Simulation Science at the National Institute for Fusion Science[*)]

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Based on the past two-decades activities at the Theory and Computer Simulation Center (TCSC) and the Department of Simulation Science (DSS) in the National Institute for Fusion Science (NIFS), the Numerical Simulation Research Project (NSRP) has been launched to continue the activities in TCSC and DSS, and evolve them in a more systematic way for the re-organization of NIFS in 2010. In this study, the progress of simulation science at NIFS in the past two decades is reviewed and an overview of the NSRP for the foreseeable future is reported.

Keywords: simulation science, multi-scale/multi-hierarchy simulation, numerical simulation research project, science of complexity, numerical test reactor, fusion plasma simulation

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1. Introduction

There are three important aspects in the study of fusion plasma simulation. First, fusion plasma is a multi-hierarchy system that encompasses the macroscopic transport phenomena, magnetohydrodynamic (MHD) phenomena, and the microscopic ion and electron dynamics. Second, fusion plasma is covered by multiple areas of physics including not only plasma physics but also atomic physics such as nuclear reaction, and material sciences such as plasma-wall interaction. Large-scale numerical simulation is a powerful tool to explore physics in complex fusion plasmas. Third, to investigate such a complex system via numerical simulation we need to introduce and develop the state-of-the-art technology in simulation science to effectively utilize the most powerful supercomputer available for fusion research. Therefore, interdisciplinary collaboration between simulation science and computer science researchers is also needed.

Thus, for the complete understanding of fusion plasmas, we need to not only investigate the mechanisms of all element physics in each hierarchy of both core and periphery plasmas, but also develop innovative simulation technologies to interlock all hierarchies and physical elements, in accordance with the progress of the supercomputer available for fusion simulation. To promote fusion simulation science more effectively, we have recently launched a new simulation project at the National Institute for Fusion Science (NIFS), called the Numerical Simulation Research Project (NSRP). In this study the progress of simulation science at NIFS and an overview of the NSRP are reported briefly.

2. History of Simulation Science at NIFS

Simulation science at NIFS was initiated by the foundation of the Theory and Computer Simulation Center (TCSC) in 1989, based mainly on the research activities at the Institute for Fusion Theory in Hiroshima University. TCSC had two purposes: one is to understand complex phenomena in fusion plasmas and to systemize their physical mechanisms; the other is to explore the science of complexity in plasmas as a basic research to support fusion plasma studies. Because fusion plasma as our research target is a complex system consisting of multi-scale nonlinear processes in each hierarchy and multiple physical processes, it is extremely important to establish hardware and software environment to explore such a complex system and extract underlying physics. Professor Tetsuya Sato, who was the first director of TCSC, constructed the basis of simulation science at NIFS.

One of the typical examples of simulation research environments established at NIFS is a Grand Man-Machine Interactive System for Simulation (MISSION), which consists of a super-computer, Mass Data Processing System (MDPS), Research Lab, Simulation Lab, Graphic Lab, and CompleXcope. Here, the CompleXcope is a three-dimensional analysis system for complex simulation data, based on the virtual reality system “CAVE” [1]. For scientific visualization, we have modified the original CAVE system and developed the additional functions [2]. A supercomputer system for large-scale plasma simulation at NIFS, the Plasma Simulator, has been installed and periodically upgraded to support various research activities. The present Plasma Simulator, HITACHI SR16000, has the total peak performance of 77 Teraflops (TF) and the total main memory of 16 Terabytes (TB); it will be upgraded to the total peak performance of 315 TF and the total main memory of 32 TB in 2012. MISSION supports every step

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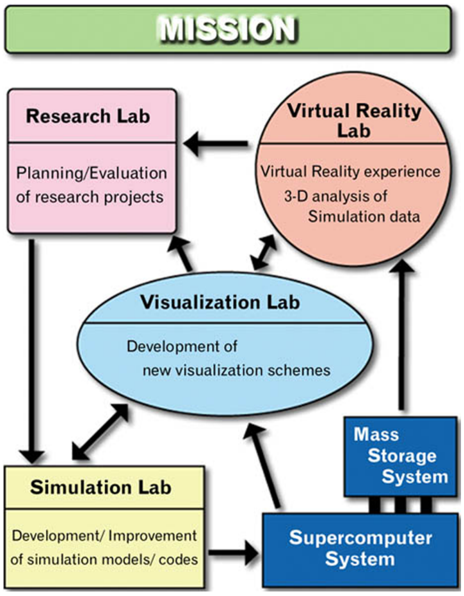

Fig. 1 Flowchart of MISSION.

of the numerical simulation research, which includes planning of simulation projects, developing physical models, coding, executing simulation jobs, and performing three-dimensional analysis of obtained complex simulation data (Fig. 1).

By utilizing MISSION, a series of large-scale numerical simulations were performed to explore the dynamical evolutions in open, non-equilibrium systems consisting of multiple hierarchies, and numerous cutting-edge results in plasma and nuclear fusion sciences were obtained, which also contributed to construct the basis of the science of complexity. The simulation studies of island formation in 3D equilibria [3], relaxation phenomena in spherical tokamak [4], toroidicity-induced Alfven eigen modes [5], ITG turbulence [6], tilt disruption of a field-reversed configuration plasma [7], spheromak merging [8], collisionless driven reconnection [9], punctuated reversals of dipole magnetic field [10], and structure formation of short chain molecules [11] are the typical examples of large-scale numerical simulations.

The Department of Simulation Science (DSS) was established in 2007, by merging two centers, i.e., TCSC and the Computer and Information Network Center, to continue and expand the simulation research activities of TCSC. Three Simulation Research Projects were launched in DSS at the same time, i.e., the Large Helical Device (LHD) and Magnetic Confinement Simulation Project, the Laser Fusion Simulation Project, and the Plasma Complexity Simulation Project [12]. The tasks of the three projects are as follows.

(1) In the LHD and Magnetic Confinement Simulation Project, various researches on multiple physical processes and their mutual interactions occurring in core and edge plasmas have been studied based on fluid and kinetic simulations. The aim is to realize of the Numerical Test Reactor (NTR) to develop the concept of helical magnetic confinement fusion reactor [12].

(2) The Laser Fusion Simulation Project has been promoted to completelly clarify the physics of Fast Ignition and to design targets for Fast Ignition Realization EXperiment (FIREX) project at Osaka University by the Fast Ignition Integrated Interconnecting code (FI^3) simulation under the closed domestic collaboration [13].

(3) The Plasma Complexity Simulation Project aims to clarify magnetic reconnection phenomena, which are controlled by various physics from micro to macro-scale in solar and magnetosphere plasma and fusion plasma, and to clarify the physics of plasma-material interaction in compound physics system.

The research activities in TCSC and DSS also extended in multiple directions. First, the direction bridging different hierarchies, i.e., macroscopic, mesoscopic and microscopic hierarchies. Second, the direction bridging the different domains of a fusion plasma system, i.e., core, edge, and periphery domains. Third, the direction toward multiple compound physics of plasma, atomic, and material sciences. Fourth, the direction toward its diversity covering basic, fusion, and computer sciences.

3. Numerical Simulation Research Project

A new simulation project, called the Numerical Simulation Research Project (NSRP), has been launched to continue the tasks in TCSC and the subsequent simulation research activities in DSS, and evolve them in a more systematic way for the re-organization of NIFS in 2010. Based on large-scale numerical simulation researches utilizing the complete capability of the supercomputer, the NSRP is aiming to understand and systemize physical mechanisms in fusion plasmas and to ultimately realize the NTR, which will be an integrated predictive model for plasma behaviors in the entire machine range. The concept of the NSRP is illustrated in Fig. 2. To realize the NTR, we need all element physics controlling fusion plasmas and innovative numerical technologies to interlock them, along with powerful supercomputing resources at the petascale level or more as a common platform of simulation science. We should also assemble all obtained results to upgrade integral transport model and approach the final NTR in the synergy of LHD experimental groups and fusion engineering groups. In other words, all the simulation tools in the NTR should be experimentally validated to enable predictive simulations with considerably improved physics fidelity for exploring future magnetic confinement systems. Thus, the verification and validation studies of simulation models against LHD experimental results are very important processes to construct the NTR.

In order to realize this approach we assembled nine

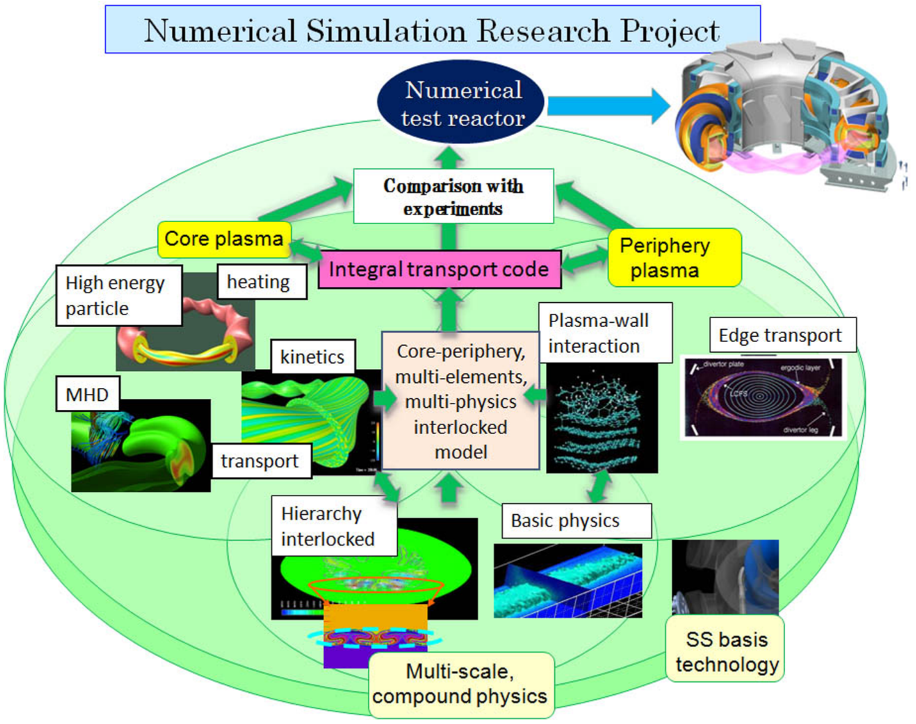

Fig. 2 Concept of the Numerical Simulation Research Project.

research groups responsible for the tasks in the NSRP under closed domestic collaborations, which cover a wide range of simulation subjects including 3D equilibrium of core plasmas and its stability, high energy particle physics, plasma heating, plasma transport, micro and macro turbulence, burning plasma physics, periphery plasmas, plasma-wall interaction, other basic plasma physics supporting fusion science, and simulation methodology such as multi-scale simulation modeling, scientific visualization.

The tasks of the nine research groups in the NSRP and the typical examples of their simulation results are as follows.

(1) "**Plasma fluid equilibrium stability group**" studies macroscopic physics of core plasmas such as MHD equilibrium, MHD stability, the nonlinear global evolution of core plasma, and pellet injection using nonlinear MHD and extended MHD models. The evolution of beta-increasing plasma without any serious disruption is simulated for the LHD plasma [14]. We succeeded in revealing the saturation mechanism of moderate wave number ballooning modes, which grew from unstable $R_{ax} = 3.6$ m inwardly shifted MHD equilibrium [15].

(2) "**Energetic particle group**" investigates physics issues related to energetic particles in toroidal plasmas such as Alfven eigenmodes, neoclassical transport of alpha particles in burning plasmas, and NBI/ICRF heating. Based on the comparison studies of linear and nonlinear simulation runs of a $n = 4$ TAE evolution, it is found that the saturation level is reduced by the nonlinear MHD effects [16].

(3) "**Integrated transport simulation group**" works to develop core transport code in 3D configuration (TASK3D) and to apply it in order to predict the overall time evolution of observable physics quantities in the plasma core. In this research several integrated modules have been developed for the accurate three-dimensional physics [17]. The verification simulations by the application to LHD experimental results have been performed [18].

(4) "**Fluid turbulence transport simulation group**" studies physics issues related to turbulent transport in toroidal plasmas by using the theory and simulation based on fluid model. Turbulence Diagnostic Simulator has been developed for understanding the mechanism of the turbulence structure formation based on the demonstration of experimental measurement and the correlation analysis [19]. By using a set of reduced two-fluid model the excitation of the macro-MHD mode has been demonstrated owing to the multi-scale interaction in a quasi-steady equilibrium formed by the balance between micro-turbulence and zonal flow [20].

(5) "**Kinetic Transport Simulation Group**" investigates anomalous transport mechanisms, collisional transport mechanisms and the multi-scale physics of transport, and predicts the transport level for achieving efficient confinement of high-temperature plasmas based on kinetic modeling. By using flux tube gyrokinetic codes (GKV/GKV-X) the kinetic plasma dynamics

in the five dimensional phase space has been investigated for the LHD plasmas [21, 22]. Collisional transport mechanisms have been studied using Delta-f Monte Carlo codes (FORTEC-3D/KEATS) to directly solve the drift kinetic equation with the finite-orbit-width effect [23, 24].

(6) The objective of "**Peripheral plasma transport research group**" is to construct the model of boundary plasma between the scrape-off layer (SOL) and the divertor plate, and to use this model to investigate impurity transport near a plasma facing wall in LHD. Comparison study of modeling by the EMC3 code to experimental observation on impurity screening of high density plasmas in LHD has been reported [25]. By using the modified ERO code the redeposition profiles of impurities from the divertor plates have also been studied [26].

(7) "**Plasma-wall interaction group**" aims to investigate dynamical process on the surface of plasma facing materials such as chemical spattering of divertor plate and yielding hydrocarbon, via molecular dynamics (MD) simulation, and its extended model. Mechanism of yielding hydrocarbon for graphene, graphite, diamond and amorphous carbon has been investigated using MD simulation [27]. Physical and chemical reactions between hydrogen and graphite in sub-micrometer have been studied using the MD-AC∀T hybrid code [28].

(8) "**Multi-hierarchy physics group**" investigates complex multi-hierarchy phenomena related to fusion plasmas by developing various multi-scale or multi-hierarchy models and numerical techniques. In this study multi-hierarchy simulation models based on domain decomposition method [29–31] and equation-free projective integration method [32] have been developed and successfully applied to the propagation of ion acoustic wave [32], plasma inflow process across the micro-macro domain boundary [30, 32], and collisionless driven reconnection [31].

(9) "**Simulation science basis group**" aims to develop innovative analysis tools of complex simulation data such as scientific visualization on CompleXcope, and various numerical techniques for utilizing powerful supercomputing resources. The softwares developed for this purpose are the modified VFIVE for the analysis of reconnection simulation data [33], AIScope for the analysis of molecular dynamics simulation data, and the simultaneous visualization tool of simulation and experimental device data based on AVS and Fusion VR [34].

Various large-scale numerical simulations have so far been carried out for the analysis of one or two element physics by utilizing the Terascale supercomputer with approximately 10000 CPU cores. Furthermore, as a step toward the realization of the NTR, the NSRP is now promoting the R&D of multi-scale/multi-hierarchy simulation models to assemble several element physics that mutually interact with each other. After the verification and validation studies of simulation models and tools against LHD experimental results, all the obtained results will be used to upgrade the integral simulation model with considerably improved physics fidelity and approach the final NTR.

Significant progress in the NSRP will be achieved by the access to powerful supercomputing resources at the Petascale level and beyond, together with innovative advance in analytical and computational methods. We are now planning to use three supercomputer systems in Japan for this project. The main supercomputer is the NIFS plasma simulator which will be upgraded to the total peak performance of 315 TF and the total main memory of 32 TB in 2012. The other two are the Japanese Next Generation supercomputer "K" at the Kobe Port-Island with the total peak performance of approximately 10 Petaflops (PF), and the ITER-BA supercomputer with the total peak performance of approximately 1 PF, which will be available for public use in 2012.

4. Summary and Discussions

We have reported the progress of simulation science at NIFS within the past two decades and its future direction. The research activities on the science of complexity at TCSC have evolved to those on multi time/spatial scale physics in fusion plasmas and related academic fields at DSS. The research activities in TCSC and DSS also extended in multiple directions, i.e., those bridging different hierarchies and different domains, towards multiple compound physics of plasma, atomic, material sciences, and toward its diversity covering basic, fusion, and computer sciences. These activities and their products form the basis for a new simulation project at NIFS, called the NSRP, which started in 2010 with the ultimate goal to realize "Numerical Helical Test Reactor." Furthermore, to make this approach more effective, nine simulation research groups responsible for each task in the NSRP are assembled under closed collaboration.

Because fusion simulation science is a long-term project, we need to promote education and training programs of simulation science for students and early career researchers who will support the research activities in the foreseeable future. In addition, various R&D programs toward Exascale computing have been started in the field of computer science [35]. However, many problems are yet to be solved in the scientific applications, such as data management, development of hybrid-type/multi-scale simulation codes optimized for machine architecture and user-friendly programming language suitable for complicated architecture of supercomputer with numerous CPU cores and chips. Thus, under the interdisciplinary collaboration with computer science researchers, we need to introduce and upgrade hardware and software environments supporting various collaboration researches on simulation science in accordance with the progress of supercomputing technology available for fusion simulation.

[1] D. Pape, IEEE Comp. Graph. Appl. **16**, 44 (1996).
[2] A. Kageyama, in Proceedings of the Sixteenth International Conference on Numerical Simulation of Plasmas (UCLA, Los Angeles, 1998), p. 130.
[3] T. Hayashi, A. Takei, N. Ohyabu and T. Sato, Nucl. Fusion **31**, 1767 (1991).
[4] N. Mizuguchi, T. Hayashi and T. Sato, Phys. Plasmas **7**, 940 (2000).
[5] Y. Todo, T. Sato, K. Watanabe, T.H. Watanabe and R. Horiuchi, Phys. Plasmas **2**, 2711 (1995).
[6] T.-H. Watanabe and H. Sugama, Phys. Plasmas **9**, 3659 (2002).
[7] R. Horiuchi and T. Sato, Phys. Fluids B**2**, 2652 (1990).
[8] T.-H. Watanabe, T. Sato and T. Hayashi, Phys. Plasmas **4**, 1297 (1997).
[9] R. Horiuchi and T. Sato, Phys. Plasmas **1**, 3587 (1994); W. Pei, R. Horiuchi and T. Sato, Phys. Rev. Lett. **87**, 235003 (2001).
[10] J. Li, T. Sato and A. Kageyama, Science **295**, 1781 (2002).
[11] S. Fujiwara and T. Sato, Phys. Rev. Lett. **80**, 991 (1998).
[12] S. Sudo *et al.*, J. Physics, Conference Series **133**, 012025 (2008).
[13] H. Sakagami, T. Johzaki, H. Nagatomo and K. Mima, J. Phys. IV France **133**, 421 (2006).
[14] K. Ichiguchi and B.A. Carreras, Proc. 23rd IAEA Fusion Energy Conference (11-16 October 2010, Daejeon, Republic of Korea), THS/P5-08.
[15] H. Miura and N. Nakajima, Nucl. Fusion **50**, 054006 (2010).
[16] Y. Todo, H.L. Berk and B.N. Breizman, Nucl. Fusion **50**, 084016 (2010).
[17] A. Wakasa *et al.*, Contrib. Plasma Phys. **50**, 582 (2010).
[18] Y. Nakamura *et al.*, Plasma Fusion Res. **3**, S1058 (2008).
[19] N. Kasuya, S. Nishimura, M. Yagi, K. Itoh and S.-I. Itoh, Plasma Fusion Res. **6**, 1403002 (2011).
[20] A. Ishizawa and N. Nakajima, Phys. Plasmas **14**, 040702 (2007).
[21] T.-H. Watanabe, H. Sugama and S. Ferrando-Margalet, Phys. Rev. Lett. **100**, 195002 (2008); H. Sugama and T.-H. Watanabe, Phys. Plasmas **13**, 012501 (2006).
[22] M. Nunami, T.-H. Watanabe and H. Sugama, Plasma Fusion Res. **5**, 016 (2010); M. Nunami, T.-H. Watanabe, H. Sugama and K. Tanaka, Plasma Fusion Res. **6**, 1403001 (2011).
[23] S. Satake, R. Kanno and H. Sugama, Plasma Fusion Res. **3**, S1062 (2008).
[24] R. Kanno, M. Nunami, S. Satake, H. Takamaru, M. Okamoto and N. Ohyabu, Plasma Phy. Control. Fusion **52**, 115004 (2010).
[25] M. Kobayashi *et al.*, Fusion Sci. Technol. **58**, 220 (2010).
[26] G. Kawamura, Y. Tomita M. Kobayashi, M. Tokitani, S. Masuzaki and A. Kirschner, Contrib. Plasma Phys. **50**, 451 (2010).
[27] A. Ito, H. Nakamura and A. Takayama, J. Phys. Soc. Jpn. **77**, 114602 (2008); A.M. Ito, H. Okumura, S. Saito and H. Nakamura, Plasma Fusion Res. **5**, S2020 (2010).
[28] S. Saito, A.M. Ito, A. Takayama, T. Kenmotsu and H. Nakamura, J. Nucl. Mater. (in press) doi:10.1016/j.jnucmat.2010.12.233; S. Saito, A. Takayama, A.M. Ito, T. Kenmotsu and H. Nakamura, Progress in Nuclear Science and Technology (accepted).
[29] S. Usami, H. Ohtani, R. Horiuchi and M. Den, Comm. Comput. Phys. **4**, 537 (2008).
[30] S. Usami, H. Ohtani, R. Horiuchi and M. Den, J. Plasma Fusion Res. **85**, 585 (2009).
[31] S. Usami, H. Ohtani, R. Horiuchi and M. Den, Plasma Fusion Res. **4**, 049 (2009); R. Horiuchi, S. Usami, H. Ohtani and T. Moritaka, Plasma Fusion Res. **5**, S2006 (2010) .
[32] S. Ishiguro, S. Usami, R. Horiuchi, H. Ohtani, A. Maluckov and M.M. Skoric, J. Physics, Conference Series **257**, 012026 (2010).
[33] H. Ohtani and R. Horiuchi, Plasma Fusion Res. **3**, 054 (2008).
[34] H. Ohtani, N. Ohno, N. Mizuguchi, M. Shoji and S. Ishiguro, Plasma Fusion Res. **5**, S2109 (2010).
[35] W.M. Tang, J. Physics Conference Series **125**, 012047 (2008).