Innovation in Atomic Energy Research through Advanced Computational Science and Technology

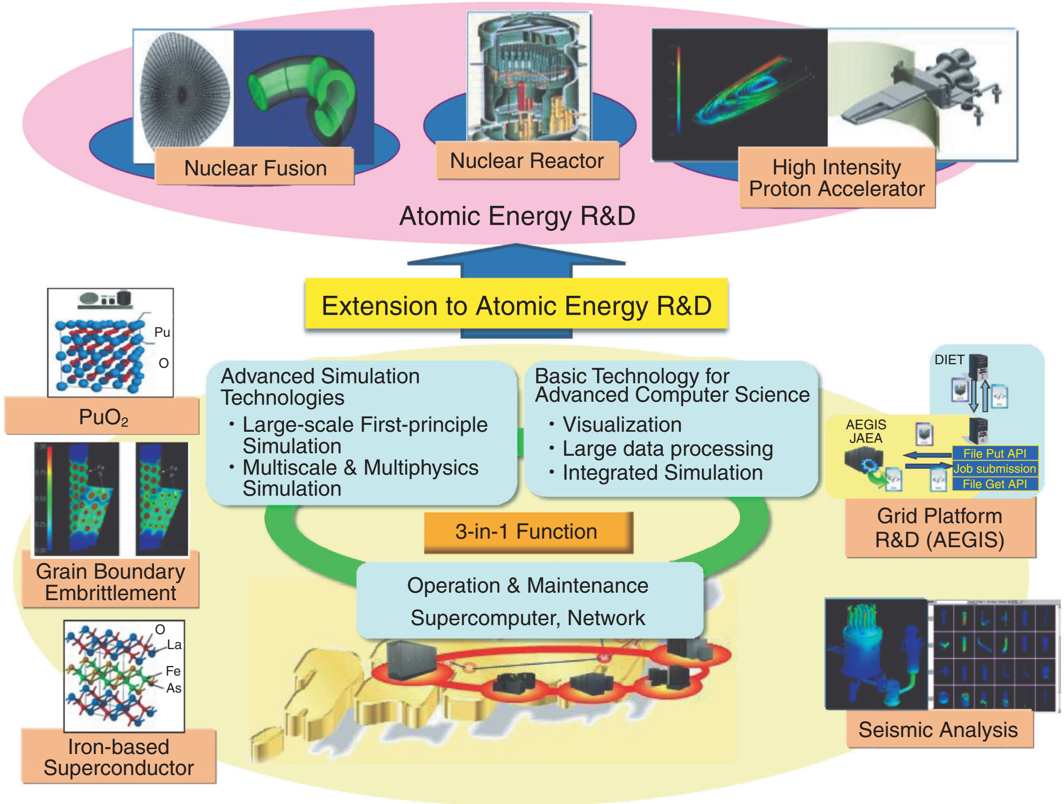

Fig.12-1 Role and achievements of computational science in atomic energy R&D
CCSE leads and supports development of computer science for the atomic energy field by promoting three missions, “Development of basic technology for computer science”, “Development of advanced simulation technologies” and “Support for operation & maintenance of computer systems”. Our achievements in 2008 include the development of Grid middleware, the elucidation of the mechanism of the grain boundary embrittlement, and the discovery of strong-lattice coupling in iron-based superconductors.

Computational science has made remarkable progress since the computer was invented in the 1940’s. At present, computer simulation is a third method by which to pursue R&D together with “theory” and “experiment”. Computer simulation especially has an important role in the atomic energy research, because experiments are difficult to perform due to budget and safety considerations. This being the case, the Center for Computational Science and e-Systems (CCSE) carries out three missions, “Development of basic technology for computer science”, to promote use of supercomputing in atomic energy research, “Development of advanced simulation technologies” to perform realistic simulations, and “Support for operation & maintenance of supercomputer systems” as depicted in Fig.12-1. We believe that the combination of these three missions is the course of R&D making the most effective use of the latest supercomputers. Two typical issues taken up by CCSE R&D in 2008 were as follows.

One was R&D on AEGIS (Atomic Energy Grid Infrastructure), which is Grid middleware for atomic energy research. We connected AEGIS to DIET (Distributed Interactive Engineering Toolbox), which is the Grid middleware in France, through the Internet. The interoperable system we developed enables us to efficiently utilize the computer resources in both Japan and France. Details are reported in Topic 12-2.

The other is a first-principle study by computer simulation of the electronic properties of iron-based superconductors, which were discovered in 2008. We calculated the electronic structures of various iron-based superconducting compounds. Moreover, we compared these structures with measurement data obtained by SPring-8, and confirmed that the magnetic order and the lattice vibration cooperatively contribute to achieve superconductivity. Details are reported in Topic 12-3.

In the future, CCSE will explore more advanced simulation technologies to make more effective use of the latest supercomputers. Furthermore, we will extend these technologies to significantly contribute to the advance of atomic energy R&D.