

Introducing FACETS, the Framework Application for Core-Edge Transport Simulations

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Abstract. The FACETS (Framework Application for Core-Edge Transport Simulations) project began in January 2007 with the goal of providing core to wall transport modeling of a tokamak fusion reactor. This involves coupling previously separate computations for the core, edge, and wall regions. Such a coupling is primarily through connection regions of lower dimensionality. The project has started developing a component-based coupling framework to bring together models for each of these regions. In the first year, the core model will be a 1 1/2 dimensional model (1D transport across flux surfaces coupled to a 2D equilibrium) with fixed equilibrium. The initial edge model will be the fluid model, UEDGE, but inclusion of kinetic models is planned for the out years. The project also has an embedded Scientific Application Partnership that is examining embedding a full-scale turbulence model for obtaining the cross-surface fluxes into a core transport code.

1. Introduction

The approval of the ITER project [1] brings to the fusion sciences community an exciting new time. ITER is an international project to build the largest tokamak magnetic plasma device. Its parameters (6.2 m major radius, 2.0 m minor radius, 500 MW power, 15 MA plasma current, and a burn time in excess of 400 s) are far beyond those of any current tokamak. It is expected to have a fusion triple product (the performance parameter $n\tau T$, where n is the plasma density, τ is the energy confinement time, and T is the plasma temperature) exceeding the best tokamaks extant by a factor of 20-30.

Computational modeling will be critical for the performance of ITER. Current estimates are that each shot will cost of the order of \$1 M. Hence, it is important that each shot be carefully planned,

with the outcomes predicted to the greatest possible degree, so that maximum knowledge can be gleaned. Computational modeling will be necessary for this planning. Computational modeling will allow multiple scenarios, including calculations of alternate, competing theories, to be generated. Moreover, computational modeling is important for experimental analysis, as it is often how one determines where, e.g., the energy from neutral beams and/or radiofrequency (rf) power is deposited.

While the fusion community has a long history of computation for the prediction of plasma dynamics, the fusion community, through the SciDAC program, is moving towards a new computational challenge, that of computational modeling of the entire device in one simulation – a simulation that would require petascale resources to complete. There are several projects (FACETS [2], SWIM [3], CEPS [4]) that are exploring different ways of coupling and different aspects of the coupling problem. The FACETS project is working in the space of direct coupling through messaging (rather than file-based transfers) using the Message Passing Interface (MPI), and it is concentrating in the early years of the project in surfacial coupling, i.e., the different models are applicable in different spatial regions, and they meet in a region of lower dimensionality. The specific application is core-edge coupling [5].

The FACETS project therefore has set up teams in each of the areas of the project. The Framework team has the task of putting together the coupling framework that will bring in each of the components. Similarly, there are teams for each of the component areas – Core, Edge, and Wall. Cross cutting areas include Performance, Algorithms, and Coupling Research, the latter from the point of view of physics, applied math, and computer science. Finally, there is a Scientific Application Partnership dealing with embedded turbulence computations.

2. Plasma core

The magnetic field lines in a tokamak have two different topologies (*cf* Fig. 1). Inside the *separatrix*, the magnetic field lines lie on dense, nested *flux surfaces*. Outside the separatrix are the *open field lines*, which intersect the walls. Sufficiently inside the separatrix is the *core*, the region where the local plasma thermodynamic intensive quantities are nearly constant on flux surfaces. This occurs because the rapid transport along magnetic field lines causes equilibration within a flux surface. In the core, the dynamics is well represented by a 1D reaction-diffusion-convection-like equation.

The difficulty in core computations thus comes not from the basic form of the equation, but instead from the complexities of computing the coefficients and sources for the transport equation. The transport itself largely originates from turbulence. Reduced models (e.g., [6]) provide the fluxes of particles, heat, and angular momentum given the local plasma parameters, such as the density, density gradient, temperature, temperature gradient, etc. Reduced models are important given that the turbulence calculations to compute the fluxes for a single set of local values require high-performance computing resources. However, even so, the current reduced model calculations are compute intensive, such that the computation of the local flux can be parallelized over of the order of 10 processors, and fluxes must be computed over of the order of 100 surfaces. In addition, the computation of sources of particles and energy through, e.g., neutral beam ionization and slowing down [7] and propagation of rf waves into the plasma requires high-performance computing resources. Thus, fully descriptive core computations themselves can benefit from high-performance computing. For coupling with the edge, the requirements are even greater.

3. Plasma edge

The edge region (just inside and outside the separatrix to the wall in Fig. 1) plays various key roles: (1), it distributes the escaping plasma exhaust power to the walls to avoid excessive local heat fluxes;

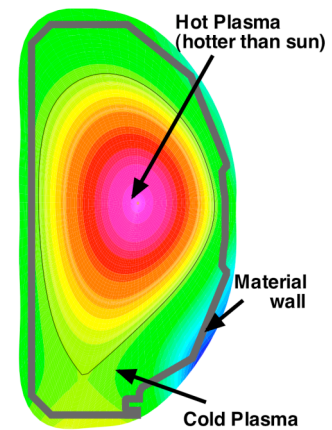


Fig. 1. Cross-section of a tokamak plasma.

(2), it partially shields the core from contaminating impurities sputtered from the walls; and (3), it determines the plasma density and temperature at the edge of the core, which has a very strong influence on fusion power gain. The geometrical complexity of this region is greater than in the core because outside the separatrix, as noted above, the magnetic field lines intersect material surfaces rather than forming isolated flux surfaces, and a magnetic X-point is formed (Fig. 1). Consequently, plasma parameters are no longer approximate constants along the field lines, but have variations that must be computed even for transport calculations. Hence, even the fluid transport models such as UEDGE [8] are 2D. Furthermore, owing to steep gradients, large ion orbits, and the presence of the separatrix, neoclassical collisional transport cannot be treated analytically, thus requiring 4D transport codes now being developed that add two velocity-space dimensions to describe the non-Maxwellian distribution functions. A crucial phenomenon of the edge region is the Edge Localized Mode (ELM) that is a 3D MHD instability. As in the core, microturbulence can be described by 3D fluid codes and 5D kinetic codes. In addition, there are substantial neutral gas components in the edge (hydrogen and impurity) that arise from the walls that must be consistently modeled with the plasma.

4. Plasma-wall interactions

Plasma ion species interact with plasma facing components (PFCs) via collisions with plasma particles penetrating and diffusing into the wall. The first few nanometers of wall are known to contain more hydrogen than the whole plasma volume. Even small inventory variations in the wall can have a strong impact on the plasma, including experimentally observed Multifaceted Asymmetric Radiation from the Edge (MARFE), transition to a detached divertor state, and plasma disruption. Coupling to edge plasma transport will allow us to assess the tolerable heat and particle loads in a steady-state operation, the lifetime of PFCs, the effect of plasma contamination by impurities, as well as the level of tritium retention, all of which are vital issues for ITER.

We are presently developing a new code - the Wall and Plasma-Surface Interactions (WallPSI) module - to model wall temperature and concentrations of adsorbed, mobile and trapped particle species in the wall. The plasma-wall interactions are strongly non-linear. The characteristics of elementary wall processes such as desorption, trapping, detrapping, diffusion, and chemical reactions depend exponentially on wall temperature and implicitly on plasma parameters. Our goal is develop infrastructure and algorithms for coupling the WallPSI module to the edge plasma transport code UEDGE so as to resolve the short time scales known to cause abrupt thermal plasma instabilities in response to changing magnetic equilibrium, incident plasma flux or wall temperature.

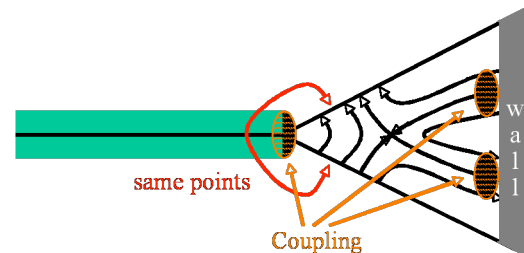


Fig. 2. Topological representation of the plasma

5. Couplings and the framework

Topologically, the plasma coupling can be represented as in Fig. 2. As noted above, the dynamics can be considered one-dimensional in the core, but then as the separatrix is approached, variation along field lines arises. Taking the coupling to be at the outer limit of where variation with a flux surface can be ignored, then the coupling between core and edge is at a point, the rightmost extreme of the thick green line in Fig. 2. Similarly, at the termination of the field lines that hit the wall in Fig. 2, there are point couplings between the edge plasma and the wall.

Each of the components in this model must be advanced implicitly, as there are local time scales, such as those associated with rapid relaxation of small scale perturbations in the core diffusion equation, that are very fast compared with the time scales of interest. From this, it is believed that the fully coupled system must be advanced implicitly.

So far, we have been discussing this system as if the magnetic field, which determines the topology, is static. However, in fact the equilibrium is determined by the pressure profiles which are

determined by the core dynamics as well as by pressure gradients and currents in edge plasma, both inside and outside the separatrix. Thus, the coupling framework will have to deal with volumetric in addition to surfacial coupling, as the core and edge dynamics are intimately tied to the magnetic topology throughout the plasma volume.

To bring all of this together, we need a flexible coupling framework, which is under development now, with an initial implementation to be presented at our first meeting in Boulder Aug 9-10. The framework must handle surfacial couplings, but in the out years it will need to handle volumetric couplings. It will need to work with implicit and explicit couplings. Moreover, since the computational requirements are large, we are developing a framework that can disperse the many calculations across multiple processors and, at the same time, set up the determined but irregular communication paths among the components.

6. Embedded Turbulence Computations

The goal of the Steady State Gyrokinetic Transport (SSGKT) Project SAP is to develop a prototypical code that integrates micro-scale gyrokinetic turbulence simulations into a macroscopic transport system. This multi-scale simulation will be used to predict the performance (the fusion energy gain, Q) given the H-mode pedestal temperature and density. At present, projections of this type rely on transport models like GLF23 [6], which are based on rather approximate fits to the results of linear and nonlinear simulations. SSGKT will address a key problem of critical scientific importance; namely, predicting the performance of ITER given an edge boundary condition – but now using embedded turbulence calculations. The key scientific advance will be crucial: to show that gyrokinetic codes (simulating microscales) can be run practically within a transport code (simulating the macroscale).

The method of approach is to develop a lightweight master code TGYRO that will coordinate feedback between a transport module and multiple independent (each massively parallel) gyrokinetic simulations using GYRO [9]. Each instance of GYRO will compute local radial fluxes that will be periodically communicated through TGYRO to the transport module. Figure 3 shows preliminary results from the TGYRO prototype.

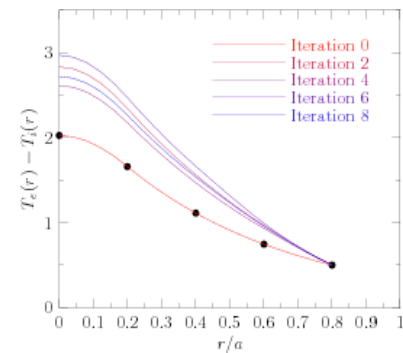


Fig. 3. Computation of the temperature profile from four embedded turbulence computations using GYRO.

7. Performance activities

Performance analysis and improvement of the FACETS components and framework are important to reach the timing and scaling goals of the project. The TAU parallel performance [10] system is being used for instrumentation and measurement of the NUBEAM, UEDGE, and WALL components, including their parallel implementations (performance testing of parallel NUBEAM is currently underway), with TAU's profile and trace analysis tools used to interpret performance inefficiencies and opportunities for tuning. A performance database and a web-based portal is being created to track performance data throughout the project. In addition to FACETS component analysis, the performance infrastructure is being integrated in the FACETS framework to observe and understand performance of the coupled simulation. Performance evaluation activities will include experiments on large-scale computing platforms at NERSC, ORNL, and Argonne. Particular performance studies will focus on simulation scaling and exposing performance bottlenecks within and between components on the different platforms.

8. Algorithmic improvements

The solution of (non)linear partial differential equations (PDEs) pervades several aspects of the coupled core-edge simulations, including core transport, edge transport, edge turbulence, and neutral transport. In present-day uncoupled models, a significant fraction of overall simulation time for edge computations is often devoted to linear and nonlinear solvers. We are thus addressing algorithmic issues in collaboration with the TOPS project [11], whose mission is to develop a set of compatible toolkits of open-source, optimal complexity solvers for nonlinear PDEs. Initial work focuses on incorporating TOPS expertise in scalable nonlinear algebraic solvers into the base physics codes that provide the foundation for the coupled models, with emphasis on achieving scalable performance using preconditioned Newton-Krylov methods. We developed an interface between UEDGE and the nonlinear solvers in PETSc [12], and experiments are currently underway with various preconditioning algorithms and variants of matrix-free Newton methods.

9. Coupling research

As noted earlier, the FACETS project involves both surfacial and volumetric coupling of physics components that differ in spatial and/or temporal scales and/or dimensionality. The algorithm chosen for coupling may have a significant impact on the speed, accuracy, and stability of the overall calculation. Various coupling strategies must be examined for the potential impact on the accuracy and stability properties of the resulting numerical method as well as the efficiency of solution. In some cases, new coupling integration schemes need to be developed.

Two examples of near-term interest for FACETS are the coupling of core and edge transport (a surfacial coupling) and the calculation in either region of transport with self-consistent turbulence. The transport equations in the core and edge are both diffusive in nature, though the solutions evolve over vastly different scales. Employing a coupling strategy introduces new kinds of discretization error, e.g. the numerical error in the solution of one component enters as modeling error in the other component, and affects overall stability, e.g. defining an implicit scheme becomes difficult since the core and edge are solved at different scales. These can affect the convergence of the iteration between the core and edge solutions and the accuracy of a computation over time. Past efforts in coupling iteration include both fixed point and Newton iterations to achieve consistency of the common boundary conditions. We are pursuing Newton approach to try to preserve implicitness in the overall solution. We are developing *a posteriori* error estimates based on variational analysis and the solution of adjoint equations to quantify the effects of numerical error and coupling on overall accuracy. This will lead to quantitative information about the expected accuracy of various coupling schemes and provide a guide for balancing resources, e.g. between advancing the physics in time and coupling the physics at a given time. As part of this project, we are exploring the implementation of adjoint-based analysis tools for peta-scale simulations.

10. Summary and future directions

The FACETS project has outlined the issues and has begun developing new software and adapting existing software to provide a full, core-edge-wall model of a tokamak plasma. The FACETS project is concentrating on surfacial couplings during the first period of the project, but it will need to allow for volumetric coupling once dynamic equilibrium has been brought into the system. The FACETS project also has a research component that is looking at coupling issues from physics, applied math, and computer science points of view.

References

- [1] <http://www.iter.org>.
- [2] <https://facets.txcorp.com/facets/>
- [3] <http://www.cims.nyu.edu/cpes/>
- [4] <https://cswim.org/>
- [5] Fichtmuller M, Mertens V, Neuhauser J et al. 1998 Czech J. Phys. **48** Suppl. 2, 25

- [6] Waltz R E, et al., 1997 Phys. Plasmas **4** 2482
- [7] Goldston RJ et al. **1981** J. Comp. Phys. **43** 61; Pankin A, McCune D, Andre R et al. 2004 Comp. Phys. Comm. **159** 157
- [8] Rognlien T D and Rensink M E 2002 Fusion Eng. Design **60** 497
- [9] Candy J and Waltz R E 2003 J. Comput. Phys. **186** 545
- [10] S. Shende and A. Malony, "The TAU Parallel Performance System," International Journal of High Performance Computing Applications, Volume 20, Number 2 Summer 2006. Pages 287-331.
- [11] Keyes D E (PI), TOPS SciDAC project, <http://www.scidac.gov/math/TOPS.html>.
- [12] Smith B et al., PETSc library, <http://www.mcs.anl.gov/petsc>