3. Numerical Simulation Reactor Research Project

Fusion plasmas are complex systems which involve a variety of physical processes interacting with each other across wide ranges of spatiotemporal scales. The National Institute for Fusion Science (NIFS) has conducted the Numerical Simulation Reactor Research Project (NSRP) by utilizing the full capability of the supercomputer system, Plasma Simulator, and propelling domestic and international collaborations. Missions of the NSRP are (i) to systematize understandings of physical mechanisms in fusion plasmas for making fusion science a well-established discipline and (ii) to construct the Numerical Helical Test Reactor, which is an integrated system of simulation codes to predict behaviors of fusion plasmas over the whole machine range.

The Plasma Simulator “Raijin (雷神)” (Fig. 1) began operations in July 2020. It consists of 540 computers, each of which is equipped with eight “Vector Engine” processors. The 540 computers are connected to each other by a high-speed interconnect network. The computational performance is 10.5 petaflops. The capacities of the main memory and the external storage system are 202 terabytes and 32.1 petabytes, respectively.

Presented below in Figs. 2 and 3 are examples of successful results from collaborative simulation research in 2022-2023 on the Ion Cyclotron Range of Frequency (ICRF) heating of LHD plasmas and on ion velocity distribution functions formed in magnetic reconnection, respectively. Also, highlighted in the following pages are achievements of the NSRP research task groups on energetic-particle physics, turbulent transport, integrated transport code, and plasma-wall interaction. The NSRP was completed in March 2023 and its legacy is being carried over to the new organization of NIFS starting from April 2023.

(H. Sugama)

Fig. 1 The Plasma Simulator, “Raijin (雷神)”

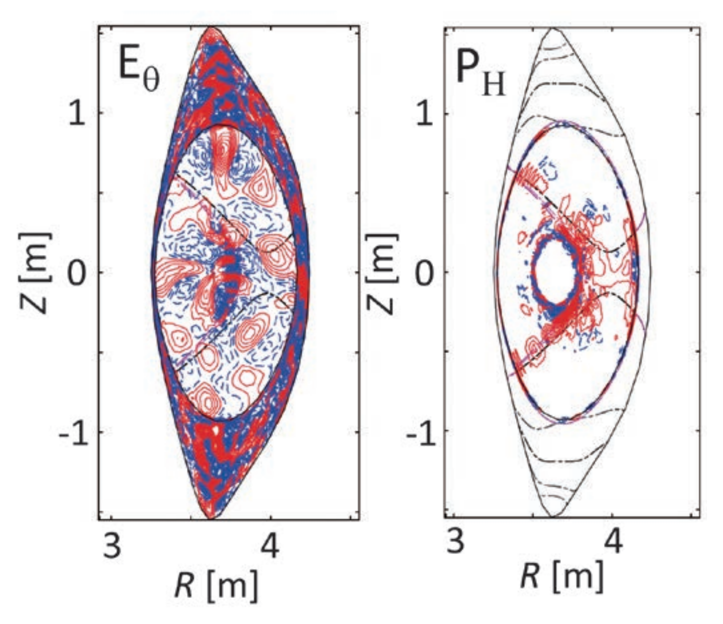

Fig. 2 Distributions of the electric field (left) and the absorbed power (right) obtained by the simulation of the Ion Cyclotron Range of Frequency (ICRF) heating of an LHD plasma [presented by Dr. R. Seki (NIFS)]. The TASK3D/WM code (A. Fukuyama and T. Tohnai, in 5th IAEA Technical Committee Meeting on Alpha Particles in Fusion Research, IAEA, Vienna, 1997) is used for the simulation.

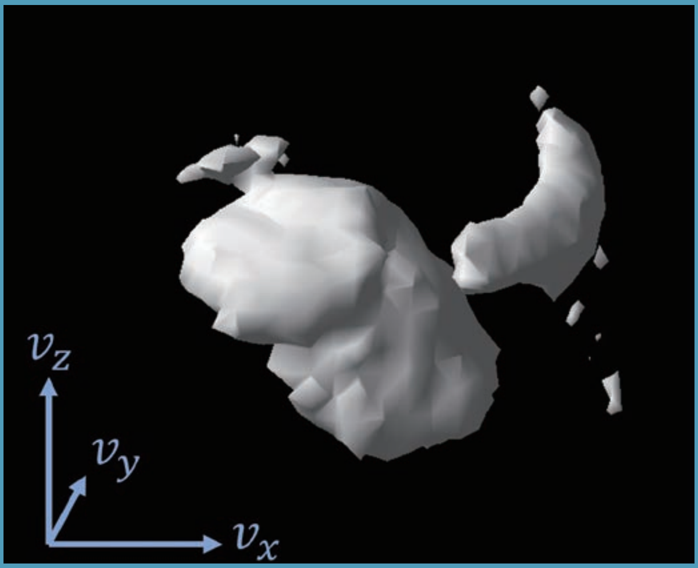

Fig. 3 An isosurface of the ion phase space density obtained by particle simulation of magnetic reconnection [presented by Dr. S. Usami (NIFS), Reference: S. Usami and S. Zenitani, in the Physical Society of Japan 2023 Sprint Meeting, Online, 2023]. This simulation was performed by using the PASMO code.

Energetic-particle Driven Instabilities and Energetic-particle Effects on Magnetohydrodynamic Instabilities

Highlight

Self-consistent simulations of ICRF-induced Alfvén eigenmodes in LHD

Self-consistent simulations which include ion-cyclotron-range-of-frequency (ICRF) acceleration and collisions were conducted with MEGA, which is a kinetic-magnetohydrodynamic (MHD) hybrid simulation code, to investigate the ICRF minority heating scenario in the LHD. Alfvén eigenmodes (AEs) were studied for the first time based on a realistic phase-space distribution of minority ions. It was shown that an AE can be driven unstable during on-axis ICRF heating, where ICRF-generated energetic localized trapped minority ions play a significant role in the AE destabilization. Firstly, a hundred-millisecond classical simulation, where the MHD perturbation is turned off, was performed to obtain the minority ion distribution in a steady state. Figures 1(b) and (c) show the energy distribution functions of minority ions in on-axis and off-axis heating cases, respectively. A considerable number of localized trapped (helically trapped) minority ions are accelerated to high energy (~MeV) in the on-axis (off-axis) heating case, as shown in Figs. 1(b) and (c). A localized trapped particle is toroidally trapped between two adjacent vertically elongated plasma cross-sections in the LHD, whose toroidal precession motion is almost zero, as shown in Fig. 1(a). Then, AE stability was investigated via a hybrid simulation based on the steady-state minority ion distributions. An unstable mode can only be found in an on-axis heating case. The unstable mode is identified as an energetic particle mode (EPM) localized in the plasma core with toroidal mode number $n=1$ and dominant poloidal harmonics $m=2,3$. The mode frequency is mainly between 80~100kHz, propagating in the ion diamagnetic drift direction. The resonance condition shows that localized trapped minority ions with energy 400~1000keV contribute to the EPM drive, whose poloidal drift orbit frequencies can match the mode frequency. Recent experimental observations of ICRF-induced modes during 2.5 MW on-axis ICRF heating in the LHD show good consistency with the simulation results of the mode frequency and both toroidal and poloidal mode numbers.

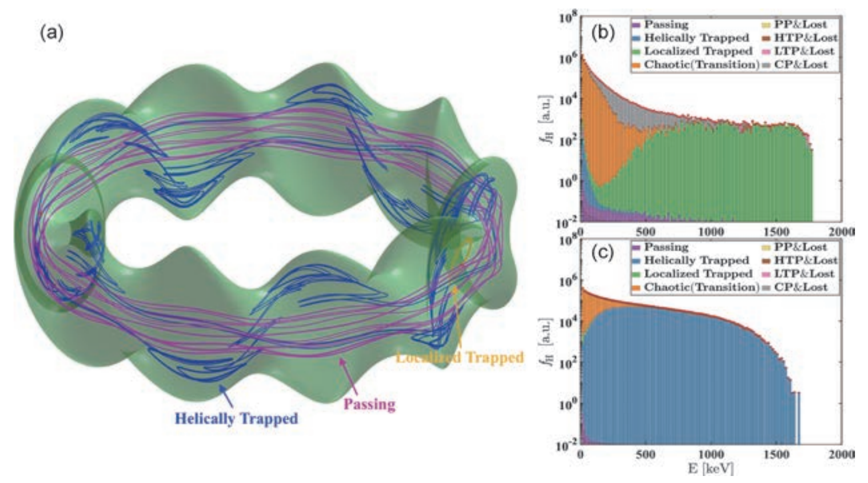

Fig. 1 (a) Typical ICRF-accelerated minority ion trajectories in the LHD. Minority ion energy distribution functions (red solid circles) in steady states for (b) on-axis heating (B_{ax}=2.55T), and (c) off-axis heating (B_{ax}=2.80T). Proportions of particles with different orbit types in each energy band are marked with different colors in panels (b) and (c).

[1] J. Wang *et al.*, “Self-consistent Simulations of ICRF-induced Alfvén Eigenmodes in the Large Helical Device”, in the 28th Meeting of ITPA Topical Group on Energetic Particle Physics (Nov. 21–25, 2022, ITER Headquarters).

(J. Wang)

Simulation study of interaction between energetic particles and magnetohydrodynamic modes in the JT-60SA inductive scenario with a flat q≈1 profile

Interactions between energetic particles (EPs), an internal kink mode, and other MHD instabilities in the JT-60SA inductive scenario were simulated with the MEGA code [2]. In this scenario, it was predicted by TOPICS, an integrated transport code, that the internal kink mode can be unstable, and the sawtooth relaxation results in a flat safety factor (q) profile with $q \approx 1$ for $r/a \leq 0.6$. In this equilibrium, it was found in the simulation results that the MHD stability depends strongly on the bulk plasma pressure gradient. In a simulation where toroidal mode numbers with $n \leq 8$ are retained, the most unstable modes are high-n interchange modes with a poloidal number $m=n$. The mode's frequency is less than 1 kHz because the toroidal and poloidal orbit frequencies of the co-passing EPs are approximately equal to each other within the $q \approx 1$ surface. During the linear growth phase, EP transfers energy to the mode. Due to the low mode frequency and the approximately equal toroidal and poloidal orbit frequencies, all passing EPs within the $q \approx 1$ surface can resonate with the mode. The resonance layer in the energy and canonical toroidal angular momentum phase space is parallel to the flux surfaces. The overlapping of these modes creates a stochastic magnetic field, leading to stronger EP and bulk plasma pressure redistributions. During the nonlinear phase, the transition from the high $m=n$ modes to the low $m=n$ ones is observed, as shown in Fig. 2, where the dominant mode is the $m/n=1/1$ mode with an internal kink-like structure. These low $m=n$ modes are generated by the nonlinear coupling of the high $m=n$ modes. The EP kinetic effect has a minor contribution to the dynamics of these nonlinearly generated $m=n$ modes.

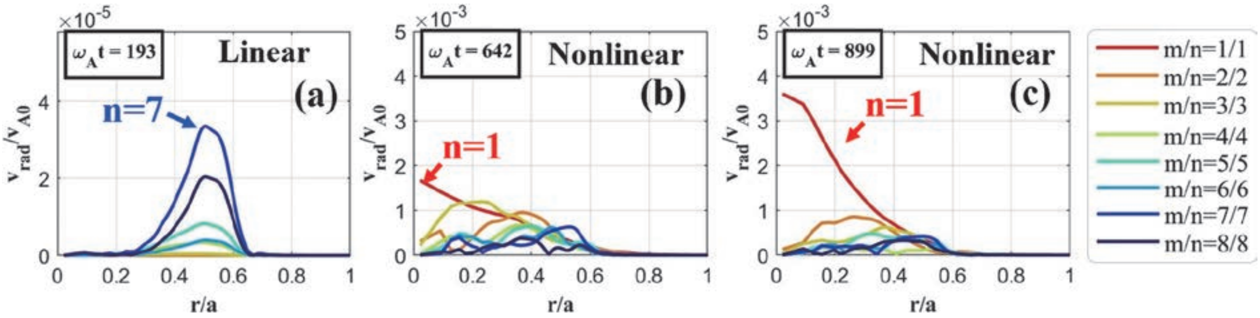

Fig. 2 Radial MHD velocity profiles for the $m=n$ modes in the JT-60SA inductive scenario at (a) the linear growth phase ($\omega_A t=193$), (b) the beginning of the nonlinear phase ($\omega_A t=642$), and (c) the final time of the simulation ($\omega_A t=899$).

[2] P. Adulsiriswad *et al.*, "Simulation Study of Interaction between Energetic Particles and Magnetohydrodynamic Modes in the JT-60SA Inductive Scenario with a Flat q≈1 Profile", submitted to Nuclear Fusion.

(P. Adulsiriswad)

Waveform distortion of off-axis fishbone instability in the nonlinear magnetohydrodynamic evolution in tokamak plasmas

We conducted kinetic-MHD hybrid simulations to investigate the waveform distortion of off-axis fishbone modes (OFMs) driven by energetic particles in tokamak plasmas [3]. Building upon our previous work [4], we extended the simulations to include higher-n harmonics in the MHD fluid, where n represents the toroidal mode number. The simulations successfully reproduced the waveform distortion in both magnetic and temperature fluctuations which were observed in the experiments. Our analysis revealed that the waveform distortion originates from the combination of n = 2 harmonics and fundamental n = 1 OFM, while the n = 2 harmonics are generated by MHD nonlinearity resulting from the n = 1 OFM. Depending on the phase relationship between the n = 1 and n = 2 harmonics, as well as the relative amplitude of the n = 2 harmonic, two types of waveform distortion can occur, as shown in Figure 3. Lissajous curve analyses demonstrated that wave couplings between the n = 1 and n = 2 harmonics, with phase-lock approximately equal π and 0, lead to “rising distortion” and “falling distortion,” respectively. These two waveform distortions can be attributed to the strong shearing profile of radial MHD velocity with n = 2 around the q = 2 magnetic flux surface. Additionally, we investigated the dependence of waveform distortion on viscosity and found that the viscosity required to reproduce the waveform distortion is higher than the classical value in the experiment.

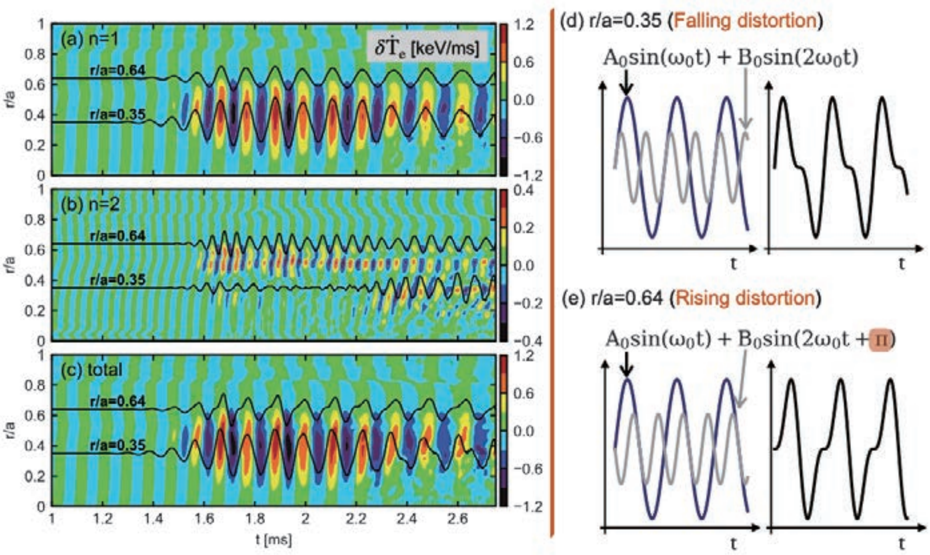

Fig. 3 Temporal evolution of the radial profile of the time-derivative of temperature perturbation at φ = 0 on the outboard midplane for (a) n = 1, (b) n = 2, and (c) total with the oscillations at r/a = 0.35 and r/a = 0.64. Additionally, schematic figures (d) and (e) demonstrate how the phase difference between two sinusoidal waves generates two types of waveform distortion.

[3] H. Li *et al.*, Nuclear Fusion **63**, 086012 (2023).
[4] H. Li *et al.*, Nuclear Fusion **62**, 026013 (2022).

(H. Li)

A Novel Simplified Model to Predict Nonlinear Turbulent Transport

Highlight

Nonlinear turbulent flows and transport in fusion plasmas are predicted by combination of mathematical model and linear computations.

One of the most important achievements toward realizing a fusion reactor is the clarification and prediction/control of “turbulence” in magnetically confined plasmas. Many efforts have been devoted to studies on the turbulent transport of thermal energy and particles, by means of large-scale numerical simulations based on kinetic and fluid models. Although supercomputing is a powerful approach, the high computational cost often discourages investigation of a wide range of physical states/conditions in the plasma. A simplified mathematical model is thus required to extract the predominant components in the turbulence dynamics.

To this end, our research group has successfully constructed a novel, simplified model to predict nonlinear turbulent transport in plasmas. By applying mathematical optimization techniques to the big data obtained from large-scale “nonlinear” turbulence simulations, the newly developed mathematical model can predict the turbulent heat transport level only by a simplified “linear” calculation, which is about 1500 times faster than the conventional large-scale simulations. The mathematical model with linear-calculation quantities, e.g., the instability growth rate and the zonal-flow decay time, captures the complex functional structures of the turbulence simulation data, and resultingly the applicability and accuracy are significantly improved in comparison to those in previous studies (Fig. 1). Also, the present model can estimate the zonal-flow amplitude, which has a great impact on transport suppression. These studies not only accelerate turbulence research in fusion plasmas, but also the present method of predicting complex dynamics from simple calculations is expected to contribute to various research fields.

The results have been published as two papers [1-2], and further application to the development of a new global turbulent transport simulation is also underway.

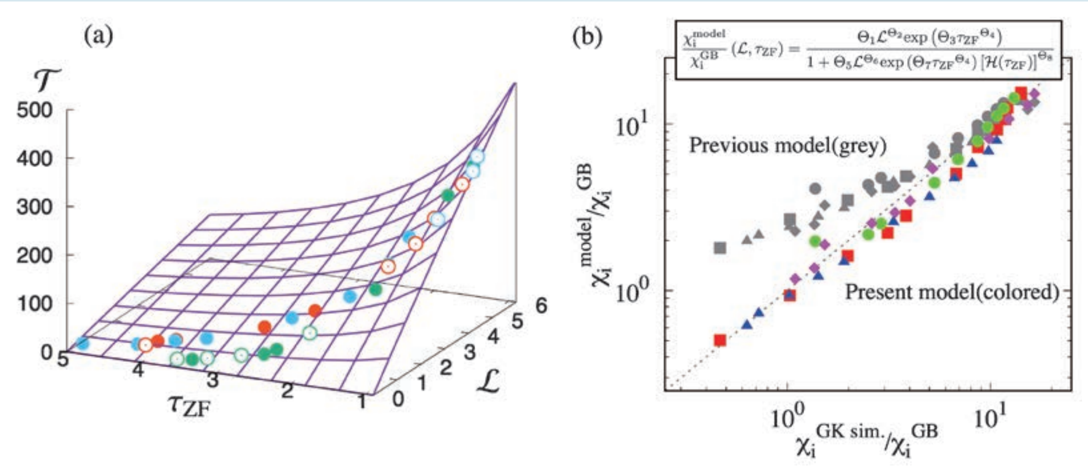

Fig. 1 (a) Nonlinear function (surface) to interpolate the turbulence simulation data (symbols). (b) Accuracy of the present simplified model.

[1] T. Nakayama, M. Nakata, M. Honda, M. Nunami, and S. Matsuoka, Plasma Physics and Controlled Fusion **64**, 075007 (2022).
[2] T. Nakayama, M. Nakata, M. Honda, E. Narita, M. Nunami, and S. Matsuoka, Scientific Reports **13**, 2319 (2023).

(M. Nakata)

Prediction of plasma profiles in helical plasmas by integrated code coupled with gyrokinetic transport models

Transport simulation is a challenging task, using the turbulent transport level evaluated by gyrokinetic simulation results. In this study, the transport simulation is performed by an integrated code using reduced gyrokinetic models [3]. Especially, the quasilinear flux model is used in helical plasmas. The turbulent transport is evaluated by reduced models using the linear gyrokinetic simulation results for kinetic electron response at each step of the integrated simulation. By performing the integrated simulation with the gyrokinetic models installed, multi time-scale simulation can be performed. The multi time-scale simulation is performed in the standard and inward shifted field configurations of the Large Helical Device (LHD). The multi time-scales consist of those for the gyrokinetic simulation (~1μs) and for the transport simulation (~100ms). The simulation using the quasilinear flux model based on the gyrokinetic simulation results, including effects of zonal flows and kinetic electrons, is performed for the first time to predict temperature profiles in the LHD. This is achieved by combining two codes, the integrated code, TASK3D and the local flux tube gyrokinetic code, GKV, developed for helical plasmas. The quasilinear flux model includes a cross-phase effect between fluctuating potential and temperature in addition to the linear growth rate and the zonal flow decay time. The stationary temperature profiles obtained by the transport simulation, using the reduced models, which reproduce the nonlinear simulation results, are predicted within a difference of 30%, at most, from the experimental results in the LHD, where the ion temperature gradient (ITG) mode is unstable. Some validations in the adiabatic electron condition for the other discharge in the LHD are done.

In this study are the cases for fixed heating power to obtain a stationary state where the power balance holds are focused. Validations over energy confinement time where the heating power varies in time are left for future research.

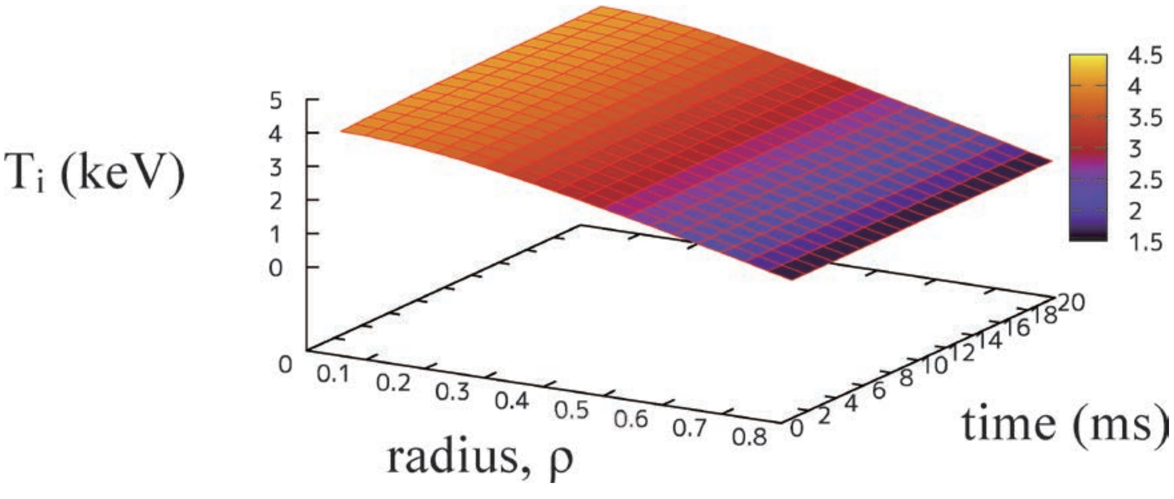

Fig. 1 Simulation results for time evolution of ion temperature profile, T_i are shown. State at t=20ms is stationary.

[3] S. Toda *et al.*, Plasma Phys. Control. Fusion **64**, 085001 (2022).

(S. Toda)

Functional Extension of Integrated Transport Analysis Suite

Highlight

Developed Integrated Transport Analysis Suite, TASK3D-a, has been the Basis for Physics Analysis and Transport Modelling of LHD Plasmas

On the occasion of formulation of the Numerical Simulation Reactor Research Project, the first version of the integrated transport analysis suite for LHD plasmas, TASK3D-a01, was released in September 2012, after integrating various elemental analysis codes (modules) such as three-dimensional equilibrium, NBI heating, and heat transport processes. The construction of TASK3D-a01 has greatly advanced the automation of heat transport analysis. It is now possible to provide the results of dynamic transport analysis that take into account the temporal changes in temperature and density profiles. To apply TASK3D-a to a wider range of LHD experimental conditions, we have continuously added modules and improved the accuracy, and released it as TASK3D-a02. In TASK3D-a02, we incorporated a module to evaluate neoclassical thermal and particle diffusion fluxes. As a result, a neoclassical energy flux analysis was performed simultaneously with experimental energy balance analysis, which could provide a turbulent transport contribution in energy flux. In addition, by introducing ECH modules, energy balance analysis incorporating ECH absorption power could be performed, and then the analysis target was significantly expanded from the NBI-only heated plasmas to NBI and ECH-heated plasmas.

For large-scale simulation codes that are difficult to integrate in the framework of TASK3D-a, due to large differences in required computational resources, we have established a linkage function to provide LHD plasma equilibrium, temperature and density profiles, etc. from TASK3D-a to those simulation codes. As a result, TASK3D-a has enabled smooth implementation of LHD plasma analysis by large-scale simulations and furthermore enhanced international code benchmarking activities.

The third and fourth versions of TASK3D has enabled the capabilities of NBI heating calculations in the presence of multiple ion species: hydrogen, deuterium, and helium. The functions were expanded one after another, and TASK3D-a05 supported density profile measurement calibration based on Bayesian statistics. Including other upgrades, a version of TASK3D-a has now existed up to a07. This extension of functions has greatly contributed to the creation of an analysis database that serves as a basis for research on isotope effects. It also serves as a base for neutron measurement and quantitative evaluation of high-energy particle behavior in the LHD deuterium experiment. To improve the user's convenience, the TASK3D-a English manual was revised (in May 2021) and distributed to users in Japan and overseas.

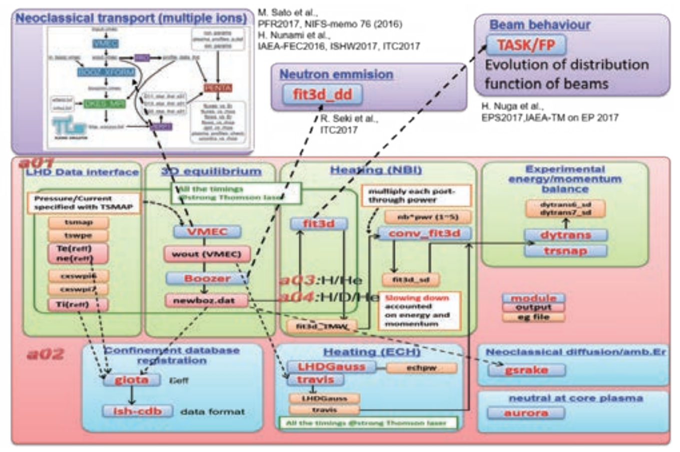

Fig. 1 Evolution of functional expansion of the integrated transport analysis suite, TASK3D-a, for LHD plasmas. From the first version (TASK3D-a01) shown in a horizontal row in the center, the function expansion (TASK3D-a02) written in the lower part, has been made to accommodate the existence of multiple ion species (hydrogen, helium, deuterium) for an NBI heating module (a03, a04). Other extensions have been made for Bayesian-calibrated density profiles, linkage with large-scale simulation codes, and energetic particles' behavior (upper part). (Reprinted from Ref. [1])

[1] M. Yokoyama *et al.*, Journal of Plasma and Fusion Research **96**, 610 (2020).

(M. Yokoyama for TASK3D-a Users and Developers)

Development of ICRF Module for Further Extension of TASK3D-a

We are developing TASK/WM for evaluating wave propagation and heating of ICRF for non-axisymmetric configurations such as the LHD. In TASK/WM, the wave propagation is calculated by solving the wave equation with electric field components being spectrally expanded in toroidal and poloidal directions and being radially differentiated. Currently, to solve the wave propagation including second harmonic heating, we are applying a hot plasma model that considers the thermal motion of the plasma, and introducing a permittivity tensor in a differentiational form in which a wave number can be given consistently with the wave electric field. After these implementations, results provided by TASK/WM will be verified against the experiment results in the LHD.

(R. Seki)

Integrated Transport Simulation of Fusion Plasmas based on the Data Assimilation Technique

We have developed a fusion plasma control method using data assimilation. First, we developed a new data assimilation framework, DACS [2], which integrates the optimization of the integrated simulation by assimilating the observation information and the estimation of the control input which is required to realize the target state. We extended the data assimilation system ASTI [3] to a control system based on DACS (adaptive model predictive control) and investigated its control capability by conducting numerical experiments to control virtual plasma created with the integrated code TASK3D. In addition, ASTI was accelerated so that it could be calculated in real time, and the control experiment of ECH plasma in the LHD was performed. The controllability of ASTI has been demonstrated in experiments in which the central electron temperature is controlled to approach the prescribed target temperature. This framework DACS can easily incorporate various observational information and control problems and is the basis for constructing a general-purpose and robust control system. Furthermore, while proceeding with a demonstration of the actual experiments, we will consider the development towards real-time plasma control.

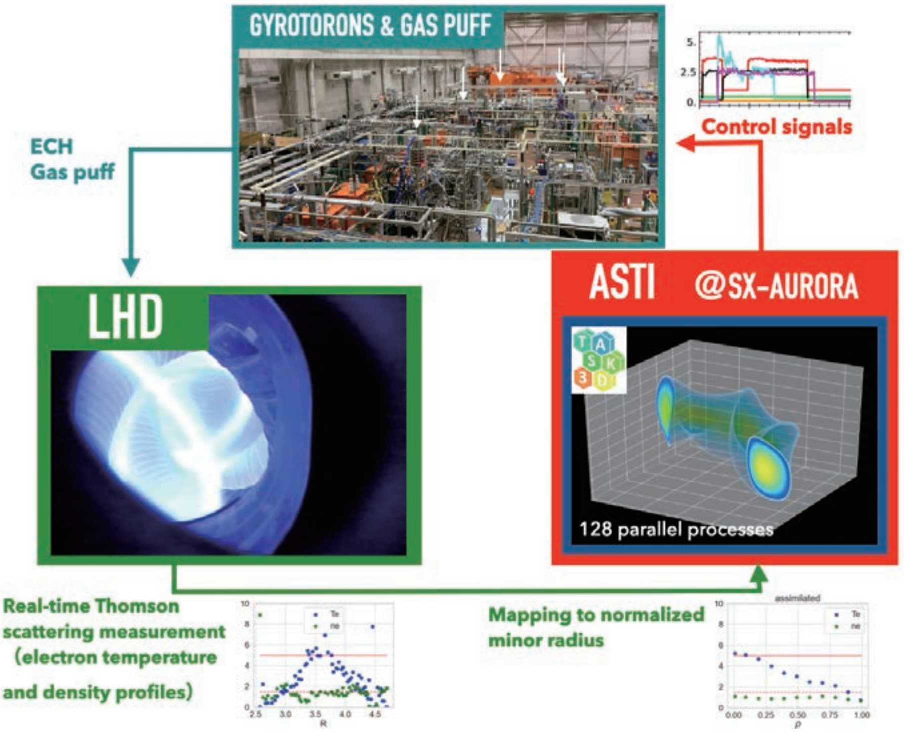

Fig. 2 Overview of the data assimilation-based control system for fusion plasmas (LHD in this case). The control signals for the gyrotrons (and the gas puff system) are estimated in the data assimilation system, ASTI, based on the prediction by the integrated code, TASK3D. In addition to the control estimation, ASTI processes Thomson scattering measurement data in real time to optimize the transport model sequentially along with the actual plasma experiment.

[2] Y. Morishita *et al.*, Computer Physics Communications **274**, 108287 (2022).
[3] Y. Morishita *et al.*, Journal of Computational Science **72**, 102079 (2023).

(Y. Morishita, Kyoto University)

Reactive Force Field Molecular Dynamics Simulations on Various Structural Transition Phenomena

Highlight

Molecular Dynamics Simulation on Hydrogen Trapping on Tungsten Vacancy

Tungsten (W) with its high melting point and thermal conductivity is one of the most promising candidates for plasma-facing materials including the divertor plate. In addition, W has lower hydrogen isotope solubility than carbon materials and is less prone to wear and tear due to hydrogen isotopes. On the other hand, defects such as atomic vacancies and voids in metals are known to act as trapping sites for hydrogen isotopes, and it has been suggested that tritium retention may be increased by neutron irradiation, which is a product of nuclear fusion.

Because hydrogen isotopes contain tritium, which is a radioactive material, this retention is limited in fusion reactor operation. Therefore, it is necessary to control this retention in the steady-state operation of fusion reactors. Elucidating the interaction between tungsten, vacancies, and hydrogen isotopes is one of the key issues, and various studies have been conducted through numerical calculations and experiments. The novel findings here, which were obtained in collaboration with Yamagata University, have been published in JASSE [1].

However, the effect of different exposure temperatures of hydrogen isotopes on the interaction between vacancies and hydrogen isotopes has not been fully elucidated. Therefore, we clarify the interaction effects between vacancies and hydrogen isotopes at different hydrogen isotope exposure temperatures using Molecular dynamics (MD) simulation. To achieve the objective of this study, we developed the tungsten-hydrogen code, developed and performed simulations of neutron-irradiated W with and without hydrogen isotopes shown in Fig. 1. Furthermore, the effects of varying the number of hydrogen isotopes and the temperature during hydrogen isotope irradiation on the displacement, fluctuation, and density distribution of W and H atoms are shown in this study.

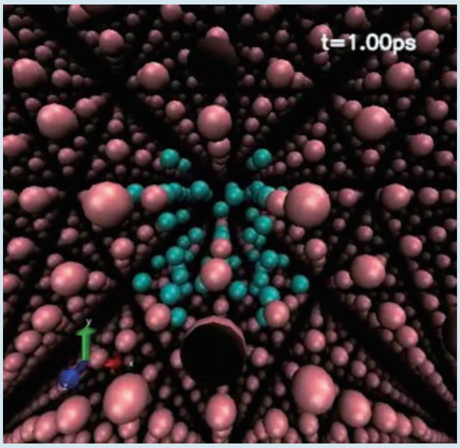

Fig. 1 Snapshot of hydrogen (green) filling a vacancy in a tungsten (brown) crystal.

[1] H. Nakamura, K. Takasan, M. Yajima and S. Saito, J. Adv. Simulat. Sci. Eng. **10**, 132 (2023).

(H. Nakamura)

Molecular dynamics simulation on fabrication of chiral nanoneedle by optical vortex

Toyoda *et al.* fabricated chiral nanoneedles by vortex laser ablation. They used 2 mm thick polished tantalum (Ta) as the target. According to their result, an optical vortex produced a chiral nanoneedle with a spiral conical surface at the center of the ablation zone. Inspired by this result, we attempted to elucidate the chiral nanoneedle structural formation process by the molecular dynamics (MD) simulation.

We have successfully generated tantalum chiral nanoneedles in silico using three-dimensional MD simulation to calculate the time evolution of the motion of atoms [2] shown in Fig. 2. Since current computer capabilities do not allow this nanostructure formation to be calculated at the electron level, the interaction between the optical vortex and tantalum atoms is approximated by a pseudo-electric force field, which is proportional to the electric field. The embedded atom method potential "2013_aem.alloy" is used for the interatomic forces between tantalum atoms. The dependence of a topological charge and helicity of the optical vortex beam on needle geometry, such as needle height and screw orientation, is quantitatively demonstrated. This dependence partially agrees with experimental measurements. Furthermore, we found that the presence of structure formation can be evaluated by extracting only the radial component of the force field and solving the one-dimensional equation of motion in the radial direction.

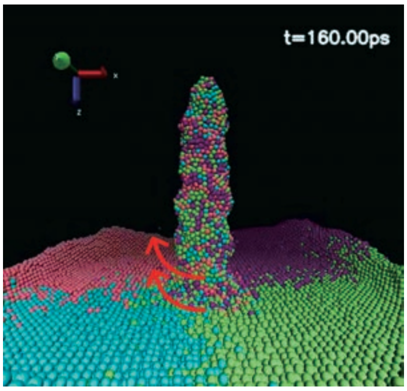

Fig. 2 Tantalum surface structures in the final state. The chiral structure is recognized, which is the same helicity of the force fields.

Isotope effect of the rovibrational distribution of hydrogen molecules desorbed from amorphous carbon

Plasma confinement experiments were carried out using deuterium in the LHD, and the isotope effects were reported. Motivated by these isotope experiments at the LHD, we aim to extend neutral transport and molecular dynamics codes, which had been developed for light hydrogen, to handle not only deuterium but also tritium.

When the hydrogen isotope atom is injected into amorphous carbon with the incident energies E of 20, 50, and 80 eV, we obtain the following physical quantities of hydrogen isotope atoms/molecules emitted from the amorphous carbon using molecular dynamics and heat conduction hybrid simulation [3]. The physical quantities are the time evolution of the emission rate, the depth distribution of the original location of the hydrogen emitted from the target, the polar angular dependence, and the translational, rotational, and vibrational energy distributions. In addition, the approximate analysis yields the emission distributions at vibrational (v) and rotational (J) levels (Fig. 3). Using these distributions, we evaluate the rotational temperature T_{rot} for $v = 0$ and small J states. From the above, it is found that molecules with higher rotational levels J tend to be emitted as E in increases or as the mass of hydrogen isotope increases. Moreover, the isotope effect appears in the mass dependence of T_{rot}.

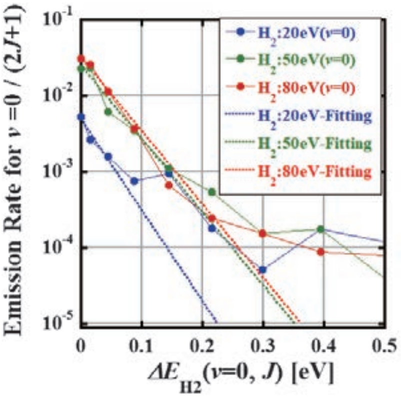

Fig. 3 The emission rate of hydrogen molecules from the graphite surface. The Boltzmann distribution is used as a fitting function. Fitting with the Boltzmann distributions is well done for low energy. However, for high energy, fitting is not well done with the Boltzmann distribution.

[2] H. Nakamura and S. Habu, Jpn. J. Appl. Phys. **62**, SA1013 (2022).

[3] H. Nakamura, S. Saito, T. Sawada, K. Sawada, G. Kawamura, M. Kobayashi and H. Hasuo, Jpn. J. Appl. Phys. **61**, SA1005 (2022).

(H. Nakamura)