Simulation science for fusion plasmas

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Abstract. The world fusion effort has embarked into a new age with the construction of ITER in Cadarache, France, which will be the first magnetic confinement fusion plasma experiment dominated by the self-heating of fusion reactions. In order to operate and control burning plasmas and next generation demo fusion reactors, an advanced capability for comprehensive integrated computer simulations that are fully verified and validated against experimental data will be necessary. The ultimate goal is to predict reliably the behaviour of plasmas in toroidal magnetic confinement devices on all relevant scales, both in time and space. In addition to developing a sophisticated integrated simulation codes, directed advanced research in fusion physics, applied mathematics, computer science and software is envisaged. In this paper we review the basic strategy and main research efforts at the Department of Simulation Science of the National Institute for Fusion Science (NIFS)- which is the Inter University Institute and the coordinating Center of Excellence for academic fusion research in Japan. We overview a simulation research at NIFS, in particular relation to experiments in the Large Helical Device (LHD), the world’s largest superconducting heliotron device, as a National Users’ facility (see Motojima et al. (1)). Our main goal is understanding and systemizing the rich hierarchy of physical mechanisms in fusion plasmas, supported by exploring a basic science of complexity of plasma as a highly nonlinear, non-equilibrium, open system. The aim is to establish a simulation science as a new interdisciplinary field by fostering collaborative research in utilizing the large-scale supercomputer simulators. A concept of the hierarchy-renormalized simulation modelling will be invoked en route toward the LHD numerical test reactor.

1. Introduction
With the start of the construction of International Thermonuclear Experimental Reactor (ITER) in Cadarache, France, a multi-national collaborative, multibillion dollar effort, as the first in the next generation of burning fusion plasma experiments, a need for comprehensive integrated fusion plasma simulations is becoming crucial. Advances in simulation science enable us to critically evaluate and test our basic theoretical understanding through comparison with experiments. However, a future capability for integrated predictive whole machine modelling will bring about peak scientific
objectives together with highest experimental productivity and the reduced operational risks. It is estimated that one ITER discharge will cost about 1 M$ with operational limits < 2000 pulses per year.

Here, we overview simulation research at the National Institute for Fusion Science (NIFS)- of the National Institutes of Natural Sciences (NINS), in particular relation to fusion plasma experiments in the Large Helical Device (LHD), as the National Users’ facility. NIFS was established as an Inter-University Research Institute in 1989, and the coordinating Center of Excellence for academic fusion research in Japan, with the Mission to promote nuclear fusion science and research on its application, in particular, (1) To promote both experimental research based on the world largest superconducting device: Large Helical Device (LHD) and theoretical and simulation research. (2) To promote collaboration research with universities and institutes all over the country and also international collaborations. (3) To educate graduate students in the department of nuclear fusion science of the Graduate University for Advanced Studies, and also in the other universities. At NIFS, the current performance of the LHD experimental program toward a steady operation, reveals remarkable progress in terms of the proton temperature of 79 Million degree at the density of 20 Trillion/cc, peak density of 1100 Trillion/cc with the internal diffusion barrier (IDB), and the highest ever achieved, steady average beta of 5% and the largest total input energy of 1.6 GJ, in all magnetic confinement fusion devices (see, Motojima, [1]). More recently at NIFS, by merging the former Theory and Computer Simulation Center with the Computer and Network Center, new Department of Simulation Science (DSS) has become among the world largest research groups studying by theory and simulation science, properties of high-temperature fusion plasmas. Main goals of the simulation research are twofold: firstly, Understanding and Systemizing physical mechanisms in fusion plasmas and exploring Complexity science of a plasma, as a nonlinear, non-equilibrium, open system, as a basic research supporting fusion plasma studies. Secondly, the aim is to establish a Simulation Science as a new interdisciplinary field through collaborative research in utilizing the large-scale high-performance supercomputer simulators. Three simulation projects; namely, LHD and magnetic confinement simulation project, Laser fusion simulation project and Complex plasma simulation project have been launched. By developing predictive hierarchy-renormalized simulation model, each of above research goals is expected to be achieved in future, ultimately realizing the LHD Numerical Test Reactor (LHD-NTR) toward the concept of helical magnetic confinement fusion reactor, as priority for steady state operation revealed at NIFS, as a demonstration reactor after ITER. The hierarchy-renormalized simulation model is developed under active domestic and international collaboration; and it consists of the hierarchy-integrated simulation model and hierarchy-extended simulation model. The former is based on the transport model, which is suitable to describe the entire temporal behavior of experimentally observed macro physics quantities, while the latter model is focused at mutual interaction among neighboring hierarchies, as shown in Figure 1. The hierarchy-integrated simulation will be performed by renormalizing the results of the hierarchy-extended simulations, eventually leading toward the LHD-NTR. A basic strategy is schematically shown in Figure 2 [3].

Figure 1 Schematics of physical hierarchies in a plasma
2. Multi-scale models and physical hierarchies

Multiscale modeling in magnetic fusion plasmas are among the most challenging tasks in the contemporary simulation science research. Multiphysics processes governing fusion plasmas span over a huge range of temporal and spatial scales resulting in intractability of direct brute force simulations, in any foreseeable future. In the extreme cases, one finds the ratio of the transport time scale to the electron cyclotron time scale of \(O(10^{14})\) and the device radius to the electron gyroradius of \(O(10^4)\). At the same time extreme anisotropy in the mean free path along and across the magnetic field can reach \(O(10^{10})\), which together with high-dimensionality (3+3=6D) in real and velocity space, intrinsic nonlinearity and sensitive geometry present fundamental challenges to fusion simulations. Currently, scale separation is exploited to a large extent by solving the separate physical (hierarchy) models. Still, in reality, plasma phenomena are coupled since sharing same particle distributions and electromagnetic fields. Moreover, large number of critical cases is identified in fusion plasmas, where essentially coupling between multiscale and multiphysics problems must be performed (Figure 1). En route to developing a hierarchy-renormalized simulation model we present several examples of successful applications to gyrokinetic Vlasov simulations of turbulent transport, nonlinear simulations of energetic particle physics, two-fluid macro-instability simulation with inclusion of micro-turbulence effects, developing a high-resolution MHD code and pellet ablation. The complexity plasma simulations are illustrated with multi-hierarchy magnetic reconnection, blob transport, molecular dynamics and new numerical methodology for multi-scale plasmas. For analyzing huge simulation data, Virtual Reality (VR) system is developed for interactive visualization in 3D space and real time.

**Hierarchy-renormalized simulation**

- **Hierarchy-integrated simulation approach** to interpret and predict plasma behavior under continuous external control (diffusive transport model \(1D\) conf.)
- **Hierarchy-renormalized model** (numerical renormalization) (boundary condition)
- **Core fluid plasma model** (3D configuration space) (closure)
- **Core kinetic plasma model** (5D phase space) (transient dynamics) (turbulent transport model)
- **Peripheral plasma model** (3D/6D phase space)
- **Inside/surface of wall**
- **Boundary layer**
- **SOL/diverter plasma** (interaction of hierarchies and compound physics processes in configuration space)
- **Interconnecting model** (interaction of hierarchies and compound physics processes in configuration space)
- **Hierarchy-extended simulation approach** to understand cross-hierarchy interactions (predictability of hierarchy-integrated simulation significantly depends on this.)

**Figure 2**

2.1. Gyro-kinetic simulation of the reduction of turbulent transport and zonal flow generation in Helical systems

In order to investigate effects of helical magnetic configurations on the ion temperature gradient (ITG) turbulence and zonal flows (ZF), we have performed gyrokinetic Vlasov (GKV) simulations [4,5] by utilizing the Earth Simulator at the Japan Agency for Marine-Earth Science and Technology (JAMSTEC) and the Plasma Simulator at NIFS. The GKV simulation code is extended so as to incorporate magnetic configuration models relevant to LHD experiments. In our recent work [6] for experimentally relevant conditions, we confirmed that an initially given zonal flow kept a higher level for a longer time in the inward-shifted configuration of the magnetic axis than that in the standard one. This is consistent with our analytical theory of zonal flows [7,8]. It should be emphasized that the inward-shifted case is optimized for reducing the neoclassical transport but with more unfavorable stability property than the standard configuration.
In the present study, the nonlinear GKV simulation implemented with the specified magnetic field parameters for the inward-shifted and standard plasma positions successfully confirms generation of large zonal flows enough to reduce the ion heat transport in the former case [9]. Contours of the electrostatic potential in the steady ITG turbulence are shown in Figure 3. For the inward-shifted configuration shown in Figure 3 (left), we clearly see radial structures of poloidal $\mathbf{E} \times \mathbf{B}$ zonal flows in the turbulent flow patterns on the poloidal cross section, while more isotropic $\mathbf{E} \times \mathbf{B}$ vortices are observed in the standard case [Figure 1 (right)]. The larger zonal-flow generation in the inward-shifted case agrees with the linear analysis of the zonal-flow response [6-8] which predicts a larger zonal-flow response to a given source in neoclassically optimized helical configurations such as the inward-shifted one. The obtained results agree with our theoretical prediction, and are consistent with experimental observation of better confinement in the inward-shifted LHD plasma [10].

![Figure 3](image)

**Figure 3** Contours of the electrostatic potential of ZF and ITG turbulence from GKV simulation for inward-shifted (left) and standard (right) LHD configurations. Normalization is chosen as $e\phi L_n/T_e\rho_i$.

2.2. Interaction between Alfvén eigenmodes and energetic particles

Alfvén eigenmodes are well known MHD type of oscillations in magnetically confined plasmas. However, in burning plasmas, fusion products in a form of alpha particles born in the 3.5 MeV energy range can resonate with Alfvén eigenmodes. This may further lead to (inverse) Landau growth and excitation of Alfvén eigenmodes and undesirable transport of energetic alphas. Many experiments using energetic ion beams generated during Neutral Beam Injection (NBI) or Ion Cyclotron Resonance Frequency (ICRF) heating of fusion plasmas have been performed in order to understand the interaction between Alfvén eigenmodes and energetic particles [11].

2.2.1. Simulations of Alfvén eigenmodes with an extended Ohm’s law for ITER-like plasma.

The simulation code for MHD and energetic alpha particles, MEGA [11-12], has been extended with the drift model with the ion finite Larmor radius effect. In addition, the Ohm’s law is extended with the effective resistivity where the electron damping is accounted by the Landau fluid model. The extended MEGA code [13] is benchmarked with respect to the linear growth rate and the damping rate of the alpha-particle-driven n=4 toroidal Alfvén eigenmode (TAE) in the TFTR D-T plasma shot #103101. The initial energetic particle distribution is similar to that of a previous particle simulation reported in Ref. 14, where an isotropic distribution for the energetic alpha particles is used in the velocity space. The number of marker particles used is $5.2 \times 10^7$. The number of grid points is $101 \times 16 \times 101$ for the cylindrical coordinates $(R, \varphi, z)$ where $R$ is the major radius coordinate, $\varphi$ is the toroidal angle coordinate, and $z$ is the vertical coordinate. The simulation domain in the toroidal angle coordinate is $0 < \varphi < \pi/2$ for this benchmark test of n=4 TAE. First, the linear growth rate was investigated with the effective resistivity turned off. The destabilized mode has a TAE spatial profile which consists of two major harmonics $m/n=6,7/4$ and frequency 215kHz. These results are consistent with the calculation with the NOVA-K code [5]. The linear growth rate obtained from this simulation,
is $8.7 \times 10^3$ of the mode frequency. This linear growth rate is close to what is observed in the previous particle simulation [14] and calculated in the NOVA-K code [15]. Next, the damping rate was investigated with the alpha particle effects turned off and the effective resistivity turned on in the linear growth phase. The damping rate is $\gamma_d/\omega = 4.8 \times 10^{-3}$, while we found $\gamma_d/\omega = 1.6 \times 10^{-3}$ with the conventional MHD model. The increase in damping rate in the drift model arises from the effective resistivity. The damping rate with the effective resistivity is roughly half of the NOVA-K results [15].

We investigated an ITER-like plasma with the extended MEGA code [13]. The plasma profile investigated is based on the non-inductive scenario reported in ITER Technical Basis [16]. The major and minor radii are $R = 6.35$ m and $a = 1.85$ m. The ellipticity and the triangularity are 1.85 and 0.4, respectively. The toroidal magnetic field at the plasma center is $B = 5.18$ T. The number density is assumed to be uniform $6.7 \times 10^{19}$ m$^{-3}$. The safety factor is $q_\Theta = 3.5$ at the plasma center, $q_{\text{min}} = 2.2$ at $r/a = 0.7$, and $q_{\text{edge}} = 5.3$ at $r/a = 1.0$. The thermal pressure profile is assumed to be uniform to focus on the instabilities driven by the alpha particles. The beta value of the thermal plasma is $\beta = 2.5\%$. The electron temperature is 12.3 keV, which is employed in the electron Landau damping model. The birth velocity of the alpha particle corresponds to $1.48v_A$; $v_A$ is the Alfvén velocity at the plasma centre.

The spatial profile of the alpha particle beta value is calculated with the plasma profile of the non-inductive scenario taking account of the D-T reaction rate and the slowing-down of alpha particles. The alpha particle beta value at the plasma centre is $\beta_{\alpha,0} = 2 \times 10^2$. The nonlinear evolution of toroidal Alfvén eigenmodes (TAE) in the ITER-like plasma was investigated [13]. The number of marker particles used is $2.1 \times 10^6$. The number of grid points is $101 \times 100 \times 101$ for the cylindrical coordinates. The TAEs with toroidal mode numbers $n = 2-5$ are destabilized. The TAEs peak around $r/a \approx 0.3$. The toroidal electric field profile of $n=3$ TAE is shown in Figure 4. The saturation levels are $\delta B_r/B \approx 10^{-3}$. The redistribution of alpha particles leads to the change in alpha particle beta profile by $\delta \beta_{\alpha} \approx 10^{-3}$.

### 2.3. Nonlinear evolution of MHD instability

We have been carrying out direct numerical simulations of the fully three-dimensional, compressible and nonlinear magnetohydrodynamic (MHD) simulations in the geometry of LHD. Purpose of the research is clarifying how hot plasma survives the interchange/ballooning instability in the LHD. For this purpose, the MHD In the Non-Orthogonal System (MINOS) code is developed. In the MINOS code, variables are described by the contravariant component on a helical-toroidal coordinate system. The 8th order compact finite difference code is adopted in the MINOS code to separate variables into directions parallel and perpendicular to magnetic field lines.

Direct numerical simulations by the use of the MINOS code are carried out for linearly unstable magnetic configuration, which is characterized by the position of the magnetic axis $R_{ax}=3.6$ m and the beta-value of 3.7% at the peak position. Number of grid points range from $(97, 97, 640)$ to $(385, 385, 64)$ depending on the Reynolds number in the simulation. By the numerical simulations, we have found three mechanisms which can help the hot plasma to overcome the instability: (1) the local flattening of the pressure, (2) the kinetic energy release into the direction parallel to the magnetic field lines, and (3) the compressibility effect to reduce the linear growth rates. [16-20]

While these computational works have been carried out carefully, the influences of the small-scale motions on large-scale motions remain unknown. The difficulty comes from the characteristics of the interchange/ballooning instability. Because of these short-wavenumber instability, we need infinite

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**Figure 4.** Toroidal electric field profile of $n=3$ TAE for ITER-like plasma.
number of grid points for ideal simulations. A simulation study with a large number of grid points (and thus a large Reynolds number) is now under progress [21].

2.4. Multi-scale interactions among micro-turbulence, macro-MHD instability, and zonal flows

Multi-scale interactions in magnetically confined plasmas were investigated analytically and numerically. The interaction between micro-turbulence and zonal flow is a typical multi-scale interaction because toroidal and poloidal mode numbers of micro-instabilities are much larger than one, while these numbers are zero for zonal flow. There are another multi-scale interaction between different instabilities which are independent in linear evolution when their free energies are different, for instance, there are interactions between micro-instability due to pressure gradient and macro-MHD instability that is caused by current density gradient and has low toroidal and poloidal mode numbers.

In our recent study we considered a situation in tokamak configuration that a current driven macro-MHD instability arises in a quasi-equilibrium including micro-turbulence and zonal flow. This is because a macro-MHD instability is destabilized when there arises one or more resonant q surfaces where the safety factor q is equal to a small rational number, while micro-instabilities can arise even if there is no integer q surfaces. Thus, micro-turbulence almost always exists before destabilization of macro-MHD instability. In order to examine this situation we carried out a three-dimensional numerical simulation of a reduced set of two-fluid equations and investigated mutual interaction between micro-turbulence and macro-MHD mode (double tearing mode) [21,22]. In the simulation micro-instabilities (kinetic ballooning mode) are destabilized at first, and then turbulent state is formed as shown in the left frame of Figure 6. We found that the excitation of macro-mode by the micro-turbulence is different from macro-MHD instability because the spatial profile of the former is significantly different from the spatial profile of double tearing mode. The energy transfer from micro-turbulence to macro-mode is similar to the energy transfer from micro-turbulence to zonal flow [22]. The macro-mode is a part of turbulence in the turbulent state. After a certain period of time, then, the induced macro-mode by the turbulence becomes eigenfunction of double tearing mode and grows up with magnetic reconnection as shown in the right frame of Figure 6, in the case that the equilibrium has free energy of macro-MHD instability such as a current density gradient [21]. When the free energy is small the double tearing mode saturates, and then we have a new quasi-equilibrium including not only the micro-turbulence and zonal flow but magnetic islands [21]. The magnetic reconnection of double tearing mode is caused by non-ideal effect due to turbulent mixing of magnetic flux at the
resonant surfaces [23]. The effect of zonal flow produced by micro-turbulence on the stability of double tearing mode is not clear [24], while the zonal flow shear is suppressed by the appearance of double tearing mode as implied in Ref. [21].

![Image of color-contour of electrostatic potential]

**Figure 6.** Three-dimensional color-contour of electrostatic potential. The quasi-steady state including electromagnetic turbulence is formed in the left frame. After the appearance of macro-MHD instability the spatial structure of turbulence is altered in the right frame.

2.5. Pellet ablation in a plasma

There are many important physics processes in connection with pellet fueling, not the least in the prediction of the pellet ablation rate and penetration distance in the plasma. Pellets ablating in hot plasma are surrounded by a cold, dense neutral ablation cloud which expands in all directions near the pellet, and then after the flow ionizes, it becomes constrained to follow the magnetic lines. To gain a fuller understanding of those atomic processes and multi-dimensional effects, a time-dependent code CAP has been developed which can rigorously treat the dynamical coupling between interior pellet motions and the exterior ablation flow [25]. The code uses an Eulerian approach based on the cubic-interpolated pseudoparticle (CIP) method [26].

In order to examine 2D effects resulting from anisotropic heating imposed by the magnetic field, the cylindrical axisymmetric coordinate system (r, z) is used. No effect of the magnetic field, except for setting the direction of the electron heat flux inducing the ablation, is included in the study. A deuterium pellet with an initial radius of 2 mm is used. Plasma electron temperature and density are 2 keV and $10^{14}$ cm$^{-3}$, respectively, which are assumed to be constant throughout the temporal evolution. The pellet surface pressure differential is of course due to the fact that the heat flux following magnetic field lines intercepting the pellet near the polar axis is entirely blocked by the pellet and thus fully absorbed, while the heat flux following field lines just grazing the pellet surface is partially transmitted across the equatorial midplane, so there is less absorption at the equatorial points. As a result, since the areal ablation rate is more enhanced at the poles than at the equatorial points, the ablation cloud becomes thicker in the polar direction than it is along the radial coordinate in the equatorial midplane. This leads to the ovalshaped density contours elongated in the polar direction as shown in Figure 7 at different times. The contour of the pellet density (which is uniform inside the pellet) has the opposite shape. Since the shear stress induced by the anisotropic pressure distribution can exceed the yield strength of the solid, the solid pellet becomes fluidized and deformed into an oval shape flattened in the polar direction and elongated in the radial direction. After a longer time, the pellet becomes flattened into a thin pancake while losing mass by ablation.

One of the key results of the study is that pellet deformation can shorten the lifetime of the pellet. The area of the pellet projected normal to the magnetic field lines increases at first, reaches a peak, and then falls to zero later on as shown in Figure 7; it reveals the essential dynamics of 2D pellet ablation. It is seen that the 2D ablation rate versus time curve (thick solid line) depends on the projected area
because the total heating power available for driving ablation is simply proportional to the area. On the other hand, the dashed line plots the ablation rate for the 1D spherical symmetric isotropic heating. The ablation rate steadily decreases in accordance with the monotonically decreasing pellet size. The dashed line agrees with the thin solid line obtained by the transonic flow model [27]. In result, it is found that the effect of the pellet deformation can shorten the pellet lifetime.

Figure 7. (left) Isodensity contours in the r-z plane in the 2D cylindrical axisymmetric coordinate system. Frames correspond to the time at 10, 20, 30, 40, 50 and 60 µs. Black lines indicate first sonic, shock and second sonic surfaces. (right) Time dependence of the pellet ablation rate for a constant heat flux over the pellet lifetime. The solid curve shows 2D cylindrical geometry and the dashed curve is 1D spherically symmetric case. The thin solid line is the ablation rate from the transonic flow model.

2.6. Multi-hierarchy simulation model for magnetic reconnection

Magnetic reconnection, which is a multi-scale phenomenon bridging between macroscopic and microscopic hierarchies, is widely believed to be one of important mechanisms controlling energetically active phenomena observed in high temperature, magnetized plasmas such as the solar flare, the magnetosphere, and fusion plasmas. For example, a microscopic process leading to the generation of electric resistivity such as wave-particle interaction and binary collisions is needed to excite magnetic reconnection. On the other hand, global plasma transport and global change of field topology take place as a result of magnetic reconnection, which, in turn, affect reconnection mechanism itself through complex nonlinear processes. Thus, its whole picture should be clarified by solving both microscopic physics and macroscopic physics consistently and simultaneously.

We are now developing multi-hierarchy simulation model for magnetic reconnection under MARIS (MAgnetic Reconnection Interlocked Simulation) project [28, 29]. The simulation model is based on domain decomposition method and consists of three parts (see left panel of Figure 8), i.e., MHD model to describe global dynamics of reconnection phenomena in the region far from reconnection point, electromagnetic PIC model (PASMO) to describe the microscopic processes in the vicinity of reconnection point, and interface model to describe the interaction between micro and macro hierarchies in the interface region. Both multi-time scale scheme [29] and shake-hand scheme [30] are also adopted for this interface model. Right panel of Figure 8 demonstrates the propagation of one-dimensional Alfven wave using developed simulation model where a uniform external magnetic field exists in y direction, mass ratio $m_i/m_e=100$, PIC domain is located in the center of the simulation box $(96<y<160$, spatial coordinate $y$ is normalized by $c/\omega_A$), MHD domains in both sides of PIC domain $(0<y<64, 192<y<256)$, and the interface domains exist between MHD and PIC domains $(64<y<96, 160<y<192)$. It is clearly seen in Figure 8 that Alfven wave is propagating from MHD domain to PIC domain, and from PIC domain to MHD domain smoothly. Thus, it is concluded that the developed interlocked scheme works well.
2.7. Three dimensional PIC simulation of blob dynamics

Recently, transport of edge plasma in magnetic confinement fusion devices has been recognized to be mostly convective and intermittent. As a theoretical explanation, blobs which are long-living macroscopic coherent structures have been referred. Some theoretical and numerical studies which are using two-dimensional modelling have been performed and their dynamics and stability have been revealed. However, these works have employed some assumptions to reduce the equations and the validation is not clear. We have planned three dimensional particle-in-cell (PIC) simulation studies to reveal detailed physical picture. The configuration of our 3D PIC simulation is following: an external magnetic field is pointing into the z-direction. Particle absorbing boundaries corresponding to diverter plates are placed at both ends of the z-axis. A particle absorbing plate corresponding to the first wall is also placed at one end of the x-axis, while a particle reflecting plane at the other one. Particle impinging onto the absorbing boundaries are removed from the system. In the y-direction, periodic boundary conditions are applied. Initially, a high density blob, like a piece of spaghetti, is placed along the magnetic field line in the center of the system. Figure 9 shows the temporal evolution of the ion density profile in the x-y plane at the center of the system. The blob moves across the magnetic field due to EXB drift, where electric field is self-consistently created by grad B drift. Its speed is about 0.1 c_s, where c_s is the ion acoustic speed [31]. More detailed study is under consideration.

2.8. Molecular Dynamics Simulation of Hydrogen Atom Sputtering on a Graphite (0 0 0 1) Surface

Hydrogen atom sputtering on a graphite surface of divertor in the LHD was investigated using molecular dynamics (MD) simulation. Because graphite has a layer structure, two kinds of potential models were used. One is the modified Brenner reactive empirical bond order potential to represent a covalent bond when a distance of particles is shorter than 2.0 Å [32, 33]. The other potential model is
the interlayer intermolecular potential developed by us to represent the layer structure with ‘ABAB’ stacking [34]. Time is developed by the second order symplectic integration. Because the farmer potential model is a complicated function, a time step is very small time $5 \times 10^{-18}$ s. In this simulation, layered graphite is composed of eight graphene layers in which an interlayer distance is of 3.35 Å under the periodic boundary condition except for the direction perpendicular to graphene surfaces. Hydrogen atoms are injected onto a graphite (0 0 0 1) surface at a flux $2.5 \times 10^{30}$ atom/m²s. The MD simulation follows conditions of constant energy and volume, that is, temperature is not controlled.

The following dynamics of erosion was found by the MD simulation. The graphene layers were peeled off one by one from the surface when the bombardment of hydrogen atoms continues (Figure 10). However, under graphene layers maintained the layer structure of graphite. This phenomenon is called ‘graphite peeling’. On the other hand, the graphite peeling did not occur in the MD simulations of graphite with vacancies and graphite without the interlayer intermolecular interaction. Both of these graphite change into an amorphous structure due to the bombardment of hydrogen atoms. This fact implies the following mechanisms. The repulsion of the interlayer intermolecular interaction defends against approach of the graphene layers and then the layer structure is maintained. However, a vacancy does not cause the interlayer intermolecular interaction and carbon atoms around the vacancy which have only two covalent bonds become more stable to create the third covalent bond with a carbon atom of the other layer than to keep the layer structure. In addition, it is also important that hydrocarbon molecule created from the graphite peeling had mainly a chain structure. The ends of the carbon chains were often terminated by the hydrogen atom, while the center of carbon chain does not attach hydrogen atoms.

![Figure 10](image)

**Figure 10.** Graphite peeling when incident energy is 5 eV. White and green spheres indicate hydrogen and carbon atoms. Green lines indicate covalent bonds.

2.9. *Macro Projective Integration- EFREE- Method for Multiscale Plasmas*

Multiscale problems are difficult to simulate due to interconnected physics of micro- and macro-scales which defies direct brute force numerical computations. A potential of a novel simulation framework in plasmas, Macro Projective Integration (called, Equation-free) method has been investigated [35]. Based on a micro-physics simulator (kinetic, i.e., particle-in-cell code-PIC), the macro-scale dynamics is determined by repeatedly extrapolating forward macro variables obtained from short bursts of micro simulations [36]. Different schemes for reconstruction and mapping between high-dimensional (micro) and low-dimensional (macro) phase space, using: moment representation, cumulative distributions, wavelets, etc., are analyzed [37-38]. Starting with proof-of-principle studies of simple one-dimensional nonlinear plasma paradigm, i.e. the ion sound waves, it is expected to be able to eventually move to more realistic multiscale fusion plasma models, as visualized in Figure 11.
3. Conclusions

In conclusions, computer simulations are increasingly envisioned as the third methodology of science aiming to bridge a gap between the traditional theory and experiments by taking advantages in rapid progress in applied mathematics, computer science and high-performance computers. Moreover, the development of validated predictive simulation codes is understood to be crucial to ensuring the success of future burning plasma experiments, such as ITER. The future role of Petascale toward Exascale computing capability will be becoming of strategic importance for achieving above goals, as stressed in the comprehensive long-term proposal for a leadership Fusion Simulation Project (SciDAC) in US [39]. At NIFS, the present supercomputer is shortly to be replaced by the new Plasma Simulator system (Figure 12) in the competitive 100 teraflops range to be in the second stage upgraded to 315 TF. In particular, it may be stressed that in contrast to other leading supercomputer systems which typically share resources within the broad scientific community, NIFS Plasma Simulator, is likely the largest supercomputer system entirely committed to research on plasma and fusion science.

![Figure 11. Concept of EFREE projective integration in a plasma (left), and electron and ion kinetic energy (right) in ion sound waves from a standard PIC (red) and EFREE method.](image)

![Figure 12. New Plasma Simulator supercomputer system at NIFS](image)

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