# 5. Theory and Computer Simulation Project

Various computer simulation researches have been pursued in the framework of the simulation science, which include simulations related to magnetic fusion plasma physics, laser fusion plasma physics, space plasma physics, basic plasma physics, physics of molecular dynamics and so on, and also related aria supporting computer simulations such as numerical technique, visualization technique, virtual reality technique, and network technique. Some of them are originally initiated by NIFS, and the others are initiated through the NIFS collaboration program. The NIFS collaboration program is important in order to deepen physics understanding and extend the range of the simulation science. With the progress of the computer performance, the simulations based on the reduction to the elements or simulations in the mono-hierarchy are leading to the states that the simulations could explain and interpret the individual experimental phenomena. Thus, as a natural tendency, the paradigm shift is beginning from the simulations based on the reduction to the elements to those based on the integration of elements or simulations interconnecting various space-time scales or hierarchies in order to understand and predict a whole structure of the natural phenomena.

In order to develop such a predictive simulation code system, a hierarchy-renormalized simulation model is being developed, which consists of hierarchy-integrated simulation approach and hierarchy-extended simulation approach. The former model, - which is mainly based on a transport model with simple theoretical models representing physical processes in various hierarchies -, is suitable to investigate the entire temporal behavior of experimentally observed macro physics quantities, and the latter model, - which is mainly distinguished into: fluid core plasma description, kinetic core plasma description, and peripheral fluid/ kinetic description with various physical processes -, is focused on the mutual interaction among neighboring hierarchies.

Simulation codes in the hierarchy-extended simulation approach are intensively developed from two ways; one way from macro to micro scales, and the other way from micro to macro scales. In the way from macro to micro scales, the nonlinear evolution of the interchange and ballooning modes is investigated in comparison with LHD experimental results, which might lead to understanding the validity range of the MHD theory. Resistive Wall Mode (RWM) is one of the key issues in ITPA MHD physics. In order to perform the nonlinear RWM simulations with multiple- helicity under the condition of the small current quench observed in JT-60-U, the simulation code based on the reduced equation is improved, so as to use Bi-conjugate gradient method and MPI. As a result, it is found that the number of used Fourier modes significantly affect nonlinear behaviors.

The interaction between MHD modes and energetic particles is considered to be one of interconnecting phenomena in the hierarchy-extended simulation approach. Properties of energetic-particle continuum modes (EPM) in tokamak plasmas were investigated using the hybrid simulation code for MHD and energetic particles; MEGA. It has been clearly shown that the energetic-ion orbital frequency determines the EPM frequency. A new gyro-kinetic plasma simulation model for electromagnetic phenomena has been constructed. In this model, the total characteristic method, where the $\delta f$ particle-in-cell simulation model is complemented with the fluid model to satisfy the conservation properties, is applied to electrons. Both the real frequency and damping rate of kinetic Alfvén wave have been computed correctly for various electron beta values.

In order to extend the MHD fluid model into multiple- phases including gas, liquid, and solid phases, the CAP code, which is originally developed for investigating atomic processes related to the pellet injection, is being extended so as to include MHD phenomena in the general toroidal magnetic configurations. The difference of the pellet penetrations between tokamak and LHD is being explained.

The effects of microscopic scales such as the Hall term, pressure anisotropy, electron inertia, and wave-particle interaction as well as flow on properties of equilibrium are being investigated, in order to understand the basis of the extended MHD and consider the closure problems of fluid equations. Multiple scale nonlinear interactions among microscopic turbulence, macroscopic MHD instabilities, and zonal flows have been examined, where a reduced two-fluid model is used. The simulation firstly demonstrates that a macroscopic MHD mode is excited, as a result of multiple scale interaction, in a quasi-steady equilibrium formed by a balance between microscopic turbulence and zonal flow. This multiple scale simulation is more comparable to the experimental observation of growing macroscopic MHD activities than earlier MHD simulations starting from linear macroscopic instability growth in a static equilibrium, because plasmas in experiments inherently include turbulent fluctuations and zonal flows, and they apparently affect the growth of macroscopic MHD modes through multiple scale interactions.

In order to understand the anomalous transport by toroidal ITG modes in the helical configurations such as LHD, the gyrokinetic simulation code GKV with high resolution in velocity space is extended into the non-axisymmetric toroidal geometry. It is clearly observed that the zonal flow generated by the ITG turbulence leads to reduction of the ion heat transport in the nonlinear saturation phase of the ITG instability, and that the ion heat transport in the inward shifted model, which has the larger linear growth rates of the ITG instability, is observed in a level comparable to the standard case. This is attributed to the stronger zonal flows generated in the inward-shifted model configuration.

To study peripheral (edge) plasmas near the separatrix or the last close flux surface, and SOL plasmas including divertor function is one of the key ingredients for understanding the plasma as a whole. The induced charge of the spherical dust particle on the plasma-facing wall and the resultant electrostatic potential due to the induced charge are analytically and numerically evaluated. Moreover, gravitational effects on release conditions of dust particle from plasma-facing wall are investigated in the aspects of acting force on dust and critical radius. In order to consider the interaction between core and peripheral plasmas, a dynamic five-point model of the peripheral plasma (scrape- off-layer (SOL) - divertor plasmas) and an integrated code TOPICS-IB based on the 1.5-dimensional core transport code TOPICS extended to the integrated simulation for burning plasmas are developed. It is shown by using the TOPICS-IB to the study of the energy loss caused by ELMs that the ELM energy loss decreases with increasing the collisionality.

Research project is reported aiming to propose the experimental plan for the steady state operation of the high-beta FRC plasma to realize $\alpha$ particle simulation by using a particle simulation, an equilibrium analysis and a MHD stability analysis based on the experimental database.

A Fast Ignition Interconnected Integrated ($FI^3$) project is continuously being promoted for evaluating fast ignition with cone-guided targets. In this project, the arbitrary Lagrangian Eulerian hydro code (PINOCO), the collective Particle-in-Cell code (FISCOF1), and the relativistic Fokker-Planck code (FIBMET) are integrated via data exchanges. Dependence of electron energy spectra on the scale length is investigated. Two-dimensional PIC simulations were used to study strong laser-plasma interaction with cone targets and generation of fast particles

In order to investigate the dynamical evolution of collisionless driven reconnection, electromagnetic PArticle Simulation code for a Magnetic reconnection in an Open system (PASMO) is being developed. In this model, the interaction between macro system and micro system is expressed by the plasma inflow and outflow through the system boundary. Using developed simulation code, both fast electron inflow channel and force balance in electron dissipation region are investigated. Structure of ion dissipation region is also examined from the aspect of off-diagonal components of pressure tensor term due to ion meandering motion. In order to clarify triggering mechanism of collisionless magnetic reconnection, anomalous resistivity associated with drift kink instability and lower hybrid drift instability in a thin current sheet are studied in detail by using particle simulation. Simultaneously, multi-scale simulation algorism for connecting microscopic and macroscopic regions is being developed based on MHD and PIC codes. Three-dimensional MHD simulation code with dynamic AMR (Adapted Mesh Refinement) and Roe or Roe-MUSCL (Monotone Upstream-centered Scheme for Conservation Laws) method is being developed for treating shock structure exactly. Also, in relation to a real-time earth magnetosphere simulator for forecasting space weather, kinetic effects in geomagnetic disturbance are studied. Particle acceleration due to strong electromagnetic fields in shock waves is extensively investigated continuously. The evolution of the rotating accretion disks is examined by using global 3D MHD code, by which it has been found that when an inner torus is formed, the disk shows sawtooth-like oscillation with period about 10 rotation time of the torus. Structures of the magnetic field and velocity in stars are discussed based on the mean field MHD equations. As a special case, the solution constructed by the Beltrami solution in the stellar convection zone with the symmetry in the azimuthal direction is presented. Moreover, effects of multiple-species ions on plasma-flow velocity-shear-driven instabilities are investigated.

Molecular Dynamics simulations might become one of key simulations for NINS collaborations. To clarify the yielding mechanism of small hydro-carbon molecules in chemical sputtering between hydrogen and graphene sheets, classical MD simulation with modified Brenner's REBO potential has been used in a more realistic physical system. It is found that momentum transfers from incident hydrogen to graphene causes to destroy graphene structure and that almost all fragments of graphene sheets form chain-shaped molecules, and that yielded hydrocarbon molecules are composed of carbon chain and single hydrogen-atom. The similar type of simulation is done for hydrogen isotope for more simple system. Related to divertor or wall heat load, graphene melting by rise in temperature is studied, from which creation of chain-like carbon molecule is found. Amphiphilic molecule possesses hydrophilic (water-loving) groups chemically bonded by hydrophobic (water-disliking) groups. Under certain condition, amphiphilic molecules spontaneously self-assemble in water to form small aggregates called "micelles", which are generally represented as small compact globules. The interior of micelle is composed of hydrophobic groups and protected from water by the outer corona of the hydrophilic groups. With a view to investigating micelle formation in amphiphilic solution at the molecular level, MD simulations of coarse-grained amphiphilic molecules with explicit solvent molecules are performed, leading to the identification of micellar shape. Aiming at the quantum transport phenomena in the non-equilibrium system in the strong magnetic field, the Nernst effect in the regime of the ballistic conduction is studied. Moreover, a hydrogen neutral transport code for LHD plasmas is under developed, in order to analyze spectroscopically measured atomic and molecular emission line intensities and profiles.

Multifractal tools have been employed in order to test the universality of the edge turbulence properties in various magnetic confinement devices. It was shown that Large Deviation Spectra (LDS) could represent a powerful tool enabling advanced insight into the multifractal processes and provide information that is sensitive to the data and hence to the confinement device in which the date were generated. An ensemble of the vortex rings in the super fluid is simulated in terms of the vortex element method, to examine the spatial distribution law, energy spectrum and energy dissipation of the ensemble. Also, mechanism of energy cascade in NB turbulence is examined by using massive parallel DNS. Simulation study of scale hierarchy in plasma turbulence is done in the framework of Hall MHD by using shell model. The structures responsible for generation of dissipation of the turbulent energy in homogeneous isotropic and shear turbulence are investigated in the case of incompressible flows. Such structures are considered to be similar to Lundgren stretched-spiral vortex. The large scale turbulent structures with heat transfer are reported.

The concept of the hierarchy-renormalized simulation model and status of development of the hierarchy-integrated simulation approach as a part of the hierarchy-renormalized simulation model are reported. An alternative coarse projective integration method; so-called Equation-Free method, for multi-scale plasma simulation is also reported. A 3D electrostatic Particle- in-Cell (PIC) code together with Monte Carlo collision technique is being developed in order to investigate peripheral transport. The numerical method for solving the partial differential equation by completely separating the analytic definition of interpolants from the geometric elements is being developed, where the new finite node methods (FNM) and the boundary node methods (BNM) to resolve the accuracy degradation problem are introduced. The parallelization of FDTD method in terms of OpenMP is reported. Orthonormal divergence-free wavelet analysis is used in order to investigate nonlinear interactions in a rolling-up vortex sheet, so that it is found that the active nonlinear interactions are very closely distributed around the coherent structures irrespective of the forward or backward transfers and that the dominant nonlinear interactions are “local” in the sense of distance.

The design using large-scale virtual reality (VR) device like CAVE is tried in various fields. There are two main purposes to use the VR system in design. One is to observe objects in real three-dimensional space and the other is to be used in the operation of assembling parts. The aim to build the virtual realty system with the collision and the interference detection function in real time is reported. This system consists of two computers, one is for the virtual environment and the other is for collision detection and these computers are connected on the network. The research is reported about 3D shape representation of detailed shape models for immersive virtual systems. One of the goals of this study is to implement virtual laboratory. In the system, an effective and efficient way of the shape representation has been required in order to establish experiments using photorealistic objects.

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