nucleosome in vitro form the so-called 30nm fiber, which is stabilized by linker histone proteins, H1 and H5. Fluctuations of nucleosome system are important for gene expression and regulation. For mono-nucleosome dynamics, several interesting experiments are performed, but for multi-nucleosome case, the structure of 30nm fiber is highly controversial. Recently, we combined a coarse-grained (CG) protein model and a DNA model, in which the protein model can simulate folding processes and large conformational changes, and the DNA model reproduces mechanic properties of DNA duplex and melting behavior. In this study, we simulate multi-nucleosome systems that include 2 to 20 nucleosomes with and without linker histone proteins as a first step to address the structure and dynamics of higher level nucleosome structures via molecular simulations.

1C1448 B-Z DNA ジャンクション構造の分子動力学シミュレーション Molecular dynamics simulations of B-Z DNA junction structure

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B- to Z-DNA transition is one of the most complex conformational changes in biomacromolecules. It is important to clarify the mechanism of the transition because it is involved in gene transcription and some kinds of diseases. However the atomistic details of the mechanism remained unclear. In 2005, an x-ray crystal structure of the B-Z DNA junction in complex with four Z-DNA binding proteins was determined. This revealed the following characteristic features of the B-Z DNA junction structure: (1) Hydrogen bonds of one base pair at the B-Z boundary were broken and the bases were extruded from the double helix structure. (2) Nevertheless, base stacking was continuous from the part of B-DNA to the part of Z-DNA.

To investigate the atomistic mechanism of the transition, we performed molecular dynamics simulations for the B-Z DNA junction structure with and without the Z-DNA binding proteins in explicit solvent. We used the parmbsc0 force field parameter for DNA. We analyzed fluctuations of DNA and proteins and interactions between protein and DNA. At present, a transition model termed "stretched intermediate model" has been proposed. This model has been supported by several computational studies. We will discuss the validity of this model based on our simulation results. While the past computational researches did not consider the effect of the proteins on the transition, we will discuss their roles by comparing the trajectories obtained from the simulations with and without the proteins.

1C1512 DNA 回文配列に対するレトロウイルスの特異的挿入：反応特異性と DNA 局所構造変化の定量的考察

Site-specific integration of retrovirus onto palindromic sequence: Analysis of integration selectivity in relation to DNA local structure

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Integration into the host cell genome by retrovirus plays the critical roles in many physiological and pathological processes. Especially the influence to oncogenes expression is one of the most talked-about topics nowadays. It has been debated long time that whether the integration of murine leukemia retrovirus (MLV) occurs selectively on certain base-sequence or not. Recently, we have shown that MLV has the potential to selectively integrate into a specified sequence via the experiments both on levels of whole animal and of in vitro model system; i.e., large enhancement of the integration for a palindromic sequence (T. Tsuruyama, et al, PLoS ONE. 5, 11 (2010)). It is known that palindromic sequences in a double string DNA can form specific secondary structure called as cruciform under certain condition in vitro system. In the present paper, we have performed the quantitative analysis on the experimental data given by Dr. Tsuruyama concerning the base specificity on the integration reaction around the palindromic region. It will be argued that the integration selectivity is attributable to the occurrence of cruciform structure on the palindromic sequence generated in living cells. This study is expected to provide a new insight on the mechanism how infection of retrovirus is caused in living cells depending on the specific DNA structure induced by the environmental change.

1C1524 生きた細胞の分裂期染色体の動的なクロマチン構造

**How can we know the chromatin environment in living cells?
-Structural analysis of mitotic chromosomes in living cells -**

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Mitotic chromosomes are essential structures for the faithful transmission of duplicated genomic DNA into two daughter cells. So far the structural analyses on mitotic chromosomes have been performed using 'dead chromosomes' like chemically fixed ones. How can we know the chromatin environment in living cells? To address this question, we used a combination of Fluorescence Correlation Spectroscopy (FCS) and Monte Carlo Brownian computer simulation. FCS reveals mobility of fluorescent molecules in a small volume by measuring their intensity fluctuations. Monte Carlo Brownian simulation is a tool for reconstruction of chromatin environment. For FCS measurement, we established a cell line stably expressing EGFP (fluorescent molecule for measurement) and H2B-mRFP (marker for chromatin regions). From the obtained FCS data, we calculated the diffusion coefficients of the EGFP in cytoplasm, interphase nuclei and mitotic chromosomes in living cells. To our surprise, the EGFP mobility in the mitotic chromosomes, which are highly condensed structure, was not significantly different from that in the interphase nuclei. Next, based on the obtained and known physical parameters, we reconstructed the living chromatin environment using the computer simulations. Our FCS and computer simulation results suggest that the chromatin environment during mitosis would be considerably dynamic to ensure accessibility for the diffusing proteins.

1C1536 Fluorescence microscope study of DNA motion near silicon based nano scale pore

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Silicon based solid state nanometer scale pore, called nanopore is one of powerful tools for rapid single DNA molecule detection. The translocation threading DNA through nanopore electrophoretically produces ionic current changes and provides the information of DNA i.e. length. One of issues in this detection method is clogging DNA molecules into nanopore. Once DNA molecules are clogged, the molecules are not able to be removed by just varying the applied bias voltages across nanopore. We have been studying how a DNA molecule move, trap and translocate or clog into nanopore by directly observing the DNA using a fluorescence microscope. By analyzing the DNA motion, the current induced electric field around nanopore was estimated. Interestingly, the field is not spherical around nanopore and the field strength reduces regions less than 2 μm away from the nanopore surface. Furthermore, electrically modified nanopore surface was prepared by coating Au and the profile of the electric field around nanopore was estimated. In this presentation, we will discuss the influence of surface conductivities, applied voltages and ionic concentrations on the electric field profiles around nanopore and the probability of the clogging DNA under these field profiles.

1C1548 Direct observation of P1 plasmid movement on an optical microscope

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The segregation of genome DNA is critical process for living organisms. In order to maintain faithful inheritance of genetic information, the replicated genome DNAs should be partitioned to the daughter cells properly before cell division. The same is true for low-copy-number plasmid. Plasmids are useful for investigating these processes. P1 plasmid is a low copy plasmid in *Escherichia coli* and the plasmid segregation system is simple. Only two P1 plasmid encoded proteins, ParA and ParB and a cis-acting centromere-like DNA, *parS* are required for the P1 plasmid segregation. ParA is a Walker-type ATPase, interacts with DNA non-specifically *in vitro* and colocalize with the bacterial nucleoid *in vivo*. ParB is *parS* specific DNA binding protein and ParB-*parS*