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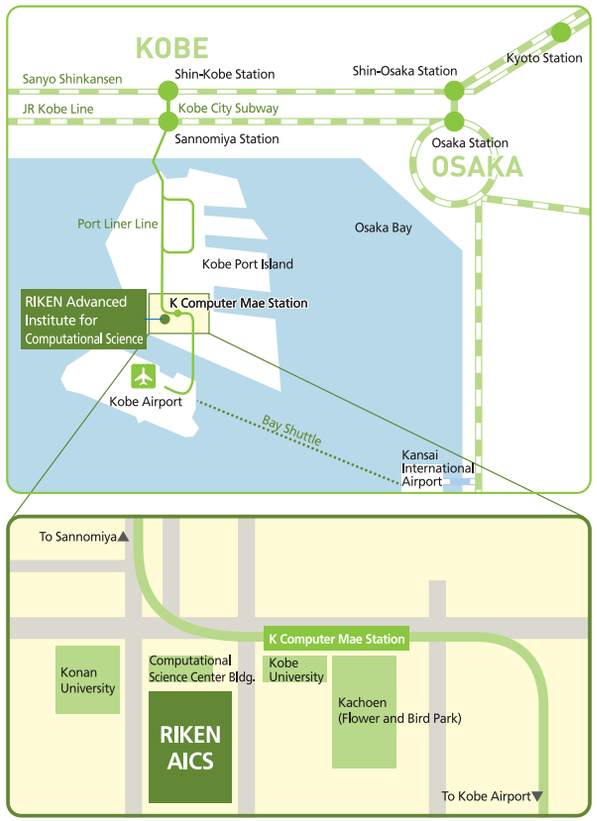

Strategic Programs For Innovative Research Field 1

Supercomputational Life Science

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K computer

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Strategic Programs For Innovative Research Field 1

Supercomputational Life Science

For Better Health

Simulating the Human Body

SCLS

What can the K computer do?

What do you mean by supercomputational life science?

Under this approach, simulations are created that allow us to look at biological phenomena at the level of molecules, cells, and entire organisms. By doing this, we can make discoveries that can lead to a healthier future for everybody.

※**K computer**

The K computer can perform more than ten quadrillion mathematical calculations per second. We will use this power to make extremely detailed simulations of various phenomena. For example, it will be used to help decode genetic information, which can be likened to a jigsaw puzzle with ten billion pieces!

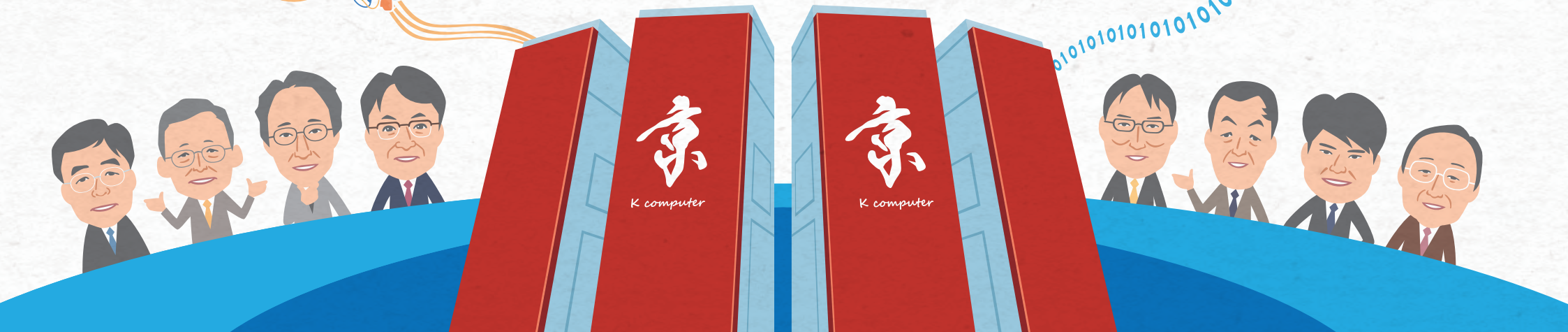
We can understand life using computers!

The biological phenomena that make up life start from events that take place at scales so small we cannot see them. We build models of biological phenomena using sciences such as physics, chemistry, and mathematics, and reproduce them as models inside the K computer. The K computer will allow us to do this more accurately than ever before.

How will this research change our future?

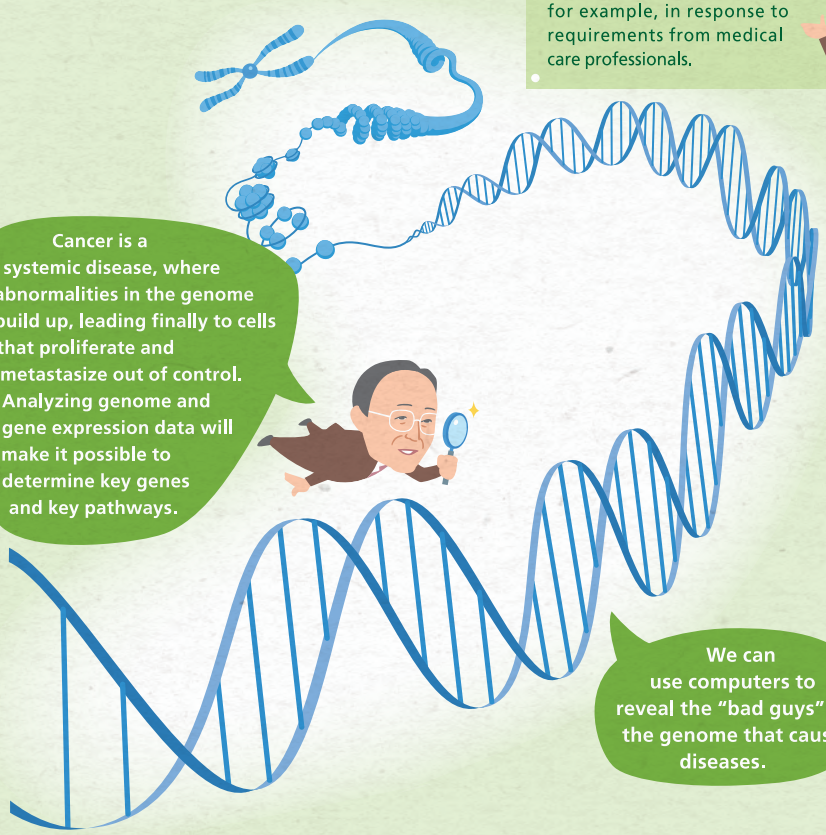
Computational life science can help us discover new drugs and treatments. This will not only help us to cure diseases, but will also make it easier to understand the health conditions of individual people, and to prevent diseases before people get sick.

We will use the K computer to better understand complex biological phenomena, with the goal to help us all live healthier and more prosperous lives.



1 Large-scale Analysis of Life Data

High-speed computers can contribute to the development of personalized medicine because they can quickly analyze huge amounts of data, such as genomic information. This will make it possible to quickly determine the proper amount of a drug to give to an individual patient, to minimize side-effects, and to develop new vaccines, for example, in response to requirements from medical care professionals.

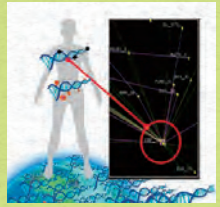


Cancer is a systemic disease, where abnormalities in the genome build up, leading finally to cells that proliferate and metastasize out of control. Analyzing genome and gene expression data will make it possible to determine key genes and key pathways.

We can use computers to reveal the "bad guys" in the genome that cause diseases.

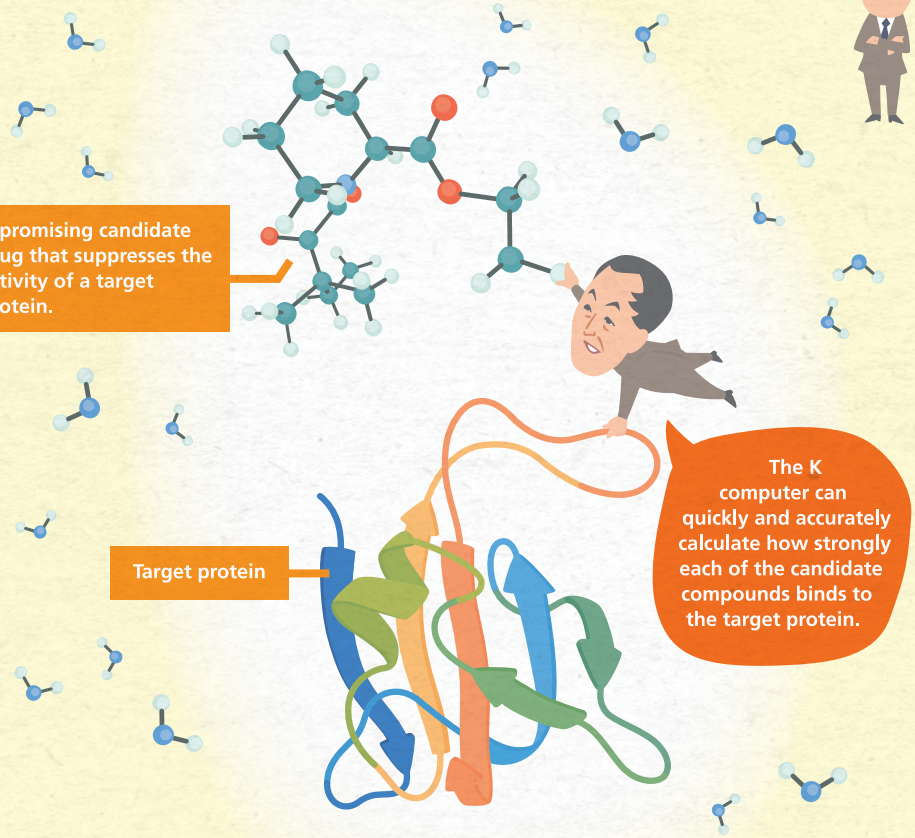
? How can the K computer help? Bringing personalized medicine closer to reality!

Personalized medicine is a concept that involves providing tailor-made treatment and health management to individual patients, based on an understanding of their health condition and lifestyles, along with information on their genetic makeup. The goal is to provide the most appropriate treatment for each patient, in a way that is efficient and gives the patient a sense of security.
In the area of personalized cancer therapy, scientists from around the world are cooperating to decode the genome of cancer tissues in order to develop better ways to prevent, diagnose, and treat the disease. The K computer is being used to analyze this genomic data.



2 Drug Development

With the hope of creating medical drugs that work well but have few side-effects or burdens on patients, we are working to understand the mechanism of diseases and to design new drugs based on this understanding. Through this, we are accelerating drug development.



A promising candidate drug that suppresses the activity of a target protein.

Target protein

The K computer can quickly and accurately calculate how strongly each of the candidate compounds binds to the target protein.

? How can the K computer help? Accelerating the early development process!

In order to calculate how strongly a single candidate compound binds to the target protein, a typical personal computer would take 300 days. The K computer, if all its resources are concentrated on the task, can analyze 250 compounds in a single day! We are putting the new computer to work to accelerate the early process of drug development.

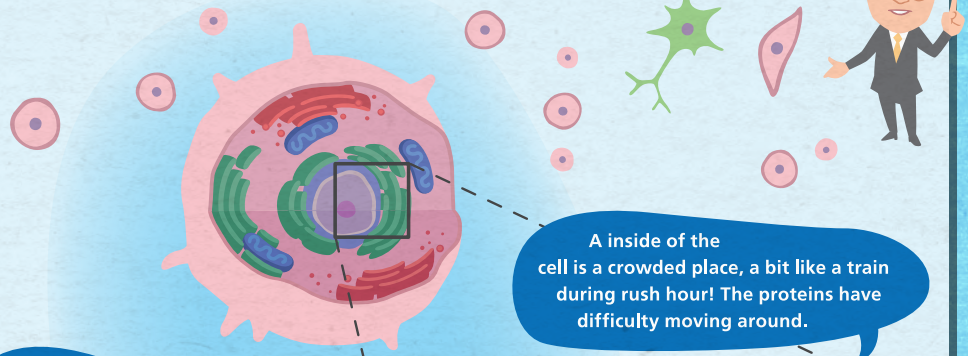
The drug development process

Into the hands of patients!

Target selection → Compound design → Compound screening → Preclinical trials → Clinical trials → Sales → Post-marketing surveillance

3 Molecular-level Simulations

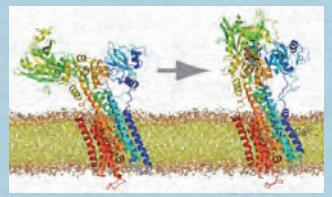
By developing molecular-level simulation methods and carrying out research on potential applications, we are working to elucidate biological phenomena at the cellular level, and by doing to make possible new therapies and develop new drugs.



Most of the inside of a cell is water, but proteins actually take up 30%, and are constantly rubbing up against one another.

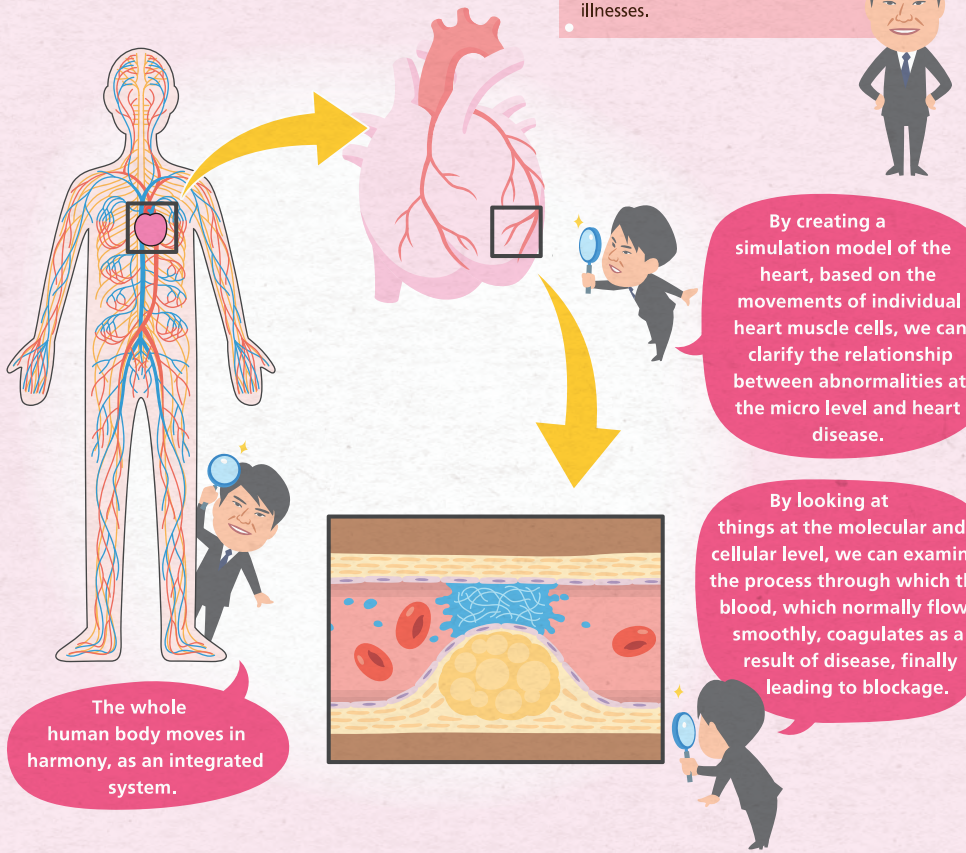
? How can the K computer help? Simulating cells "just the way they are"!

Many diseases begin when a protein is no longer able to fulfill its proper function. Because we understand this, a lot of modern research aims to get an accurate picture of the behavior of proteins in the cell. Analysis of the behavior was in practice impossible with the relatively slow computers of the past. We were limited to modeling the behavior of a single protein within a solution. The K computer will, for the first time, make it possible to model the behavior of proteins within the cellular environment.



4 Integrating Simulations at Various Levels

Simulations have been developed for different organ systems, such as the circulation, musculature, skeleton, brain, and nervous system. By integrating them, we will be able to gain an understanding of complex conditions such as heart disease and movement disorders, and to develop optimal personalized medicine to treat these illnesses.



? How can the K computer help? Simulating the body as a whole!

In the past, computers have been used to study individual organs such as the brain, nerves, muscles, heart, and blood vessels. With the K computer, it is possible to study those systems not in isolation, but together. We are engaged in a collaborative effort, with medical professionals, to create a new system of medical science. Based on the results of that research, we aim to make possible detailed consideration of medical treatment and prediction of prognosis.