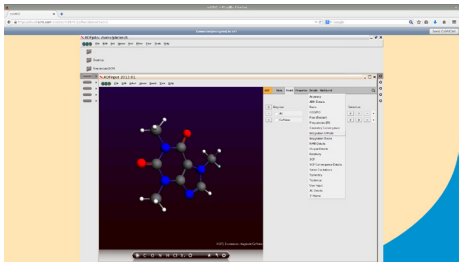
Fortissimo Case Study

FORTISSIMO

HPC-Cloud-based molecular modelling

Fortissimo Experiment Facts:
- Segment: Chemical Engineering
- Application Domain: Molecular Simulation
- Application: ReaxFF



The Company

The Albemarle Corporation is a globally leading developer, manufacturer, and distributor of highly engineered speciality chemicals for a wide range of sectors, including petroleum refining, automotive, transportation, pharmaceuticals and food safety. It serves customers in approximately 100 countries. Molecular modelling is a proven powerful tool, providing key information for the design of new chemicals and materials. The software for modelling large-scale molecular systems has applications in sectors such as electronics, organic chemistry, food, paints, dyes, adhesives and alloys and ceramics for the aerospace industry. Albemarle already uses HPC in the development of its products. However, it wants to improve its capability in this area through the use of CPU-GPU hybrid HPC platforms which offer significant benefits in terms of price-performance and power-performance, but to take advantage of this, the simulation codes used need some reprogramming.

The Challenge

The challenge is to port an existing simulation code so that it will run on a hybrid HPC platform. To demonstrate the successful porting and the benefits of using a hybrid HPC system a test case was chosen from the petroleum refining sector which involved the use of catalysts in the removal of sulphur from vehicle fuels.

The Solution

The solution involved not only the porting of the simulation code for the target computer system, but also the development of a simple user interface to prepare the models and their submission to the HPC system.

Fortissimo Experiment Partners:
- Albemarle (End-user)
- Scientific Computing and Modelling (ISV)
- SURFsara (HPC Expert and Service Provider)

More Information:
www.fortissimo-project.eu
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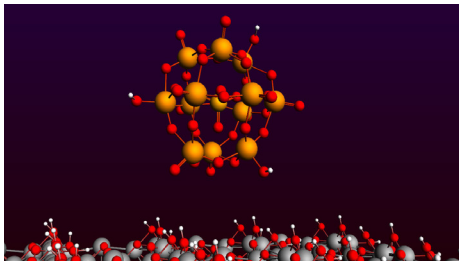

The Benefits

The case study demonstrated a successful port of a molecular modelling package to a hybrid HPC system with resultant cost benefits. The case study also demonstrated that the annual costs for the use of a Cloud-based HPC system on a pay-per-use basis was approximately half that of owning and maintaining a sufficiently powerful in-house system, representing a yearly saving of €38,000. As a result of this case study, Albemarle has allocated a significant budget for Cloud-based HPC computing for its next business year.

The Fortissimo Project

Fortissimo is a collaborative project that enables European SMEs to be more competitive globally through the use of simulation services running on a High Performance Computing cloud infrastructure. The project is coordinated by the University of Edinburgh and involves 123 partners including Manufacturing Companies, Application Developers, Domain Experts, IT Solution Providers and HPC Cloud Service Providers from 14 countries. These partners are engaged in 53 experiments (case studies) where business relevant simulations of industrial processes are implemented and evaluated. The project is funded by the European Commission within the 7th Framework Programme and is part of the I4MS Initiative.

I4MS Fortissimo is part of I4MS ICT Innovation for Manufacturing SMEs: www.i4ms.eu

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