5. Theoretical and Simulation Researches

Various theoretical and simulation researches have been pursued in the framework of NIFS collaboration program, which include theoretical studies and 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 techniques, visualization techniques, virtual reality techniques, and network techniques. 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 field of the theoretical works and simulation science.

With the progress of the computer performance and theoretical background, 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 in the department of simulation science. In the case of the LHD and magnetic confinement simulation project, the hierarchy -renormalized simulation model 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. Knowledge obtained by the hierarchy-extended simulation approach is introduced into the hierarchy-integrated simulation approach as hierarchy-renormalized model, which leads to improvement of the predictive performance of the hierarchy-integrated simulation approach and realization of the LHD numerical test reactor. The whole structure of the hierarchy -renormalized simulation model is reported.

Relating to the fluid models of core plasma in the hierarchy-extended simulation approach, various researches are reported. A new numerical matching scheme for linear MHD stability analysis is proposed in a form that the numerical implementation is tractable, where full implicit scheme is used for time derivative. The pressure-driven instabilities like interchange and ballooning modes have a general tendency that the growth rate increases with the mode number. Since reduced equations can not treat instabilities with high mode numbers (because of using the averaging method), the direct numerical simulation code which can handle such instabilities with high mode numbers are under developing by using the 8-th order compact finite difference scheme.

The influences of microscopic scales such as ion skin depth, FLR, electron skin depth, and wave-particle interaction as well as flow on properties of equilibrium state are being investigated, in order to understand the basis of the extended MHD and consider the closure problems of fluid equations. The equations for high-beta axisymmetric equilibria with flow comparable to the poloidal Alfvén velocity in the reduced two-fluid model with FLR and flow comparable to the poloidal sound velocity in the single-fluid model are derived by using asymptotic expansions in terms of the inverse aspect ratio. Multiple scale nonlinear interactions among microscopic turbulence (kinetic ballooning modes), macroscopic MHD instabilities (double tearing modes), and zonal flows have been examined, where a reduced two-fluid model is used. By examining energy transfer from micro-turbulence to macro-MHD, it is found that the micro-turbulence does not cause the macro-MHD instability, but the turbulence just produces a seed of macro-MHD instability. The multi-scale interaction between plasma blob and SOL turbulence is investigated using 2-dimensional Hasegawa-Wakatani equations with a density source term. It is reported that intermittent convective transport is generated by the plasma blob and that formation of the 2nd SOL, whose thickness depends on the intensity of turbulence, is observed.

In order to extend the MHD fluid model into multiple-phases including gas, liquid, and solid phases, the CAP code is being extended so as to include MHD phenomena in the general toroidal configurations. It is reported that the plasmoid moves to the high field side after expanding along the filed line and moving to the low field side.

The interaction between MHD modes and energetic particles is one of typical interconnecting phenomena in the hierarchy-extended simulation approach. Simulation study of energetic ion transport due to Alfvén eigenmodes in LHD plasma has been performed in comparison with experimental data. By using the experimentally estimated transport distance of energetic particles and numerically obtained linear Alfvén eigenfunctions, the amplitude of Alfvén eigenmode is evaluated.

In order to investigate effects of helical magnetic configurations on the ion temperature gradient (ITG) turbulence and zonal flows, gyrokinetic Vlasov simulations have been performed 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 the Large Helical Device (LHD) experiments. The larger zonal-flow generation in the inward-shifted case agrees with the linear analysis of the zonal-flow response, 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 the theoretical prediction, and are consistent with observation of better confinement in the inward-shifted LHD plasma. Since the electron temperature gradient (ETG) turbulence is considered as one of the possible candidates causing the anomalous electron heat transport in a core region of magnetic fusion plasmas, the gyrokinetic Vlasov simulations of the ETG turbulence in a 2D slab geometry with high velocity space resolution have been performed by utilizing the Plasma Simulator at NIFS. The transition of the potential structure from turbulent to coherent and of the transport level from high to low, which are not observed in the simulation results of the slab ITG turbulence, have been observed.

In the peripheral plasma region, so many physics processes mutually interact that this region is treated by separating it into three regions; namely, SOL/Divertor region, plasma facing material region, and the boundary layer region between them. In the boundary layer region, the behaviors of dust particles are examined. In order to evaluate the forces on the dust particle, the particle flux, the ion flow velocity and the electric field at the wall are investigated taking account of effects of truncation of electron distribution. Also, The effects of truncated electron velocity distribution on the release conditions of the spherical dust particle are discussed in the case of the gravitational force directing toward or from the conducting wall. The integrated divertor code system

SONIC, developed in JAEA, consists of the 2D fluid code (SOLDOR), the neutral Monte-Carlo code (NEUT2D), and the impurity Monte-Carlo code (IMPMC). Extension of the SONIC toward 3 dimensional modeling for full-scale analysis of divertor experiment of LHD is under going. As one example, IMPMC code is used under the concept of LHD equivalent axisymmetric plasma, in order to understand the behaviors of impurities in SOL /Divertor region of LHD.

As a hierarchy-integrated simulation code for toroidal helical plasmas, TASK3D is being developed under the strong collaborations with Kyoto University. TASK3D is based on the TASK (Transport Analyzing System for tokamaK) for two dimensional toroidal configurations developed in Kyoto University. The TASK3D has a module structure, allowing us to carry out simulations by using an individual module or combination of some modules for the user's purpose. The TASK3D has modules inherent to 3-dimensional configurations, and now it is used for evaluating the time evolutions of the radial electric field and the rotational transform.

An integrated code between core and peripheral plasmas; TOPICS-IB has been developed in JAEA on the basis of the 1.5-dimensional core transport code TOPICS extended to the integrated simulation for burning plasmas. In the TOPICS-IB, a dynamic five-point model of the peripheral (SOL/Divertor) plasma is coupled with TOPICS. The experimentally observed collisionality dependence of ELM energy loss is successfully reproduced.

The laser fusion simulation project is based on the Fast Ignition Interconnected Integrated (FI^3) project, which 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. Scaling law for fast electron beam intensity in fast ignition is investigated by using FI^3. In the case of the short scale length preformed plasma, the average core temperature quickly rises but shortly saturates because the fast electron beam intensity decreases. With the longer scale length preformed plasma, the beam intensity of fast electrons are maintained and the core heating is sustained for a longer time, and finally the core reaches higher average temperature.

Plasma complexity simulation project roughly consists of two parts; researches on collisionlless magnetic reconnection and researches related to plasma material interactions.

In order to investigate various aspects of the dynamical evolution of collisionless driven reconnection, electromagnetic PArticle Simulation code for a Magnetic reconnection in an Open system (PASMO) has been developed. In this model, the interaction between macro system and micro system is expressed by the plasma inflow and outflow through the system boundary. By using PASMO, electron force balance in the inflow direction, conversion process of electron kinetic energy in the electron dissipation region, and generation of anomalous resistivity are investigated. Simultaneously, in order to connect the PASMO to MHD code in the downstream side, a new boundary condition has been successfully developed. Furthermore, a multi-scale simulation algorithm for connecting microscopic (PASMO) and macroscopic (ideal MHD) regions is being developed by using the domain division method. The propagation of shear Alfven wave is confirmed.

Three-dimensional Particle-In-Cell (PIC) simulation code with particle absorbing boundary has been developed, and used for investigating the blob transport.

Researches on plasma material interactions might become one of key elements for NINS collaborations. Interaction between hydrogen atoms and graphite in atomic scale has been examined by using molecular dynamics simulation, where the hydrogen atom is injected into a graphite (0 0 0 1) surface at the incident energy of less than 30 eV. As the incident energy increases from 5eV to 30eV, adsorption, reflection, and finally intercalation of hydrogen occur.

Collisional-radiative models of atomic and molecular hydrogen and a neutral transport code for hydrogen species have been constructed in comparison with experiments. Intensities and profiles of atomic hydrogen emission lines from LHD edge plasmas have been analyzed by the codes in order to study the particle balance and the energy balance of the plasmas.

The prediction of quasi-bound states (resonant states with very long lifetimes) that occur in the eigenvalue continuum of propagating states for certain systems is reported in which the continuum is formed by two overlapping energy bands. Unlike the bound states in continuum predicted by von Neumann and Wigner, these states occur for a wide region of parameter space.

In order to investigate the transport phenomena of charged particles and the thermal transport phenomena in the non-equilibrium quantum system, the quantum Nernst effect is studied in the electron gas system in the regime where the ballistic conduction is almost realized. The Nernst coefficient of Bi crystal is estimated by considering contribution from holes in Bi.

With a view to investigating mesophase formation in amphiphilic solution at the molecular level, the molecular dynamics simulations of coarse -grained amphiphilic molecules with explicit solvent molecules are performed and the mesophase formation process is analyzed.

Effects of degrees of freedom in subgrid scale (SGS) on grid scale (GS) are examined from the viewpoints of dynamics, statistics, and renormalization. The contributions from SGS components may be written in the form of Langevin type equation, however, the random force is not white noise in time and its probability density function is not Gaussian at all. Also the topological dimensions of the singular structure in classical and quantum turbulence in 4 dimensions are studied in terms of Direct Numerical Simulation, in order to understand the energy cascade and energy dissipation.

Whether the non-dimensional dissipation coefficient obtained from Taylor's relation is universal or not is investigated. It is found out that the coefficient is non-universal.

Fundamental factors determining the characters of turbulence in steady shear flow are studied by using the shell model. When the total energy in the turbulence is large, the energy spectrum has -5/3 power law. When the total energy in the turbulence is small, however, a linear term coming from shear flow plays a role, and so the index of the power law is not unique.

In order to investigate the properties of the energy spectrum in turbulent flow in a statistically stationary state, the averaging conditioned on the temporal variations of the dissipation rate is applied to the ensemble of the energy spectra. It is shown that the entire cascade process is divided into the two phases.

Ortho-normal divergence-free wavelet analysis is applied to both the energy spectrum and the nonlinear energy transfer spectrum. It has been shown that the nonlinear energy transfer is relatively more intensified in some narrow region.

The fully developed turbulent flow with heat transfer under the magnetic field is studied by using DNS code with hybrid spectral finite difference methods. It is shown that the mean temperature profiles become laminar profile, as the strength of magnetic fields increases.

By using particle simulations, have been studied 1) parallel electric fields in nonlinear magnetosonic waves, 2) shock formation processes in a collision of two plasmas with their relative velocity oblique to the magnetic field, 3) evolution of oblique shock waves in a reversed external magnetic field and associated electron acceleration, 4) effects of ion composition on the propagation of nonlinear magnetosonic waves in a two-ion-species plasma, and 5) detrapping of energetic electrons from curved shock front.

The global 3D MHD simulations are carried out to study the dependence of time variabilities of black hole accretion flows on the temperature of the accreting gas.

The power spectral density (PSD) of time variations of accretion rate starting from a cool torus has a narrow width, which is consistent with the observation.

In order to better understand processes and support experiments planned at INRS-´EMT with a new 200 TW laser system (Advanced Laser Light Source-ALLS), a series of 2D relativistic EM PIC simulations has been carried out to study generation of high harmonics and atto-second pulses in the interaction of high intensity laser beams with over-dense plasmas. Also, relativistic compression of a laser pulse reflected from a moving plasma is considered.

Effects of multiple-species ions on plasma-flow velocity-shear-driven instabilities are investigated. It is reported that the introduction of the two kinds of positive ions regulates the growth of the fluctuations.

The ion kinetic effects on wide range of experimentally generated FRC plasmas have been discussed. Based on such theoretical, numerical and experimental investigations, experimental plan for the steady state FRC operation has been constructed.

Effects of non-axisymmetric magnetic field on characteristics of axisymmetric cusp direct energy converter of FRC have been discussed, where non-axisymmetric magnetic field is treated as a perturbation. Effects of the equilibrium electric field are also discussed.

When present simulation codes are used in near future super computers, many problems will be expected. Such problems and the methods to resolve them are discussed.

The code for automatically calculating optimal parameters for the design of the photonic crystal with photonic band gap is under developed, where simulated annealing (SA) being one of probabilistic algorithms for optimization problem and finite -difference time domain (FDTD) method are used.

The boundary node method (BNM) is a method for solving the boundary-value problem of a partial differential equation. Since the BNM is one of meshless approaches, elements of a geometrical structure are no longer necessary and, hence, the preparation of data is considerably simplified. However, the BNM has been plagued by its inherent difficulty: the boundary must be divided into a set of cells to evaluate contour integrals. Hence, a concept of elements is partly included into the BNM. The boundary node method without using any integration cells (BNMWC) is formulated, and its performance is investigated by comparing with the boundary element method (BEM).

Three-dimensional MHD simulation code is being developed with dynamic Adapted Mesh Refinement (AMR) and Lax or Roe, one of TVD methods, or Roe-MUSCL (Monotone Upstream-centered Scheme for Conservation Laws) for a flux part in order to capture discontinuities without artificial numerical viscosity. The method to remove remaining noise problems is also discussed.

A method that enables us to construct 3D detailed shape models suitable for immersive virtual systems and to carry out psychological experiments on the system is being developed. It is called 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 such as face model reconstructed from 3D point measurements. The shape modeling method based on implicit surface representation has become an indispensable technique yielding fast and accurate modeling from massive amount of points on a surface.

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