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PROGRESS IN FIRST-PRINCIPLES BOUNDARY SIMULATIONS OF PLASMA TURBULENCE AND NEUTRAL DYNAMICS WITH THE GBS CODE

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Abstract

We present recent progress in boundary plasma simulations with the GBS code, which self-consistently evolves plasma and neutral species in three dimensions. Simulations show that negative triangularity stabilizes turbulence and affects the width of the scrape-off layer, while power sharing in double-null configurations is governed by drifts, turbulence, and geometry, captured by a validated scaling law. Simulations at high-density reproduce detachment dynamics, revealing the importance of molecular processes and E×B drifts. Flux-driven simulations with resonant magnetic perturbations demonstrate reduced divertor heat loads, and stellarator studies highlight distinct turbulence features with respect to tokamaks.

1. INTRODUCTION

The past years have seen major improvements in the modelling of the boundary region that regulates the exhaust in tokamaks and stellarators, an issue of vital importance for the design and operation of future fusion devices. In particular, the improvement of physical models and the increase of computational power have allowed for first-principles, turbulent simulations of experimentally relevant scenarios, where the plasma dynamics is self consistently simulated with the dynamics of neutral particles.

In the present work, we report on recent progress in the understanding of the physics mechanisms and predictive capabilities obtained with the GBS code. GBS [1] simulates self-consistently plasma turbulence and neutrals in the boundary of magnetic confinement devices in three-dimensions with no separation between fluctuating and equilibrium quantities. In its most general formulation, GBS evolves three charged species (electrons, D^+, D_2^+) and two neutral species (D and D_2), interacting through ionization, charge exchange, recombination, and molecular dissociation, which are subject to recycling phenomena at the wall. Plasma species are modelled with drift-reduced fluid Braginskii equations, while a kinetic model is used for the neutral dynamics. GBS flexible numerical algorithm allows simulations in arbitrary magnetic configurations, including complex wall geometries.

In the past years, GBS numerical scheme has been significantly improved. Thanks to the use of advanced meshing tools, it is now possible to carry out simulations that considers TCV first wall in baffled configurations. Advanced linear algebra techniques are used to solve the elliptic equations addressed by GBS, while advanced time stepping schemes are being developed to remove the constraints of the explicit schemes.

GBS flexibility is used to simulate the tokamak boundary in configurations that are alternative to the positive-triangularity lower-single-null configuration of ITER. Significant improvement of our understanding of the plasma dynamics in negative configurations is allowed by GBS simulations. We report our studies of the double null configuration, focusing on the mechanisms behind the power equipartition among the four divertor legs. The dependence of turbulent transport and the power decay length on the scrape-off-layer connection length is also being studied via leg-length scans.

For the first time, access to detachment conditions is studied through turbulent simulations. The relative role of different collisional processes that yield detachment are disentangled. The simulations point out that the E×B drift could play an important role in detachment access, and that a longer outer leg length makes detachment easier in both experiments and simulations. GBS reproduces the trends observed in experiments, such as increased turbulence in the divertor region for detached plasmas.

The flexibility of GBS has allowed the first simulations of plasma turbulence in the stellarator boundary. Simulation of the TJ-K stellarators were validated against experimental results. Ongoing effort is focused on the simulation of W7-AS, HSX and LHD stellarators.

2. ADVANCES IN NUMERICAL SCHEMES

Recent efforts have focused on overcoming the main computational bottlenecks of GBS by introducing advanced numerical techniques that target the most expensive parts of the code. A subspace acceleration method [2] was developed for efficiently solving the large-scale linear systems arising at each time step of the plasma model, which originate from the discretization of the field equations imposed upon the Braginskii fluid equation. The fields evolve smoothly in time, a property that can be exploited to generate high-accuracy initial guesses for iterative solvers by constructing a reduced-order subspace from the history of past solutions and using randomized linear algebra techniques to efficiently compress it. The initial guess for the next time step is then obtained by solving the linear system projected onto this compressed subspace. A rigorous convergence analysis, which extends the classical polynomial extrapolation theory to a vector-valued setting, show that the accuracy of the predicted initial guess improves rapidly as the size of the solution history increases. When applied to GBS, this approach significantly decreases the number of GMRES iterations required to solve the plasma elliptic systems, leading to a substantial reduction in the overall simulation time while preserving accuracy.

A hierarchical matrix approximation [3] strategy was implemented to accelerate the kinetic neutral model. In its deterministic formulation, the method of characteristics reduces the neutral dynamics to a set of two-dimensional integral equations with dense non-local operators. Upon discretization, these equations generate large dense matrices, making both their assembly and storage prohibitively expensive, especially in high-resolution simulations relevant to reactor-scale devices. The new algorithm hierarchically partitions the physical domain and identifies matrix blocks where the interaction kernel is smooth, allowing selective low-rank approximations via adaptive cross approximation. This reduces both computational complexity and memory requirements from quadratic to nearly linear in the number of grid points. Integrated into GBS, the method achieved over 90% savings in both time and memory, enabling unprecedented high-resolution simulations of neutral dynamics and providing a fully resolved picture of plasma–neutral interactions.

A globally stiffly accurate Implicit–Explicit (IMEX) Runge–Kutta scheme [4] is implemented in GBS, where the fastest plasma phenomena are integrated implicitly. IMEX methods offer a balanced approach by treating stiff terms implicitly and non-stiff terms explicitly, thus enabling larger time steps than the Courant–Friedrichs–Lewy limit, while avoiding the full cost of fully implicit integration. The fastest plasma dynamics are characterized by shear Alfvén waves (SAWs) [5] and parallel diffusion, which are consequently treated implicitly. To improve the spatial discretization of the SAWs, we introduce a finite difference method on staggered grids, specifically designed for wave-like problems, which is both rigorously energy-preserving and highly accurate [6]. This method mimics key features of the summation-by-parts framework, in particular the discrete preservation of the divergence theorem. To accelerate the implicit solution of the SAW system, we construct a 3D physics-based preconditioner tailored to this system, inspired by techniques developed in the magnetohydrodynamic context [7]. Both the solver and preconditioner are implemented using the PETSc library. By combining stable spatial discretization with an efficient IMEX time integration strategy, we demonstrate both numerical stability and significant computational efficiency in simulating two-fluid edge turbulence.

In order to capture wall shape effects on boundary turbulence, the GBS implementation is generalized to handle realistic first wall geometry. This extension is then used to perform the first set of plasma edge turbulence simulations in baffled TCV configurations. Leveraging curvilinear finite differences, plasma profiles are solved on boundary-fitted single-block structured meshes. Mesh generation is enabled by a spline-based elliptic solver stemming from isogeometric analysis applications, and supports goal-oriented optimizations, such as ensuring homogeneous cell volumes [8]. In order to capture the impact of first wall geometry on neutral species, the kinetic neutral solver of GBS is extended to use "Chimera" meshes, combining high resolution boundary segment data and a coarsely discretized interior vessel volume. The implementation is checked for correctness using a set of unit tests and direct comparison against existing simulations in rectangular geometry. First turbulence simulations of a half-size TCV configuration in baffled geometry are performed. Results are found to be well characterized by the separation between last-closed flux surface and outer baffle tip, as previously seen in numerical and experimental studies [9,10]. In particular, an increased ratio between particle flux received by the baffle surface with respect to the vessel floor is measured as the baffle tip is placed closer to the separatrix. In baffled geometries, a decrease of density fluctuations is attributed to a reduction in perpendicular transport caused by baffle insertion. When including neutral dynamics, an increased neutral compression ratio is retrieved with increasing divertor closure, alongside a decrease in upstream neutral density, in line with previous numerical transport studies [10].

2. ALTERNATIVE EXHAUST CONFIGURATIONS

The numerical flexibility of GBS enables the study of various alternative divertor configurations to the ITER positive-triangularity (PT) lower single-null (LSN) scenario. These include negative triangularity (NT), double-null (DN), and even non-axisymmetric configurations such as tokamak with resonant magnetic perturbations and stellarators. We first investigate the effect of triangularity on tokamak boundary plasma turbulence [11], focusing on NT plasmas. Nonlinear simulations show that NT stabilizes interchange-type turbulence, while linear analyses indicate that this stabilization arises from a reduced magnetic curvature drive of the resistive ballooning mode (RBM). As a result, the pressure decay length L_p, which is linked to the scrape-off layer power fall-off length λ_q, is strongly affected by triangularity. Building on the analytical scaling law for L_p in L-mode plasmas derived in Ref. [12], we extend the theory to include triangularity effects. The extended scaling predicts a reduced λ_q due to weaker RBM drive, consistent with nonlinear simulations and multi-machine experimental databases, including recent TCV discharges dedicated to triangularity effects in L-mode diverted plasmas.

We then examine L-mode double-null (DN) configurations, where four divertor targets may help distribute power across multiple strike points [13]. To analyse power sharing at the upper and lower outer targets, we perform parametric scans where we vary plasma resistivity and magnetic imbalance. The results show that power asymmetry in DN plasmas arises from the combined influence of diamagnetic drifts, turbulence, and geometrical effects. Even in balanced DN scenarios, heat deposition is not evenly distributed between upper and lower targets; instead, the interplay between radial transport scales, magnetic imbalance, and diamagnetic contributions determines the up–down power asymmetry.

Finally, we explore the combined influence of triangularity and DN geometry on power exhaust [14]. Similar to the SN case, NT plasmas in DN geometry exhibit reduced RBM drive at the outer midplane. Blob detection analyses further reveal that NT reduces both blob size and radial propagation velocity, leading to mitigated plasma-wall interactions. These findings suggest that combining NT shaping with DN geometry may offer significant advantages for divertor power exhaust in future devices.

We also focus on the long-legged divertor configuration. A set of half-size TCV simulations scanning the divertor leg length of a LSN configuration is performed. The peak of the parallel heat flux at the low-field target decreases as the leg length increases. The profiles also show a weak increasing trend in the profile widths. These trends agree with the experiments performed in TCV. A detailed analysis of energy conservation in the divertor region reveal that the main drive of the reduction in peak heat flux is the turbulent cross-field transport. In addition, we observe that the strength of cross-field transport decreases along the leg. The set of simulations is now being repeated including monoatomic neutrals to assess the importance of plasma-neutral interaction in the particle and heat exhaust properties of the long leg configuration.

By taking advantage of the numerical algorithm implemented in GBS, the first results of three-dimensional, flux-driven, electrostatic, global, two-fluid turbulence simulations of a diverted tokamak configuration with applied resonant magnetic perturbations generated by a set of saddle coils are presented [15]. The simulations of an L-mode plasma show that the heat flux pattern on the divertor targets is affected by the resonant magnetic perturbations, because of the interplay between turbulent cross field transport and parallel flows. The simulation results reveal the potential of resonant magnetic perturbations to reduce the heat flux to the wall. In fact, the peak of the toroidally-and time-averaged heat flux as well as its value integrated over the divertor decrease as the amplitude of the magnetic perturbation increases, while the plasma sources are held constant.

3. DETACHMENT

In order to study the physics of detachment, simulations of high-density deuterium plasmas in a lower single-null magnetic configuration based on a TCV discharge are performed [16]. To control the divertor conditions, a gas puffing is used. The increase in fuelling leads to an increase of density in the scrape-off layer and a decrease of the plasma temperature. At the same time, the particle and heat fluxes to the divertor target decrease and the detachment of the inner target is observed with varying divertor leg length and constant power. As observed experimentally, a longer leg leads to detachment at lower upstream plasma density. The analysis of particle and transport balance in the divertor volume shows that the decrease of the particle flux is caused by a decrease of the local neutral ionization together with a decrease of the parallel velocity, caused by the lower plasma temperature and the increase in momentum losses. The relative importance of the different collision terms is assessed, showing the crucial role of molecular interactions, as they are responsible for increasing the atomic neutral density and temperature, since most of the neutrals are produced by molecular activated recombination and dissociation. The presence of strong electric fields in high-density plasmas is also shown, revealing the role of the E×B drift in setting the asymmetry between the divertor targets.

Simulation results agree with experimental observations of increased density decay length, attributed to a decrease of parallel transport. Quantitative comparisons between GPI measurements and synthetic diagnostic results show good agreement, indicating that GBS simulations can reproduce both the fluctuation levels observed in experiments and the trend of increasing turbulence with higher plasma density. The simulations further reveal larger plasma blobs and higher radial velocities, consistent with the experimental findings.

4. BIASING

A polarized electrode is now implemented in GBS to perform the first voltage biasing turbulence simulations in a realistic diverted magnetic geometry [17]. The first GBS voltage biasing simulations are performed targeting RFX-mod diverted experiments, where the biasing electrode is used to generate a significant level of E×B flow shear that enables the access to the high-confinement (H-mode) regime [18]. The GBS simulations show a strong turbulent transport reduction when the tokamak edge is biased, which is caused by the large E×B flow shear that forms across the separatrix. Consequently, the pressure gradient across the separatrix increases by almost a factor of two when the electrode is polarized to experimental voltage values, thus reproducing the transition to the H-mode found experimentally. The flow shear radial profile across the separatrix and the value of the current drained by the electrode are in qualitative and quantitative agreement with the experimental measurements [19]. By leveraging the results of the GBS simulations with voltage biasing, the analytical theory-based scaling law for L_p in L-mode plasmas, derived in Ref. [12], is extended to include the effect of the E×B flow shear.

The E×B flow shear turbulence suppression is particularly effective at large density, where the turbulence fluctuations driven by resistive ballooning modes at the tokamak edge are very extended in the radial direction and therefore are subjected to a large differential poloidal velocity. Consequently, the very large turbulent transport observed in high-density GBS simulations [20] is reduced substantially when the tokamak edge is biased to drive moderate values of E×B flow shear. The results of this numerical investigation suggest a possible important effect of the flow shear on turbulence-based density limit scaling laws, such as the one derived in Ref. [21].

5. STELLARATOR

Finally, the geometrical operators appearing in the drift-reduced Braginskii equations evolved by GBS are expanded considering the typical parameter ordering of stellarator configurations [22]. Simulations of an island divertor stellarator show that, although the island magnetic field-lines divert the plasma towards the strike points of the walls, the islands do not seem to have a significant impact on the turbulence properties. The dominant mode, identified as interchange-driven, is field-aligned and breaks the stellarator toroidal symmetry. The radial and poloidal extensions of the mode are of the same order, in contrast to typical tokamak simulations.

A first validation exercise was carried out against measurement from the TJ-K stellarator, a low temperature plasma experiment ideally suited for turbulence measurements [23]. More recently, we focus on the comparison with local turbulent measurements from the HSX stellarator [24], the largest quasi-symmetric stellarator in operation. Using synthetic Langmuir probes, we find very good agreement with experimental turbulence properties, including power spectra, local poloidal wavenumbers, and correlation lengths. Turbulence is observed to be field-aligned and driven by pressure gradients and magnetic curvature. Radial transport is driven by the E×B drift, consistently with measurements.

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