

HDF File-based interoperability for multiscale modelling

Fabio Sacconi and Stefano Bellocchio

Tiberlab srl, Rome, Italy

e-mail: fabio.sacconi@tiberlab.com, web page: <http://www.tiberlab.com>

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ABSTRACT

We present the possible choice of the Hierarchical Data Format (HDF5) for implementation of interoperability in multiscale and multiphysics modelling. HDF5 has many important characteristics for scientific data storage. It offers platform-independent binary data storage with optional compression and hierarchical data ordering. Data are stored with alphanumeric tags, so that one can examine a HDF5 file's contents with no knowledge of how the file writing program was coded. Abstractly, an HDF5 file is a container for an organized collection of objects. The objects are groups, datasets, and other objects in a hierarchical structure. The objects are organized as a rooted, directed graph. We can say that HDF file format provides several features which can make it a good choice as a common data format for interchange of material data through different simulation tools, such as:

- Platform-independent binary data storage with optional compression
- Hierarchical data ordering
- Self-describing tags
- Support for complex data relationships and dependencies through Datasets (multidimensional arrays) and Groups (container structures)
- Direct access to parts of the file without first parsing the entire contents
- Efficient support for a parameter database
- Possible embedding of post processing of output results, data plots, etc.

We will show how an open source Common Data Format (CDF) based on HDF5 standard has been defined and implemented to allow the exchange of data of different kind and the coupling of numerical simulations in the framework of the OS software environment developed in the FP7 Project DEEPEN. The aim of this project is to develop an integrated multiscale simulation capability for predictive design of novel materials and nanostructures, such as LEDs based on InGaN/GaN nanowires and InGaN/(Al)GaN quantum wells, as well as nano-scale electronic devices including new channel materials for sub-10 nmCMOS.

REFERENCES

- [1] www.hdfgroup.org/HDF5
- [2] <http://www.nmp-deepen.eu>