# Toward a first-principles integrated simulation of tokamak edge plasmas

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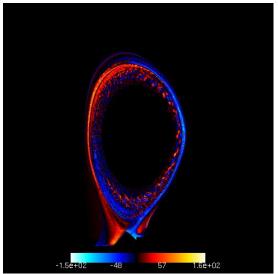
**Abstract.** Performance of the ITER is anticipated to be highly sensitive to the edge plasma condition. The edge pedestal in ITER needs to be predicted from an integrated simulation of the necessary first-principles, multi-scale physics codes. The mission of the SciDAC Fusion Simulation Project (FSP) Prototype Center for Plasma Edge Simulation (CPES) is to deliver such a code integration framework by (1) building new kinetic codes XGC0 and XGC1, which can simulate the edge pedestal buildup; (2) using and improving the existing MHD codes ELITE, M3D-OMP, M3D-MPP and NIMROD, for study of large-scale edge instabilities called Edge Localized Modes (ELMs); and (3) integrating the codes into a framework using cutting-edge computer science technology. Collaborative effort among physics, computer science, and applied mathematics within CPES has created the first working version of the End-to-end Framework for Fusion Integrated Simulation (EFFIS), which can be used to study the pedestal-ELM cycles.

## 1. Introduction

The mission of the SciDAC Fusion Simulation Project (FSP) Prototype Center for Plasma Edge Simulation (CPES) is to develop of an integrated predictive plasma edge simulation package that will simulate the edge pedestal buildup and subsequent large-scale edge localize mode (ELM) crash for existing magnetic fusion facilities as well as for next-generation burning plasma experiments such as ITER [1]. Timely

progress on this formidable scientific challenge demands a well-coordinated effort involving experts in plasma physics, computer science, and applied mathematics. The performance of ITER depends sensitively on the ability to achieve H-mode operation [2] with a high-edge pressure pedestal while suffering minimal damage from ELM instabilities [3]. Many nonequilibrium physical processes on different spatiotemporal scales in the edge region demand large-scale integrated simulations based on as much first-principles physics as possible using high-performance computers.

The local equilibrium of the edge plasma is nonthermal, for which kinetic models are required. For the first time, a special full-f distribution function (full-f) kinetic transport code suite, consisting of the codes XGC0 and XGC1, has been developed for real tokamak edge geometry. The existence of ion-temperature-gradient (ITG) turbulence in the real geometry pedestal region was demonstrated using the XGC1 code: a particle-in-cell (PIC) approach on a massively parallel, high-performance computing platform (see figure 1). A production run normally uses 10,000-20,000 Cray XT4 processing cores for 20 hours. The resulting ion thermal transport rates are at experimentally estimated level [4]. An effective team effort among the physics, applied mathematics and computer science has been critical for this rapid progress. The XGC1 code benefits from the state-of-the-art applied mathematics tools of the SciDAC Center TOPS and Courant Mathematics and Computing Laboratory (CMCL) and highperformance software engineering from the SciDAC Performance Engineering Research Institute (PERI). XGC1 will be further enhanced to investigate electromagnetic turbulence. XGC0 is a simplified version of XGC1 for carrying out experimental timescale simulation of the



**Figure 1.** ITG turbulence in a real geometry DIII-D edge with a mild L-mode type pedestal. The temperature gradient is strong enough for ITG instability at the pedestal top but not in the pedestal slope. Still, the ITG grows at both locations.

kinetic pedestal buildup, which will utilize the turbulent transport information from XGC1. The XGC0 code, using a coarse-grained PIC approach with only a radial electric field solution, shows that the pedestal is routinely built up from neutral ionization resulting from wall-recycling of neutrals and from heat/momentum/particle flux from the core.

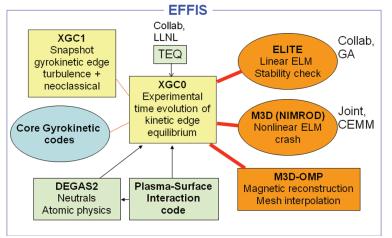
Our new End-to-end Framework for Fusion Integrated Simulation (EFFIS) has successfully been used to automate integrated simulation of XGC0 kinetic pedestal buildup, Elite [5] stability-boundary check, M3D [6] edge localized mode crash, and back to XGC0 pedestal build up, for multiple ELM cycles. EFFIS uses highly advanced inter-operating computer science tools that include workflow management, fast presentation of image data on a web-based dashboard, speedup of I/O operations, collection and management of provenance metadata, and wide-area data transfer. EFFIS facilitates efficient integration of different fusion codes running on multiple and nonlocal platforms, provides users with real-time dynamic tracking of simulation progress through graphs and images on a dashboard, and has already been used on tens of thousands of processors in secure environments. EFFIS demonstrates the initial aspects of the FSP within the CPES project. Code performance optimization is achieved in collaboration with SciDAC Institute PERI. The performance information is displayed on the dashboard.

## 2. Pedestal buildup and ELM crash

Even though the full-f 5D gyrokinetic code XGC1 includes equilibrium physics [7], it is prohibitively

expensive to use XGC1 to study experimental timescale equilibrium evolution (i.e., pedestal development) together with turbulence physics on the present-day high-performance computers. Use of XGC1 will thus be limited to snapshot studies of critical turbulent transport until faster-than-petascale computers are available. Accumulation of errors in a gyrokinetic code is another issue to be resolved in an experimental timescale simulation. Development of the XGC0 code has been accelerated to fulfill the demand of experimental timescale kinetic pedestal buildup [8]. The XGC0 code, which is a simplified version of the XGC1 code, computes the kinetic equilibrium physics (based on neoclassical physics including orbit loss and wall interaction) in real geometry by solving only the radial electric field  $E_r$  in one-dimensional radial cells, instead of the 3D turbulence field in three-dimensional cells. This leads to a reduction in particle number by a factor >1,000. The plasma sheath/presheath solution in the scrape-off region is simplified with the logical sheath algorithm [9]. Since XGC0 is not a turbulence code, it does not perform the gyrokinetic four-point averaging operation, leading to additional significant savings in computing time. As a result, XGC0 is ~1,000 times faster than XGC1. The Lagrangian equations of motion used in XGC0 are identical to those in XGC1.

XGC0 simulates not only the electrons and ions but also the Monte Carlo neutral particles with a wall recycling model. An electron subcycling technique is used to simulate the electron dynamics efficiently. Non-axisymmetric magnetic perturbations are another input, taking advantage of the 3D nature of the particle dynamics. XGC0 incorporates magnetic and limiter geometry information from the g-eqdsk files, as in XGC1. XGC0 accepts the heat, torque, and particle fluxes from the core. It uses a radial profile of



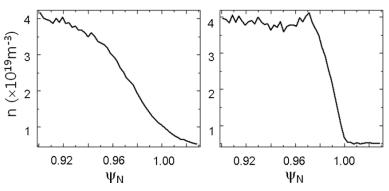
**Figure 2.** Schematic diagram of code integration in CPES. Thick red lines represent nonlocal data coupling, thin arrow lines show subroutine coupling, and thin red lines indicate manual transport coupling.

anomalous transport coefficients and converts them into radial random and convective walks superimposed on the Lagrangian particle motions. The anomalous transport coefficients can be prescribed analytically, based on experimental validation, or they can be based on simulation results from turbulent transport codes such as XGC1. At the present time, XGC0 is used for pedestal buildup only without any ELM activities. The ELM crash is completely described by the nonlinear resistive MHD code M3D-MPP (cross-verified against NIMROD). Systematic verification of the XGC0 code has been carried out to ensure that the code is accurate to the desired level. XGC0 is a mature code, with validation against experimental data underway.

The kinetic-dominated pedestal buildup followed by the nonlinear evolution of the MHD-dominated ELM crash is routinely simulated within EFFIS. This is accomplished by data coupling four separate codes: XGC0 for kinetic simulation of the pedestal buildup, M3D-OMP [6] for equilibrium reconstruction and mesh interpolation, ELITE to determine the ideal MHD linear stability of the evolving profiles, and M3D-MPP (without the two-fluid effects) to simulate the nonlinear resistive MHD evolution during an ELM crash when the profiles are deemed unstable by ELITE. (We also use NIMROD for cross-verification.) The density, temperature, and current profiles along with the equilibrium configuration files in g-eqdsk format are transferred among the codes, which employ very different spatial meshes and

resolution. The entire process in EFFIS is automated using the Kepler workflow framework, the ADIOS data I/O technology, and the Dashboard run-monitoring, visualization and run-control (see Section 3). Additional necessary integrations are achieved by including them into XGC0 as subroutines (see figure 2).

Below an example of a specific integrated simulation is described. The kinetic equilibrium simulation code XGC0 was run on 128 processing cores on the Cray XT4 at ORNL, the M3D-OMP equilibrium

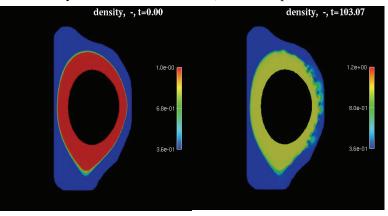


**Figure 3.** Density profiles at t=0 (left), and t=42 (right) showing the pedestal edge buildup. The times are normalized by the ion transit time.

reconstruction and ELITE stability checks were done on one processor of a Linux Opteron cluster called ewok at ORNL, and the nonlinear resistive MHD code M3D-MPP was run on 128 cores of ewok. During the kinetic simulation, it is assumed that the edge plasma is already in H-mode, where the neoclassical and the neutral atomic physics are important. A small prescribed level of anomalous transport is superimposed on the Lagrangian particle motion as a radial random walk and convection steps. The magnitude is determined by comparison with experimental pedestal shapes. (Turbulent transport information from XGC1 will be integrated into the

XGC0's random walk and convective steps in the future.) The edge pedestal builds up in XGC0 from neutral ionization; that is, the density and pressure gradients at the edge get steeper, and the electrical current density becomes higher from the kinetic bootstrap effect (see figure 3 for the pedestal buildup during an example simulation). The pressure and current density profiles are examined periodically by the ELITE code through the end-to-end data coupling network to determine if they are unstable to ideal MHD peeling-ballooning modes. Before the linear stability check, the magnetic equilibrium is automatically reconstructed from the profiles with a free-boundary Grad-Shafranov solver, which is part of the M3D-

OMP code. If the profiles are ideal MHD unstable, then the nonlinear resistive MHD code M3D-MPP takes over the simulation of the nonlinear development of the ELMs and the subsequent relaxation. Figure 4 shows a 2D plot of the density perturbation that emerged from the example integration, illustrating the fast expulsion of plasma into the surrounding region by a ``ballooning" instability. The instability type saturates as the density gradient in the plasma edge is reduced below a critical level and the plasma begins to relax back towards the original configuration, but with a broader edge pressure pedestal. Once the flux



**Figure 4.** Density images at t=0 (left) and t=103 (right) showing the nonlinear development of the ELMs in the example integrated simulation. The times are normalized by the Alfvén time, and t=0 is at the beginning of the ELM crash.

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surfaces have adequately healed, a new equilibrium is computed along with profiles by toroidal averaging and poloidal smoothing of the full 3D fields. The end of the ELM crash is checked using an input parameter specifying a threshold level of density fluctuation. The relaxed plasma profiles and magnetic equilibrium information are then used to initiate a new pedestal buildup in the XGC0 code and automatically repeat the ELM cycle.

## 3. Computer science in End-to-end Framework for Fusion Integrated Simulation (EFFIS)

In this section several computer science technologies that have been integrated into the single framework EFFIS are described, which facilitates real-time dynamic monitoring of simulations while they are running, code integration of simulations, and dynamic generation of images that help visualize and track the simulations as well as various data movement activities. EFFIS has been successfully performing automated integrated simulation of XGC0 kinetic pedestal buildup, ELITE stability-boundary check, M3D edge localized mode crash, and back to XGC0 pedestal build up, for multiple ELM cycles. EFFIS uses highly advanced interoperating computer science tools that include workflow management, fast presentation of image data on a web-based dashboard, speedup of I/O operations, collection and management of provenance metadata, and wide-area data transfer. EFFIS facilitates efficient integration of different fusion codes running on multiple and nonlocal platforms, and has already been used on tens of thousands of processors in secure environments. CPES researchers recognized that they needed a framework as powerful as EFFIS, since they commonly run simulations on thousands of processors and I/O becomes a bottleneck. Additionally, because the simulations run for a long periods of time, there is a need for easy way to monitor the simulations, which includes invoking analysis and visualization during the monitoring stage.

The EFFIS framework is organized in terms of "foundation technologies" and "enabling technologies (see figure 5). The three foundation technologies are stacked into three layers: the Adaptable I/O System

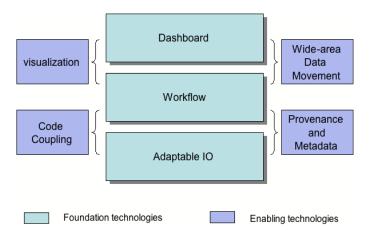


Figure 5. EFFIS foundation and enabling technologies.

(ADIOS), which is designed to achieve high I/O bandwidth, is at the foundation, the Kepler workflow system is on top of ADIOS, and the Dashboard is on top of the workflow system, indicating that workflows use the ADIOS technology and that the Dashboard displays the results generated by workflows. The enabling technologies interact with these layers to collect provenance and metadata into database repositories and to provide efficient data coupling, advanced visualization, and widearea data movement. We focus the rest of this section on our Adaptable I/O system, our workflow system, and our Dashboard.

One of the main goals of the computer science work in CPES is to facilitate running

workflows that will perform dynamic monitoring of simulations and the dynamic analysis of the time steps in order to track the simulations. This required the use and development of special components (called "actors") of the Kepler workflow system, through collaboration with the SDM (Scientific Data Management) center [10]. Such workflows incorporate many other tasks, such as generation of images and movies, data transformation on-the-fly as the data is generated, and combining of multiple small files into a larger file for archiving. The workflows developed not only support "monitoring workflows," but also support "integration workflows" across machines.

A diagram of the Kepler coupling workflow is shown in figure 6. In this figure, the M3D-OMP pipeline (top of figure) realizes the loose cyclic coupling between XGC0 and M3D-OMP. From XGC0, a small data file *m3d.in* is transferred to the processing site where M3D-OMP is executed as a batch job. The new magnetic equilibrium is then transferred back to the simulation's directory. The result also triggers the execution of the ELITE pipeline, which transfers the p-eqdsk data (plasma density profile) from XGC0 and runs ELITE (also via the job queue). A wrapper script around ELITE performs all the tasks: prepare and submit job and wait for results, check all output files for errors or problems, generate output plots using IDL, and determine whether the XGC0 simulation has become MHD unstable. (All of these subcomponents could also be realized as sub-workflows in Kepler if more detailed control were needed inside the workflow.) The result of the script is a simple "control file" containing the string stable or unstable, which is checked in the last actor of this sub-workflow. If XGC0 is determined to be MHD unstable, the M3D-MPP code is launched, while the workflow stops XGC0 completely and releases the **CPUs** until after the M3D-MPP run is finished. а new start

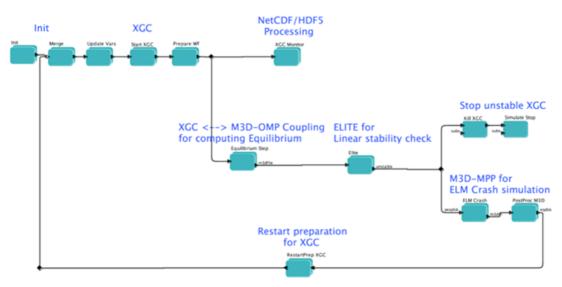


Figure 6. Coupling pipelines performing the M3D-OMP, ELITE, and M3D-MPP steps.

The *M3D-MPP* pipeline is fairly complex and can be run as a stand-alone workflow to execute M3D-MPP and monitor it. This workflow generates images from the HDF5 output of M3D-MPP using AVS/Express, so the structure is similar to the *HDF5 Processing* pipeline that we use in our monitoring workflow. The AVS/Express job is submitted directly from the workflow, not from a script. Thus, the workflow is able to wait for the AVS/Express job to start, perform other tasks while the job is running, and stop the job at the end of the processing. This capability is provided by a set of job-related actors in Kepler that support several job managers (PBS, LoadLeveler, SGE, Condor, and "process fork") and use SSH to connect to remote computing sites. Finally, the coupling workflow completes the cycle by detecting the end of the M3D-MPP simulation, processing the new equilibrium data, and returning it to XGC0 for the next pedestal buildup simulation.

Simulation monitoring and effective code integration are critical tasks in EFFIS. Because of the scarcity and costliness of supercomputing resources, it is very important that any large-scale simulations be well monitored. Such monitoring may include data sorting, filtering, transformation and/or reduction, as well as

graphical representations or visualizations and simple remote access to these outputs. Most of these tasks are data-centric and can be automated and thus are amenable to the use of scientific workflows. The main purposes of simulation monitoring are tracking the progress of a run, detecting possible errors in the simulation setup or behavior, and recording selected code diagnostics of interest in real time. Such monitoring can prevent the waste of precious resources and instead focus simulations on key physics insights as identified by the scientist in the setup phase and even while a simulation is in progress. For our workflows, we choose the Kepler scientific workflow management system [11] largely due to its support of advanced computational models such as pipeline-parallel execution. We prefer Kepler over other scientific workflow systems because the majority of them are grid-oriented (where each component must be realized as a job) or web-based (where a component is a web service call). The resources at hand are not part of any grid or web-based software infrastructure. Even if they were, in a grid infrastructure there is no access to a job's output on the fly unless all output is first put onto external storage elements. The quick access to and processing of data and the fast turnaround in the execution of operations are essential for efficient kinetic-MHD code integration and are not achievable using grid-based job submission. Another advantage over many other systems is that Kepler development is community-driven. Thus, the many different projects and teams such as CPES and the SciDAC SDM Center that use Kepler can collaborate to share development tasks and system improvements.

We developed ADIOS [12] in conjunction with Sandia, for the improvement of I/O speed for dumping data from the compute engines. The original idea was to provide fast, scalable and portable I/O for the large data producing codes used in this project. The approach taken is to remove the load from the application codes by permitting generic I/O calls which invoke libraries that use the desired properties of the I/O (type of data, parallelism, etc.) captured in an XML file. This work, the Adaptable I/O System (ADIOS), provides great improvements of the I/O speed, as well as elegant separation of the I/O details from the application code. As a result, the application code does not have to be modified if changes to the I/O properties are desired; the changes are recorded only in the XML file that the I/O libraries use. Since

one of the goals under the CPES work was to facilitate code integration, ADIOS also allows us to componentize this layer so that we can move data quickly from different components inside of the CPES framework, and to communicate directly with our integration and monitoring workflows. This allows a CPES scientist to abstract the data movement from CPES components, placing this burden our EFFIS infrastructure. on ADIOS has recently been used in large XGC1 simulations, which have produced over 50 TB in 24 hours on the Cray XT at ORNL on 28,672 cores, writing the data at over 24 GB/sec.

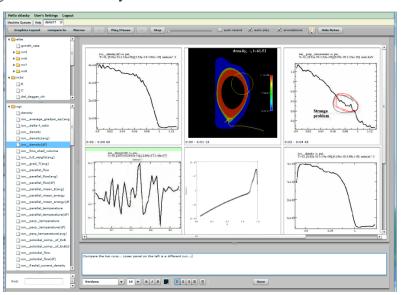


Figure 7. Simulation monitoring via Dashboard.

The eSimMon (electronic Simulation Monitoring [13]) dashboard is a web-based interface that presents several views of simulation resources and results, including an overview of activity on the computers of

interest at DOE, a means to monitor data provenance and analytics related to either current or previous runs (or *shots*), and a display of other provenance information and status tools. The purpose of eSimMon is to provide the user a simple "one-stop shopping" access to view the status of simulations (see figure 7), launch new simulations, and analyze or revisit existing runs. It is a lightweight front end for comprehensive end-to-end data and workflow management that provides users with access to large simulation datasets, as well as provenance information and performance records for simulations and their associated workflows. Users can examine the evolution and outputs of their runs or drill down into runtime processes, workflows and system information. More recently, we have added wide-area file movement to the physicist's site through requests made on the Dashboard, using a Storage Resource Manager (SRM) technology used in the SDM center called SRM-lite.

#### 4. Conclusion and discussion

End-to-end Framework for Fusion Integrated Simulation (EFFIS) has been built to perform the pedestal-ELM cycle, aiming to bring together first-principles physics codes and reduced transport model codes running on multiple nonlocal platforms, as well as the physics data information saved on disk. To date, the XGC0 kinetic code for pedestal evolution, M3D-OMP for mesh interpolation and magnetic reconstruction, ELITE for linear ELM stability check, and M3D-MPP for nonlinear resistive ELM crash to relaxation have been integrated in EFFIS. In the future, the XGC1 gyrokinetic turbulence code will be integrated with XGC0 to provide turbulent transport information. M3D-MPP will be improved to perform a more robust two-fluid ELM crash all the way to relaxation. In addition, EFFIS will be used for another urgent ITER problem, namely, prediction of the resistive MHD response to an external resonant magnetic perturbation (RMP), kinetic pedestal behavior, and ELM control.

The physics integrated simulations carried out in EFFIS will be systematically verified and validated. The simulations will be used to analyze edge data in existing tokamaks and to predict edge performance, including the pedestal width and height, and the divertor heat load in ITER. A core turbulence code will be integrated into EFFIS to allow an edge integrated simulation of core turbulent transport. EFFIS will be enhanced to collect and provide system and data provenance information through the Dashboard, as well as additional analytical capabilities. The ADIOS system will be enhanced to include experimental data for comparison with simulation data through the Dashboard.

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