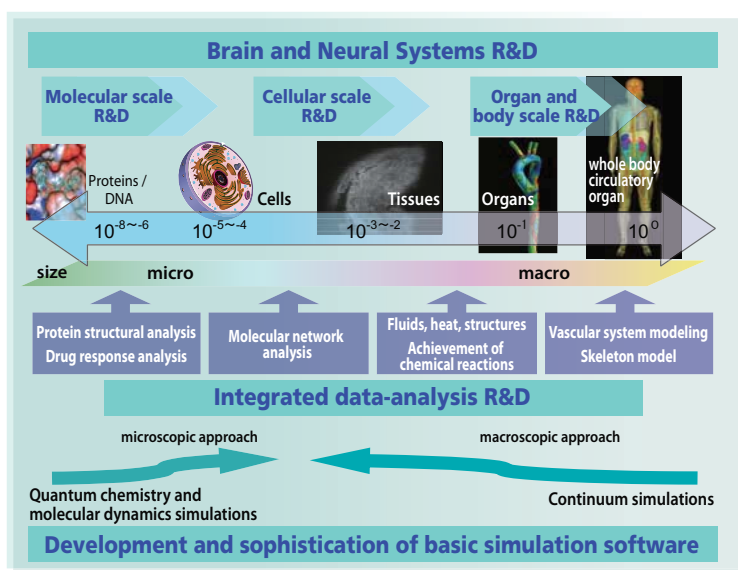## The "Grand Challenge" software applications

One goal of the Next-Generation Supercomputer project is to develop major software applications for the life sciences and nanotechnology and to deploy those applications on a wide range of platforms. We call the software for these two fields the "Grand Challenge" software applications.

The Next-Generation Integrated Simulation of Living Matter

RIKEN is developing new simulation software that will make full use of the Next-Generation Supercomputer's potential in helping us to understand a wide range of diverse phenomena, from the level of the molecule to that of the entire organism. In developing this new petaflop-scale simulation software, we adopt both an analytic approach, where we study phenomena through basic principles, and a data-analysis approach, where we attempt to discover new processes and laws by analyzing large quantities of experimental data. The new software we are developing takes full advantage of the Next-Generation Supercomputer's potential by integrating research results from across diverse scales with micro- to macro-scale experimental data. In addition, RIKEN also plans to actively collaborate with industry in applying research results to the real world in areas such as medical diagnostics, drug discovery and health science.

Brain and Neural Systems R&D

Molecular scale R&D	Cellular scale R&D	Organ and body scale R&D

Proteins / DNA — Cells — Tissues — Organs — whole body circulatory organ

$10^{-8}\sim^{-6}$ $10^{-5}\sim^{-4}$ $10^{-3}\sim^{-2}$ 10^{-1} 10^{0}

size   micro   macro

Protein structural analysis / Drug response analysis	Molecular network analysis	Fluids, heat, structures / Achievement of chemical reactions	Vascular system modeling / Skeleton model

Integrated data-analysis R&D

microscopic approach   macroscopic approach

Quantum chemistry and molecular dynamics simulations   Continuum simulations

Development and sophistication of basic simulation software

Research and Development on Next-Generation Integrated Nanoscience Simulation

This project, based at Institute for Molecular Science (IMS), is developing theoretical and computational methodologies in molecular and materials science which aim to analyze and predict various properties of nanoscale materials through extensive and accurate computations. The project must therefore develop simulation software for computational nanoscience based on theoretical processes, which will be optimized for the Next-Generation Supercomputer. Research activities are being conducted in collaboration with academic and industrial researchers in Japan, and focus on three fields: "Next-Generation Functional Nanomaterials for Information Technology", "Next-Generation Nano Biomolecules", and "Next-Generation Energy", which we refer to as the grand challenge targets.

Grand Challenges in Next-Generation Integrated Nanoscience

Next-Generation Integrated Nanoscience Simulation Software

Cooperation with experimental and industrial researchers
Human resources development

Next-Generation Nano Biomolecules
Medical & Medicinal Creation, Drug Delivery System Infrastructure
· Viruses
· Cell Membranes
· Nanoprocesses for Drug Delivery Systems
· Protein Control

· Nonlinear Optic Components
· Nanoquantum Devices
· Spin Electronics
· Super High-density Storage Devices
· Compound Electronic Devices
High-speed, Powerfully-featured, Energy-serving Electronic Devices

Next-Generation Functional Nanomaterials for Information Technology

Novel materials   Solid surface
Photo-induced phase transition   Magnetic properties

Next-Generation Energy
Green Energy
· Solar Energy Storage
· Alcohol Fuels
· Fuel Cells
· Electrical Energy Storage

Image of Next-Generation Supercomputer facility

T4 bacteriophage   Polio Virus   Liposome

Nafion   Water   15nm   Nafion mesoscale film structure   Cellulolytic enzymes