



HDF5: A New Approach to Interoperability in Finite Element Tools

Internship Report

Introduction

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 wide variety of engineering problems.

However, most of these tools had been developed independently by academicians, research centres and companies for solving problems of a particular kind, by particular methods on a particular scale, which lead to some limitations. One of these limitations, interoperability, was to be researched about and a methodology had to be proposed to resolve it for a small use-case of finite element problems at a continuum scale.

The main idea revolved 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 [1]. So during the internship the major task was to enable the interoperability among tools, and propose a methodology to export data from Abaqus Output Database (ODB) [2] directly to HDF5 [3] containers in form of an example.

Main tasks

- 1. Create Metadata:** An elaborate list of keywords which will be used as metadata in the HDF5 files, and will serve as communication standard among tools eventually. The list was prepared using Abaqus documentation as a reference, taking thermo-mechanical problems as an example. The list comprises of key words, their small useful description, quantity type described by keywords eg. integers, alpha numeric etc., tensorial order, and units.
Status: The task was successfully finished to evaluators satisfaction. Further, I have been invited to co-author two chapters in the ICMEg book, but that is out of the scope of this internship.
- 2. Enable Communication:** The next task was to customize HDF5 containers for thermo-mechanical problems using h5py, a Python API for HDF5 files. Using the previously collected metadata for the problem from Abaqus v6.14, a methodology for the export of data from Abaqus to HDF5 containers was defined. Detailed description of methodology and the scripting procedure will be published in a paper titled “HDF5: A new approach to interoperability”, co-authored by myself, Prof Carlos, Prof Chiumenti, and Prof Cervera.
Status: The task was successfully finished, as a result of which material properties were input into Abaqus directly from HDF5 containers.



3. **Presentation:** To present the work done in **Metadata and Interoperability in Integrated Computational Materials Engineering (ICME) and Multiscale Materials Modelling (MMM)**, 2nd workshop held in Brussels.
Status: Presented the work done to the project leader of ICMEg as a part of the deliverables of CIMNE in the ICMEg project.
4. **Write and Publish a Paper:** A paper was written and submitted to the project committee, which is pending approval.

Results and Experience

The internship work was successfully finished by delivering all the requirements of the project. As the results of the project were quiet encouraging, I have been invited to Brussels to attend the project meeting in March'16 and also I have been invited as a speaker at the Second International Workshop on Software Solutions for Integrated Computational Materials Engineering.

During the internship, Prof. Carlos was very supportive in describing the problem, and helping me understand the bigger scenario of the project. He also carefully guided me and encouraged me at every step while I was trying to develop methodology. Encouraged by his in-depth knowledge of the subject and his incredible experience in the field I have decided to extend this internship into my master thesis under his guidance.

Submitted by,

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REFERENCES

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- [3] The HDF Group, <https://www.hdfgroup.org/HDF5/doc/index.html> (2016).