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Project Title: Center for Plasma Edge Simulation (CPES)

Final Technical Report for the Period 1/15/2006 to 1/14/2012

The Center for Plasma Edge Simulation (CPES) project was a multi-institutional research effort funded jointly by the Office of Advanced Scientific Computing Research (OASCR) and the Office of Fusion Energy Sciences (OFES) within the Department of Energy's Office of Science. The effort was led by our Principal Investigator, CS Chang, at the Courant Institute for Mathematical Sciences at New York University. The Center included participants from Oak Ridge National Laboratory, Princeton Plasma Physics Laboratory, Lawrence Berkeley National Laboratory, California Institute of Technology, Columbia University, Lehigh University, Rutgers University, University of Colorado, Massachusetts Institute of Technology, University of California at Davis, University of California at Irvine, North Carolina State University, and Georgia Institute of Technology. This report concerns the work performed by Dr. Julian C. Cummings, who was the institutional Principal Investigator for the CPES project at Caltech.

The overall goal of the CPES project was to develop a new integrated and predictive plasma edge simulation code package. This new capability was to consist of a fully kinetic model of neoclassical and turbulent transport in realistic tokamak edge geometry and a two-fluid MHD model of fast-growing plasma instabilities such as edge-localized modes (ELMs) that can reduce tokamak plasma performance. These two plasma modeling tools would be integrated via modern scientific workflow software. The role of Caltech within this project was to provide expertise and practical experience, both in terms of the gyrokinetic particle simulation techniques to be incorporated within the kinetic edge plasma model and the use of workflow tools to coordinate the actions of several high-performance computing applications.

The first three years of CPES were primarily focused on developing the gyrokinetic edge plasma simulation capability. The project started from an existing XGC code that could model gyrocenter drift motions in realistic tokamak edge geometry including the magnetic X-point. Significant work was needed to add the gyrokinetic effects to the ion equations of motion and to add a gyrokinetic Poisson solver to compute the self-consistent electrostatic potential and allow for turbulent transport processes. This work was primarily carried out by code developers at NYU, but Caltech provided critical assistance in the areas of code diagnostics and portability. Specifically, a configure-and-build system based upon the GNU Autoconf and Automake tools was created for XGC and associated sub-packages, making it easier for both the primary code developers and less familiar code users to build versions of the code on high-performance computing platforms at the National Center for Computational Sciences (NCCS) and the National Energy Research Supercomputer Center (NERSC). (Note: NCCS is now known as the Oak Ridge Leadership-class Computing Facility, or OLCF.) In addition, new code diagnostics were added and existing diagnostics were modified to utilize new data I/O formats specially engineered for performance on the HPC platforms. In the first two years, we primarily relied upon the Bzip library, research software from Rutgers University for binary packing of output data and conversion into standardized formats like HDF5 for later visualization. In later years, the Adaptable I/O System (ADIOS) library,

primarily developed at Georgia Tech, became the primary tool for transferring data in and out of XGC and other CPES codes. Caltech provided the bulk of the support for adapting XGC I/O and diagnostic routines first to use the binpack library and later ADIOS. In addition, much of the testing of new ADIOS releases and features with the XGC application was performed by Dr. Cummings at Caltech. This testing and feedback was critical to the early success of the ADIOS development process, and ADIOS has since gone on to become a key piece of software infrastructure for many other HPC application code efforts across the Department of Energy and other Federal research funding agencies.

Besides the ongoing development of XGC into a fully gyrokinetic model for edge plasma turbulence, the other focus of our CPES work in the first three years was the creation of an automated workflow for studying the so-called pedestal ELM cycle. A prominent feature in tokamak edge plasma is a *pedestal* in the radial density and temperature profiles, as the plasma transitions from the hot, dense core region to the scrape-off layer (SOL) plasma in the open field line region near the device wall. Since these radial profiles tend to be “stiff” in the plasma core, the height of the edge pedestal (i.e. the value of the density and temperature at the top of the pedestal) correlates strongly with the core density and temperature and thus regulates the fusion output. In the preferred “H-mode” operation, turbulence in the edge region is reduced and an “internal transport barrier” is created, allowing the edge pedestal to grow significantly. (This process is not completely understood and is a topic of ongoing research.) The sharp pressure gradient associated with a steep edge pedestal can help to drive MHD instabilities known as edge-localized modes or ELMs that lead to sudden or bursty losses of plasma density and energy and cause the edge pedestal to drop or “crash”. After an ELM crash, the edge pedestal may then begin to slowly build up once again and repeat the cycle.

Understanding the dynamics of this pedestal ELM cycle required the interaction of multiple plasma models. Our concept was to link the XGC kinetic edge model of the pedestal buildup with a linear MHD model to look for ELM-unstable edge profiles and a nonlinear MHD model to analyze the ELM development and subsequent changes to the plasma profiles. For the linear stability analysis we deployed the ELITE code developed primarily by Phil Snyder at General Atomics. The nonlinear MHD modeling of the ELM crash was done using the parallel M3D code, with expertise provided by Linda Sugiyama at MIT. In addition, a serial version of the M3D code was needed to transform the plasma profile data from XGC into a form that was suitable for analysis with ELITE and the fully parallel M3D. The actions of these four separate application codes needed to be highly coordinated in order to track the pedestal ELM cycle, and this orchestration was managed with the help of the Kepler scientific workflow engine developed at UC San Diego. The Kepler system is Java-based and contains “actor” scripts that work together to process a data-driven workflow. Norbert Podhorzski at UC Davis (now at ORNL) was the primary developer of the Kepler workflows for the pedestal ELM cycle studies, and Dr. Cummings worked extensively with him to design and test these workflows on several generations of HPC systems at NCCS. The creation of this workflow-driven multi-physics simulation of the pedestal ELM cycle was a novel accomplishment in tokamak plasma simulation and led to several conference presentations and journal publications (*e.g.*, J. Cummings *et al.*, Commun. Comput. Phys. **4** 675).

The early success of these workflow-driven coupled simulations encouraged CPES to pursue a grander integration of several software technologies under development at this time. The aforementioned

ADIOS library was utilized to facilitate data I/O on HPC platforms and efficient data transfers between parallel application codes such as XGC and parallel M3D. Another critical technology was developed at ORNL called eSiMon: a Web-based portal for viewing HPC resources, monitoring ongoing simulations, visualizing simulation results, and storing and accessing these results in a shared project database. Dr. Cummings was an early tester of eSiMon for XGC and coupled-code simulations and worked closely with developers at ORNL to debug and improve this tool throughout the CPES project. Together, the Kepler scientific workflows, the ADIOS library and the eSiMon tool became known as EFFIS: the End-to-end Framework for Fusion Integrated Simulation. The notion was to provide a complete solution for the design, performance and analysis of an integrated simulation of fusion plasma. The EFFIS tools could be used to combine multiple types of simulation codes in a variety of ways to address different needs. The EFFIS concept and several generations of these tools were documented in a series of journal articles and conference presentations (e.g., J. Cummings *et al.*, 2010 PDP Conf. Proc., pp. 428-434).

When the initial three years of the project concluded, CPES competed for and was awarded a two-year renewal of funding by DOE. In the next two years, our goal was to expand upon the pedestal ELM cycle studies that had been completed previously, both in terms of the physics and the computer science involved. On the physics side, we introduced new code diagnostics to examine the particle and heat loads being transported radially out of the plasma and along the scrape-off layer onto the divertor. The divertor heat loads experienced before and during an ELM crash are a critical factor in the design of modern tokamak devices and hence were of importance as a topic of interest here. In addition, we wanted to examine the effects of electromagnetic perturbations due to the development of ELMs on the plasma kinetic behavior. In other words, we planned to extend the “one-way” interaction of our kinetic and MHD models to become a “two-way” interaction with MHD perturbations feeding back into the kinetic code in real time. This latter extension of the EFFIS code-coupling system required new computer science techniques to allow for easier data sharing between the codes and was a key driver for the DataSpaces software developed at Rutgers University. DataSpaces allowed the user to declare a shared space for certain data arrays in memory that could be accessed by multiple applications using RDMA technology (see C. Docan *et al.*, 2010 CCGrid Conf. Proc., pp. 293-301). The incorporation of DataSpaces as a native data transfer method available via the ADIOS read/write APIs made this new tool readily accessible to the kinetic and MHD codes of CPES. Dr. Cummings at Caltech became one of the early users of DataSpaces and verified its value in enhancing the efficiency of inter-code data transfers and making integrated simulations with frequent and large data transfers feasible.

In 2010 the CPES project requested and was granted funding for a final one-year extension to complete its research mission (in coordination with the two other proto-FSP centers, SWIM and FACETS). During the last 12 months, Caltech continued its involvement with the CPES project by pursuing collaborations in the areas of simulation software technology and extending previous work on coupled kinetic-MHD simulations of ELM events. In June of 2010, Dr. Cummings participated in a workshop and technological exchange at the CEA facility in Cadarache, France, to discuss the use of the Kepler scientific workflow system and other software technologies for tokamak whole-device modeling. The European participants included researchers from the Euforia project and the Integrated Tokamak Modeling (ITM) group. This discussion helped to clarify the current directions of ITER discharge modeling in Europe and exposed

some interesting new software tools, such as the Consistent Physical Object (CPO) representation for experimental and simulated diagnostics. The meeting in Cadarache led to a further technological exchange between the European researchers and the CPES team in December.

At the 2010 APS/DPP meeting in Chicago, Dr. Cummings presented a poster of results from coupled kinetic-MHD simulations of divertor heat loads during ELM instabilities. The study compared output from a divertor heat load diagnostic in XGC0 for runs with and without the imported ELM perturbation data from M3D. The purpose of this study was to better understand how Type I ELM events modify the expected divertor heat load profiles. At this meeting Dr. Cummings was also co-author of a presentation on EFFIS, and he presented a second poster on kinetic simulations of the dependence of divertor heat load profiles on plasma current and heating power. This latter work was part of the 2010 Joint Research Target (JRT) studies involving comparisons of similar discharges in the DIII-D, NSTX, and Alcator C-Mod tokamak devices, and it led to a journal publication (A.Y. Pankin *et al.*, Prob. Atom. Sci. Tech. **2011** (1) pp. 8-12).

After returning from a medical leave in mid-March 2011, Dr. Cummings gave a talk on the ongoing coupled kinetic-MHD simulation studies during the 2011 Transport Task Force (TTF) meeting in San Diego. This talk was essentially a review of prior work, but the meeting provided a valuable opportunity for modelers and experimentalists to discuss how to better work together on such studies of the divertor heat load profiles and ELM effects. Around this same time, Dr. Cummings co-authored a paper on the ActiveSpaces system for code coupling with CPES collaborators at ORNL and Rutgers, which was presented at the 2011 IPDPS conference in Anchorage, Alaska.

At the CPES Spring 2011 All-Hands Meeting in May, Dr. Cummings presented further work on the coupled kinetic-MHD simulation in which the issues of tighter code coupling and time synchronization of the XGC0 and M3D codes were more fully explored. Orchestrating the concurrent operation of these two parallel codes requires a detailed study of the performance and wall-clock efficiency of each code, so that computing resources can be properly balanced between them. In addition to working on these computational studies, Dr. Cummings also co-authored a paper on in situ data processing for large-scale simulations that was presented at the 2011 SciDAC conference in Denver.

The CPES project has produced significant advancements in both computer science and plasma physics as they relate to simulation of the edge region of tokamak fusion plasmas. Several critical new pieces of HPC software, including the ADIOS library, DataSpaces, and the eSiMon web portal, were created and enhanced via applications driven by the specific needs of CPES. Dr. Cummings of Caltech played a key role as the liaison between software developers and physics application users, insuring that the tools worked as advertised and met all the requirements of the simulations. With these new technologies, we were able to perform novel code-coupling simulations on leadership-class computing facilities and make contributions to tokamak performance studies of current interest to the international fusion research community. Moreover, these software tools are also finding use across multiple DOE application areas such as combustion and global climate modeling.