# TOWARD AN INTEGRATED SIMULATION PREDICTIVE CAPABILITY FOR FUSION PLASMA CHAMBER SYSTEMS

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*The fusion environment is inherently complex, in which an adequate understanding of response from a plasma chamber system requires integrated (and in some areas coupled) analysis across multiple disciplines (neutronics, thermo-fluids, structural mechanics, electromagnetism etc). An integrated simulation predictive capability, which utilizes a computer based single CAD geometric model where a detailed simulation of the multi-physics phenomena occurring in a fusion plasma chamber system is performed, is under development and is described in this paper.*

## I. THE NEED FOR AN INTEGRATED SIMULATION PREDICTIVE CAPABILITY FOR PLASMA CHAMBER

The trend of using advanced numerical simulation for solution of complex problems is growing rapidly. The development of an integrated simulation predictive capability stands on this advanced simulation technique that is capable to treat geometric complexity, integrate multi-scales ($\geq$mm) in the simulation, include multi-disciplinary models and as a result interpret phenomena from many scientific disciplines. The actual behavior of a plasma chamber component in the fusion environment is extremely complex. Neutron and other forms of radiation emerging from the plasma core of the reactor are incident upon the geometrically complex shapes of the divertor/first wall and blanket component assembly [as illustrated in FIG. 1]. The effects of plasma radiation and fusion neutrons include heating of the components; production, transport and permeation of tritium; and deformation of the structure. Structural deformation in its turn influences flow and heat transfer, and results in strong coupling of physics. The flowing liquid metal breeder experiences magneto-hydrodynamic (MHD) forces, which alters liquid velocity characteristics according to the local flow component [see FIG. 1] [1]. Diffusion and convection processes result in property gradients that influence heat distribution and species concentrations.

As we progress toward ITER and beyond, it is imperative to develop an integrated simulation predictive capability (ISPC) allowing for the realization of a fusion simulation environment optimized for the plasma chamber environment, enabling integrated multi-physics modeling in 3D complex geometries under transient and steady-state conditions. The envisioned virtual plasma chamber systems integrated predictive capability will be instrumental in providing information that is not easily obtainable through experiments. It helps develop knowledge with fewer experiments and interpret information gained from experiments.

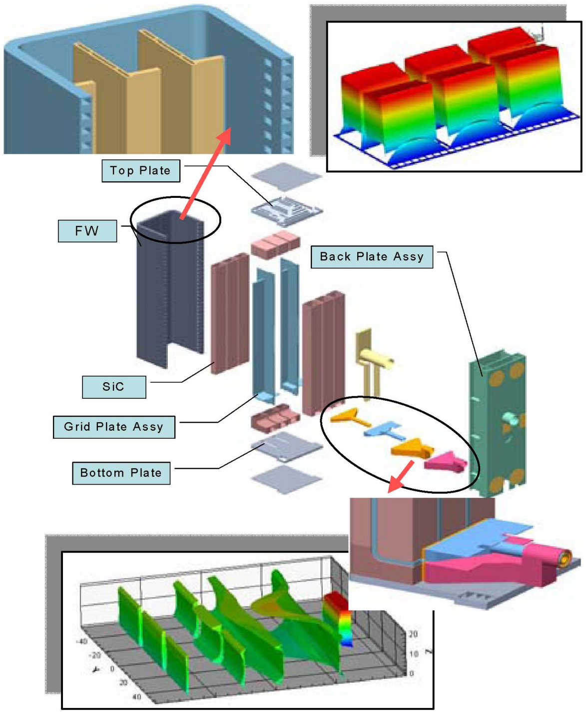

*Figure 1 A liquid metal (DCLL) blanket involves complex geometric elements and associated MHD flow characteristics*

### I.1 Approaches/Objectives

The ISPC has been envisioned for the fusion plasma chamber systems for near term machines (ITER/CTF- a component test facility) as well as DEMO. The goal is to develop a predictive capability which utilizes a single computer based geometric model (CAD), in which simulation of the multi-physics phenomena occurring in a fusion plasma chamber system is performed. Specifically, the CAD-based solid model is the common element across physical disciplines. The simulations will be geared progressively towards allowing for design optimization, performance evaluation, failure mitigation, and operational control of ITER/CTF components in the near term and DEMO in the future. This will be accomplished as a staged approach where the initial stage will focus on the component level modeling. In the next stage the component level analyses will be integrated with system level modeling for global performance and safety analyses. The development of this ISPC will be pursued with the mindset of providing a link to the Fusion Simulation Project (FSP) [2]. Ultimately the vision for ISPC leads towards development of a predictive capability for DEMO, which has been strongly benchmarked with the experimental data obtained from the ‘real fusion environment’ on ITER and CTF.

## II. ISPC COMPONENTS

The ISPC will be built upon four fundamental underpinnings. The first component in the simulation tool will be the integration and assimilation of state of the art analysis codes from the various disciplines involved. The key physical phenomena characterizing the plasma chamber systems encompass the disciplines of neutronics, electro-magnetism, plasma material interaction, thermo-fluids, species transport, and structural mechanics. There exist analysis codes that can cater to these individual physics to a large extent, but these codes have to be enhanced and tuned to be applicable in the realm of fusion plasma chamber environment with regards to phenomenon, materials and interfaces. For example, constitutive equations need to be added to the existing codes describing the thermal-physical properties of a heterogeneous medium in breeding pebble bed. The liquid metal MHD, tritium permeation and PFC melt layer dynamics modeling, have to be incorporated in the form of in house research codes or specialized user sub routines. A unique feature of the ISPC is that the CAD-based solid model alone is the common element across physical disciplines, which warrants a consistent assessment for the performance evaluation.

The second component includes advances in data translation, involving efficient and high fidelity data mapping across various analysis codes to enable integrated or coupled simulations in a multi-physics environment. A sample list of codes with numerical and mesh schemes that are frequently used in plasma chamber analysis is shown in Table 1. If the computational discretization for the different physical analyses (for example: fluid flow and structural dynamics) are nearly identical, the transfer and interpolation of data like forces and moments is straightforward. However, in most realistic calculations, the computational meshes used for different physical analyses are very different in nature. Numerical modeling of individual physics has its own unique mesh resolution requirements. This is illustrated in FIG.2.

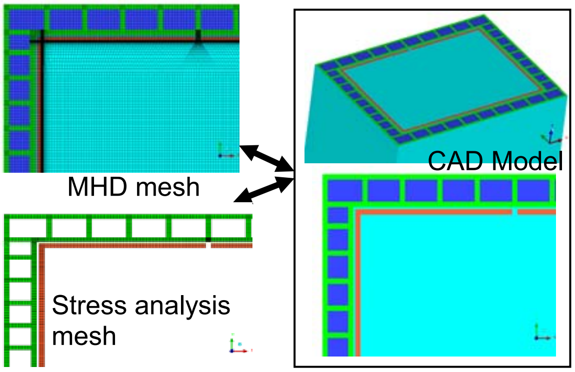

*Figure 2 MHD flow solution on a hexahedral mesh requires much finer meshes at the fluid and solid interface*

| Physics | Analysis code | Mesh specification |
|---|---|---|
| Neutronics | MCNP | Particle in cell (PIC) |
| | Attila | Unstructured tetrahedral mesh (node based) |
| Electro-magnetics | OPERA | Unstructured Hex/tetra-hedral mesh (node based) |
| | ANSYS | Unstructured Hex/Tet mesh (node based and edge based formulations) |
| Thermo-fluids | SC/Tetra | Unstructured hybrid mesh (node based) |
| | Fluent | Unstructured hybrid mesh (cell based) |
| | CFdesign | Unstructured hybrid mesh (node based) |
| MHD | HIMAG | Unstructured hybrid mesh (cell based) |
| Structural analysis | ANSYS/ ABAQUS | Unstructured second order Hex/Tet mesh (node based) |

*Table 1: The sample analysis codes and mesh requirements*

The third component in the ISPC is the computational analysis management. An important role that is served by the ISPC is that of a simulation process management system, whereby all of the data relevant to each aspect of the simulation is stored and transmitted to multiple solvers in an appropriate format, as well as made available for post-processing and debug utilities. Furthermore, it is desired to provide an interactive visualization, allowing real time lifelike representation of the system response, which forms the fourth main component and its progress relies on the computer graphic science/ technology advancement. In the following sections, example details on implementation will be discussed; while current state of ISPC development on various integrated simulations will be presented in section III.

### II. 1 Coupling across Physical Disciplines- High Fidelity Data Mapping/Translation

The computational discretization for different physical analysis has different requirements and results in diverse computational meshes. Data mapping and loads transfer interpolation across analysis codes and dissimilar meshes have to be accurate. In general, based on physical principles, the data interpolated (or shared at a boundary as in fluid-structure interaction,) must satisfy certain physical conservation laws or preserve profiles of the parameters of interest. These include the conservation of net force, moment, mass flow rate and energy, and the preservation of temperature or displacement profile, as applicable to any given problem. Accuracy of interpolation procedures can be judged by the extent to which such conservation/ preservation is enforced. To cite an example, the total heat deposition $q$ computed from a neutronics solver going into a fluids solver must be conserved (in each material,) even though the fluids meshes may be too coarse to resolve the sharp gradients in $q$ that are present. Such a conservative interpolation on arbitrary meshes may be performed by projecting solution data in a least-squares sense. Higher order accuracy can be achieved by using appropriate basis functions to interpolate the solution within computational cells.

It must be noted that the enforcement of conservation has never been guaranteed in existing multiphysical environments. As illustrated in FIG. 3, the following techniques, , are generally used for data interpolation: (a) Point-element relations for standard interpolation, (b) Element-element relations based on intersection, and (c) Point-point relations for matching grids/nearest neighbor. In addition, fast search engines such as octree approaches are available for use to alleviate the inefficiency search when the number of nodes increases.

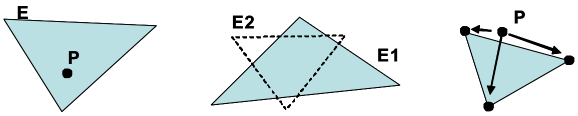

*Figure 3 Example interpolation schemes used in existing multi-physical solvers*

### II.2 Morphing Capability

When there are deformations of solid walls resulting from a structural analysis calculation, this change must be propagated across the solvers to achieve a satisfactory coupling of these analysis fields. This capability is specially needed during the modeling of liquid metal MHD in channels under fusion magnetic field conditions, as any change in channel geometry affects the flow field significantly. The most natural method of propagating geometry changes is through the CAD model, which is common to all solvers. We intend to use a non-uniform rational B-spline (NURBS) based procedure to accommodate structural deformations, and require that the initial CAD data be specified or modified in order to enable this functionality [3-4].

A CAD-based approach is being pursued to transfer geometry change information to the physical analyses:

1. The surface is decomposed into non-uniform rational B-spline (NURBS) curves;
2. Deformation data is mapped onto the CAD model;
3. A new set of NURBS coefficients is computed using least squares to match the deformed surface from a set of sample points; and
4. Corrections are made to ensure that surface discontinuities are not created as a result of the newly calculated NURBS coefficients.

## III. PRESENT STATUS- EXAMPLE APPLICATION STUDIES

The aforementioned CAD integrated numerical approach is being applied to the US ITER FW/ shielding blanket design as well as a test blanket module (TBM) design optimization. In addition, the induced currents and subsequent EM forces and structural loads under disruption scenarios have been evaluated with the ITER 40 degree CAD model for shielding blanket and vacuum vessel [5].

### III. 1 Neutronics, Thermo-fluid Integration for ITER FW/Shielding Blanket Design Analysis

High-fidelity coupling of neutronics and thermo-fluid analysis has been performed on a model of an ITER first wall panel, using CAD-based Monte Carlo neutronics analysis to generate the nuclear heating source term for a detailed thermo-fluid analysis. The Direct Accelerated Geometry Monte Carlo (DAGMC) capability developed at the University of Wisconsin was integrated with MCNPX v2.6b to allow simulation of radiation transport directly on the CAD-based solid model of the first wall and shield components, without translation to the native MCNPX geometry format as illustrated in FIG. 4 [6]. In this analysis, volumetric nuclear heating results were collected on a cylindrical mesh with a 3mm x 3mm x 3mm resolution over the entire geometry, resulting in nearly 20 million mesh elements. A single orthogonal structured grid was used for the entire problem, which does not conform to the geometry.

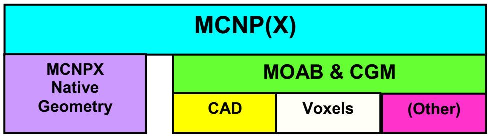

*Figure 4 Performing MCNP on directly CAD-based geometry using MOAB and CGM utility: Direct Accelerated Geometry Monte Carlo (DAGMC) scheme illustrations*

The thermo-fluid analysis uses an unstructured mesh that conforms to the geometry of the model and is resolved to capture the fluid flow boundary layers as well as the strong gradients in temperature and flow based physical quantities. The first wall model contains four different material regions and as a result, there are four distinct meshes, one for each of the materials. The typical size of the mesh is of the order of 10 million elements. The source term for the thermo-fluids calculation is the nuclear heating generated in each of the elements of the meshes, which is obtained from the neutronics calculation.

Because the neutronics mesh is not conformal, each mesh cell can comprise of more than one material. MCNPX offers two options for generating nuclear heating in such cases: the volume averaged total nuclear heating in the mixture of materials, or separate neutron and photon heating in the entire cell, assuming a single material. In either case, the neutron transport solution is calculated using the full detail of the material compositions independent of the mesh used for collecting results. However, in the case of volume averaged nuclear heating, the results for a particular mesh cell are not representative of any of the particular materials in the cell and therefore not useful as the source term for the thermal analysis. In order to supply nuclear heating data in the four material zones for the thermo-fluids analysis, eight separate heating results were calculated on the same high-fidelity neutronics mesh, one for neutron heating and one photon heating tally for each of the four materials used in this model: Be, CuCrZr, stainless steel, and water.

For each material, the neutron and photon heating data was summed and that data was interpolated to the corresponding CFD mesh using one of a number of sampling strategies. In the simplest strategy considered, the geometric centroids of each CFD tetrahedral mesh element was matched with the corresponding grid element of the MCNPX mesh, and the associated volumetric nuclear heating value was assigned to the entire tetrahedral mesh element. A better strategy performs a similar lookup for each of the vertices in the tetrahedral mesh, and then uses standard finite-element integration/ quadrature techniques to determine the total heating in each element. Finally, the most accurate approach determines the volume fraction of each tetrahedral element that overlaps with each MCNPX mesh cell and sums the MCNPX heating values according to those volume fractions to determine the total heating in a tetrahedral mesh element.

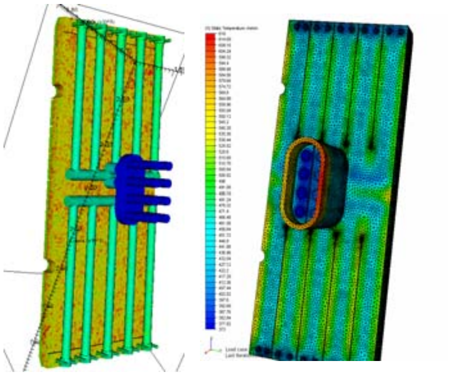

*Figure 5 MCNP calculated nuclear heating (left) mapped to CFD meshes (right) for thermo-fluid temperature calculations*

### III.2 Neutronics, Thermo-fluid and Thermo-mechanics Integration for TBM Design Optimization

A simple coupling procedure between the volumetric nuclear heating, thermo-fluids analysis and structural analysis has been developed to aid in the Helium Cooled Ceramic Breeder (HCCB) ITER test blanket module (TBM) design [7]. The effective thermo-physical properties of beryllium pebble bed in the HCCB design depend on the temperature and the strain level inside the pebble bed. The temperature increase as a result of nuclear heating leads to thermal strain development in the bed. The thermal strain in the beryllium pebble bed then alters the thermo-physical properties and heat transfer patterns. As a result new temperature and strain fields are created. An integrated neutronics, thermo-fluids and thermo-mechanics structural simulation capability is required to accurately model the temperature and stress states in the pebble bed. A high fidelity simulation with correct phenomenological modeling capability (strain dependant physical properties) can lead to an optimized HCCB design. In this particular example the volumetric nuclear heating rates were obtained at an orthogonal MCNP tally grid. These were computed using a CAD base translator scheme developed at ASIPP in China [8] for MCNP (Monte Carlo analysis) and were translated onto a thermo-fluids hybrid mesh (tetrahedral and prismatic) in a way that the total nuclear heating rate in each material domain is preserved after the mapping. The temperature field was solved by the thermo-fluids solver iteratively with the stress analysis solver in a coupled manner to capture the effect of strain dependence of pebble bed thermal conductivity based on the flow chart described in FIG. 6.

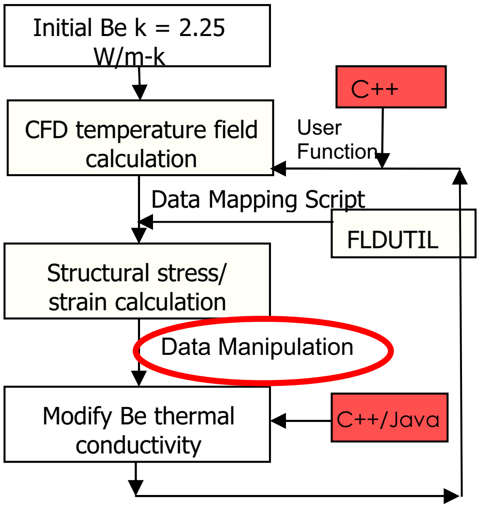

*Figure 6: Flowchart representing the iterative coupling procedure between the thermo-fluids and thermal stress analysis.*

The mesh used in structural analysis is different from the thermo-fluids mesh as it is more localized in the region of interest and is comprised of second order elements (thermo-fluids mesh has first order elements). The ability to model strain dependent thermal conductivity gives a much more accurate prediction of the temperature and stress field. It was observed that the predicted maximum temperature in the beryllium region of the HCCB module was over 40C lower [7] if the correct strain dependent physical property variation is taken into consideration. This provides the designers with a much better predictive capability to make better informed design decisions.

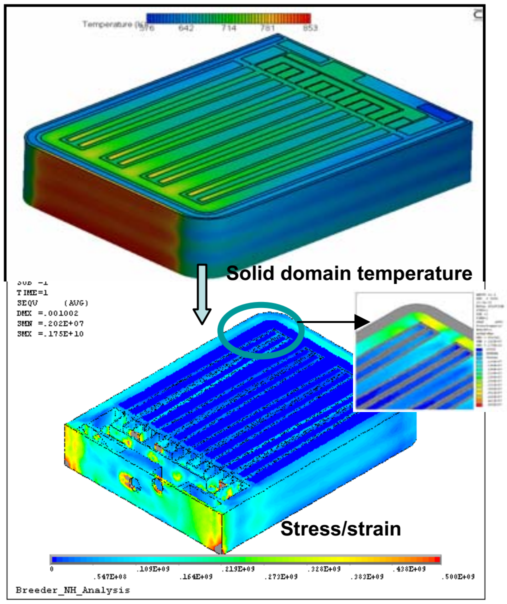

*Figure 7 Solid domain temperatures from CFD analysis imported to a structural code for stress/strain estimations in the HCCB TBM design*

## IV. SUMMARY AND FURTHER DEVELOPMENT

The ISPC represents a paradigm shift in the manner in which multidisciplinary simulations are performed. In this paper a basic framework of ISPC has been laid out and some examples demonstrating progress in a few important areas have been presented. As the next step, several tasks have been identified to further enrich this development. The future development of ISPC should closely follow the development of the fusion simulation project (FSP) to ensure compatibility. The ISPC when linked to the simulation capabilities being envisioned in the FSP would be able to simulate the plasma chamber responses to various fusion plasma shots.

1. Fusion Specific Research Code Advancement: The third party simulation software, that form a substantial component of the ISPC are typically well established existing solvers. These codes have been considered because of robustness and fast numerical schemes and an ability to handle large and complicated geometries. Regardless of that, the validation of these codes coupled together in fusion operating conditions is undoubtedly necessary. Nevertheless, there remains a requirement for development of simulation capability of critical

phenomenon that is very unique to fusion such as such as high Hartmann number liquid metal MHD modeling, pebble bed thermo-mechanics, melting and subsequent molten layer movement of plasma facing surfaces etc. The advancement of modeling capability to incorporate these fusion specific simulation challenges is foreseen as an important part of the ISPC mission.

2. A Hierarchical Simulation Framework: In a complex physical system like fusion reactor, several situations arise that warrant the need for a hierarchical simulation framework. The modeling of accident scenarios, in particular require the simulation of the affects of an individual component with the entire system. This calls for a simulation framework with a hierarchy built into it so that codes that perform global system level modeling can interact and obtain inputs from and tender output to codes that carry out detailed component level modeling. Development of this hierarchical framework, providing ability for systems and component level modeling to interact will be a part of the ISPC.

3. Common Domain Representation: A multi-physics integration has been enabled by the ability to perform all analyses on geometric models that are derived from an identical representation i.e. the CAD-based solid model. As described in the examples in this paper, the neutronics calculation were performed directly on the same solid model as was used to generate the CFD mesh. As a result there is confidence that the results can be mapped onto each other robustly, despite the limitations of the orthogonal MCNPX tally grid used in the neutronics calculations. This common domain representation points to a strategy for expanded multi-physics applications where the internal representation of the geometry is common across the simulation tools. This example adopted the MOAB [9] mesh database implementation of the ITAPS [10] interfaces. The MOAB representation is used internally in DAGMC for the radiation transport calculation. In addition, the mesh interpolation was performed by reading both the MCNPX and CFD mesh into a tool based on MOAB. While ad-hoc solutions can be generated to allow interaction among physics analyses, relying on a common domain representation can facilitate both the re-use of methods developed within a project and the use of methods developed outside a project.

4. Support for heterogeneous, high performance computing: By construction, the ISPC will contain a resource management utility and the ability to run on multiple operating systems and communicate across platforms. High performance computations, requiring parallel processing and access to remote data and resources will be possible.

5. Efficient use of open-source software: As an example, MOAB [9] is currently under active development to support efficient parallel mesh representations, domain decomposition and generalized interpolation of field data between meshes. Furthermore, tools are being developed within the ITAPS framework [10] for mesh refinement, shape optimization and other services, using a common interface to MOAB and similar implementations.

## ACKNOWLEDGEMENTS

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