Summary of the US-Japan Workshop on Integrated Modeling (with European participation) held at PPPL Sept. 21-24, 2004

Whole Device Modeling Codes
There was general agreement on the need to emphasize modularization of integrated modeling codes, with the need for more unified standards and sharing modules internationally, as well as the need for the use of more sophisticated modules for turbulent transport, extended MHD, scrape-off-layer, ELMs and pedestal. A significant number of results were shown from existing codes such as JETTO (JET), TSC (PPPL), BALDUR (Lehigh), TOPICS (JAERI), TRANSP (PPPL), ASTRA (Garching), and TASK (Kyoto University). Modeling code initiatives in Japan include the Burning Plasma Simulation Initiative (BPSI), which includes the Transport Analysis System for Tokamaks (TASK), the 2-D SOLDOR code, and the CSD reduced core-edge modeling code. Initiatives in Europe include the integration of transport and MHD codes at JET (JETTO, CRONOS, and ASTRA under a unified working environment) and the EU Integrated Modeling Task Force, which includes the Code Platform Project, Data Coordination Project, and five integrated modeling projects. In the US, initiatives include the National Transport Code Collaboration (at http://w3.pppl.gov/NTCC) and the Fusion Simulation Project (FSP), which is expected to receive initial funding next year.

The ability to deal with physical processes on disparate time scales and regions with different space dimensionality is another important ingredient of integrated modeling. Full modeling should include the core plasma (which is mainly 1-D), the 2-D scrape-off-layer and 3-D neutrals, as well as the plasma-wall interaction. Previous examples of fully integrated modeling include simulations of ITER using the coupling of JETTO with EDGE2D/NIMBUS and CORSICA with UEDGE. Such a fully integrated approach is an extremely complicated task and many modelers adopt a more simplified, focused approach, which reduces the level of complexity to a bare necessary minimum. Examples of the coupling of core and edge plasmas have been demonstrated during this meeting by R. Hiwatari (Divertor Modelling with Simple Core-SOL-Divertor Model), T. Rognlien (Modelling encompassing both the pedestal and SOL region), T. Takisuka (Divertor simulations), and G. Bateman / A. Kritz (Pedestal height and ELM frequency in tokamaks). This approach appears to be very reasonable and practical, and it should be encouraged.

MHD and Extended MHD
The 3D resistive MHD model has been used for quantitative comparison of MHD modes in a small tokamak device. It has been found that the 3D MHD codes predict the existence of a large number of resistive ballooning modes that are not seen in the experiment. The resolution may be that a more complete extended MHD model is necessary [ie, two-fluid and stress tensor], or it may be that a more complete treatment of the nonlinear effects of the high-n modes may yield perpendicular thermal conductivity that stabilizes these modes.

3D Hybrid particle/fluid model of TAE modes in tokamaks were presented. There was generally good agreement with measured mode-frequency, and qualitative agreement with nonlinear behavior. Presently, full integration (eg, alpha particle effect on thermal particles) is not included in the simulations

The application of an Extended MHD model to stellarators was shown to give qualitative explanation of several anomalies: Beta limits can be higher than predictions of high-n ideal ballooning because of the stabilizing effects of the "omega-star" terms. Resistive interchange modes, predicted by the pure resistive MHD model to be unstable, are stabilized by "extended MHD terms". Also, the observed faster growth of magnetic islands in the Extended MHD model is consistent with soft beta limits that are observed experimentally.

Progress is being made in the development of specific physics oriented models for inclusion in "Whole Device Modeling" codes. It was shown that complete ELM modeling is very challenging in that it must incorporate transport, linear MHD stability, non-linear MHD analysis including effect of filaments, and SOL transport. NTM models are in place using Rutherford equation for the growth of an island. Also presented were models of beta-collapse and the current hole phenomena.

Presentations on 3D configurations showed the srong link between equilibrium, stability, and transport. In particular, the field line structure outside the LCFS was shown to play an important role.

Global MHD studies with the gyrokinetic model may be feasible in the future. The reduced gyrofluid model shows the importance of ion landau damping

Turbulence Simulations
There were presentations on the existing global gyrokinetic codes: In the US, therse were GTC (Lin et al.), and GYRO (Candy et al.)**.** In Japan, this was GT3D (Idomura et al.)**.** Physics issues discussed were the ITG, ETG, ITG/ETG coupling, finite-beta efftecs, and transition from Bohm to gyro-Bohm.

There were presentations and discussion on **s**teady state simulation issues that need to be addressed for long time simulations needed for integrated modeling. These include velocity-space nonlinearity, and collisional effects . Some of the other integration activities discussed were turbulence and kinetic-MHD integration, turbulence and neoclassical simulation integration, core-edge simulation integration, and the coupling of initial value codes with modeling codes with equilibrium codes.

Global gyrokinetic particle codes (e.g., GTC at PPPL and GT3D at JAREI) has been used successfully for core transport simulation for tokamaks in the past few years. Recent advances in understanding Alfven waves, edge physics and steady state transport based on gyrokinetic formalism has enable us to propose particle simulation algorithms suitable for integrated simulation between core and edge, as well as for transport time scale simulation based on kinetic MHD.

There was a presentation on ETG turbulence based on the gyro-fluid model. It was shown that magnetic shear is the key to control amplitude of electron thermal diffusivity, bursting ion transport (ITG) was due to ETG zonal flow (high k noise), and that ntegration of simulation results was necessary for integrated modeling.

A presentation showed that turbulence spreading could reduce turbulence intensity and modify mixing length formula for ITG modes. It was suggested that the effect of turbulence spreading on ETB and core boundary interaction should be evaluated.

The Edge-Plasma Integrated Modeling

The edge is defined as the region near the plasma boundary that encompasses both closed magnetic field-lines (the pedestal for tokamaks) and open field-lines [the scrape-off layer (SOL)], including plasma/wall interactions. Because of the strong radial gradients in this region and relatively large neutral densities, implementation of continuous, integrated physics models are likely very important. Furthermore, the geometrical complexity presented by the magnetic separatrix and material structures increases the need for numerical solutions. It is very desirable to develop validated reduced models that capture the essential physics, but that are more easily and efficiently integrated together and joined with models of other regions. Also, benchmarking of integrated models with other models and experiments is an essential activity.

A variety of edge codes were discussed that themselves perform some physics integration and are possible components for more comprehensive integration packages. Transport codes discussed are as follows: for edge transport; (1), CSD, a fast, reduced model of the core (0D), SOL (2-pt.) , and divertor recycling (2-pt); (2), 2D full-geometry fluid codes SOLDOR and UEDGE. Neutrals and impurities are included to yield SONIC, which combines SOLDOR, IMPMC (Monte Carlo for impurities), and NEUT2D (MC for neutrals). On the other hand, UEDGE integrates neutrals and impurities as fluid components, or alternately, the DEGAS-2 MC neutral code has been iteratively coupled. For kinetic plasma transport, the PARASOL code evolves PIC ions, electrons, and neutrals with collisions in 1D and 2D divertor configurations; extension to toroidal effects in 2D is planned. A continuum kinetic transport code is under development in the U.S. that includes one spatial dimension (along B) now, and will add radial transport next year, and 3D turbulence is the following year. Turning to edge turbulence, 2D (IFS code) and 3D (BOUT) resistive (Braginskii) fluid treats microturbulence. BOUT includes toroidal geometry and X-point effects, and is beginning to nonlinearly evolve long wavelength ELM-like modes. By 2006, the continuum kinetic code mentioned above will be able to consider turbulence as well.

Integration and application of the above components include using CSD to model LHCD in HT-7U, and plans are couple CSD with a 1D core transport code to analyze L-H transitions for ITER. A self-consistent iterative coupling between BOUT turbulent fluxes and UEDGE profile evolution was illustrated to yield a self-consistent steady state. An initial nonlinear ELM simulation with BOUT shows localized features suggestive of predicted explosive nonlinear growth, but more analysis is required. The impact of strong convective transport in the SOL in producing strong charge-exchange loss was illustrated by combining calculations from UEDGE for the plasma and NUT for kinetic neutral transport. Coupling between the near-surface MC ion code WBC and UEDGE for a lithium divertor surface indicates that core Li contamination should not be excessive. The SONIC package was used to model an X-point MARFE in JT-60U and for the divertor design of the National Centralized Tokamak Facility. For kinetic effects, the temporal response of the SOL to an ELM energy pulse was demonstrated by results from the PARASOL code in 1D. In fitting the PARASOL results to a simpler flux-limited heat-flux model, it is found that the heat flux is a larger fraction of the electron thermal limit than typically found previously.

For future plans, the purpose and structure of the newly formed U.S. Edge Coordinating Committee for identifying key issues and fostering edge collaborations was discussed. There are many crucial and poorly-understood edge issues that integrated modeling will play a key role to fully resolve. These include the L-H transition, nonlinear ELM crash, transport, and pedestal recovery, the density limit, and material erosion (with redeposition and dust formation) and accompanying impurity transport. For the next few years, there are plans to make the following advances: extend edge-plasma integration include ExB and time dependence for turbulence/transport coupling, bridge the range of turbulence wavenumbers from microturbulence to MHD ELMs, improve coupling between sputtering/SOL-transport simulations, complete kinetic edge equation formulation, extend kinetic simulations including continuum and PIC (PARASOL) models, and re-activating/extending core/edge coupling.

Sources and Software:

Comprehensive suites of advanced radio-frequency (RF) and neutral beam (NB) source codes have been assembled in Japan, the European Union (EU) and the United States (US). Closed loop (integrated) computations between full-wave ICRF and Fokker Planck solvers were presented (AORSA2D and CQL3D). Full-wave LHRF (TORIC) and 3D ICRF (AORSA 3D) simulations were also reported, although these simulations employed Maxwellian particle distributions. RF source modules in the IC, LH, Alfven, and EC range of frequencies have been combined with stability and transport codes within the TASK code structure in Japan. The TASK architecture is set up for large scale code integration in that it was developed using CVS, employs parallel processing, and stresses high portability of libraries. Results from TASK for EC current drive using beam and ray tracing analyses were also shown. Integrated modeling that combines advanced ICRF antenna modules with full-wave solvers is only now starting. An example of one such effort was discussed which combines the TOPICA antenna code and the TORIC full-wave solver. As of yet, the majority of the most advanced ICRF and LHRF wave propagation and Fokker Planck codes have not been run within closed loop computations with transport and stability packages. Exceptions to this are the Monte Carlo NB package in TRANSP and the LHCD code in CRONUS. Self-consistent closed loop RF calculations with TASK and TRANSP are planned for the near future. However these types of simulations will require complete or partial use of MPI.

The importance of modular structure and standard data set in integrated modeling is now widely recognized. At this meeting an approach using Common Component Architecture was described by researchers at ORNL and TechX, which gave rise to active discussions. The importance of standard, well defined interfaces, to enable different people to work on different parts of a software project was noted. Preliminary considerations for a common data set and program interface for the Burning Plasma Simulation Initiative (BPSI) was also presented. Finally it was agreed that an international framework for module and data exchange should be discussed in the near future.