INTEGRATED TOKAMAK MODELLING : THE WAY TOWARDS FUSION SIMULATORS

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1. Introduction

In parallel to the construction of ITER, many initiatives are needed to address complementary technological issues relevant to a fusion reactor, as well as many remaining scientific issues. One of the next decade's scientific challenges consists of merging the scientific knowledge accumulated during the past 40 years into a reliable set of validated simulation tools, accessible and useful for ITER prediction and interpretation activity, as well as for the conceptual design of DEMO and future reactors. Obviously such simulators involve a high degree of "integration" in several respects: integration of multi-space, multi-scale (time and space) physics, integration of physics and technology models, inter-discipline integration etc. This very distinctive feature, in the framework of a rather long term and world-wide activity, constrains strongly the choices to be made at all levels of developments. A European Task Force on Integrated Tokamak Modelling (EU-ITM-TF) has been created with the long-term aim of providing the EU with a set of codes necessary for preparing and analysing future ITER discharges, with the highest degree of flexibility and reliability.

The task force was initiated in late 2003 with a long term work plan along the following lines:
- structure the EU modelling effort for both the existing devices and ITER
- address the modelling issues which require a high degree of integration (physics integration, code integration, discipline integration)
- identify the theory and modelling development needs
- strengthen the collaborative modelling activity between EU and other ITER partners and promote EU modelling activity at ITER level
- provide EU modellers with a code platform structure, which enables easy coupling between codes and models, provides access to device geometries and databases, strengthens systematic code comparisons and confrontations with data.
- implement a systematic verification and experimental validation procedure for the task force modelling activities, as well as documentation and reporting.

The task force is structured under five Integrated Modelling Projects addressing integrated physics issues (IMP1: Equilibrium and Linear MHD Stability, IMP2: Non-linear MHD and Disruptions, IMP3: Transport Code and Discharge Evolution (incl. core-edge coupling issues), IMP4: Transport Processes and Micro-stability and IMP5: Heating, Current Drive and Fast Particles) and two Support Projects (CPP: Code Platform Project, responsible for developing, maintaining and operating the code platform structure, and DCP: Data Coordination Project, supporting IMPs and CPP for Verification and Validation aspects and standardisation of data interfaces and access). The seven projects are working in close collaboration with each other, establishing the foundations of the simulators.

2. Equilibrium and Linear MHD; Data Structuring.

IMP1 has now identified a full list of equilibrium codes (free and fixed boundary, low and high resolution) as well as a list of linear MHD codes and flux surface reconstruction tools. The contributed codes are standardised to avoid any internal information on machine or diagnostic data. All geometry/diagnostic data come from external databases. As consequence of the adaptation of the codes to be machine independent, the same version of the code can be applied to all machines from which a machine description is available. For example, a new version of EFIT has been applied to Tore Supra, JET and ITER equilibria (FIG.1).
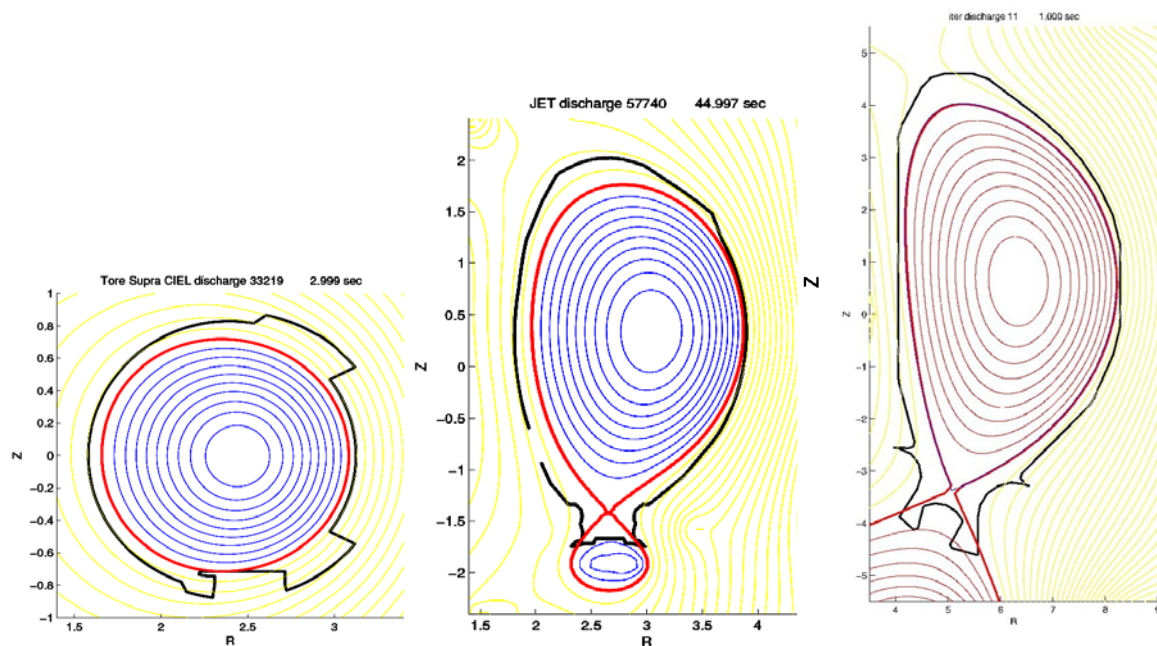

FIG.1. Tore Supra, JET, and ITER equilibria computed with the ITM tools

To enable the description of the geometry of a generic tokamak and its diagnostics, data structures have been defined in collaboration with the DCP project. Data structures have also been defined, with the aid of XML schemas, for the transfer of data between the codes. Notably a complete description of an 'equilibrium' and the coordinate systems necessary for the MHD stability codes. The current phase 3 of the data structures is operational and used for the IMP1 verification and validation activities. Of course the data structures are in continuous development. A phase 4 implementation addressing issues identified in the implementation of the phase 3 data structures is under development. The initial database systems is based on MDS+ technology supported by XML tools. Local file access (e.g. HDF5 or NetCDF) will be further evaluated in particular with respect to compatibility with XML tree definitions. MDS+ read and write routines are now available to access the data structures at the level of the structures (like a complete equilibrium). These are now actively used and form the basis for the API specification for the Universal Access Layer. The driving force behind the Universal Access Layer (UAL) is the need for the TF to have "Device independent" access to data. With a generic API targeting the TF data structures, it will act as a transparent layer providing a single interface to many data sources. It is essential that the data access, which sits in the heart of most applications, is sufficiently extensible (through plug-in technology) to be easily adapted to new data sources. Initially the UAL should incorporate MDS+ access with a local

file access option being made available. A survey recommending HDF5 (over netCDF) as the choice for local file format (to be used as restart file format, scratch area and in situations where MDS+ may be unsuitable due to bandwidth problems or other limitations) has been performed. Actual and real work towards the specification and the implementation of the UAL needs further resources and expertise being made available.

A Validation and Verification exercise is now running under IMP1 to perform comparison between equilibrium and MHD stability codes on benchmark cases and then apply such codes to relevant experimental problems/data. The physics problem selected for the validation exercise is the MHD stability of disruption in plasma with an internal transport barrier.

The high-resolution equilibrium codes CHEASE, HELENA and CAXE have been adapted to the ITM data structures. The codes now have the same interface so that they can easily be exchanged. The linear MHD stability codes KINX, CASTOR and MISHKA have also been adapted. The first benchmark cases on a Soloviev equilibrium and on an ITER standard scenario have been completed. The different versions of the linear MHD codes CASTOR and MIHSKA have been moved into a combined framework, named ILSA. As a result, one can now chose the MHD physics model (from ideal incompressible MHD to resistive compressible MHD) and the different numerical solutions methods available. The new ILSA framework has been verified on a number of synthetic benchmarks. The extension of the existing equilibrium toolbox FLUSH (JET), to be adapted to ITM requirements, is also underway. A first version will soon be available for testing.

3. Development of a Code Platform

In parallel, CPP has evaluated several frameworks for efficient coupling of codes and modules in order to select and then develop a beta version of a code platform during the course of 2006. The platform is the ultimate user interface where modellers will find user-friendly access to codes, modules, geometries, databases, documentation, as well as computer resources. Access to this material should enable them to build and run their own simulators. The platform definition is closely related to the actors (code developers, end users & administrators) needs.

The Code Platform Project major goals are:
·   Deliver a framework/toolkit for Fusion simulation applications
·   Define the interface between the codes
·   Define and deliver an integrated system for version handling of the codes
·   Define the computer resources needs for the platform and its use

A long lasting architecture is requested: open source, formal or industry standards, components and layers. A high level draft of requirements has been released.
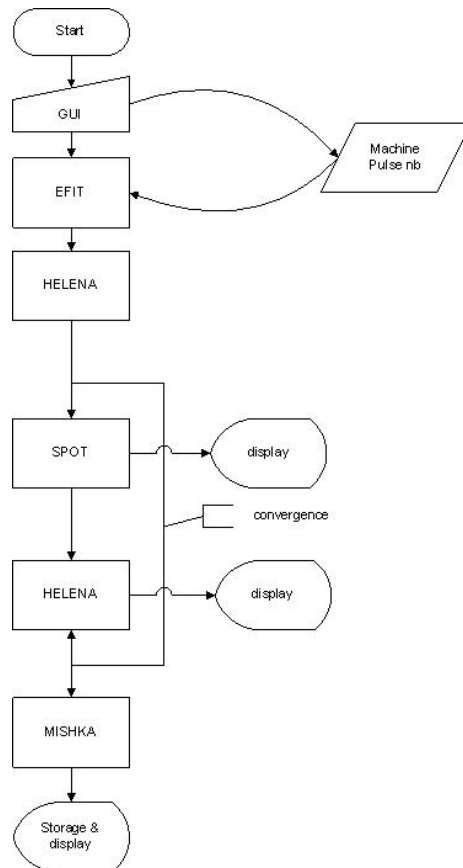
FIG.2. Workflow for Platform tests

The frameworks evaluation is now under completion, triggering the beta testing of a prototype platform in the coming months [B. Guilerminet et al., this conference]. This prototype platform will address a prescribed simple workflow, chaining equilibrium (EFIT and HELENA), MHD (MISHKA) and Orbit Following Monte Carlo (SPOT) solvers (FIG.2)

4. Non linear MHD and Disruptions

The other four IMPs have also defined their working tasks and constituted their teams, in very close connection with IMP1, DCP and CPP.

IMP2 identified four physics problems where relevant integration work could be undertaken.
- Predicting the behaviour of Sawtooth Oscillations
- Predicting the destabilization of Resistive Wall Modes
- Impact of Edge Localized Modes on tokamak performance
- Possible improvements on the modelling of Neoclassical Tearing Modes

Actual progress was obtained in the area of sawtooth oscillation, where a standardized numerical module is nearly finalized. This module provides a prescription for the occurrence of sawtooth crashes, based on a realistic linear stability threshold for m=1 internal kink modes (of the reconnecting type), and a prescription for the relaxed state as a consequence of the nonlinear evolution of these modes. Versions of this module have been implemented in various transport codes, such as ASTRA, JETTO, TRANSP, BALDUR. The effort will now be to ensure that a standard version is identified that can serve as a reference for possible future developments. In parallel, work has been initiated on two important aspects of sawtooth modelling. The first aspect concerns the determination of the fast ion distribution function

during sawtooth activity. Fast ions, either produced by ICRF, NBI or fusion reactions, are known to affect importantly the sawtooth behaviour, and indeed are included in our sawtooth trigger condition. Therefore, knowledge of the fast ion distribution function is very important in predicting the sawtooth period and amplitude. On the other hand, fast ions are redistributed by sawtooth crashes. A study of fast ion redistribution has initiated, using a development of the HAGIS code, which computes fast particle orbits in realistic toroidal geometry, interfaced with the HELENA equilibrium code and the CASTOR code, the latter providing a realistic profile for the internal kink magnetic and electric perturbations. These study is revealing a complex behaviour of fast ion orbits during kink perturbations and will hopefully be completed in 2007 with a relatively simple prescription on how to recalculate the fast ion distribution function at each sawtooth crash. Other relevant information of the fast ion evolution will come from codes like PION (a combined ICRF power deposition and Fokker-Planck solver) and from codes evaluating the scattering of fast ions during TAEs and fishbones. An overall review of this sawtooth modelling effort is presented at this conference by F. Porcelli.

5. Transport Codes and Discharge Evolution

IMP3 is actively preparing the integration of the four major transport codes operated in Europe (ASTRA, CRONOS, JETTO and RITM) in the task force framework, as well as their validation and verification. A core transport code benchmarking will be initiated in November by IMP3. This long term activity is developed in close collaboration with the JET Integration of Transport Codes Project and is utilizing JAMS, the code management and launch system used at JET for transport and MHD codes. Significant benchmarking of existing edge codes has also occurred within the ITM, EFDA-JET, ITPA and European Laboratories frameworks. Results from early stages have already been reported by D. Coster at the 2004 PSI conference. Together with the JET code improvement effort, a new coupling of the edge plasma code EDGE2D with the Monte-Carlo code EIRENE has been successfully performed (as an addition to the long standing EDGE2D-NIMBUS option). Finally, an initial version of possible interfaces for various edge code interactions has been created and placed on the EFDA-TF-ITM website.

6. Transport Processes and Micro-stability

The first instalment of Transport Processes and Micro-Stability code catalogue is available on the IMP4 website. It covers the turbulence simulation codes, whether fluid or kinetic, in three spatial dimensions. A total of eleven codes from seven Associations are currently listed. Three codes are gyrokinetic and the rest are fluid (whether gyro-fluid with Landau closures or based on the Braginskii equations). Most codes are specialised to simulate either the core or the edge plasma, but certain codes in the catalogue can treat both situations. The cross verification of codes within each of the main categories (micro-stability, micro-turbulence, and neoclassical transport) has started. Reference test cases have been defined. Specifications are inspired by the US Cyclone project (1997-2000). Three cases were identified, one being the original Cyclone test case, for turbulence in the tokamak core. The second is a small device test based on FT-2 parameters, for cases with reduced scale separation. The third is an L-mode ASDEX-Upgrade test case, for edge turbulence codes (FIG.3).
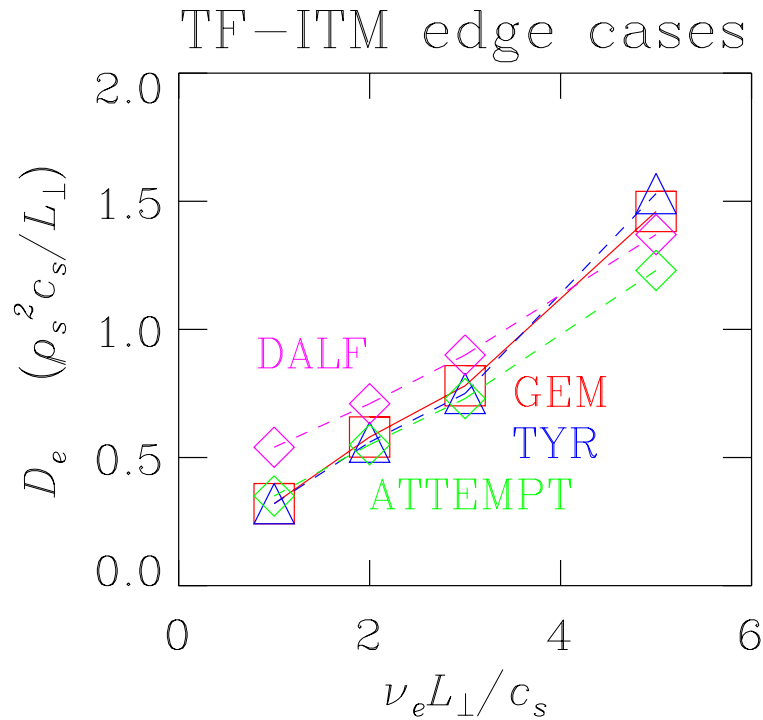
TF−ITM edge cases

FIG.3. The L-mode ASDEX Upgrade test case was used for this comparison. All codes use electromagnetic local equations with local flux-tube geometry. The results show the normalised electron diffusivity De (in gyro-Bohm units $\rho_s^2 c_s/L_\perp$, with $L_\perp$ the perpendicular scale length) against the normalised electron collision rate (here given in units $c_s/L_\perp$)

In parallel, IMP4 addresses issues in plasma theory, physics theory and numerical mathematics that are needed to go beyond present-day models and codes. This task is considered of strategic importance, since it would give impulsion to key areas of research that may shape code development in the years to come.

7. Heating, Current Drive and Fast Particles

Finally, the work carried out within the framework of IMP5 is concentrated on developing a package of codes for prediction and interpretation of heating, current drive and fast particles instabilities. Twelve different tasks have been initiated in these domains, and IMP5 is presently working closely with DCP to include in the phase 4 data structure the schemas related to heating, current drive and fast particles issues.

8. Hardware & Collaboration issues

In parallel with the development of simulation tools and software environment, the long term evolution of hardware needs is also under preparation at several levels (EU, broader approach, high performance computing, grid technology, data access etc.).

Concerning the present development activity, local fusion computers and facilities are provided by European fusion laboratories to the Task Force. To support the need for data storage and access for the IMP1 activity for instance, an MDS+ server has been installed in Frascati. Currently this has a capacity of ~1.5TB storage area. This will provide reasonable coverage for the short term needs of the TF with the exception of the higher volume data set

needs of the IMP4 Turbulence code verification activities which is expected to need 5-10Tb of data before end of 2006, stored in heterogeneous files formats ranging in size from ~200Mb to several Gbytes. A draft of the longer term needs in terms of a database hardware infrastructure and support have been circulated through DCP.

Regarding the near future evolution, from the present activities and resource needs emerges the importance of a rapid implementation of a modelling Gateway. In terms of concept, the Gateway is expected to offer to European modellers all the elements necessary to allow them to run fusion simulations. This ranges from full sets of necessary input data to documented codes, and to computer access and the archive management. The Gateway should also provide a minimum set of visualization tools. Essential elements of the Gateway should include: a front server enabling secure connection to all services, a central code repository, a data repository and its Universal Access Layer, the Code Platform server, and it should offer the necessary high-speed connection links to the various fusion devices and computers.
Obviously, from the point of view of computing resources, Grid Computing should be available from the Gateway, as needed by the different applications. The accessible computers will range from European Fusion Laboratories computers, to a (set of) central high performance computer(s) dedicated to fusion applications (presently under discussion), and up to top range computers dedicated to "millennium runs", also under preparation at moment in Europe.

Finally, the ITM task force is also setting up and pursuing regular collaborative efforts with similar integrated modelling structures which already exist or are being put in place by the other ITER partners. A coordinating structure ensuring dialogue to address various practical/legal issues [e.g. exchange of codes and models, compatibility between structures (data access, languages and formats, portability, code platforms, libraries, etc.), the need for an Integrated Fusion Modelling Workshop/Conference, copyrights and licensing] has been decided together with the ITPA Confinement DataBase & Modelling topical group. An international expert working group is now in charge of such questions. The working group is referred as IMAGE (Integrated Modelling - A Global Effort). Its primary focus is the technical aspects of integrated modelling that are not presently covered by the Topical Group, or the various efforts of the Topical Groups that already consider detailed physics issues. As the new EU-ITM-TF leader, Dr Par Strand was asked to chair IMAGE. The related actions will be conducted under the umbrella of the various bilateral agreements between EFDA and the other ITER partners. The ITM-TF also regularly liaises with ITER and the ITPA groups, in order to update the code modules and relevant data as necessary.

9. Conclusions

In conclusion, the route towards magnetic thermonuclear fusion simulators is now open, mobilizing a large part of the world-wide fusion research community. Two major lines are followed, one using massive computing to solve first principle models at the forefront of new physics discoveries and the other progressively integrating the existing knowledge into the most complete description of a fusion plasma within its environment. One can reasonably expect rapid progress on both lines, together with the necessary cross-fertilization, as well as the existence of validated simulators delivered to ITER prior to its first plasma.

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