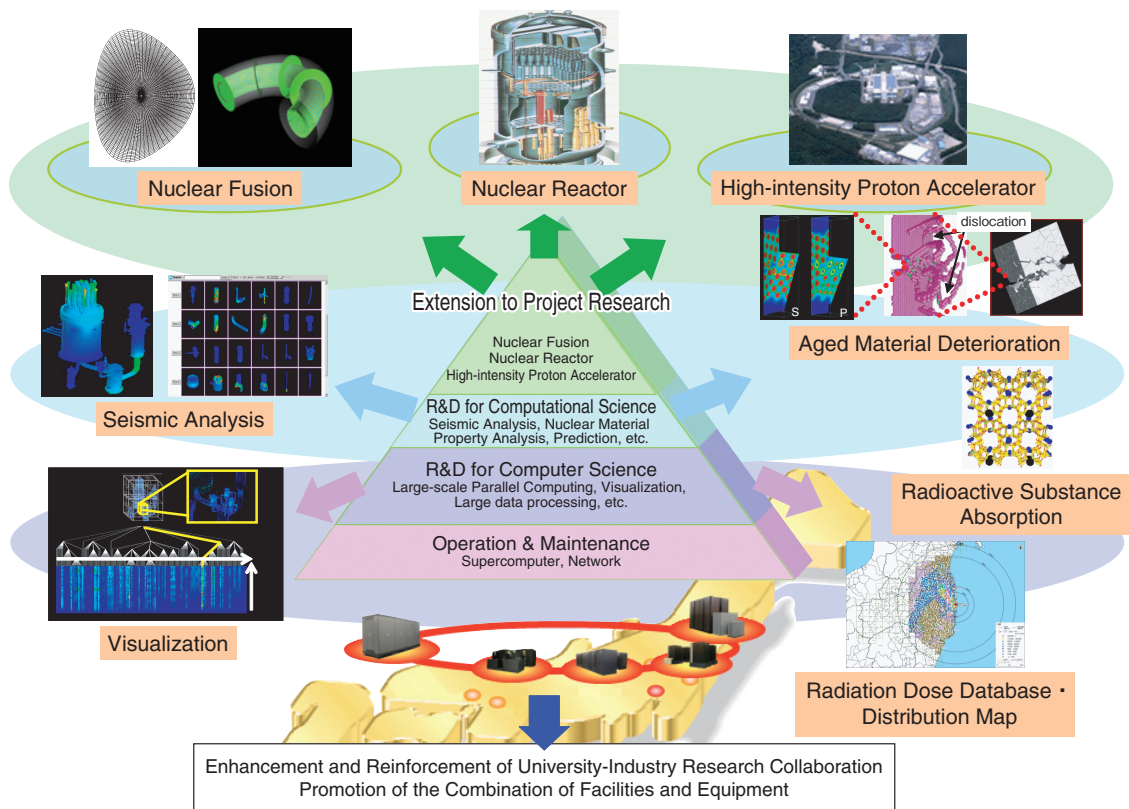


## Role and Potential of Nuclear Computational Science



**Fig.11-1 Development of nuclear computational science research in JAEA**

Nuclear computational science research is utilized not only for research projects in JAEA but also for the enhancement and reinforcement of university-industry research collaboration. In addition, we are promoting its application to research and development for Fukushima support.

Computational science is the third research methodology, following “theory” and “experiment,” and has made remarkable progress by becoming a field that is indispensable for the elucidation and prediction of phenomena difficult to observe or replicate in experiments. The next-generation supercomputer “K” was developed as a national project and has begun to be used. A change in the environment surrounding computational science has allowed its growth to accelerate.

We study important issues in the nuclear field, including those related to earthquake-resistance strength and deterioration of aged material, which cannot be sufficiently investigated without making full use of advanced computational technology, as shown in Fig.11-1. In addition, we are involved in various research and development activities and we develop and maintain the super-large-scale parallel computational technology required as a generic technology for such research. We ensure that the results of this research support broad research themes, such as fast reactor or nuclear fusion research, and allow for further development in this field.

The elucidation of the mechanism and the prediction of the deterioration of nuclear reactor structure materials are important problems faced in the research on aged material deterioration. Therefore, it is necessary to predict the segregation of atomic impurities that lower the material strength. In Topic 11-1, we introduce an example study that evaluates the segregation quantity at the grain boundary of phosphorus in irradiated materials by solving the diffusion rate equation using the coefficient obtained by the first-principles calculation.

In the research cooperation with the Quantum Beam Science Directorate, it is an important problem to analyze the data for the neutron dispersion strength of an iron-based high-temperature superconductor observed in J-PARC and to elucidate the superconducting structure. We introduce a research example of a virtual experiment on a scale that only a supercomputer can handle using the modeling by the first-principles calculation in Topic 11-2.

In the earthquake-resistance research for nuclear facilities, improving the precision to simulate the dynamic behavior of an extra-large earthquake is an important problem. First, it is important to model the elastic-plastic behavior of a connection and the neighborhood structure expected to achieve the plastic state. In Topic 11-3, we introduce one of the research examples of the elastic-plastic modeling of the connections between a nuclear building and the equipment.

In the Fukushima support, we build a database that can manage the radiation dose measurement results and a distribution map system that can confirm them on a map based on the accident at the Tokyo Electric Power Company, Incorporated Fukushima Daiichi Nuclear Power Station, in cooperation with the Fukushima Environmental Safety Center, and make this available to the public. In Topic 1-3, we summarize these systems.

In future, we will continue to work hard on nuclear research and development utilizing advanced computational science and generic computer technology. We will also deepen our cooperation with organizations inside and outside JAEA as we progress in the field of nuclear computational science research.