

3. Numerical Simulation Reactor Research Project

Highlight

Plasma oscillations excited by energetic particles are reproduced and clarified by state-of-the-art simulation

In the future fusion reactors, energetic particles born from the fusion reaction will perform an important role in heating the plasma. Since the interaction between energetic particles and plasma oscillations may lead to energetic particle losses from the plasma, energetic particles and plasma oscillations are extensively studied in the LHD (Large Helical Device) experiments using energetic particles generated by the neutral beam injection. For the prediction and understanding of the behaviors of energetic particles and plasma oscillations, a hybrid simulation program has been developed at NIFS. In this program, the plasma is divided into energetic particles and a magnetohydrodynamic fluid, and their interaction is simulated self-consistently. The simulation results shown in the figure reproduce the experimental data of the plasma oscillation excited by energetic particles. They clarify the detailed behavior of the oscillation, which is not measured in the experiment, and the interaction between energetic particles and the oscillation, which amplifies the oscillation. The simulation program has been applied to many plasma experiment devices both domestic and overseas in addition to the LHD. The program has been validated through comparisons with the experimental data on energetic particle distribution and plasma oscillation. The simulation significantly improves the prediction accuracy of the energetic particle distribution in the fusion reactors.

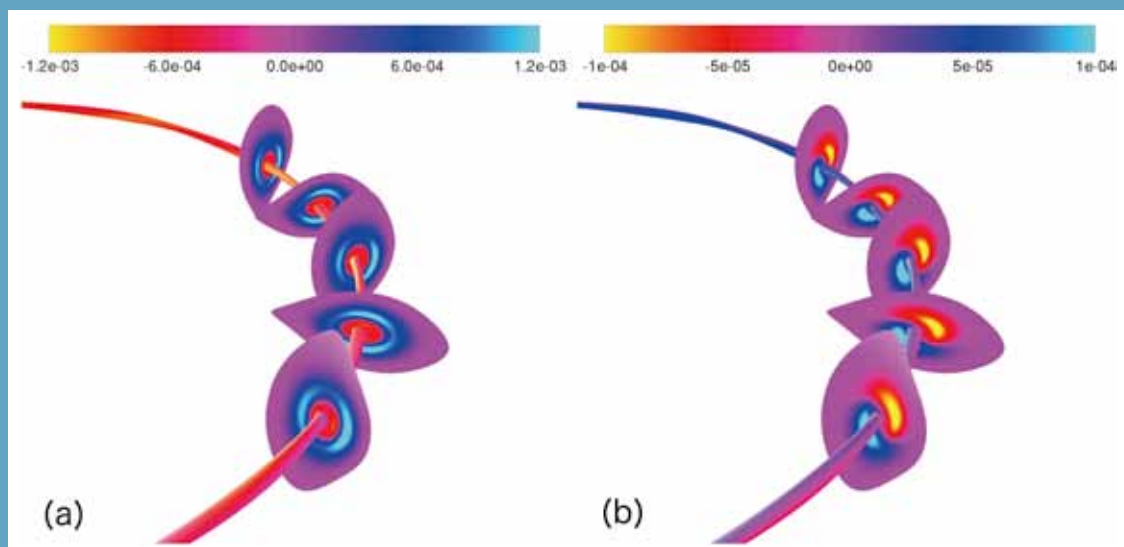


Fig. 1 Plasma oscillation excited by energetic particles in LHD. Fluctuations of (a) plasma velocity and (b) pressure on the cross-sections of the doughnut-shaped plasma are shown in the figure. The blue and red colors represent increase and decrease, respectively.

Confinement of energetic ions is critical for fusion plasmas because energetic ions heat the bulk plasma to maintain high temperature. Plasma instabilities driven by energetic particles are one of the important research issues since they lead to energetic particle transport and losses. The Numerical Simulation Reactor Research Project vigorously promotes computer simulation studies of energetic particle driven instabilities. In FY2016, 1) magnetohydrodynamic (MHD) hybrid simulations of energetic particle driven geodesic acoustic modes (EGAM), 2) comprehensive MHD hybrid simulations of Alfvén eigenmodes and energetic particle distribution formation, and 3) particle-in-cell (PIC) simulations of energetic particle driven high-frequency waves were conducted. In the MHD hybrid simulation, the plasma is divided into energetic particles and an MHD fluid. The time evolution of the energetic particles and the MHD fluid is simulated with their self-consistent interactions taken into account.

The spatial profiles of fluid velocity and pressure perturbation in 1) EGAM simulation are shown in Figure 2. Two EGAMs were observed in the LHD experiment. The primary EGAM evolves with frequency chirping, and the secondary EGAM is suddenly excited with the half frequency of the primary EGAM. The evolutions of the two EGAMs were successfully reproduced with realistic input parameters and the 3-dimensional equilibrium magnetic field. There are good agreements between simulation and experiment on the frequency chirping of the primary EGAM, on the excitation of the half-frequency secondary EGAM, on the spatial profile, and on the phase lock.

The MHD hybrid simulation code MEGA has been extended with neutral beam injection (NBI) and collisions of energetic ions with the bulk plasma for 2) comprehensive MHD hybrid simulations. The comprehensive simulations were applied to LHD and tokamak plasmas. For the LHD experiment, Alfvén eigenmodes (AEs) destabilized by the NBI were investigated. It was found that the stored fast ion energy is saturated due to the interaction with AEs at a lower level than that of the classical simulation where the MHD perturbations are neglected. Figure 2 shows the frequencies and the spatial locations of the unstable toroidal Alfvén eigenmodes (TAEs) and a global Alfvén eigenmode (GAE). The frequencies are close to those observed in the experiment. The comprehensive MHD hybrid simulations were applied also to tokamak plasmas in order to examine the distribution formation process in the collisional slowing-down time scale of energetic ions for various beam deposition power and slowing-down time. The intermittency of the TAE evolution rises with increasing beam deposition power and increasing slowing-down time (=decreasing collision frequency). With increasing volume-averaged classical energetic ion pressure, the energetic ion confinement degrades monotonically due to the transport by the TAEs. We see in Fig. 3 that the increase in the energetic ion pressure profile is saturated with increasing beam deposition power.

3) PIC simulations were conducted for the LHD experiments where the magnetic fluctuations in the high-frequency range from the ion cyclotron frequency to the lower hybrid frequency were observed. The high-frequency waves were successfully simulated with the delta-function type of initial energetic ion distribution for perpendicular velocity.

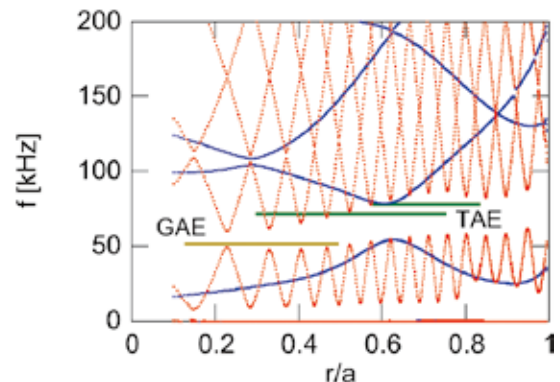


Fig. 2 Frequencies and radial locations of the unstable TAEs and GAE for an LHD plasma. The shear Alfvén continua for toroidal mode numbers $n=1$ and 11 are plotted in blue and red, respectively.

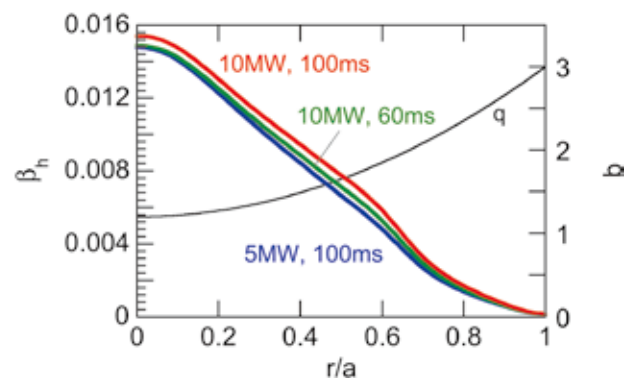


Fig. 3 Energetic ion pressure profiles for various beam deposition power and slowing-down time. Energetic ion pressure profile is saturated when the beam deposition power increases from 5MW (blue curve) to 10MW (red curve) for slowing-down time 100ms.

3. Numerical Simulation Reactor Research Project

Highlight

Peta-scale gyrokinetic Vlasov simulations provide novel theoretical findings toward full understanding of a long-standing critical issue, isotope effects on transport and confinement.

Ion mass impacts on trapped-electron-mode driven turbulence and zonal flows

Confinement performance of the energy and particle in magnetically confined high-temperature plasmas is predominantly regulated by the so-called “anomalous” transport, which is currently recognized as turbulent transport driven by microinstabilities such as ion temperature gradient (ITG) modes and trapped electron modes (TEM). Strong impacts of the hydrogen isotope ion mass on the energy confinement, which are observed in several experimental devices, have been a long-standing issue for several decades in plasma and fusion research, despite its broad interest and importance. One of the scientific goals in the LHD deuterium plasma experimental campaigns, which are recently initiated, is to explore the isotope effects on the transport and confinement, as well as further improvement of the plasma performance.

Optimizing our gyrokinetic code, GKV, for Peta-scale supercomputing on Plasma Simulator at NIFS and on K-computer at RIKEN-AICS, TEM-driven turbulence simulations in three-dimensional magnetic configuration of helical plasmas with hydrogen isotope ions and real-mass kinetic electrons have been realized for the first time, and the linear and the nonlinear nature of the isotope and collisional effects on the turbulent transport and zonal-flow generation are clarified. It is newly found that combined effects of the collisional TEM stabilization by the isotope ions and the associated increase in the impacts of the steady zonal flows at the near-marginal linear stability lead to the significant transport reduction (see figures below). This implies a reasonable agreement with the previous experimental observations indicating the opposite ion mass dependence of the energy confinement in comparison to the conventional gyro-Bohm scaling. The universal nature of the isotope effects on the TEM-driven turbulent transport has also been verified for a wide variety of toroidal plasmas, e.g., axisymmetric tokamak and non-axisymmetric helical or stellarator systems.

The novel findings here, which are obtained in collaboration with Nagoya University, have been published in Physical Review Letters [1], and the experimental verification activities in LHD have also been launched.

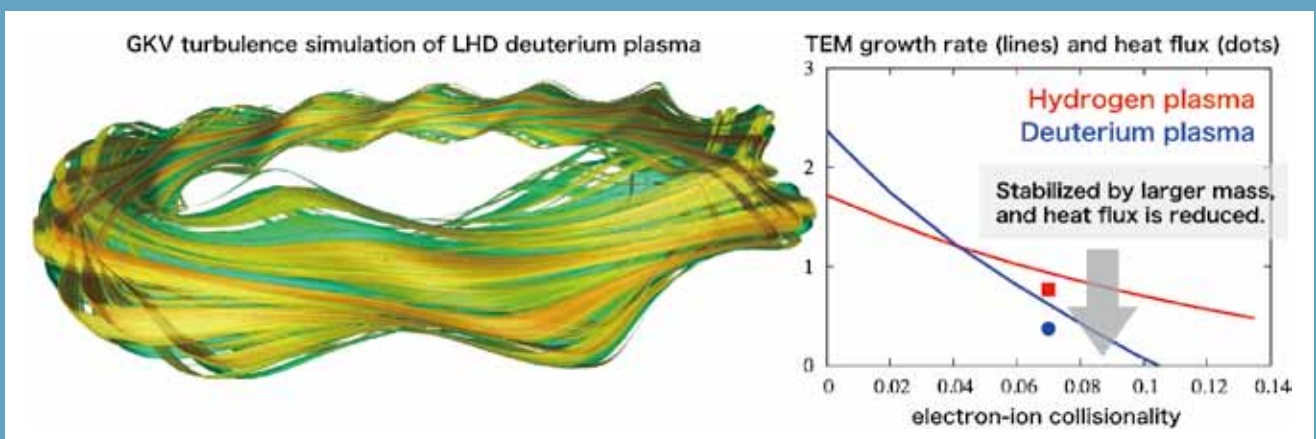


Fig. 1 GKV simulation results of TEM-driven turbulence in LHD with isotope ions.

Transport reduction of multi-ion-species LHD plasmas

Understanding of the transport phenomena in mixed plasma consisting of multi-ion-species is strongly demanded for burning plasma studies, and the deuterium experiments in LHD. In this work, we investigated the ion scale microinstability and turbulent transport of multi-ion-species plasmas in LHD by gyrokinetic simulations. Here, we focused on the LHD experiment with the multi-ion-species including hydrogen, helium, and impurity carbon ions, where it was found that the ion temperature increases with the decrease of the ratio of hydrogen density to helium density. The gyrokinetic simulations for the LHD plasmas with real-mass kinetic electron show that the linear growth rates of the ion temperature gradient mode are reduced for the helium-dominated plasma compared with the hydrogen-dominated plasma. The mixing length estimates obtained from the gyrokinetic simulations show the smaller ion thermal diffusivity for the helium-dominated plasma than the hydrogen-dominated plasma in the hydrogen gyro-Bohm unit, due to the differences of the plasma profiles of temperatures, densities, and the temperature ratio between both plasmas (see the figure on the bottom left). The findings obtained here have been published in Plasma Physics and Controlled Fusion [2].

Reduced model for dynamical simulation

A high ion temperature mode in the Large Helical Device is examined, where the ion temperature gradient mode is unstable. How to apply the reduced model of the turbulent ion heat diffusivity derived from the gyrokinetic simulation with the adiabatic electron to the transport code has been shown in helical plasmas. The transport simulation results for the ion temperature profile do not contradict the experimental observation in the figure on the bottom right [3]. The nonlinear gyro-kinetic simulation is performed for the values of the turbulent ion heat diffusivity with the kinetic electrons. The model function for the ion heat diffusivity is shown in terms of the squared turbulent electrostatic potential fluctuation and the squared zonal flow potential. The terms of the turbulent electrostatic potential fluctuation and the zonal flow potential are approximated by the terms of the mixing length estimate and the zonal flow decay time derived from the linear simulation. To reduce the computational cost for applying the model of the diffusivities to the dynamical transport simulation, a reduced model for the ion heat diffusivity is proposed. The use of the linear simulation results enables us to reproduce the nonlinear simulation results by the reduced model.

In addition to the studies mentioned above, (1) a reduced simulation model for evaluation of bootstrap current is successfully developed by S. Satake *et al.*, and (2) collisional transport of electrons in ergodized field lines is investigated by R. Kanno *et al.*

- [1] M. Nakata, M. Nunami, H. Sugama, and T. -H. Watanabe, Phys. Rev. Lett. **118**, 165002 (2017)
- [2] M. Nunami, M. Nakata, H. Sugama, K. Tanaka, and S. Toda, Plasma Phys. Control. Fusion **59**, 044013 (2017)
- [3] S. Toda *et al.*, J. Phys.: Conf. Ser. **561**, 012020 (2014)

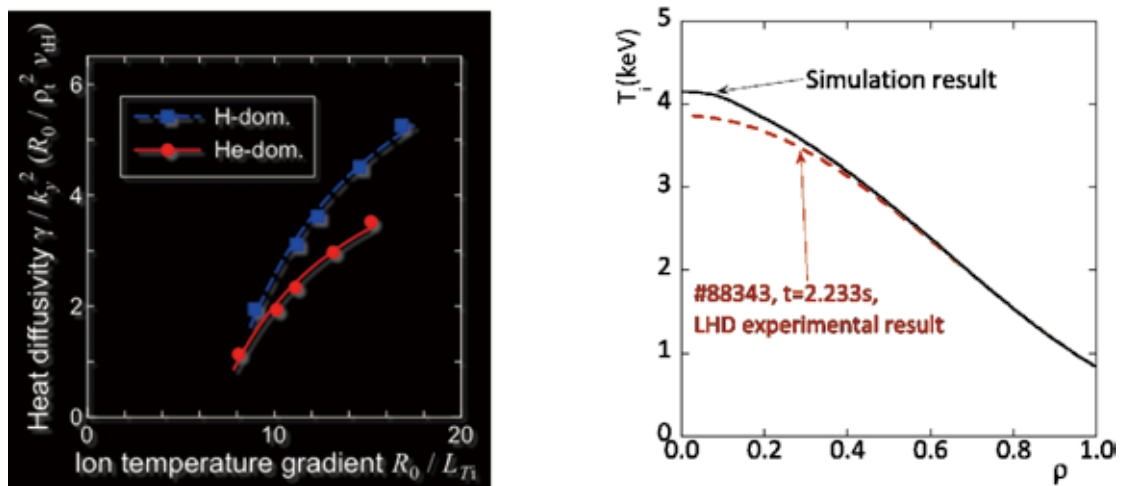


Fig. 2 Left: Ion temperature gradient dependences of the mixing length heat diffusivities in the He-dominated plasma (red solid curve) and the H-dom. case (blue dotted curve).

Right: Comparison for ion temperature profile of the simulation result with the experimental result.

3. Numerical Simulation Reactor Research Project

Highlight

Automatic Path Search for Helium Diffusion Process in Polycrystalline Tungsten

We have developed a new simulation method to automatically and quickly search migration paths of helium atoms in polycrystalline tungsten. Each path is evaluated by using molecular dynamics in a small cutout area, and the distribution of their MD calculations into many CPU cores on the supercomputer system "Plasma Simulator" is implemented by multi-program multi-data architecture.

The evaluated migration paths are used to perform kinetic Monte-Carlo simulation to research helium diffusion behavior in grain boundary region under plasma irradiation. This method is applicable to any material other than tungsten.

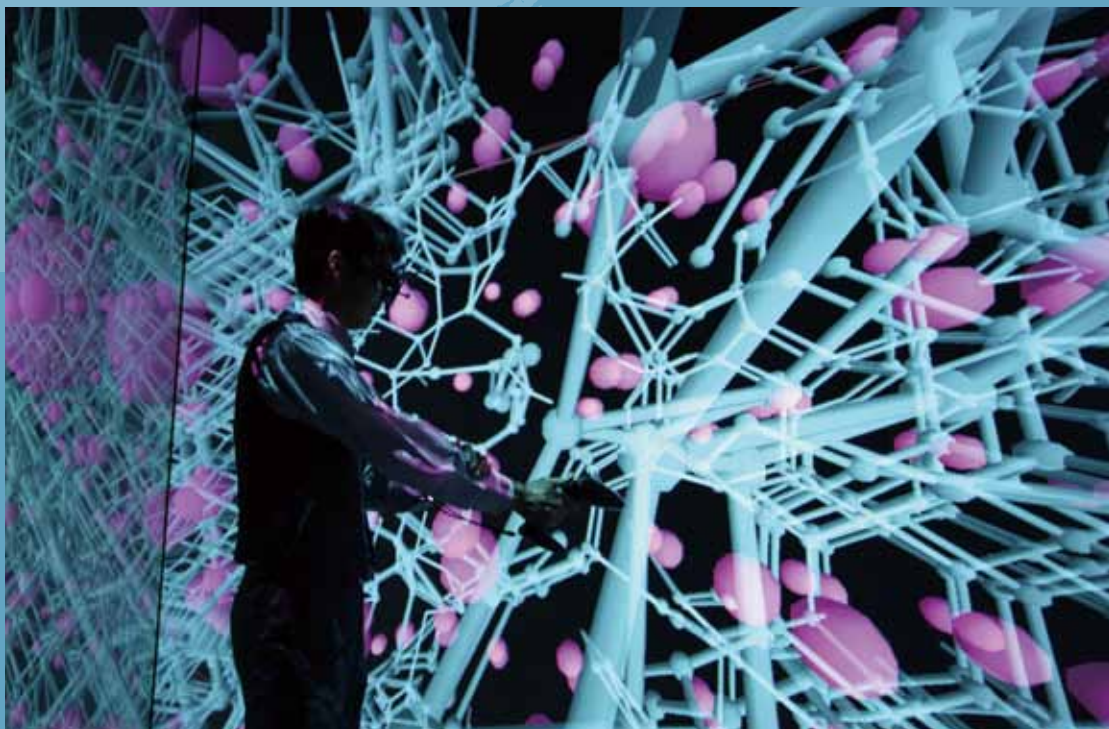


Fig. 1 Visualization using CAVE (CompleXscope) in NIFS

Diffusion process of hydrogen and helium atoms in tungsten materials, which are used for divertor plates in experimental fusion devices, is important for estimating the retention of these atoms in the tungsten materials. The retention amount is generally determined by competition between plasma injection flux and diffusion speeds of injected hydrogen and helium atoms in the tungsten materials.

In atomic simulation research on plasma-material interaction, a kinetic Monte-Carlo (KMC) simulation is generally employed to solve the diffusion process of impurity atoms. Here, impurity atoms are hydrogen and helium inserted into the tungsten materials. The calculation speed of the KMC is much faster than that of molecular dynamics, and the KMC thus can treat a long time scale of one millisecond or longer.

To execute the KMC, all possible migration paths of impurity atoms in materials and their migration barrier energies must be listed in advance. Migration paths and migration barrier energies in single crystalline materials are well researched in material sciences. Meanwhile, tungsten material used in experiments in plasma devices is poly-crystal. Although we can evaluate the migration path and the barrier energy in any structure by using the computer simulation with density functional theory (DFT), its calculation speed is insufficient to cover all of the migration paths that exist in large tungsten materials.

In this research, we have developed a new simulation method to quickly evaluate migration paths and migration barrier energies in any material. Localized molecular dynamics (MD) is used to evaluate the energies of atoms instead of DFT. The potential model used in MD was optimized to fit many reference data obtained by DFT. Each migration path is searched in a small cutout area of a nanometer scale sphere within a target material as shown in Fig. 2. Many small cutout areas are prepared to cover the entire region of the target material, and then each localized MD calculation in each small cutout area is independently performed by each central processing unit (CPU) core. Migration path finding is divided into the following two steps: first, the local minimum energy site of the impurity (helium) atom is found by structure relaxation in localized MD. Then, the migration barrier energy is estimated by nudged elastic band (NEB) method in localized MD.

Simulations with this novel method were performed on the supercomputer system in the NIFS "Plasma Simulator," which has approximately 70,000 CPU cores. Distribution of localized MD in small cutout areas into CPU cores and gathering of its results are implemented based on Multi-Program Multi-Data (MPMD) architecture. As a result, we can quickly evaluate whole migration paths and migration barrier energies.

Based on automatic migration path search developed in the present research, KMC simulation of helium diffusion process in polycrystalline tungsten material is performed (Fig. 3). By using the KMC simulation, we are tackling the clarification of helium behavior in tungsten grain boundary region under a plasma irradiation process.

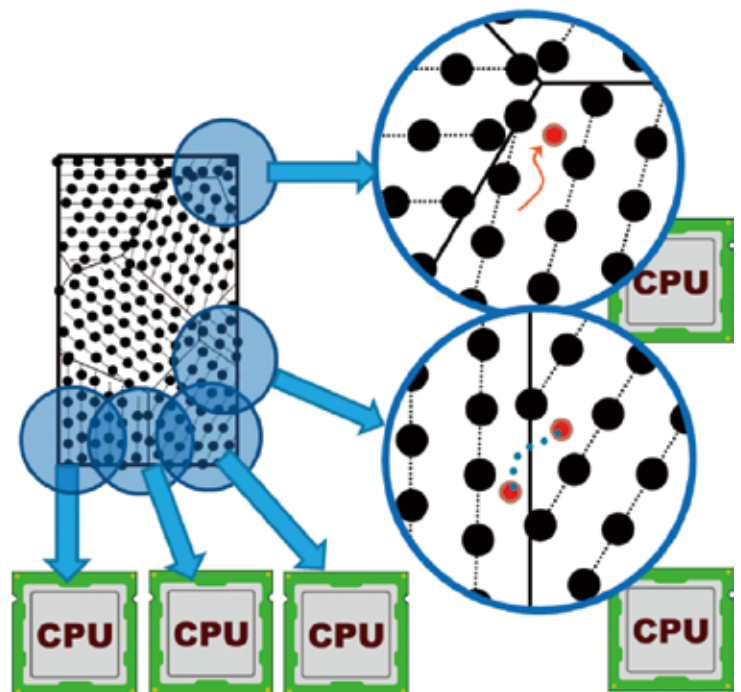


Fig. 2 Parallelization for evaluation of the local minimum energy sites and migration barrier energy by the localized MD in a small area

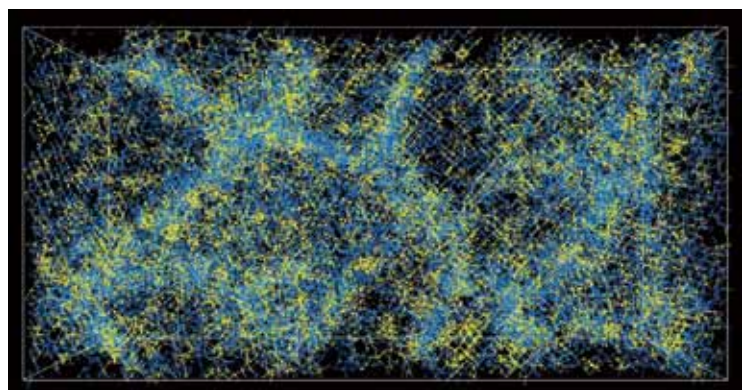


Fig. 3 Demonstration of eighteen-grain system. The blue and yellow spheres indicate the tungsten atoms on the grain boundary region. The red spheres indicate impurity atoms in KMC simulation on migration paths found by the present method, and the white lines represent their trajectories

3. Numerical Simulation Reactor Research Project

Highlight

Extension of Capabilities is Progressing: Integrated Transport Analysis Suite, TASK3D-a, for LHD Experiment

The integrated transport analysis suite, TASK3D-a (Analysis version), has been developed for routine whole-discharge analyses of plasmas confined in three-dimensional (3D) magnetic configuration such as the LHD. The routine dynamic energy balance analysis for NBI (neutral beam injection)-heated plasmas was made possible in its first version released in September 2012 [1]. The suite has been further extended by implementing additional modules for neoclassical transport and ECH (electron cyclotron heating) deposition for 3D magnetic configurations [2].

TASK3D-a has made “data integrated” transport analysis possible (compared to the conventional scheme that can be called sequential flow) by means of its automated calculations with full use of experiment database. It extracts all the time-slice information, and heating and energy balance analyses are then performed to provide transport analysis results: ion and electron heat diffusivity with two dimensions (2D, depending on time in addition to radius), as a function of radius and time.

To facilitate the application of computationally-intensive code (beyond the “module” level in current TASK3D-a servers) to LHD experiment data, a loose coupling has been established in the sense that all the necessary files for execution of large simulation code are automatically prepared by the TASK3D-a execution [3]. Users merely need to transfer this set of necessary files to a large-scale computer for executing the job. In this way, TASK3D-a will continue to establish loose-coupling to large simulations, and continue to further extend the capability of wide-ranging physics analyses of LHD plasmas.

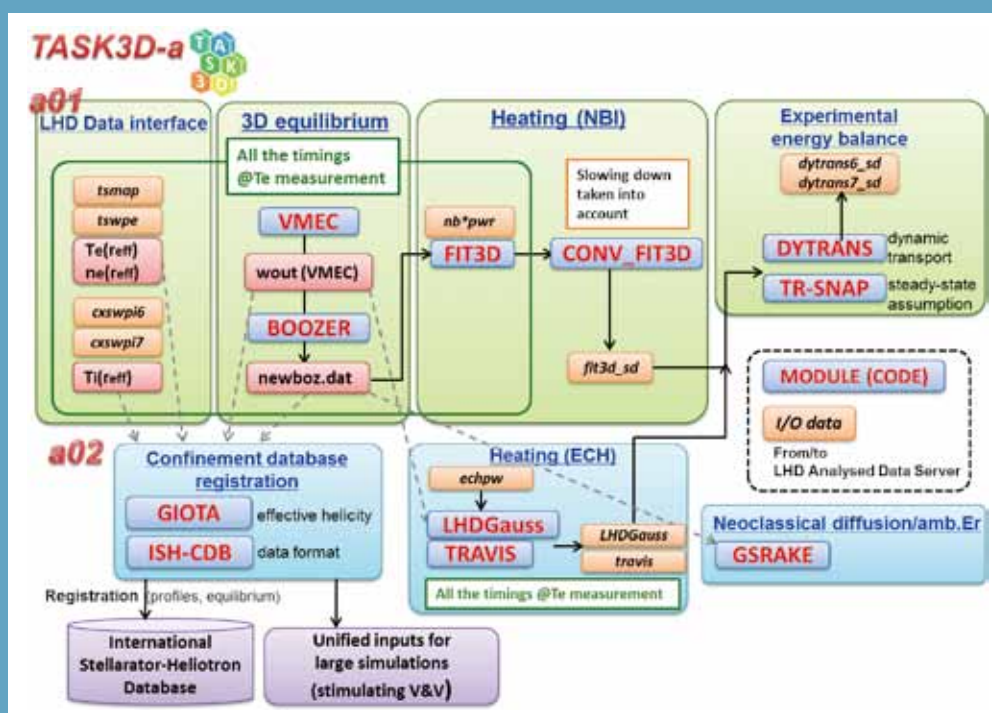


Fig. 1 The sequential calculation flow of TASK3D-a01 and a02.

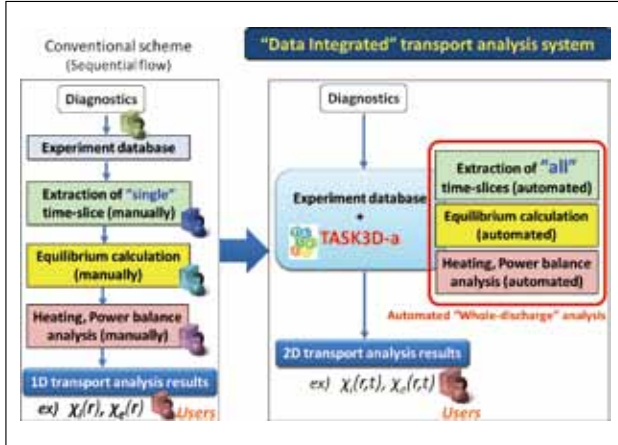


Fig. 2 Conceptual view of “data integrated” transport analysis made possible by TASK3D-a, in comparison to that of conventional scheme

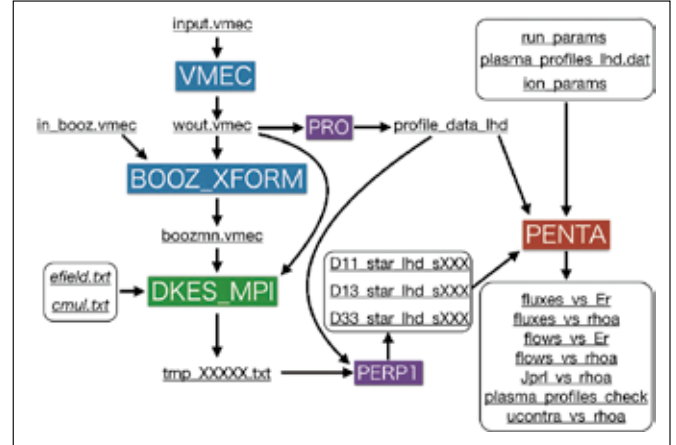


Fig. 3 Calculation flow of DKES/PENTA with a loose-coupling with TASK3D-a.

The integrated transport analysis suite, TASK3D-a, has been further extended by implementing additional modules for neoclassical transport and ECH (electron cyclotron heating) deposition for 3D magnetic configurations. The module has also been added for creating the systematic data for the International Stellarator-Heliotron Confinement and Profile Database (ISH-DB). Improvement of NBI modules for multiple-ion species plasmas is also a highlight of recent development. Provision of unified equilibrium and temperature/density profiles from TASK3D-a to several simulation codes has facilitated the verification and validation (V&V) activity, as described in Ref. [4].

TASK3D-a has made “data integrated” transport analysis possible to provide 2D (depending on time (t) in addition to radius (r)) transport analysis results, that is, ion and electron heat diffusivities; $\chi_i(r,t)$ and $\chi_e(r,t)$, as shown in Fig. 2.

Recently, there was a request to implement DKES/PENTA code [5] so that neoclassical particle fluxes of multiple ion species can be evaluated, and the accumulated measurement data for plasmas flows are systematically compared to the prediction from neoclassical transport simulations. DKES/PENTA code calculates the neoclassical parallel flows, radial particle and energy fluxes, and the radial electric field for a surface given that the plasma profiles (density and temperatures, including impurity ions), surface geometry information (from VMEC), and the mono-energetic transport coefficients are provided. This is rather computationally intensive, and cannot be applied practically to whole-discharge analysis in a TASK3D-a environment. However, to facilitate the application of DKES/PENTA to LHD experiment data, a loose coupling to TASK3D-a has been established [3] in the sense that all the necessary files for DKES/PENTA executions are automatically prepared by the TASK3D-a execution. This is also the significance of TASK3D-a, which has demonstrated one of the practical ways for broadening physics analyses with large-scale simulations in an integrated environment. The overall calculation flow of DKES/PENTA with a loose coupling with TASK3D-a is schematically summarized in Fig. 3. The VMEC part is prepared by TASK3D-a execution along with the necessary files such as execution shells and input files for successive modules. In this way, TASK3D-a will continue to establish loose-coupling to large simulations, to extend the capability of wide-ranging physics analyses of LHD plasmas.

- [1] M. Yokoyama, *et al.*, Plasma Fusion Res. Special Issue 8 (2013) 2403016.
- [2] M. Yokoyama, *et al.*, Nucl. Fusion 57 (2017) 126016.
- [3] M. Sato, M. Yokoyama and TASK3D-UD (Users and Developers), NIFS memo 76 (Aug. 31, 2016).
- [4] M. Sato, S. Satake and M. Yokoyama, J. Plasma Fusion Res. 93 (2016) 67 (in Japanese).
- [5] D.A. Spong, *et al.*, Phys. Plasmas 12 (2005) 056114.

3. Numerical Simulation Reactor Research Project

Highlight

Microscopic Dynamics on Coherent Structure in Peripheral Plasmas

By the use of the electrostatic particle simulation code which has been developed in this group, dynamics between impurity ions and a blob or a hole and impurity ion transport caused by blob and hole propagations were studied. In the case where the initial impurity ion density is spatially uniform, we have discovered that impurity ion density distribution in the blob or the hole becomes a dipolar profile. Such a profile is formed because the impurity ions experience electric field variation by blob or by hole propagation. Then impurity ions move by polarization drift, being trapped in a potential well, and are transferred with the blob or the hole.

In the case where the initial impurity ion density has a radial gradient, the blob, which is initially located in a region without impurity ions, penetrates to the impurity ion region, and sweeps impurity ions with the propagation. The impurity ions which surround the blob are then transferred in the grad-B direction as shown in Fig. 1 (a). In the case of the hole, it moves from the impurity ion region, and carries impurity ions in the grad-B direction as seen in Fig. 1 (b).

The effective radial diffusivity for impurity ions by a single blob / hole is comparable to that of the Bohm diffusion. Since the blob or the hole propagation direction in helical devices is opposite to that in the low-field side in tokamak devices, such a type of impurity ion transport might be able to account for the difference of impurity transport property between tokamak and helical devices.

These numerical results have been presented in the 26th IAEA Fusion Energy Conference (October 2016, Kyoto), as well as in the 33rd JSPF meeting (November 2016, Sendai) as invited presentations. The results were released to the press on December 13, 2016, EurekAlert! on December 21, 2016, and ITER Newsline on January 9, 2017.

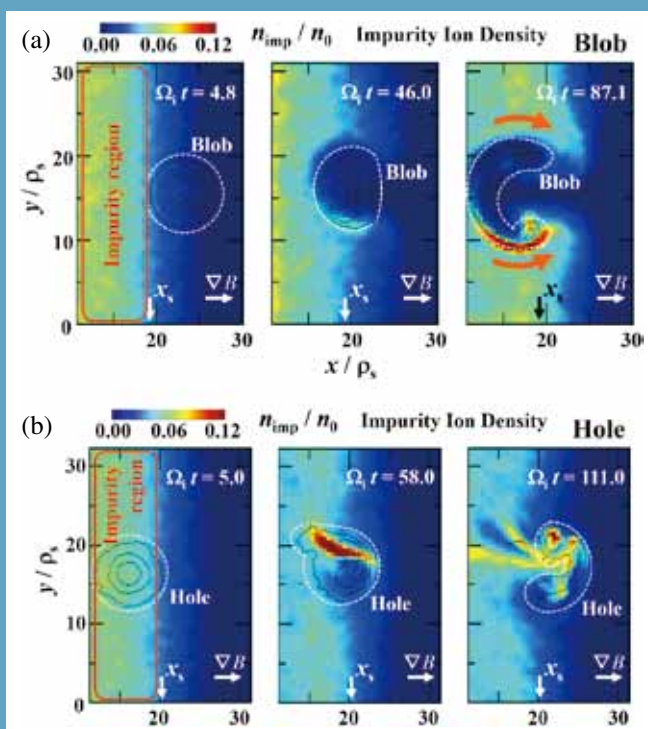


Fig. 1 Impurity ion density distributions in poloidal cross-section at various times with the blob (a) and hole (b) propagations, where the contour lines in each panel represent the electron density distributions.

Multi-hierarchy Physics Research Group Activities

The activities of the Multi-hierarchy Physics Research Group Activities can be classified in two categories, (1) extended MHD studies, and (2) micro-physics studies by the use of Particle-In-Cell (PIC) technique.

- (1) In the category of the extended MHD studies, this task group has achieved progress in two research fields. First, stability analysis of tearing modes in cylindrical plasma, by the use of both analytic theory and numerical analysis, has clarified that the power-law of the growth rate and the real frequency of the tearing mode can be quite different depending on the ion skin depth, which represents the two-fluid (micro-physics) effects to magnetic field, and resistivity. Second, two-fluid Large Eddy Simulation (LES) method for ballooning modes in LHD has been developed. Sub-grid-scale models for the LES approach have been developed. It has been shown that the LES approach provides a reasonable physical result at a very small computational cost (Fig. 2).

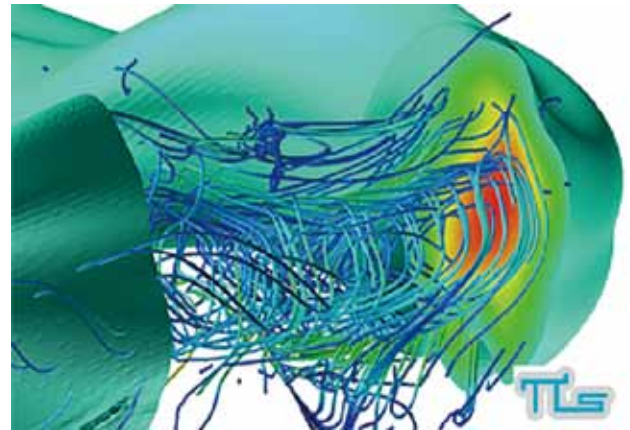


Fig. 2 Isosurface of the pressure and streamline in two-fluid LES of LHD.

- (2) Major progress has been achieved in four fields of micro-physics studies by using PIC techniques. The first achievement is the blob/hole simulations which have been introduced in the Highlight. The second achievement is in a study of particle acceleration by an oblique shock wave and the electric field parallel to the magnetic field. Magnetosonic wave in a two-ion-species plasma is shown to split into two modes. For the two regions, for which nonlinear behavior can be described by KdV equation, we have derived the electric field parallel to the magnetic field and the force to a particle along the magnetic field, and have shown that the parallel electric field in the high-frequency mode can significantly influence particle acceleration. The third achievement is understanding of the ion heating process through magnetic reconnection in plasma merging experiments in a spherical tokamak. Electromagnetic PIC simulations have shown that ion particles behave as non-adiabatic and are effectively heated. Ion velocity distributions spread mainly in the outflow direction, forming ring-like structures (Fig. 3). The ring-like formation represents effective heating. The fourth achievement is development of a PIC code for detached plasma studies. The new code, called PAMCADE, contains various aspects of plasmas such as collision of charged particles with neutral gas, Coulomb collisions among charged particles, and others. We have achieved simulation of the formation of detached plasma and have observed strong temperature gradient in the neutral gas region.

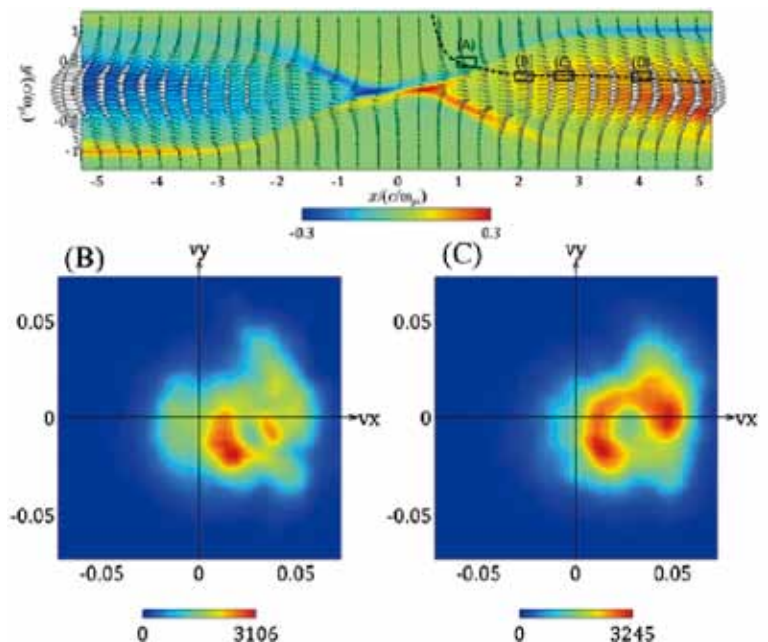


Fig. 3 Ion velocity distributions at the areas (B) and (C), which are in the downstream.

(H. Sugama)