Coupled whole device simulations of plasma transport in tokamaks with the FACETS code

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Abstract. The FACETS project aims to provide computational tools for whole device simulation of tokamak transport for use in fusion applications. The framework provides flexibility by allowing users to choose the best model for a given physics target. Our goals are to develop accurate transport solvers using neoclassical and turbulent fluxes with varying degree of fidelity and computational complexity, including embedded gyrokinetic models. Accurate sources using both ICRH wave absorption and neutral beam injection, using parallel source components, are included. Modeling of the plasma edge using a fluid based component, UEDGE, is performed and coupled to the core solver. The core region is simulated using a newly developed parallel, nested iteration based nonlinear solver while the UEDGE uses nonlinear solves from the PETSc/SNES solver package. As a first application we present coupled core–edge simulations of pedestal buildup in the DIIID tokamak.

1. Introduction

Fusion promises to be an efficient source of clean energy. The world-wide fusion community is embarking on an ambitious next step: the ITER project (`http://www.iter.org/`). ITER is a joint international research and development project that aims to demonstrate the scientific and technical feasibility of fusion power. With over 16 billion Euros investment planned in ITER from the EU, the US, Russia, Japan, China, and India, ITER is an important next step for the worldwide fusion program, and an important part of the U.S. Department of Energy mission. For this reason, ITER was listed as the highest priority in the twenty-year outlook of DOE facilities[1]. The success of ITER requires that the facility is optimally used, which not only means achieving the best operating conditions, but also achieving a thorough understanding of the experimental results.

To obtain maximal returns on this investment it is critical to have computational tools to help optimize the design and provide theoretical insights into experimental results. Several such computational efforts are currently underway, some devoted to studying detail physical processes in the plasma and others devoted to performing whole device simulations using coupled reduced physics models. The FACETS (Framework Application for Core-Edge Transport Simulations) project[2] has the goal of providing whole-tokamak modeling through coupling separate components for each of the core region, edge region, and wall, with realistic sources. This is a complex problem, as each component is parallel in its own right, and each can be made parallel in a distinct manner.

Given the large disparity in space and time scales in a tokamak, progress can be achieved only by separating physics into different parts, such that for each part, valid, reduced approximations exist. For example, in the core of the plasma, the rapid transport along field lines assures that the plasma parameters such as density and temperature are, over long time scales, constant on toroidally nested flux surfaces. This reduces the transport equation to one dimension for evolution on the discharge time scale. However, the cross-field transport coefficient are difficult to determine accurately and sophisticated models, with varying predictive capability, have been developed. The current state-of-art in core-transport modelling uses gyrokinetic turbulence calculation to account for the dominant anomalous transport processes. Although this "embedded" gyrokinetic approach is computationally expensive it is feasible with current generation of Leadership Class Facilities (LCFs). In the plasma edge, though, simulations must be global and two-dimensional. The separation of scales in the edge is not as clean as in the core region and for this reason global edge turbulence models need to be developed to achieve true predictive capability. The development of such edge turbulence models, even using fluid approximations, is still an active research area.

The complexity of whole-device simulations of tokamaks translates to requiring a software component approach, as FACETS is taking. FACETS is bringing together successively more accurate and, hence, computationally demanding components to model the complete plasma device. It is being developed to run on LCFs to be able to use the most computationally demanding components, while at the same time it is usable on laptops for less demanding models. FACETS is constructing a C++ framework for incorporating the best software packages and physics components. A description of the FACETS framework is given in[3] in which the component approach and description of key concepts in the framework is given.

In this paper we present results from coupled core-edge simulations of pedestal buildup in the DIII-D tokamak for a selected shot. The rest of the paper is organized as follows. We first describe the core and edge equations used in the analysis and also describe the coupling scheme to advance the coupled system self-consistently in time. Then we describe the shot (DIII-D shot 118897) and initial conditions and edge interpretive analysis used in the calculations. Results are then presented and discussed. We then make some concluding remarks and indicate further work on modelling the core-edge physics more accurately.

2. Core and Edge Models and Coupling Scheme

High-performance tokamak plasma discharges (so-called "H-mode" plasmas) are characterized by steep gradients of temperature and density near the plasma separatrix where open field lines separate from closed field lines. This region is referred to as the "H-mode pedestal". Experiments and core transport simulations indicate that core profiles are relatively insensitive to the overall values of density and temperature, but that the shape is set by stiff transport due to kinetic turbulence. Thus, the overall fusion gain depends sensitively on the parameters at the top of the pedestal temperature and density[4]. The pedestal height serves as a boundary condition to the core plasma region. The physics determining the formation of the pedestal (the so-called L-H transition) is not fully understood, and is the subject of active investigations[5]. As a first test of the FACETS code we have undertaken the simulation of the the pedestal buildup in a particular shot of the DIII-D tokamak. However, due to poor understanding of the edge physics and lack of availability of predictive models for the edge transport we have used an interpretive analysis to determine the edge cross-field transport coefficients. These are held constant throughout the simulation. Although not fully self-consistent, this serves to test the infrastructure and also gives insight into the time-scales over which edge transport coefficients evolve.

Well inside the separatrix the plasma is hot which leads to large disparities in the transport parallel and perpendicular to the field lines. This in turn implies that, on transport time-scales, the plasma equilibriates in the poloidal direction and the physics can now be described as a set of one dimensional equations for the perpendicular transport of density and energy

$$\frac{\partial n}{\partial t} + \frac{1}{V'}\frac{\partial}{\partial \rho}(V' F_n^\rho) = S_n \tag{1}$$

$$\frac{3}{2}\frac{\partial}{\partial t}(nT_s) + \frac{1}{V'}\frac{\partial}{\partial \rho}(V' F_s^\rho) = S_s \tag{2}$$

where $n(\rho,t)$ is the plasma number density, $T_s(\rho,t)$ are electron ($s = e$) and ion ($s = i$) temperatures, F_n^ρ is the contravariant particle flux, F_s^ρ are the contravariant thermal fluxes and $S_n(\rho,t)$ and $S_s(\rho,t)$ are the particle and thermal sources. The independent variable is the dimensionless normalized toroidal flux ρ and the radial geometry is encapsulated in $V' \equiv dV/d\rho$, where $V(\rho)$ is the volume enclosed inside the flux surface ρ.

The fluxes are computed using a combination of anomalous and neoclassical terms $F_{\mathrm{GLF}} + F_{\mathrm{CH}} + F_{\mathrm{ETG}}$, where F_{GLF} is the anomalous flux computed using the GLF23[6] model, F_{CH} is the neoclassical flux computed using the Chang-Hinton[7] model and F_{ETG} is anomalous electron transport due to Horton-ETG model[8]. The system of core transport equations Eq. (1) and Eq. (2) are highly non-linear and stiff due to the strong dependence of the fluxes on the gradients of the density and temperatures. A nested-iterations based implicit solver is implemented in FACETS to evolve this set of equations[9].

As we approach the separatrix the plasma cools and the field lines are no longer nested. This leads to two-dimensional effects and the plasma transport both along and perpendicular to the field lines now needs to be evolved. FACETS incorporates the fluid edge code UEDGE[10, 11] to solve the edge plasma equations. UEDGE includes full single- or double-null X-point geometry with a simulation domain including the region spanning well inside the separatrix and extending to the outer wall and the divertor plate region. A reduced set of the Braginskii transport equations is solved. Usually the cross diffusion terms are turned off and the Alfven waves are suppressed by not evolving the induction equation for the magnetic field. Additional assumptions are used to express the equations in a form more amenable to disabling various physics terms to allow faster solution times, or to allow better physics understanding. The specific form of the equations are found in Ref.[11].

The coupling between the core and the edge regions is performed using an explicit scheme. There are several challenges in setting up an self-consistent problem across the one-dimensional predictive core region with the two-dimensional interpretive edge region. First, the initial conditions need be to C^1 continuous across the core-edge (CE) interface. Second, the transport coefficients at the CE interface need to match. This is particularly difficult as completely different models are used to compute the fluxes in the core and edge solvers. An ad-hoc scheme is presently implemented in FACETS to enforce this. The continuity in the initial conditions is ensure by using the same set of experimental data to initialize both the core and the edge. However, this

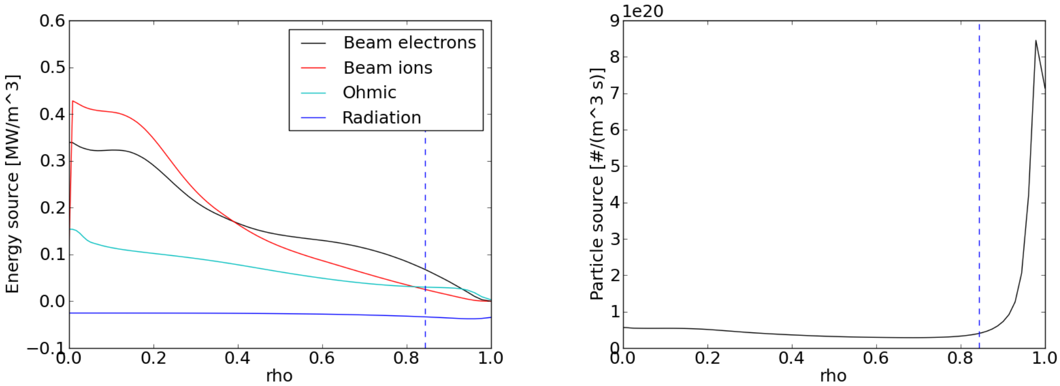

Figure 1. Power sources for electrons and ions (left) and plasma particle source (right). Total beam power for ions is 1.78 MW, for electrons 2.21 MW and Ohmic heating is 0.93 MW and radiation loss is 0.40 MW. Net particle injection rate is 2.12×10^{21} s^{-1}. Out of these, the fraction of particles into the core is 4.99×10^{20} s^{-1}. Rest (1.617×10^{21} s^{-1}) should be accounted for in the edge.

does not guarantee the continuity of slopes at the CE interface as two components use different grids and discretization schemes.

The coupled simulation is run as follows. The core and edge components are run concurrently for a specified time-step dt. Typically, both component need to sub-cycle to evolve their solutions by this time-step. The particle and energy fluxes are passed from the core to the edge, i.e. $F^{\rho}V'/A = F^{\rho}/ < |\nabla\rho| >$ is sent to the edge, where A is the area of the flux surface at the CE interface and the angular brackets indicate flux surface averaging. The flux-surface averaged temperature and number density are passed from the edge to the core. These steps are repeated and the simulation evolved in time.

The explicit coupling scheme described above is stable as long as sufficiently small time-steps are taken. Numerical experiments show that a time-step on the order of several 100 μs can be taken without the coupled solution going unstable. A fully implicit coupling scheme, although not used in this paper, is also implemented in FACETS and presently being tested for use in core-edge simulations.

3. Problem Setup and Results

Coupled core-edge simulations using the methods described in the previous section are performed to study the pedestal buildup in the DIII-D tokamak. For this we have chosen to simulate the time slice from 1555 to 1590 ms of DIII-D shot 118897. From the experimental wave forms it is seen that the neutral beams are turned on around 1490 ms and the plasma density increases from around 2.8×10^{19} m^3 to 3.9×10^{19} m^3.The beam power in the chosen interval averages to around 4.5 MW and eventually drops down to 2.5 MW around 1600 ms. The discharge is ELM free till around 2355 ms.

Beam sources are held constant during the simulation and are taken from an interpretive ONETWO simulation. See Fig. 1 for beam source heating profiles for ions and electrons. The simulation is initialized using experimental data averaged around 1555 ms into the discharge. See Fig. 2 for initial density and temperature profiles. The core component is run to $\rho = 0.85$ and the edge component from there to the wall. Note that this puts the pedestal inside the edge component. The reason for doing this is two fold: (a) the core transport models do not work very well for $\rho > 0.85$ and, (b) we want to ensure that the edge is sufficiently inside the

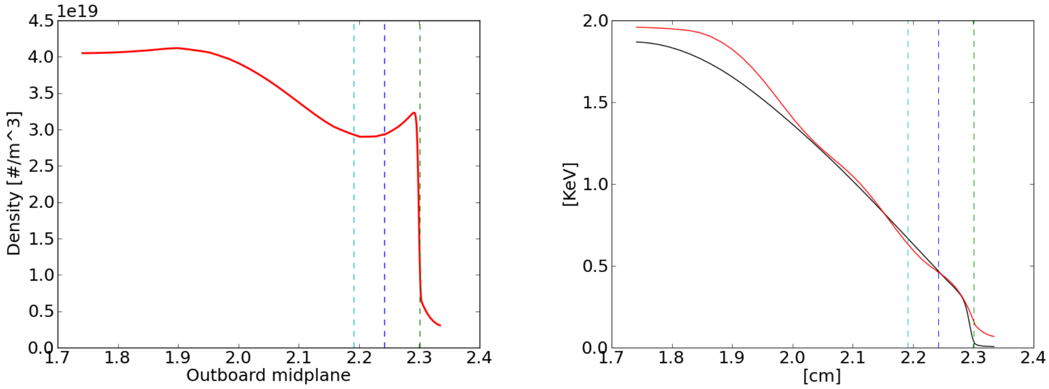

Figure 2. Initial density (left) and temperature (right) profiles for electrons (black) and ions (red) for shot 118897 at 1555 ms. The blue dashed lines indicate the core-edge interface, the green dashed line the separatrix and the cyan line the start of transition from predictive to interpretive fluxes.

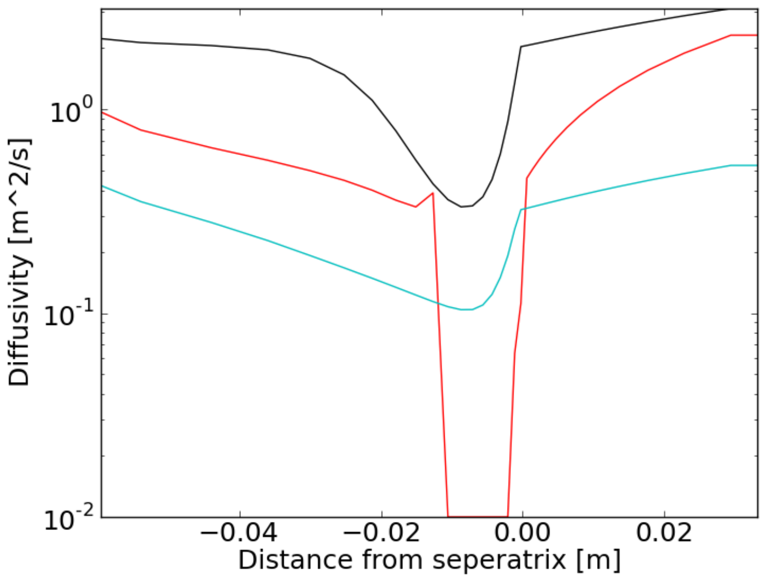

Figure 3. UEDGE diffusivities from interpretive calculations. Red line D, black line χ_e, blue line χ_i.

separatrix for the solutions to be relaxed along the poloidal direction.

An initial set of calculations using experimental profiles and sources is performed to determine the cross-field diffusivities for UEDGE. See Fig. 3. The diffusivites drop down significantly in the pedestal to create a transport barrier for the pedestal formation. As mentioned before this procedure is not self-consistent as the core is predictive, but lacking predictive edge models this method must be adopted. A fully interpretive edge model should predict a similar transport barrier. Once these diffusivities were determined they were held constant through the 35 ms simulation time.

The core and edge components were evolved using the explicit coupling scheme described

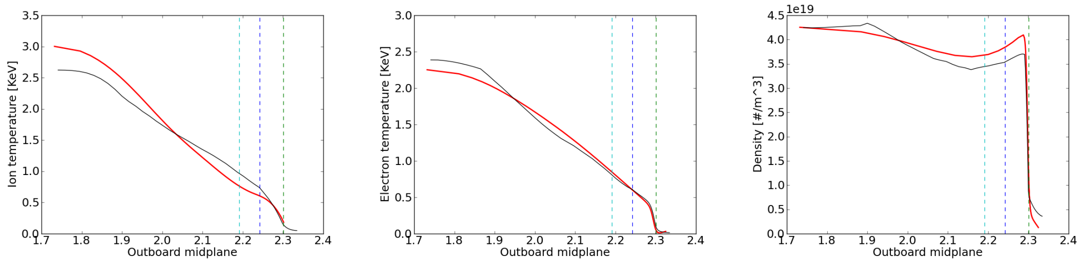

Figure 4. Final experimental (red) and simulation results (black) for ion (left) and electron (middle) temperatures at 35 ms. Final experimental density profile (red) and simulation results (black) are shown in the right panel. The ion temperature is over-predicted at the pedestal while the plasma density is under-predicted. Tuning the gas puff to supply an additional particle fueling source could lead to a higher density buildup in the edge.

above. A time-step of 200 μs was used to couple the components, although the components internally were allowed to choose their own time-steps. Plasma density, electron and ion energy equations were evolved. See Fig. 4 for comparison between simulation results and experimental profiles averaged around 1590 ms into the discharge. Our initial results show that the electron temperature is predicted better that the ion temperature. As seen in the figure the ion pedestal temperature rises beyond that seen in the experiment, indicating a greater flow of ion thermal energy into the edge. This leads to a corresponding loss in ion energy near the magnetic axis. This is behaviour is being investigated and it is believed that a proper accounting for the $\omega_{|E\times B|}$ shear profile will lead to a damping to the ion thermal flux near the CE interface and improve the ion temperature predictions. It is also seen that the density buildup in the edge is under-predicted. The reason for this could be that the neutral particle source fueling the edge is not sufficient to supply the net line-integrated density in the tokamak. An additional gas-puff source would supply this particle source and this is being investigated at present.

4. Conclusions

We have presented coupled core-edge simulations of pedestal buildup in a selected shot of the DIII-D tokamak. Our initial simulations show that FACETS can evolve the plasma density in addition to the electron and ion energy equations self-consistently using coupled core-edge simulations. Our initial calculations have shown a sensitivity of the pedestal buildup on the core-edge power balance and also to the presence of a gas-puff as a fueling source in the edge. These calculations show the ability of the framework to perform concurrent coupled simulations with multiple components and serve as a test for the explicit coupling algorithms. We expect improvements in the predicted ion temperature and plasma density with a better accounting of the shear flow profiles and a proper tuning of the gas-puff. We believe that our agreement with experiments is reasonable given the uncertainties in the core density model (GLF23) and the lack of a predictive edge model.

Our current work in FACETS is to increase the physics fidelity of the simulations. We have incorporated the NUBEAM neutral beams package that allows the self-consistent computation of the beam deposition into the core. However, before NUBEAM can be used on a production level it will have to be extended to deposit power into the edge. We have incorporated the TGLF[12] anomalous transport model to better predict the core transport coefficients. We have implemented a Newton-method based implicit coupling algorithm that we expect will allow us to take 10 ms time-steps, thus increasing the discharge time that can be simulated. We have completed the implementation of a sophisticated wall model that will be incorporated into the simulations. FACETS is now being used to simulate other DIII-D discharges to better quantify the core-edge physics.

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