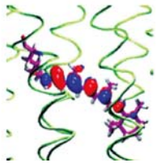
Molecular Scale Team

Molecular simulations try to elucidate the molecular basis of biological functions brought about by proteins and other biomolecules at the atomic level. Hierarchical nature of biological functions can be modeled by the multi-scale simulation combining quantum chemical (QM), molecular dynamics (MM), and coarse-grained model (CG) simulations, i.e., QM/MM and MM/CG. Developing these methods, we try to simulate large-scale systems containing long-time dynamics with high-precision. Our scope covers a wide-range of biological problems, from enzymatic reaction to molecular events in the cellular environment. These techniques should form a fundamental basis for rational drug design.

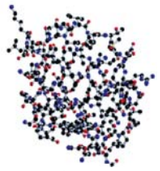
Three-Layers of Biomolecular Simulation

Quantum Chemical (QM)



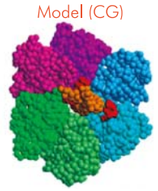
Structure changes and molecular interactions

Molecular Dynamics (MM)



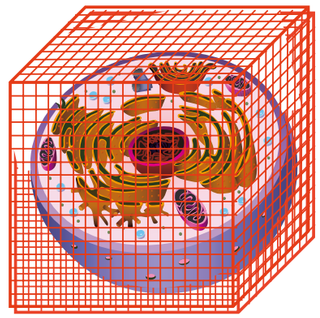
Coupling between reactions and motions

Coarse Grained Model (CG)



Large spatial/temporal scale events in cellular context

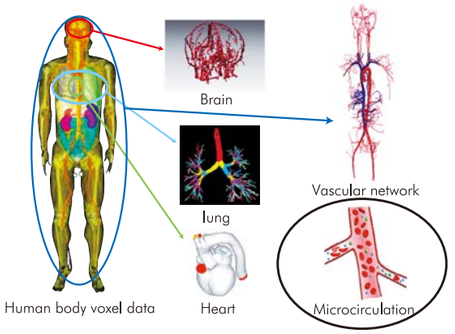
Cell Scale Team



Simulation of metabolism in various organelles and subcellular localization of material and enzyme

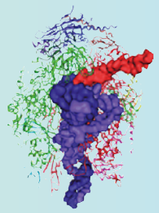
We are developing the integrated cell simulation platform which is important system of cell scale research. This platform is a common base system which takes into consideration of an intracellular place and the coupled simulation.
In the space of a fixed lattice, the model parameter obtained from experiment data can simulate various cell reactions on our platform. We section a cell in 1,000,000 voxels and take the information such as the quantity or movement of material. Then we simulate a phenomenon in the cell to various cell reactions.
Our first target is hepatocyte. We reproduce the energy metabolism or the drug metabolism based on the experimental data. We hope for the achievement of biology and the medical significant simulation. It is thought that it becomes a useful tool to understand the disease and the clinical condition.

Organ and Body Scale Team

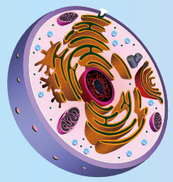


We are developing a living human body model which has the circulation system, the musculoskeletal system, all sorts of organs and the nervous system. Using this model, we are trying to develop the simulation-based supporting system for the next-generation medical treatment.
For example, as one of the blood flow simulators, thrombosis simulator is developed through the introduction of the coupling method between continuum scale simulation for blood flow and cell level simulation for the aggregation of platelets. This simulator will be used for the prediction and treatment of the thrombotic disease.

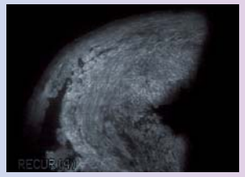
gene



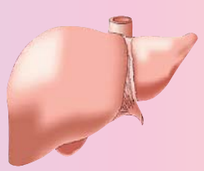
Molecule



Cell



tissue

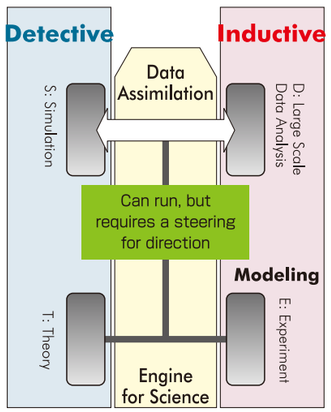


Organ

Body

Data Analysis Fusion Team

We are facing with the explosion of measurement data related to genes and genomes. This team is developing algorithms and their applications for data analysis which cannot be realized without peta-scale computing. In parallel with this data analysis challenge, we are creating a peta-scale modeling technology based on data assimilation that fuses observational data and simulation models.



In the future, these developments will form the fundamental information technology that will contribute to drug target discovery and medicine with the full scope of all human genes and their variations. Currently, by sharing "lung cancer and drugs" as a common theme in the team, the members are making a strong synergy to establish the technology that can predict large biological network structures and their dynamic models from data and will produce personalized models from "general models" with "personal data" with the innovation of data assimilation.

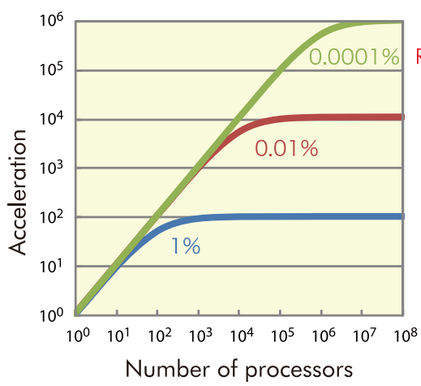
Brain and Neural Systems Team

The brain is a profound biological system where information emerges on the basis of physical molecules. We perform simulation studies of development and plasticity of single neurons, dynamics of cortical neuron ensembles, and processing of invertebrate's olfactory system and vertebrate's visual system; they will lead not only to elucidation of information processing functions of brain and neural systems but also to understanding how development/learning disorders arise in the brain.

In order to reveal the functions of processing units in the brain, we develop models and software to simulate molecular networks related to development and plasticity of single neurons, and highly-complicated cortical neural microcircuits. Moreover, we develop models, databases and software about insects' processing from odor stimuli to odor-source exploration and animals' processing from visual stimuli to eye movements, so as to simulate the real-time information processing by the brain.

High Performance Computing Team

The developments of highly-parallel software is essential to enhance the potential of the next-generation supercomputer system. We contend with the difficult problems in massive parallelization with the other research teams. Also, we develop the parallelized libraries for the basic simulation software such as molecular dynamics, molecular orbital methods and fluid/elastic mechanics, as well as visualization and work-flow tools.



Amdhal's law: a little time for serial execution greatly harms the parallelization performance in a system with massive parallel processors.