The way towards thermonuclear fusion simulators

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Abstract

In parallel to the ITER project itself, many initiatives 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 the 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 has been activated 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. In parallel with the development of simulation tools and software environment, the long term evolution of hardware needs is also discussed at several levels (EU, EU-Japan broader approach, high performance computing, grid technology, data access etc.), and progress in this domain is reported. Finally, the ITM task force is also working out the worldwide compatibility through regular collaboration with the similar integrated modelling structures which already exist or are being put in place by the other ITER partners.

Key words: plasma physics; modelling; magnetic fusion; ITER

1. Introduction

New international flag for thermonuclear magnetic fusion energy research, the ITER project was approved and sited in Cadarache, France, by June 28^{th}, 2005. Seven partners, Europe, Japan, Russia, China, USA, South Korea and India, representing more than half of the world population, participate into the project, which now enters its construction phase. The first ITER plasmas are expected by the end of 2016. ITER has a tokamak configuration (Fig. 1), where the magnetic confinement of the plasma is ensured by superconducting toroidal and poloidal magnets, allowing long pulse operation (>400s). The nominal main parameters are major radius R=6.2m, minor radius a=2m, plasma current Ip=15MA, toroidal magnetic field on axis B=5.3T, elongation ε=1.85, triangularity δ=0.85. The maximum fusion amplification gain Q is expected to reach 10, the fusion power to reach 400MW and the nominal plasma duration to reach 400s. So-called

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'advanced regimes' are also designed to maintain Q=5 on much longer time duration, pre-figurating a reactor-like behaviour.

ITER is a major technological challenge, integrating many concepts developed in the past years on fusion experiments around large superconducting magnet systems, large volume vacuum chambers, high heat flux exhaust handling and vessel cooling (plasma facing components), particle flux management (pumping and fuelling), high incoming power heat fluxes (heating and current drive systems), within a nuclear environment. The question of plasma control is obviously addressed in order to run such plasma discharges at the relevant performance and safety level. But ITER is also a formidable scientific challenge, concentrating within $1000\mathrm{m}^3$ of plasma all the complexity of fully ionized, magnetized, burning plasma physics, combined with plasma-wall interaction issues. This also represents a challenging integration issue, both experimentally and at the modelling level. The magnetic fusion modelling community is now at work in order to progressively integrate the physics models into fusion simulators, allowing plasma physicists to predict and/or interpret magnetic fusion experiments at the relevant level. The wide variety of needs, including the potentially extremely large computing resource, claim for the maximum flexibility in the tools. The present papers introduces first some of the major physics aspects challenging such an integration and then gives more details on the European initiative on so-called integrated tokamak modelling (ITM), as well as the world-wide effort around compatibility issues.

2. The major physics issues of magnetic fusion modelling

The ultimate goal of magnetic fusion modelling is the deliverance of the so-called plasma scenarios, i.e. of the full time sequence of the plasma response (temperature, density, . . .) to the prescribed parameters (magnetic field, plasma current, heating and current drive excitations, . . .). Therefore modelling naturally splits into two categories: the numerical descriptions directly derived from first principles, usually largely CPU time consuming, and the adhoc models, deduced either from them or from experiment, more suitable for fast simulations. A fully first principle description of all phenomena, though desirable, cannot be envisaged in the near future for both reasons that some of the descriptions still do not exist and a scenario computed this way would require a computer capability totally out of reach at present. It is thus interesting to carefully discriminate between the physics processes and adjust the level of the descriptions to the physics phenomena.

A tokamak discharge is first of all a transient inductive discharge from the primary of a transformer into its secondary, namely the plasma annulus. The backbone equation to solve is thus a multi-diffusion equation, giving the time evolution of the radial profiles of the temperatures (one per species), the densities (one per species), the plasma current density and the various components of the plasma rotation (Fig. 2). The geometry is intrinsic, i.e. to be computed self consistently with the plasma state, and ruled by the so-called Grad-Shafranov equation. In the core of a tokamak plasma, the toroidal axisymmetry allows the reduction to a 2-D problem and leads to a 1-D flux coordinate system, but in other magnetic configurations (stellarator, . . .) and/or in the region where the plasma directly interacts with the plasma-facing components (the 'edge') the geometry must be computed in 3-D. It is important to note that the various diffusion equations are a priori coupled, and unless experimental profiles can complement, they must be solved together. Finally, the 1-D (or 2-D) diffusion equations can be solved exactly, provided the geometry is given. The Grad-Shafranov equation requires extra constraints that either come from experiment providing information on pressure and/or current profiles, or from the self-consistent computation of the pressure and current profiles.

The second issue to be addressed is the determination of the various transport coefficients that appear in the diffusion equations (diagonal and cross terms). A large part of the first principle physics presently under active development is located here. The transport coefficients reflect for a large part the complexity of the problem, revealing the strong non linearities and coupling phenomena that rule the plasma evolution. Even when assuming that the plasma transport (heat, particle, momentum, current) is diffusive and local (which might be disputed), it is certainly impossible to ignore its turbulent nature, often involving simultaneously several turbulence sources together with the so-called neoclassical background, as naturally deduced from the effect of collisions on the confined particle trajectories. There exists a very large set of codes and descriptions for transport coefficients. This goes from ad-hoc analytical expressions, mostly deduced from experimental fits, to their derivation from first principle turbulence computation. This last version involves the resolution of the Maxwell-Vlasov equations, averaged over the fast gyro-motion of particles, i.e. 5-D time dependent descriptions with relevant time and space characteristic lengths. This nowadays restricts the use of such codes to the fundamental understanding of the turbulent transport and such descriptions are not available yet for a direct derivation of the transport coefficients as requested by scenarios. To alleviate this, several codes propose intermediate approaches, estimating the most unstable turbulent processes and proposing semi ad-hoc transport coefficients.

The following step concerns the determination of the source and sink terms which enter the diffusion equations. The first item deals with the plasma particle fuelling, achieved through gas puffing at the edge or high speed ($\sim$1km/s) ice pellet injections. Problems of gas penetration in the edge plasma configuration or pellet ablation in hot dense plasmas are of concern. Reversely, a steady-state plasma requires a constant skimming and pumping to insure the fuel renewal, and this deserves detailed modelling to optimize the configurations. Similarly, the injected power, both used to heat the plasma and bring it to ignition or to drive non-inductively part of the plasma current in order to prolong the plasma duration, must be modelled. The power can be transferred based on two different physics schemes

– the resonant absorption of wave power: this is achieved by coupling waves through antennas located at the plasma periphery. Several resonant mechanisms are used from cyclotron resonant damping (on ion and electrons) to Landau damping and transit time magnetic pumping effects. Modelling such effects require to solve the complete set of Mawxell + Vlasov equations on a priori non Maxwellian distribution functions, using the relevant geometry for the wave propagation, and in the presence of collisions. One further complication in such kind of descriptions is the strong mode coupling effect as the waves propagate into the plasma medium, leading to significant (if not dominant) alteration of the wave vectors, and even to mode conversions of the mother wave with possible deleterious effects (modification of damping channels, loss of wave directivity, ..).
– the injection of suprathermal atoms (i.e. atoms more energetic than the background plasma ions): this is achieved by generating in a cold plasma ion source either positive or negative ions, then accelerate them to $\sim$ 100kV for positive ions and up to 1MV for negative ions. These fast ions are then neutralised in a gas chamber and then injected into the tokamak plasma. Through collisional drag and scattering they thus transfer their energy. The modelling aspects are now rather well mastered and routinely used, involving extremely detailed Monte Carlo simulations basically.

On the top of such terms, one must also take into account the intrinsic sources of power and particle. The most important is obviously the alpha-particle production generated by the D-T reactions, but the various components of the power radiation (impurities, bremsstrahlung, synchrotron,. . .) are also mandatory to account for the detailed power balance. At this level, it is important to note that models might require information on individual particle trajectories as some configurations may not fully confine such high energetic ions.

The power must also be extracted as it reaches the plasma facing components. The plasma-wall interaction physics provides further modelling complications as it involves i) non axisymmetrical configuration and ii) non fully ionized plasmas. A very detailed edge plasma description is crucial to correctly connect the hot core plasma to its material environment and estimate its mutual influence with the plasma facing components (impurity production, material erosion and redeposition, hot spots, radiofrequency wave coupling characteristics, . . .).

Finally, an integrated modelling must be able to check the overall stability of the plasma discharge, subject to magnetohydrodynamics (MHD) instabilities either limiting the performance or even disrupting the magnetic configuration. This both occurs at the plasma core (periodic relaxations of the pressure profile, creation of magnetic islands, . . .) or at the plasma edge (periodic relaxation of the pressure profile towards the plasma facing components, ..). Most of the relevant MHD modelling must include non-ideal (i.e. resistive) effects and include non-linear saturation of modes, within the exact geometry, in the presence of supra-thermal particles as well. Such computations are amongst the most CPU time demanding as well.

3. Towards fusion simulators

The first challenge in planning such modelling endeavours is to reach realistic targets with realistic agendas. At the end of 2003, the European Fusion Development Agreement (EFDA) structure has set-up a long-term European task force (TF) in charge of "co-ordinating the development of a coherent set of validated simulation tools for the purpose of benchmarking on existing tokamak experiments, with the ultimate aim of providing a comprehensive simulation package for ITER plasmas" [http://www.efda-taskforce-itm.org/].

ITM is an extremely complex issue which poses at least three challenges in terms of integration. At first the physics integration challenge: after several decades spent to develop the various physics ingredients at play in a tokamak plasma, there is an actual need to foster interactions between the different physics areas such as MHD, heat & particle transport, exhaust, energetic particle physics, etc. Significant new physics is expected, for instance when coupling edge to core physics (L-H transition, ELMs, . . .), fast particle content to non linear MHD and/or to turbulent transport, etc. Most of them are expected to be dominant in ITER. The second challenge is the code integration. Developing a 'tokamak simulator' requires a significant effort in terms of creating full sets of validated and benchmarked codes, and of setting-up standardised inputs/outputs to allow modules from different codes and providers to be linked to each others and to multiple databases. This also implies to agree on a common framework for code development and operation. The complexity, the international context, and the very long term aspects of the problem further claim for standardised and user-friendly frameworks. The third challenge to face is the discipline integration. The success of the ITM relies on close cross-discipline interactions, with input from theoreticians to build/improve the appropriate mathematical models, modellers to construct efficient, accurate codes from the models and experimentalists to provide data to validate models. The obvious questions of the relevant computer resources and numerical support are also to be addressed at the proper level.

The year 2004 was dedicated in Europe to structure the task force and plan the mid- and long-term activities necessary to such an endeavour. The work broadly aimed at reviewing the current status of modelling and at developing the longer term strategy of the TF. The long term objectives were drawn along structuring the EU modelling effort towards ITER and the existing fusion devices, strengthening the collaborative efforts between EU and the other ITER partners, and implementing more systematic verification and experimental validation procedures as well as documentation. The objectives also include the development of a code platform structure, easily enabling the coupling between codes and models, providing access to any device geometries and databases, and easing the more systematic code comparisons and confrontations between data and simulations.

A working structure divided into seven projects was put in place, divided into:

- five Integrated Modelling Projects (IMPs), addressing the modelling issues of fusion plasma physics which require a sufficiently high degree of integration:
  - IMP1 in charge of equilibrium reconstruction and linear MHD stability analysis
  - IMP2 addressing non linear MHD issues
  - IMP3 in charge of providing the computational basis for a modular transport code, taking account of the core, the pedestal and the scrape-off layer. Ultimately, IMP3 will address the simulation of complete tokamak scenarios, e.g. for ITER.
  - IMP4 in charge of developing a suite of unified, validated codes to provide quantitative predictions for the linear properties of a range of instabilities, including: ion-temperature-gradient modes, trapped electron modes, trapped ion modes, electron-temperature-gradient modes, micro-tearing modes, etc.
  - IMP5 developing the computational basis for a modular package of codes simulating heating, current drive and fast particle effects
- a Code Platform Project (CPP), responsible for developing, maintaining and operating the code platform structure. Support to IMPs is included.
- a Data Coordination Project (DCP), supporting IMPs and CPP for Verification and Validation aspects and standardisation of data interfaces and access.

The seven projects are at work, with a careful time sequencing of a large number of cross-coupled tasks. As a first major milestone, to be reached in 2006, it was decided that IMP1 was in charge of providing an integrated suite of self-consistent codes (modules) for equilibrium reconstruction and linear MHD stability analysis, i) making full use of the prototype data structure and data access be put in place by DCP and ii) porting the modules on the prototype platform developed by CPP. This implies the complete disconnection of the equilibrium and linear MHD codes from the device geometry and diagnostic data, and a universal read/write access to data.

The first results already available are extremely encouraging. The TF is now in a position to propose a high performance object oriented database structure. This structure represents the full description of a tokamak experiment: physics quantities, subsystems characteristics and diagnostics measurements. It presents a high degree of organisation, being structured in various "trees" and "sub-trees", each of them corresponding to "Consistent Physical Objects". This avoids "flat structures" with never-ending lists of parameter names. The "Consistent Physical Objects" are either subsystems (e.g. a heating system, or a diagnostic) and contain structured information on the hardware setup and the measured data by or related to this object, or code results (e.g. a given plasma plasma equilibrium, or the various source terms and fast particle distribution function from an RF code) and contain structured information on the code parameters and the physics results. The database structure is based on XML schemas [http://crppwww.epfl.ch/∼lister/euitmschemas], allowing an actual programming language flexibility. The XML schemas are used to define the data structure (arborescence, type of the objects, . . .). User-friendly tools (XML editors) allow a fast and easy design of the data structure. Small scripts ("parsers") translate the schemas in many other languages (HTML, Fortran, C, . . .), allowing an automated interfacing of the structure to any programming language used in the community. The data storage problem is also addressed, both in terms of data access and in terms of hardware. A short term storage system solution (1Tb) has been put in place by the TF through an MDS+ server hosted by ENEA [http://fusfis.frascati.ena.it/FusionCell]. The IMPs storage needs are estimated around 4Tb at the end of 2006, and more than 15 Tb on a longer term basis (see below). The access layer is presently based on MDS+, which is the most widely used data access system in the fusion community at moment, and is interfaced already with many languages. MDS+ is convenient for storing multi-dimensional arrays, and has no problem with large data size, but it is not really object oriented (arrays of objects are not possible), and is rather slow for large numbers of data calls. The idea of a Universal Access Layer is thus under consideration within DCP. The access to data would become device independent, extensible through plug-in technology (MDS+, HDF5, . . .), providing a single read/write interface to any data manipulation.

In parallel, a code platform structure is under development by CPP. The idea is to provide modellers with a user-friendly environment, on which they would ultimately have access to (any) device geometry description, to the various systems and physics data bases, and to the codes, modules and models they need to solve the problem they address. The platform would then allow them, by automatically coupling these various elements, to build-up the desired computer application (i.e. the "simulator") and then get access to the necessary hardware resource (computer and storage). The terms of reference of the platform also specify that the modellers would find access to all the existing information about the verification and validation information relevant to the elements they use, as well as to all the existing documentation, pre- and post-processing tools. A complete specification document has been edited by DCP and is presently used to evaluate several frameworks, existing among the OpenSource community. The TF is now entering into a prototyping phase, making use of three selected frameworks in a beta version in charge of demonstrating the feasibility of such a concept. The prototype platform will encapsulate the embryo of device geometry descriptions, the existing versions of the data structure and data access layer (MDS+), and the suite of self-consistent codes (modules) for equilibrium reconstruction and linear MHD stability analysis provided by IMP1. It will also give access to a number of data servers and computers, large enough to demonstrate the flexibility. IMP1, DCP and CPP expect by the end of 2006 to be in a position of demonstrating a first complete chain of manipulation tools and standards, around a set of fully modularized equilibrium reconstruction and linear MHD stability codes for tokamaks.

The other four IMPs are progressing on a slightly longer term basis, keeping the full compatibility with DCP and CPP as a constraint of course. Concerning IMP2, initial work on resistive wall modes, sawteeth and edge localised modes has started. One expects on one side state-of-the-art models for such non linear MHD instabilities, to be validated and then delivered under self-standing documented modules and on the other side a dedicated development programme at the first principle resolution level. IMP3 is in charge of integrating the various codes and modules developed in the other projects into the discharge evolution codes and also to address the major integrated transport issues. At this level, an ambitious edge code benchmarking activity is underway (in connection with ITPA) involving SOLPS, EDGE2D/NIMBUS and UEDGE codes as well as JET, DIIID and AUG data, and MDS+ is used to couple SOLPS with the ASCOT Monte Carlo code. IMP4 has structured a very ambitious turbulence and micro-stability first principle code verification and code-code benchmarking exercise, both for core (based on the Cyclone case) and edge physics. Finally, IMP5 has also structured its activity and resources around ion, electron and fast particle physics, in order to develop the computational basis for a modular package of codes simulating heating, current drive and fast particle effects. The covers ECRH, ICRH, NBI, LH, alpha particle and fast particle interaction with instabilities. With the long-term goal of reaching self-consistent calculations validated against experiments, the priority is given to realistic modelling applicable to ITER standard and advanced scenarios.

On the hardware level, Europe is also pro-active and several initiatives are being worked out at moment. Let us quote, just focusing on plasma fusion activity, the joint effort between Europe and Japan (aka the 'broader approach') which contains a fusion super computer centre to be located in Japan, and the idea to support the ITM-TF activity within Europe with specific European resources such as a dedicated super computer for fusion and/or a more systematic use of GRID technology for fusion. The ITM-TF is also supporting the creation of a tokamak simulation 'gateway' concept, where modellers, by connecting, would have access to all the tools discussed before in this chapter, including data storage, computers and support.

Obviously this significant European modelling effort is to be conducted in close connection with other ITER partners, with ITER international team and ITPA. The TF has already initiated bi-lateral contacts with US and Japan, and discussions with ITER and ITPA in order to promote a common attitude towards full compatibility between the various developments and tools. A quality process is now progressively put in place in the tokamak modelling activity. This is certainly vital for ITER and the future.

4. Conclusion

The way towards magnetic thermonuclear fusion simulators is now open, mobilizing a large part of the world-wide research community. Two major lines are followed, one massively using first principle models at the forefront of new physics discoveries and one 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 its first plasma.

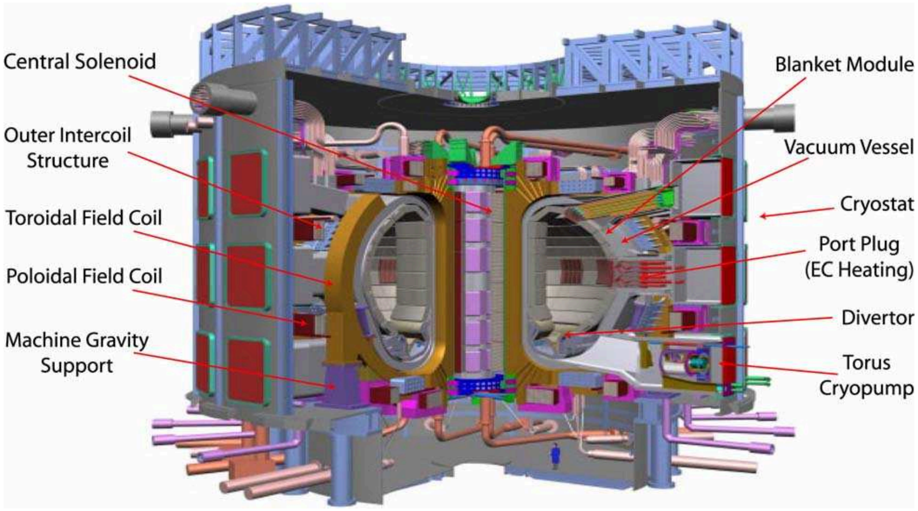

Fig. 1. The ITER main features

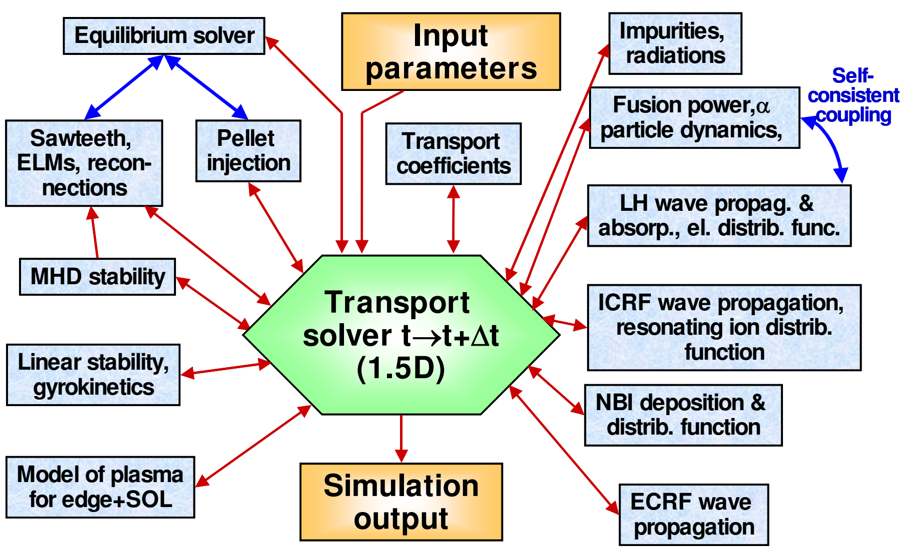

Fig. 2. Schematic structure of a tokamak simulator