# 11 Computational Science and E-Systems Research

## Computational Science Activity in Nuclear Energy Research and Development

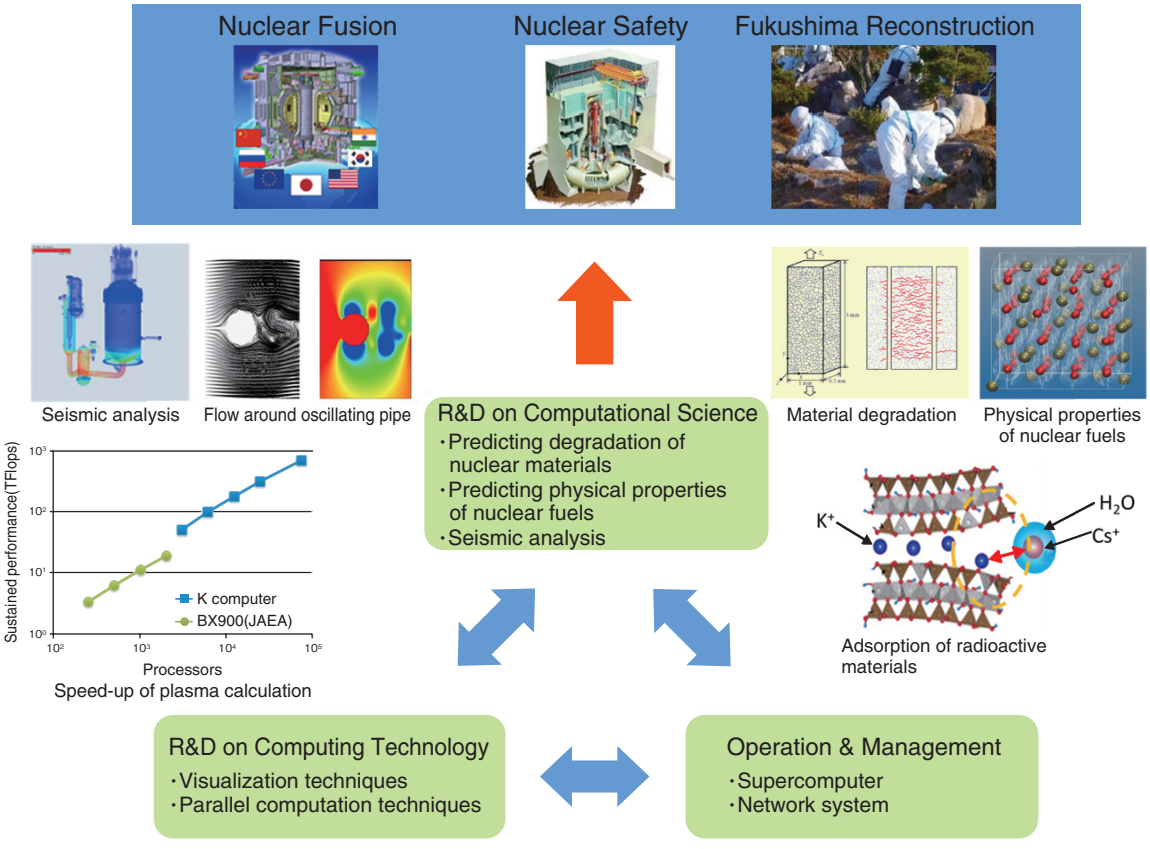


**Fig.11-1 Computational science activity in nuclear energy R&D**
The CCSE unites computational science research, computing technology research, and computer operation and management, and is creating cutting-edge knowledge and data in order to contribute to nuclear energy R&D and Fukushima reconstruction.

Computational science, which is known as the third type of research methodology after the theoretical and experimental approaches, is indispensable for understanding and predicting phenomena that cannot be resolved theoretically because of their complexity and/or that are difficult to observe experimentally because of cost and/or safety. Recently, the Ministry of Education, Culture, Sports, Science and Technology, which recognized the importance of computational science, officially announced a plan for developing a new supercomputer with a computing speed 100 times faster than that of the K computer. In addition, the news that China had successfully developed the fastest supercomputer in the world astonished the world. Such unremitting progress in computers is based on a background of increasing importance for computational science.

The Center for Computational Science and E-Systems (CCSE) manages and operates rapidly progressing supercomputers and promotes advanced research and development (R&D) on computational science using them. It grapples with important problems in nuclear energy R&D that require complicated large-scale computation, such as material degradation by aging, the high-temperature behavior of nuclear fuel, and evaluation of the earthquake resistance of structures. Furthermore, to create new knowledge about the mechanism of cesium soil pollution, the CCSE recently began a remarkable acceleration of advanced R&D by computer simulation (Fig.11-1).

In Topic 11-1, which aims at understanding the degradation mechanism of nuclear structural materials, the new concept that mobile hydrogen promotes crack growth is reported as a finding from a first principles calculation and thermodynamic analysis. In Topic 11-2, the strange thermal conductivity behavior exhibited by a new functional material, the topological superconductor, is introduced as a result obtained by a state-of-the-art computational science method. Topic 11-3 describes R&D for the international thermal nuclear fusion reactor in which the computation speed of the code for predicting plasma turbulence was materially improved using an innovative calculation method. In Topic 11-4, the effect of pipe oscillation on coolant flow is estimated as an example of seismic analysis. In Topics 1-5 and 1-19, the first principles calculation results for understanding the cesium adsorption mechanism of clay minerals and zeolites are reported as R&D for Fukushima reconstruction.

To contribute to Fukushima reconstruction and nuclear energy R&D, the CCSE will develop a state-of-the-art computer simulation technology as a key to resolving problems and strive continuously to be the leading force in computational science.