5. Theoretical and Simulation Researches

Through the NIFS collaborative research programs, various results have been produced from theoretical and simulation studies on numerous subjects including fusion and space plasmas, Navier-Stokes, MHD, two-fluid, and gyrokinetic turbulence, molecular dynamics, and quantum systems.

Magnetohydrodynamic (MHD) equations are a basic one-fluid model that is used most frequently in theoretical and simulation studies of fusion and astronomical plasmas. Nonlinear three-dimensional MHD simulations of toroidal fusion plasmas are done to investigate dynamical behaviors of ideal or resistive MHD unstable modes which sometimes lead to more stable states as found in self-organization processes of reversed field pinch plasmas. Alfven waves and magnetic reconnection processes in astronomical plasmas such as jets and solar flares are also studied by MHD simulations. Collaborative researches on solar wind and coronal mass injection are being advanced toward space weather forecast. Mechanisms of particle acceleration due to strong electromagnetic fields in shock waves are explained by theoretical and numerical analyses of electromagnetic structures in nonlinear MHD waves with particle simulations including relativistic effects.

Turbulence is a common phenomenon observed in diverse physical systems. Direct numerical simulations of Navier-Stokes and MHD turbulence are actively done to deepen understanding of universal properties of energy spectra and spatial structures of vortices. In fusion devices such as tokamaks and helical systems, anomalous transport arises from plasma turbulence driven by several types of microinstabilities, on which many theoretical and simulation researches have been done. Gyrokinetic simulation studies of turbulent transport driven by ion and electron temperature gradient modes are in progress and mechanisms of turbulence regulation by zonal flows are intensively investigated. Gyrokinetic turbulence simulation results are diagnosed by using the nonlinear dynamical system theory to mathematically characterize turbulence with and without zonal flows. In order to study interactions between drift wave turbulence, magnetic islands, and zonal flows in toroidal plasmas, several two-fluid model simulations are performed.

Equilibria with flows are another common topic in several research areas. A couple of theoretical and simulation analyses are done to study effects of flows on equilibria and instabilities in different configurations of neutral fluids and plasmas. Flow structures of a fluid system in a precessing spherical cavity are investigated by direct numerical simulations. Toroidal plasma equilibria with flows are theoretically analyzed based on reduced two-fluid equations. Effects of multiple-species ions on flow-shear driven plasma instabilities are elucidated by particle simulations.

Collisional radiative models of atomic hydrogen and molecular hydrogen are developed to construct the neutral transport code which is useful to diagnose densities, flows, and chemical reactions of the hydrogen species in LHD plasmas. For simulation of divertor plasmas in fusion devices which include various complex processes involving impurities, an integrated code is developed by combining plasma fluid and particle codes. Another integrated modeling, which treats core plasma transport and peripheral (scrape-off-layer and divertor) plasmas simultaneously, is also advanced. Collaborative studies of fusion reactor design based on a field-reversed configuration plasma are done and conditions for neutral beam injection heating and magnetic flux supply are discussed.

Molecular dynamics (MD) simulations are a powerful methodology that is applied to various fields. Microcanonical MD simulations of chemical sputtering of hydrogen atoms on graphite are done with improved spin-polarized density-functional tight-binding potential energy curves. Self-assembly phenomena of amphiphilic molecules such as lipids and surfactants, which are important biological and industrial processes, are studied by MD simulations.

The diagonal and off-diagonal components of the conductivity tensor in the quantum Hall system are calculated by using the linear response theory. Theoretical results are shown to be in quantitative agreement with experimental results obtained in the two-dimensional electron system at the low magnetic-field regime. (Sugama, H.)