Open Source Software to Visualize Complex Data on Remote CEA's Supercomputing Facilities

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Abstract

In order to guaranty performances of complex systems using numerical simulation, CEA is performing advanced data analysis and scientific visualization with open source software using High Performance Computing (HPC) capability. The diversity of the physics to study produces results of growing complexity in terms of large-scale, high dimensional and multivariate data. Moreover, the HPC approach introduces another layer of complexity by allowing computation amongst thousands of remote cores accessed from sites located hundreds of kilometers away from the computing facility.

This paper presents how CEA deploys and contributes to open source software to enable production class visualization tools in a high performance computing context. Among several open source projects used at CEA, this presentation will focus on Visit, VTK and Paraview.

In the first part we will address specific issues encountered when deploying VisIt and Paraview in a multi-site supercomputing facility for end-users. Several examples will be given on how such tools can be adapted to take advantage of a parallel setting to explore large multi-block dataset or perform remote visualization on material interface reconstructions of billions of cells. Then, the specific challenges faced to deliver Paraview's Catalyst capabilities to end-users will be discussed.

In the second part, we will describe how CEA contributes to open source visualization software and associated software development strategy by emphasizing on two recent development projects. The first is an integrated simulation workbench providing plugins for every step required to achieve numerical simulation independently on a local or a remote computer. Embedded in an Eclipse RCP environment, VTK views allow the users to perform data input using interaction or mesh preview before running the simulation code. Contributions to VTK have been made in order to smoothly integrate these technologies. The second details how recent developments at CEA have helped to visualize and to analyze results from ExaStamp, a parallel molecular dynamics simulation code dealing with molecular systems ranging from a few millions up to a billion atoms. These developments include a GPU intensive rendering method specialized for atoms and specific parallel algorithms to process molecular data sets.