

## REPORT OF THE EXTERNAL SUPERVISOR OF ANSHUMAN BHADAURIA

During the industrial training period carried out in CIMNE, Anshuman Bhadauria has been working on tasks related to the European Project “Integrated Computational Materials Engineering expert group”, ICMEg.

Integrated Computational Materials Engineering (ICME) uses a variety of software tools in a simultaneous or consecutive combination. Major developments in the area of ICME by now have successfully been driven essentially by academic and industrial users of simulation software. Even though ICME is a new and powerful discipline, coupling of different software tools is still in its infancy. If such a coupling is realized at all, major issues are significant efforts in terms of time and workforce to be spent when using the ICME approach.

Once established, an open and easily accessible formulation of a global standard for information exchange in ICME settings will:

- significantly facilitate the exchange of data between different tools
- create new options and functionalities of the present tools
- allow for easy integration between commercial and academic approaches
- provide the pathway for life-cycle modeling of components/products
- allow for global optimisation of process chains
- stimulate many further new developments

The ICMEg projects intends to set up a standard on interoperability between FE codes, With the tremendous amount of research done in the field of numerical methods for engineering, a sharp rise in the number of new algorithms and software tools (academic and commercial) have been observed in the past decades. The advent of such software tools has not only made the application of the methods easier, but it has also drastically increased the number of users and the applications of these numerical methods to engineering problems.

However, mostly these tools have been developed independently for solving problems of a particular kind, by particular methods on a particular scale, which leads to some limitations. One of these limitations, interoperability, has been addressed by Bhadauria proposing a methodology to resolve it for a small use-case of finite element problems at a continuum scale has been proposed. The main idea revolves around the fact that, popular tools use formats like VTK, STL, or XDMF, among others, for transferring data of mesh, geometry, loads, etc., and not all the tools can understand or process these formats in a useful manner. To simply state it, there is not one standard format which can enable complete interoperability among these tools. In fact, this problem of interoperability also keeps us from transferring data from one scale to another, e.g. from an RVE to a continuum scale. To enable the interoperability among tools, a methodology has been proposed to export data from Abaqus Output Database directly to HDF5 containers as an example. It has been shown that HDF5 data model is a suitable interoperability tool to be used in the Finite Element Analysis (FEA) of engineering problems.

Bhadauria has been studying the Abaqus Output Database (ODB) and its underlying hierarchical structure, and he has developed a procedure to import external libraries to Abaqus-Python. The customization of HDF5 containers has been done for thermo-mechanical problems using h5py, a Python API for HDF5 files. The metadata for the problem has been collected from Abaqus v6.14, and a methodology for the export of data from Abaqus to HDF5 containers has been defined. The developed methodology has been applied to generate an HDF5 data model

using the written scripts.

The hierarchical structure of ODB and MDB (Model Database) are similar, and they serve the two main purposes in Abaqus software. The methodology devised to extract data from ODB, can also be used to write data to a MDB, directly from HDF5 files after some alterations in the scripts. The ODB can be understood as a read-only mode, whereas MDB can be considered as read-write mode.

The work carried out by Bhadauria during this industrial training period has been very good, and he has shown a great motivation on the topic. As a result of this work, Bhadauria will participate with an invited talk in the upcoming Second Workshop on Software Solutions for Integrated Computational Materials Engineering (ICME 2016) which will be held in Barcelona on 12-15 April 2016, and we expect to write a paper on the subject to be sent to an international scientific journal.

A handwritten signature in blue ink, appearing to read 'C. Agelet de Saracibar', with a long horizontal stroke extending to the right.

Carlos Agelet de Saracibar  
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External Advisor