G8-Exascale Project Nu-FuSE to tackle Reactor Design Challenges

Nuclear Fusion Simulations at Exascale (Nu-FuSE) is the title and mission of a new global alliance between fusion science and supercomputing approved last year by G8 Research Councils Initiative on Multilateral Research Funding [1]. This ambitious project aims to push state-of-the-art simulation codes relevant for magnetic fusion energy towards the exascale performance level, allowing important physics questions to be investigated with unprecedented accuracy and realism.

Over the last century the world energy consumption has increased 20-fold, primarily enabled by readily-available fossil fuels. However, the dwindling abundance of carbon-based resources, together with their detrimental effect on the global climate, has led to an increased urgency in the search for alternatives. Nuclear fusion, the energy source of the stars, promises a sustainable, low-pollution route to large-scale power generation. For fusion to work, two or more atomic nuclei must be brought together such that their mutual Coulomb repulsion is overcome, thus forming a single, heavier nucleus. Light nuclei such as hydrogen isotopes deuterium and tritium combine to form helium, releasing neutrons with excess energy corresponding to the mass difference before and after the reaction.

To usefully exploit this process, the fuel must be brought to several million degrees long enough for thermonuclear burn to kick in – a prerequisite which poses huge scientific and engineering challenges for the development of an economically viable terrestrial reactor. In Cadarache, France, the first concerted attempt to achieve 'breakeven' – in which more energy is produced than put in – is underway with the construction of ITER, the 500 MW International Thermonuclear Experimental Reactor [3]. In this device, not only will the plasma have to be confined by specially configured magnetic fields at 100 million degrees, fundamental questions concerning the plasma-wall interaction region will have to be solved, such as how to flush impurities and helium ash from the fuel without compromising the burn process in the plasma core.

In the Nu-FuSE project three specific research areas are to be examined with the help of state-of-the-art numerical modelling: fusion core plasma, the materials from which fusion reactors are built, and the physics of the plasma edge.

Core Plasma

One of the central problems on the road to creating a working fusion power plant is understanding, predicting, and controlling instabilities triggered by unavoidable plasma inhomogeneities. One consequence is the occurrence of turbulent fluctuations, or microturbulence which can significantly increase the transport rate of heat, particles, and momentum across the confining magnetic field. This effect severely limits the energy confinement time for a given machine size and therefore the performance and economy of a tokamak device. Accurate predictions of the cross-field turbulent transport are thus vital and can only be achieved through experimentally validated simulations. To do this, the majority of researchers in this field use a gyrokinetic (ab initio) approach. Codes like GTC-P, GYSELA, and GENE solve the nonlinear equations underlying gyrokinetic theory, which lends itself perfectly to Vlasov or particle-in-cell algorithms with excellent scaling properties. The GENE team in Garching has already reported scaling on the JUGENE platform up to almost 300,000 cores, and have already implemented a hybrid MPI/OpenMP parallelization to exploit forthcoming multi-core architectures.

Plasma-wall Interaction

Plasma confinement can never be ideal, not least as it is necessary to flush the plasma flame of ash (Helium) and to replace the fuel (Hydrogen). This already sets a critical lower bound to the level of plasma surface interaction needed: the plasma core is connected to the vessel walls by a magnetically non-confined outer region, via which plasma throughput has to be maintained and in which plasma surface interactions lead to powerful exchange of matter between the plasma and the solid container. The sheer complexity of this edge physics demands multi-scale, multi-physics modelling. In particular, very near to the solid surfaces a self-consistent description for electrostatic fields and even full gyromotion-resolved kinetics is essential to follow the dynamics of the system, the plasma chemistry, and to provide consistent boundary conditions. Two codes are being deployed by the Jülich team to tackle this region: EIRENE, a well-established kinetic Monte Carlo particle transport code for the flow fields of neutral particles, impurity ions and radiation, which is generally used are in iterative combination with an edge CFD code for the bulk plasma components; and PEPC-F, a microscopic ab initio mesh-free solver for electrons and ions close to material surfaces including

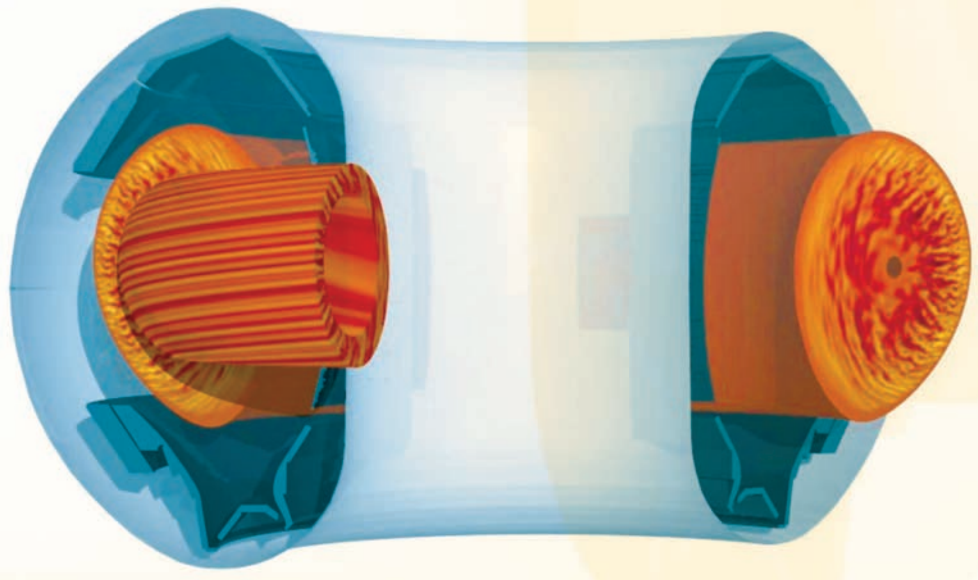

Figure 1: Snapshot from an ab initio simulation of the ITER-like fusion device ASDEX Upgrade with the sophisticated plasma turbulence code GENE.

self-consistent electrostatic fields as well as external electric and magnetic fields – Figure 2. The latter code already scales to the full 294,912 cores of the JUGENE machine [5]. The combination PEPC-F – EIRENE – edge-CFD is envisaged to provide a fully self-consistent multi-scale description of the edge region of magnetic fusion devices, from the pedestal transport barrier to the target.

Materials

Fusion reactors require very high temperatures and pressures. The fusion plasma is extremely hot and active. Whilst the magnetic field is designed to keep the plasma separated from the wall of the reactor this is not always possible and the plasma, may impact the walls of a fusion tokamak. Also, fusion energy is in the form of high energy neutrons – to convert this to electricity the neutrons have to pass through the reactor wall, heat a blanket material, which in turn drives a turbine. The neutrons cause huge damage to the wall – it is predicted that every atom in the wall of a commercial reactor will be displaced 80 times by a neutron: specially designed self-healing materials are needed to withstand this.

Reproducing the actual conditions of extended high neutron flux (such as those encountered by materials in a fusion reactor) is currently impossible in the laboratory, and there is no time to conduct 60-year experiments to mimic reactor lifetimes. Consequently materials tests will require extrapolations from experiments conducted under alternate irradiation conditions. A detailed understanding of the fundamental non-equilibrium processes involved is required, and this can only be obtained from simulation of the irradiation damage at the atomic level – Figure 3. Initially this will enable us to build models based on low-dose, short timescale experiments for reliable exploration of longer term effects; the ultimate aim is the design of radation-resistant materials for the construction of reactors with long lifespans.

In each of the above areas, the underlying algorithms are computationally intensive, and even with contemporary supercomputers cannot yet deliver realistic simulations of fusion reactor conditions. Future exascale computers will bring this possibility a step closer: however, to achieve this goal, the models

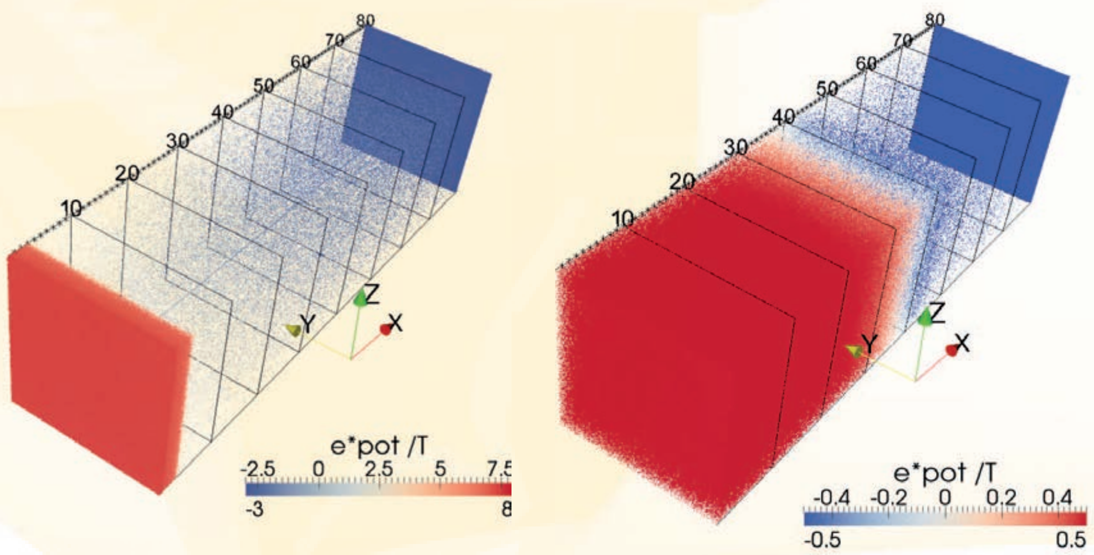

Figure 2: Formation of a plasma sheath region in the vicinity of a conducting wall with floating potential (blue) after 20 and 209 inverse plasma periods respectively

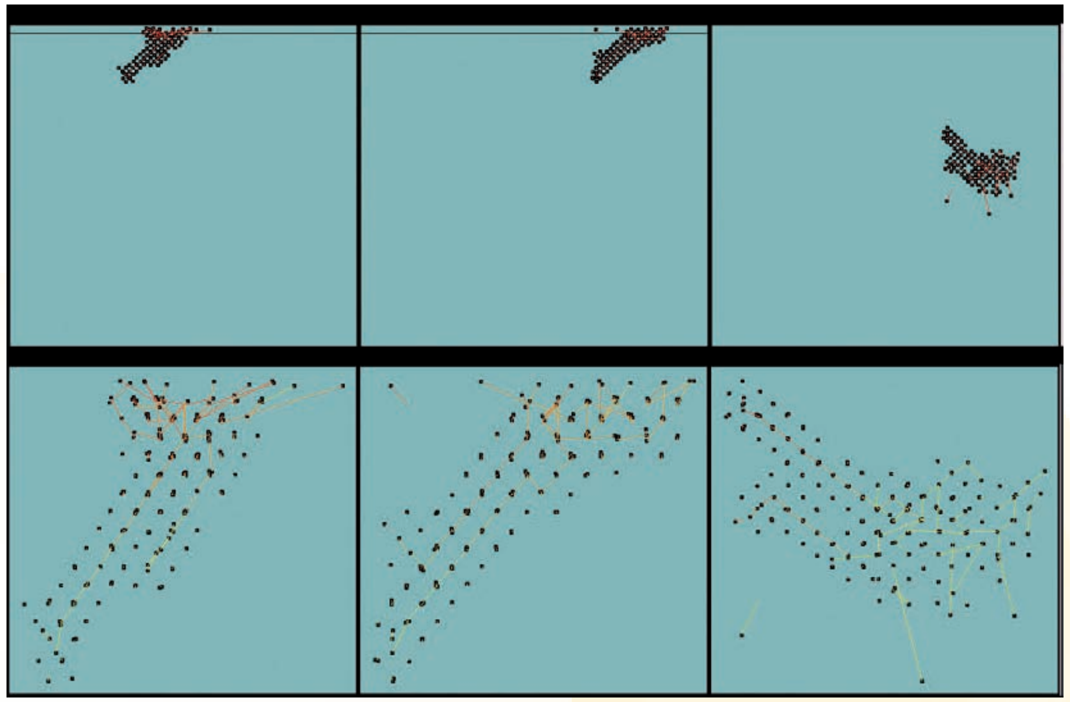

Figure 3: Damage to a reactor wall element inflicted by high-energy particles

developed by the Nu-FuSE partners must first be adapted for these emerging architectures. It is planned that the codes just described will be deployed at the supercomputing centers involved in this proposals, including the Argonne National Lab in the US and Jülich in Germany, where state-of-the-art IBM BlueGene/P systems are operative with imminent upgrades to BlueGene/Q systems. Moreover, the present consortium will also have access to the Cray XE6 system at EPCC and the IFERC (Bull with Intel Nehalem) machine at the JAEA.

Since these systems are generally considered as forerunners of future exascale computers, the implementation of our complementary set of core, edge and materials codes will require software/algorithmic advances compatible with the evolving hardware in a true "co-design" sense. Led by Prof. Graeme Ackland (University of Edinburgh), the consortium comprises researchers from Cadarache (Frankreich), Edinburgh (UK), Princeton (USA), Keldysh (Russia), Tsukuba (Japan) and Garching and Jülich here in Germany. The ultimate aim of the project is to harness the complementary expertise available within the alliance to couple these models together, creating a virtual fusion reactor capable of addressing important design issues in future power plants.

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