Atomic Energy R&D by Computer Simulation

—Toward Establishment of Advanced Technology for Atomic Energy R&D—

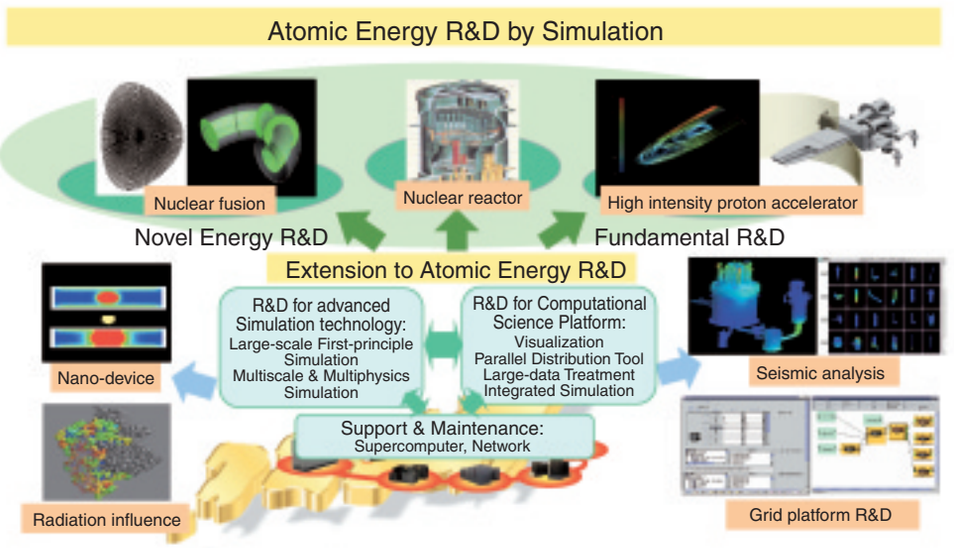

Fig.10-1 Center for Computational Science and e-Systems
Three of CCSE's missions and directions of its R&D are schematically depicted. Combining the three missions i.e., operation & maintenance of facilities, R&D for computational science platforms, and R&D for advanced simulation technology, CCSE aids users in atomic energy R&D and proposes new advanced simulation technologies.

Supercomputers which emerged in 1980's were quickly utilized for atomic energy research and development (R&D). The reason is that the computer simulation was considered to be able to replace previous techniques in atomic energy R&D, which encountered various difficulties due to economical and environmental limitations. The first of these simulations was done on computers with performance poorer than the present PC, but the supercomputer advancement has been so remarkable that they now can perform quite large-scale simulations with a parallel architecture composed of thousands of CPU's.

At the present, CCSE maintains a supercomputer and its support facilities including a network, and supports several users by allowing effective access to its rich computer resources. Moreover, CCSE developed a computational science platform to efficiently operate the parallel processing on computer resources distributed over sections and studies advanced techniques exploring a new field of atomic energy research by using massively parallel calculations.

Based on the previous experience, we believe that combining three computation technologies, for maintenance & support of facilities, a computational science platform, and advanced simulation, is crucial for promoting atomic energy research. Fig.10-1 schematically displays the R&D directions of CCSE. Following this strategy, CCSE has so far produced some achievements which have had a great impact on atomic energy R&D. The following are the latest typical results.

Firstly, CCSE has created a virtual research laboratory whose computer capacity is beyond 50 TFLOPS (1 TFLOPS=1000 billions operations per second) by participating in the ITBL project, which was carried out as a part of Japan's IT policy. Now, CCSE is utilizing this resource to study seismic activity, nanodevices, irradiation influence on the human body, etc. Especially, the seismic analysis study has successfully created 3-dimensional virtual shaking platform prototype which can evaluate 2000 parts of a nuclear plant. If such a study evolves further and we can freely construct a nuclear plant in virtual space, then dramatic reductions of the period for design and the cost for construction are expected.

Next, CCSE has succeeded in realizing a virtual strength test in atomic level simulations for reactor materials. Although the number of simulated atoms is still limited to within a few hundred atoms, a first principle simulation applying a stress into the grain boundary, in which impurities can be segregated and damage can be caused, is now executable. In such a simulation, one can examine several times how the boundary becomes fragile with the impurity segregation etc. If simulation technology progresses further, materials design based on simulations will be really possible.

CCSE continually accelerates R&D for computer science and simulation technology, which in turn dramatically advances atomic energy R&D.