Field Representative's Summary for Fusion Energy Science
SciDAC PI Meeting
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Hyatt Regency, Reston, VA
Vincent Chan and William Tang

The FES SciDAC activities are coordinated by the Plasma Science Advanced Computing Institute. Included in its portfolio are five applications projects funded by OFES and the National Fusion Collaboratory project funded by MICS.

The Extended Magnetohydrodynamics (MHD) Modeling project is managed by the Center for Extended Magnetohydrodynamics Modeling (CEMM) with Dr. S. Jardin (PPPL) as the PI. The objective of the project is to develop and deploy predictive computational models for the study of low, frequency, long wavelength fluid-like dynamics in the diverse geometries of modern magnetic fusion devices. This application has high programmatic relevance because MHD instabilities are responsible for disruptions and reconnections, which set limits for maximum current and pressure sustained by a magnetic confinement device. To enhance the predictive capability of the codes, significant improvement in the plasma models is needed, specifically in the direction of hybrid and particle-fluid models. Successful implementation will benefit from close collaboration with the computer science community. At this meeting, contacts were made with

- David Keys (TOPS) on linear solvers. Keyes and postdoc will visit PPPL on Feb 11 to begin collaboration
- Professor Glimm (TSTT) on finite elements. Two visitors from RPI came to PPPL on Jan 14-16 to start collaboration
- Phil Collela (APDEC) on adaptive mesh refinement (AMR). The two groups are sharing a staff, Ravi Samtaney and making good progress
- W. Gropp on data transfer. Discussions were initiated regarding parallel methods for writing files and transferring across network
- Arie Shoshani on data management, also involving the Fusion Collaboratory
- Mike Papka on parallel tiled rendering
- Horst Simon on visualization.

The Magnetic Reconnection Studies project is managed by the Center for Magnetic Reconnection Studies (CMRS) with Professor A. Bhattacharjee (U. of Iowa) as the PI. The primary objective is to apply the MRC code to problems of central importance in fusion science, and to explore, wherever possible, the connection of these problems to outstanding problems in space and plasma astrophysics. Physics deliverables include

- Magnetic reconnection studies in tokamaks (2002-03), magnetotail substorms (2002), and solar flares (2004)
- Error-fields studies in tokamaks (2002-03) and reverse-field pinches (RFPs) (2003-04)
- RFP and astrophysical dynamos studies
- Simulation of laboratory magnetic reconnection experiments (e.g., MRX at PPPL)

The U. of Chicago computer science department is a partner in this project. At this meeting, discussion was held with P. Collela (APDEC) on application of adaptive mesh refinement for Hall MHD. This application poses a new challenge for AMR because of the dispersive nature of Hall MHD waves. Discussion was also initiated with the SDM center on data management issues for the FLASH and MRC codes.

The Wave-Particle Interactions in Multi-dimensional Systems project led by Dr. D. Batchelor (ORNL) has the objective to generalize the physics, and to achieve computational scale-up and interconnectivity of the elements of a complete wave-plasma modeling capability. The enhanced simulation capability will be applied to study four major unsolved problems in wave-particle interactions important to ongoing experiments. A secondary goal is to explore research into completely reformulating wave-plasma problems and solution methods to expand physics scope and computational efficiency. The ORNL computer science division is a partner in this project. ISIC needs include

- Parallel linear solvers, focusing on iterative solvers with physics-based preconditions
- Applied mathematics and software tools for alternative field representation (spectral elements, wavelets, splines) to achieve adaptive grid with spectral properties.

Fusion Collaboratory supports for data access, sharing and archival has been identified.

The Terascale Computational Atomic Physics for the Edge Region in Controlled Fusion Plasmas project led by Professor M. Pindzola (Auburn U.) sets its goal to utilize state-of-the-art computational facilities to address atomic-scale problems, which present urgent needs in fusion energy research, address fundamental physics issues (atomic few-body problem), and are relevant to other applications (astrophysics, plasma processing). The two sub-projects are (1) the development of the time-independent R-matrix close coupling method for treatment of complex ions liberated from plasma-facing components, and (2) the lattice solution of the time-dependent Schrodinger equation applicable to collision data for Lithium beam charge exchange recombination spectroscopy and 3D x 3D codes for molecule catalytic recombination in divertor. Contacts made at this meeting include

- Dr. E. Ng (NERSC) who will work with this project on the scalability of an existing code, and serve as consultant in parallel complex symmetric eigensolvers
- Dr. R. Harrison (PNNL) who has suggested several quantum chemistry codes that could provide this project with bound and excited molecular orbitals to be used for electron-molecule collision calculations. Dr. Harrison has also provided a good reference on relativistic pseudo-potentials for future studies of wall erosion using complex atoms.

The Plasma Microturbulence Project led by Dr. W. Nevins (LLNL) has its main goal to integrate direct numerical simulation of plasma microturbulence into magnetic fusion energy research, and to revolutionize the fusion program's ability to interpret experimental confinement data and to test theoretical idea about turbulence. Energy confinement is a key problem in magnetic fusion energy and turbulent transport has been identified as the dominant loss mechanism. Direct numerical simulation of turbulence is a cost-effective and easily diagnosed proxy to complement very expensive experiments, necessary to develop a predictive modeling capability. Topics discussed with the computer science community at this meeting include code optimization (PERC), common component architecture (CCA), solvers (TOPS), locally structured grid (TSTT), and data management (SDM and Fusion Collaboratory).

In addition D. Schissel (General Atomics), PI of the National Fusion Collaboratory project reported a number of contacts made at this meeting

- J. Meyer (PNL), Scientific Annotation and Middleware (SAM), on comparison of electronic notebooks developed by both groups
- R. Mount (SLAC) and D. Olson, Particle Physics Data Grid (PPDG), on data security and remote job monitoring
- A. Shoshani (LBNL), Storage Resource Manager (SRM), on the coupling of SRM with MDSPlus data system
- N. Rao, network specialist, who has offered the help the Fusion Collaboratory in measurements of network bandwidth and latency for fusion applications
- D. Agarwal, Pervasive Collaborative Computing Environment, on reliable and secure group communication
- Tools for remote visualization aim at "low end" solution might also fit nicely with the fusion community.