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# Enabling validated exascale nuclear science

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**Abstract.** The field of fusion energy is about to enter the ITER era, for the first time we will have access to a device capable of producing 500 MW of fusion power, with plasmas lasting more than 300 seconds and with core temperatures in excess of 100-200 Million °K. Engineering simulation for fusion, sits in an awkward position, a mixture of commercial and licensed tools are used, often with email driven transfer of data. In order to address the engineering simulation challenges of the future, the community must address simulation in a much more tightly coupled ecosystem, with a set of tools that can scale to take advantage of current petascale and upcoming exascale systems to address the design challenges of the ITER era.

## 1 Introduction

The goal of achieving magnetically confined controlled thermonuclear fusion has been the active research of several organisations, universities and collaborations since the early 1950's. Fusion is ostensibly in the delivery era evidenced by the rapid explosion of the number of startup companies and several independent national efforts. However, several of the planned startup and international efforts face an uncertain regulatory environment; stringent fission regulation being overly restrictive, but also not quite as uncertain as the high energy physics (HEP) safety environment, for example ITER was required by the French nuclear regulator to license the reactor vacuum vessel as a fast reactor pressure vessel under the RCC-MRx regulations. Several key materials that one would likely use to build a large scale reactor relevant facility have not been pre-qualified for the fusion reactor environment, the fission environment being too different in terms of DPA and much lower operational temperature.

Given the lack of pre-qualified materials, the lack of availability of high intensity (greater than $10^{15}$ neutrons per second) 14.08 MeV neutron sources, and the current absence of a full fusion reactor relevant test facility, if we are to deliver fusion power on a short (pre 2050) timescale, we must qualify our reactor designs *insilico* with a lack of validation data and with significant uncertainty. The various load conditions experienced by components near the first wall is complex; there are neutron fluxes in excess of $10^{15}$ neutrons $cm^{-2}s^{-1}$, photon heat loads from nuclear reactions in the core of the plasma, fast (greater than 20 keV) ions, 10 Tesla magnetic fields, synchrotron radiation loads, and several others. The components near the first wall of the tokamak can expect to experience temperatures in excess of 800 ° Kelvin depending upon internal cooling rates. If we consider the range of heat fluxes seen for example on the divertor, fusion bears similarity to the materials challenges seen in advanced

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air breathing rocket engine designs, and in Formula 1 brake disc design in terms of durability requirements from very thin composite materials.

In the following section we discuss the multiphysical nature of fusion related engineering challenges, outlining the current state of the art and a vision for the way forward in *insilico* fusion reactor and component qualification. Then we consider the related aspects of multiscale simulation, necessary for accounting for the evolution of materials and their properties as they are exposed to fusion environments. Multiphysics and multiscale simulations are then combined into a fully-functioning digital twin.

## 2 Multi-Physics Approach

Our traditional analysis codes within the fusion domain are not actually born of our requirements. Being such a long multi-decadal research programme, the community has borrowed codes and software from other domains, e.g. ANSYS [1] is largely used, mostly due to its ubiquity and percieved ease of use, MCNP [2] similarly is widely used and has an extensive set of fission relevant usage and benchmarking. There has never been an effort (to the authors knowledge) that a proper requirements gathering has ever been executed. Thus in order to cover the whole range of analysis to support the design of fusion reactors from construction, through startup to full operations, dynamic behaviour during discharge, post shutdown effect and off-normal operations; we must be capable of performing the following physics coupled togther: thermo-mechanical, radiation (photons, neutrons and electrons), fluids (conjugate heat transfer and turbulence), electro-magnetics (static, quasi-static and full wave), macroscopic material deformation (solid mechanics), tritium transport, magneto-hydrodynamics, nuclear transmutation, and chemical reaction rates. This is not to say that this is an exhaustive list, as some of these collections of physics rely upon other simulations to predict coefficients and inputs.

Not only is there a computational challenge, bringing together these traditional disparate physics regimes, there are also geometric complexity requirements; fusion reactor geometries are complex *matryoshka*-like with large components adjacent to thin components, with narrow intricate 3D printed cooling channels and composite materials. Performing whole component or even whole reactor calculations may take extraordinary numbers of mesh elements estimated at between $10^{10}$ - $10^{14}$. Generating meshes in geometries with such disparate sizes is a challenge, as is generating that number of elements in a reasonable time. Generating meshes with $10^{9}$ elements could take more than 24 hours, implying that any future meshing schemes must be not only be robust, but must also scale across nodes due to memory requirements, but also across the given CPUs on a node for performance reasons. There is only one distributed parallel mesh generator that the author is aware of, BoxerMesh from Cambridge Flow Solutions, which is a hex-dominant mesh generator, but uses an octree representation of geometry to remove defects in the underlying CAD geometry.

Thus, we must simulate the collection of that physics, both in isolation for comparison with traditional Commercial Off The Shelf (COTS) software e.g. Ansys and for validation purposes. In terms of comparison, the COTS tools emply monolithic coupling of only some problems, and commercial tools are not usually HPC relevant. This means that with traditional coupling techniques, one must perform the iterative solve for a given physics solution, pass that solution by mesh transfer or by nodal result, and then converge the next physics solution, and so on until around the last physics package is reached, returning to the begining and solving the whole loop again until convergence is reached. One could imagine leaving the COTS software solution and migrating to a more easily deployed open source toolchain; using ERMES [3] for Electro-Magnetics, Calculix [4] for thermo-mechanical, OpenFOAM

[5] for fluids, and so on, but each of these codes must then be coupled using some mechanism, for example using preCISE [6]. Whilst perhaps philsophically satisfying, this solution is not particularly performant, particularly if any one of the coupled codes does not support distributed parallelism or does not scale well, producing a serial bottleneck and creating a limitation through Amdahl's law. If instead, we embrace FEA tools and libraries that have been shown to scale e.g. MFEM [7] or MOOSE [8]; we will not be limited by the slowest and non-parallel part of the sequence, since a) the sequence will be entirely block coupled and b) the fundamental libraries are MPI-hybrid (MPI & Threads) and some have GPU co-compute.

## 2.1 Multi-Scale

If we consider the failure of materials due to cracking, the origins of cavitation in fluids, or the origins of superconductivity; they are all effects whose origins are at the micro or meso-scale but their impacts are upon the macroscopic world. In particular the propagation of cracks due to microstructural defects and the nature of magnetic field propagation in superconductors is of particular concern, as these have measurable impacts upon the performance of large scale structural and magnetic components. Focusing upon materials, there are a number of macroscopic material behaviours that we ascribe, such as elasto-visco-plasticity, that have coefficients that can be determined through phase field (crystal grain) modelling and some coefficents that can be determined through DFT, an example is shown in Figure 1.

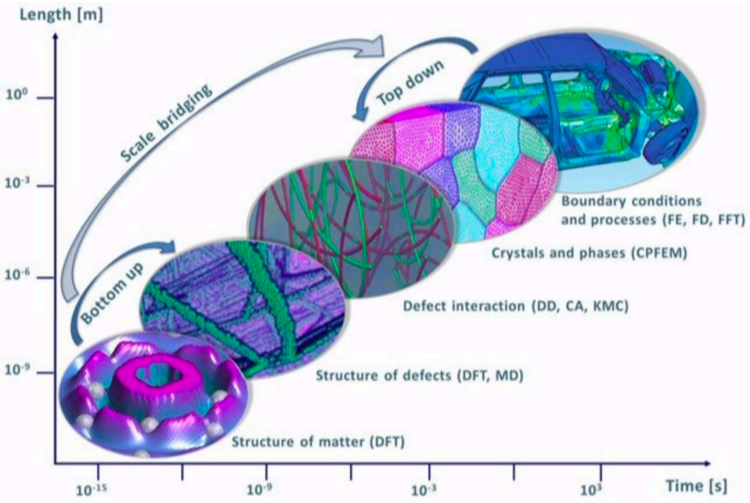

**Figure 1.** Examples of scales in plasticity modeling (Acta Mater. 58 (2010) 1152)

The simulations in which we determine the engineering response of structures need to consider these meso and micro-scopic effects, as we have many fundamental forces at play which can impact the performance of the material. Critically, it is the response of materials to the various loads present in a tokamak that determines the durability, performance and the overall economics of fusion. Further, if one considers the diffusion of tritium through materials, there are a number of concurrent processes that are driven at different scales; diffusion, porous flow through surface of materials, chemical exchange and reactions, and traditional fluid flow. The origins of magnetic flux transport through also have microscopic origins, where under certain circumstances magnetic flux flows around crystal grains, the exact onset of this driven by cooling rates on the surface around the grains, driven by macroscopic phenomena. In order to perform simulations at multiple scale lengths, there must be a way of solving the physics of the smaller subsystem multiple times under different conditions, for example the way that MOOSE solves with problem is through the "MultiApp" [9] scheme, which through parent-child links define a directed acylic graph through which the whole macro-scale problem can run, with the micro (and subsequently meso) scale functions being called several times. This type of scheme can be used to address shortcomings in macroscopic modelling, for example where two materials are bonded in traditional FEA there will be discontinuities in material response, but a multi-fidelity scheme can handled the bonded region more accurately.

### 2.2 Digital Twins

The term *Digital Twin* (DT) is a new term and has a multiplicity of definitions, The Centre for Digitally Built Britain (CDDB) [10] defines a DT as "A realistic digital representation of something physical. What distinguishes a digital twin from any other digital model is its connection to the physical twin". In the case of fusion, the current tranche of experiments are largely on machines that were built in the 1980's and the record keeping that goes with older devices is enough to remove the utility of the DT. There are, however, a number of devices world wide that ultimately should be digitally twinned; those being ITER, MAST-U (UK), NSTX (USA), DTT (Italy) and SPARC (USA private). The value of twinning these devices demonstrates that we have a sufficient understanding of the physics at play, can reproduce real results, predict the dynamic response of these devices and therefore start to use DT's to perform predictive modelling of components likely to fail. However, the simulation tools and inputs as indicated in the previous sections are far from being capable of simulating all the physics in a fully coupled manner, therefore the prospect of having a DT of a tokamak is slight. There are several other facilities in and beyond the fusion domain that one could digitally twin in the nearer term that proves out the concept. At the United Kingdom Atomic Energy (UKAEA) Culham site there are the HIVE and H3AT facilities that provide small scale tokamak relevant experiements for high heat flux and temperature. Both of these facilities could be twinned and the appropriate simulation toolchain used to predict performance, thus providing a set of validation data and some qualification of the software stack.

## 3 Digital Qualification Strategy

In terms of qualifying materials and whole systems according to regulatory requirements is a country specific endeavour and beyond the scope of this script. However, we layout arguments for the strategy for the cross validation of a suite of software tools to be used for fusion reactor design. It is clear from the timeline of fusion devices and other supporting facilities that no facility currently being planned that covers the appropriate radiation, thermal, magnetic, and plasma loads to be used to qualify materials and entire components as shown in Figure 2. There are plans to qualify materials in IFMIF [11] which will irradiate small coupons of materials to power plant relevant Displacements Per Atom (DPA) which can be used to validate findings of atomistic Density Functional Theory (DFT) predictions of performance and DPA prediction, but those materials will not be exposed to appropriate radiation, temperature or magnetic condtions.

Thus, in absence of the appropriate qualification facilities, we must find the next best set of facilities and perform overlapping validation. There are a number of operating facilities

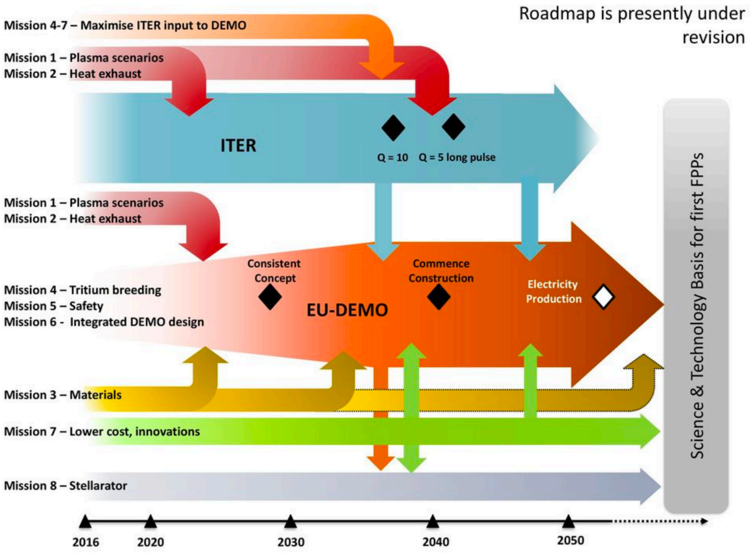

**Figure 2.** EU DEMO timeline to DEMO operations (from "The EU Fusion programme in support to ITER" by Xavier Litaudon)

**Table 1.** (non-exhaustive) List of existing (or under construction) facilities useful for cross validation note * LHC here means detailed Quadrapole simulation

| Facility | Type | EM | Fluids | Thermo-Mech | Radiation | MHD | Material |
|---|---|---|---|---|---|---|---|
| DRESDYN | MHD | X | X | | | X | |
| Diamond | Photon | X | X | X | X | | |
| MAX IV | Photon | X | X | X | X | | |
| H3AT | Fusion Test | | X | X | | | |
| HIVE | Fusion Test | X | X | X | | | X |
| Chimera | Fusion Test | X | X | X | | | |
| IFMIF | Fusion Test | | X | X | X | | X |
| SNS | Spallation | | X | X | X | | X |
| ISIS | Spallation | | X | X | X | | X |
| nTOF | HEP | | X | X | X | | |
| LHC* | HEP | X | X | X | X | | |
| MAST-U | Fusion | X | X | X | X | | |
| ITER | Fusion | X | X | X | X | | |

that can be used to validate single or dual physics, for example thermal hydraulic or liquid metal test facilities and so on, there are increasingly fewer sites that can handle multiple physics and as indicated earlier there are none that can perform all the physics (and chemistry) that we need, a list of facilities that could be used are shown in Table 1.

Fusion will need to seek collaborations and access to some of the facilities (amongst others) in order to seek validation of physics packages in regimes of interest to fusion. Non-fusion candidates include nTOF which would offer access to fluids, radiation, and thermo-mechanical data, LHC Quadrapole magnets which offers data pertinent to quench and beam divergence data. In most cases, quantities of interest are performance monitoring data such as flow rates, strain gauges, temperature monitor data, radiation count rates, currents, voltages, etc; all the data that could be used to validate real world engineering performance. These data will allow validation to occur across a range of temperatures, strains, fields and conditions and facilitate regulatory acceptence in fusion regime.

## 4 Conclusions

In order to achieve controlled magnetically confined fusion power in a short amount of time (before 2050), we must use *insilico* qualification of components in absence of experimental and operational data. We must leverage validated simulation, which itself must be cross validated with the available data and experiments from multiple domains. A key suite of experimental data across a wide range of temperatures, irradiations, magnetic fields, fluid types and flows and operational scenarios will result in the widest and most appropriate set of validation data. Fusion specifically is missing many validation experiments and thus we must look to other domains, especially spallation neutron sources and HEP experiments. These non-fusion facilities are critical to provide validation data, and to gain regulartory accepetence. We must also start to integrate mesoscopic and microscopic effects into our macroscopic domains via the use of multiscale modelling, the inclusion of such effects will allow a much more physically accurate analysis. The simulation and the design workflow must be peformed under the presence of uncertainty, and thus uncertainty propagation techniques will be important. Once we have access to a suite of validated codes, capable of performing multiphysics at large scale, wrapped with uncertainty quantification techniques; we will be able to revolutionise the way fusion engineering design is done currently, with the potential for impact on other engineering domains.

## References

[1] Gabriel J. DeSalvo and John A. Swanson, ANSYS Engineering Analysis System User's Manual, Houston, Pa., Swanson Analysis Systems, 1985.

[2] C.J. Werner, J.S. Bull, C.J. Solomon, et al., "MCNP6.2 Release Notes", LA-UR-18-20808, 2018

[3] R. Otin, "ERMES: A nodal-based finite element code for electromagnetic simulations in frequency domain", Computer Physics Communications, **184**, 11, 2588-2595pp, 2013

[4] P. A. Gustafson, F. A. Yapor Genao, et al, "Integration of MAC/GMC into CalculiX, an open source finite element code", AIAA SciTech 2019 Forum, 7-11th January 2019

[5] H. G. Weller, G. Tabor, et al, "A tensorial approach to computational continuum mechanics using object-oriented techniques", Computers in Physics, **12**, 6, 1998

[6] H.-J. Bungartz, B. Gatzhammer, et al, "preCICE - A Fully Parallel Library for Multi-Physics Surface Coupling", Computers and Fluids, **141**, 250-258pp, 2016

[7] R. Anderson, A. Barker, et al, "MFEM: A Modular Finite Element Methods Library", DOI: 10.13140/RG.2.2.10719.92322

[8] C. J. Permann, D. R. Gaston et al, "MOOSE: Enabling Massively Parallel Multiphysics Simulation", arXiv, 1911.04488, 2019

[9] D. R. Gaston, C. J. Permann, John W. Peterson, et al, "Physics-based multiscale coupling for full core nuclear reactor simulation", Annals of Nuclear Energy, **84**, 45-54pp, 2015

[10] The Centre for Digitally Built Britain, https://www.cdbb.cam.ac.uk/system/files/documents/TheGeminiPrinciples.pdf, 2019

[11] J. Knaster, P. Garin et al, "Overview of the IFMIF/EVEDA project", Nuclear Fusion, **57**, 10, 2017