Integrated Multi-physics Simulation of Nuclear Components as an Essential Element in Developing Predictive Capabilities for DEMO

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Rationale of white paper

The trend of using advanced numerical simulation for solution of complex problems is growing rapidly. The development of an integrated multi-physics simulation predictive capability (ISPC) stands on this advanced simulation technique that is capable to treat geometric heterogeneity and complexity, integrate multi-scales in the simulation, include multi-disciplinary models and as a result interpret phenomena from mutually dependent scientific disciplines, and predict performance with sufficient accuracy. 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. 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. Diffusion and convection processes result in property gradients that influence heat distribution and species concentrations. For off-normal conditions, accurate simulations of system performances are the only means of providing a-priori assurance of performance. The ISPC will significantly speed up the design and analysis process and allow predicting accurate performance features for the geometrically complex fusion systems with many synergistic phenomena.

The envisioned virtual nuclear components multi-physics integrated simulation predictive capability will serve as a vehicle to address gaps identified in the Theme areas of Fusion Power as well as Plasma Material Interface. The ISPC permits a much more thorough exploration of the design space which enables the closing of fusion fuel cycle and cuts down dramatically the huge risk and expense associated with laboratory testing of exhaust power handling for proposed fusion nuclear chamber concepts. It can be instrumental in providing scientific insight that is not easily obtainable through experiments, and helps develop knowledge with fewer experiments, define operating conditions for control, and interpret information gained from experiments.

Goal

The ISPC has been envisioned for the fusion plasma chamber systems for near term machines (ITER/CTF- a component test facility) as well as for DEMO. The central goal is to develop a integrated simulation predictive capability in a shared platform, which utilizes a single computer based geometric model (CAD). This model would represent a real component or system, in which a simulation of the multi-physics phenomena occurring in a fusion plasma chamber system is performed. 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. Ultimately the vision for ISPC leads towards development of a fully virtual design
predictive capability for DEMO, of which integrated physical models have been strongly benchmarked with the experimental data obtained from the ‘real fusion environment’ on ITER and CTF.

Accomplishing this central goal requires advances across an array of technical issues in the individual disciplines involved, including, for example, reliable predictions of nuclear features, MHD flow, structural deformation, and potential failure modes. It also requires significant improvements in system integration to deal with the complex interactions among disciplinarians, especially in a highly parallel computing environment.

Scope

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 must be validated, enhanced and tuned in order to be applicable in the realm of fusion plasma chamber environment with regards to phenomena, material properties, 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. These micro-properties as well as critical local phenomena can be modeled in a finer domain, while calculated results will be mapped and transmitted to the component scale for incorporation. Specifically, material properties in the fusion environment are to be modeled within Theme area Fusion Power Material panel mission elements including multiscale materials modeling and high-fidelity constitutive mechanical models. 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 subroutines. Experimental data (local focus or complex) will be needed to validate both individual physical models and the integrated model. The advancement of modeling capability to incorporate these fusion specific simulation challenges is foreseen as an important part of the ISPC mission.

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 multi-physics and multi-scale environments. This is because 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. 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 such as forces and moments is straightforward. Particularly, 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.

The third component in the ISPC is the computational analysis management, including geometry, mesh generation. 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. 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. Another 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 that the computed results are displayed in some comprehensible form, often through graphical visualization with interactive features, allowing real time life-like representation of the system response, which forms the fourth main component and its progress relies on the computer graphic science/technology advancement.

Strategy/Approach

The ISPC represents a paradigm shift in the manner in which multidisciplinary simulations are performed. From the outset, the emphasis will be on system integration rather than separate threads of development that might eventually come together at some point in the future. Rapid exploration of critical system integration issues entails the use of simplified-but fully integrated-models and interfaces initially, to be followed by successively refined models and interfaces as experience is gained. The ISPC can also be a fully integrated project that covers a broad aspect of activities from research in physical modeling and numerical methods, development of advanced instrumentation techniques, and performance of new experimental programs to provide data for validation and benchmarking.

The ISPC 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. In fact, such a process is at its early stage of development for the ITER first wall/shield blanket and TBM designs\textsuperscript{1-4}. 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 also be pursued with the mindset of providing a link to the Fusion Simulation Project (FSP). It 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 nuclear chamber responses to various fusion plasma shots.

References:
2. J. KOTULSKI et. al., EM Analysis Update First 40 Degree Sector, presented at SNL ITER weekly project meeting.