort out to form separate fruitingbodies depending on the identity of a locus that harbors tgrB1/tgrC1 genes that encode cell surface glycoproteins. Aggregation and morphogenesis of *Dictyostelium discoideum* cells are guided by propagating waves of extracellular cAMP that self-organize in the population. In this process, 20 to 30% of cells sacrifice themselves to form stalk that supports germ-line cells. According to the Hamilton's law, such altruistic behaviors require a mechanism to discriminate kin proximity thereby maintaining a heritable group of cell lineages that are genetically uniform. To understand the cell sorting, we study the cAMP signaling of cell populations harboring different alleles of tgrB1/tgrC1. From darkfield observation, we find that in null cells of tgrB1/tgrC1, cAMP signaling during the first 6 hrs appears normal except for ~1hr delay in the transition of the wave frequency. In cell population with tgrB1/tgrC1 (QS4,QS31) alleles, the signaling waves during the first 6hrs also appear indistinguishable from those of strains harboring the parental AX4 allele. When strains of different alleles are mixed together, the early wave formation does not appear to be altered however after ~7hr two distinct signaling centers form during mound formation. We analyze these behaviors using live cell imaging of cAMP and discuss how distinct organizing centers emerge.

2P148 細胞が上皮陥入を起こすための力学的性質
1C1420 Mechanical cell properties causing epithelial invagination

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Using the 3D cell model, invagination of the epithelial tissue was simulated, in which three cell behaviors, (1) extension and contraction of circumferential

length of apical polygons, (2) inner migration of epithelial cells and (3) "arc" arrangement of apical edges around an invagination center were included.

Based on observation of invagination of tracheal placode in *Drosophila*, we made a 3D epithelial tissue model consisting of polyhedral cells, and investigated three mechanical cell properties contributing to the epithelial invagination. Epithelial cells are intrinsically polarized in apical-basal direction. (1) Apical polygons of epithelial cells extend or contract their circumferential length. (2) Invaginating cells migrate to the basal direction along the apical-basal axis. (3) Epithelial cells produce "arc" arrangement of apical cell edges in the plane of epithelia by accumulating Myosin II in a subset of cell interface encircling the future invagination site.

Results of computer simulation using the 3D epithelial tissue model show that extension of circumferential length of apical polygons of peripheral epithelial cells and inner migration of invagination cells contribute to the three-dimensional epithelial invagination. The "arc" structure encircling the invagination center is considered to contribute to determination of the invagination center.

2P149 Three-dimensional spatial model of E. coli MinDE with Spatiocyte reveals E-ring as transiently membrane-bound MinE

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Cells have evolved to exploit the spatial dimension to perform some of the most important cellular processes such as transcription, cytokinesis, differentiation and chemotaxis. The spatial effects in these processes can manifest in the form of cell compartmentalization, dynamic localization of molecules, molecular crowding, diffusion-limited reactions and polymerization. In line with the advancement in computing hardware, detailed spatial modeling of processes with resolutions up to single molecules has become tractable. We have developed a lattice-based Monte Carlo method, called Spatiocyte, to model reaction-diffusion in and between cytoplasm (or nucleoplasm) and membrane compartments. The general-purpose stochastic method, which has been validated using analytical and numerical solutions, can also model polymerization-depolymerization of molecules and reproduce the effects of molecular crowding. In the rod-shaped bacterium *Escherichia coli*, the division site is suppressed at the cell poles by periodic pole-to-pole oscillations of the MinCDE proteins arising from carefully orchestrated RD in both cytoplasm and membrane compartments. Using Spatiocyte we could model and reproduce the in vivo MinDE localization dynamics by accounting for the previously reported properties of MinE. Our results suggest that the MinE ring, which is essential in preventing polar septation, is largely composed of MinE that is transiently attached to the membrane independently after recruited by MinD.

2P150 万能細胞の転写制御ネットワークの確率シミュレーション
Stochastic simulation of transcriptional control network in pluripotent cells

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The regenerative medical techniques have attracted much attention recently. Most prospective techniques among them are those based on pluripotent cells, such as induced pluripotent stem (iPS) cell and embryonic stem (ES) cell, which can differentiate into any specific type of cells. Molecular biological analyses of those pluripotent cells have shown that Nanog, Oct4 and Sox2 constitute a core network of transcriptional factors to maintain pluripotency. It has been also suggested that Nanog expresses either in high or low level and the dynamical fluctuation between two levels may be important features in ES cell. We construct a model of this core part of the transcriptional control network in pluripotent cells, and through stochastic simulations, the statistical features of dynamical fluctuations in expression of Nanog, Oct4 and Sox2 are discussed to characterize the pluripotent basin of dynamical state of network. These fluctuations may play roles in differentiation of pluripotent cells into lineage cells, which is the transition from the basin of pluripotent state to the other basin of lineage state, so that the relation between stochastic fluctuations and this transition will be theoretically investigated.

2P151 PAR タンパク依存的な細胞極性の方向制御
1C1435 Directional control of PAR-dependent cell polarization in C. elegans embryo

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