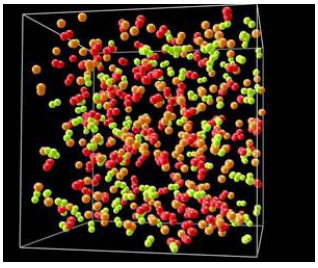
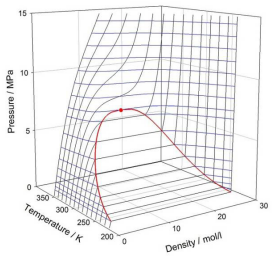
Fortissimo Case Study

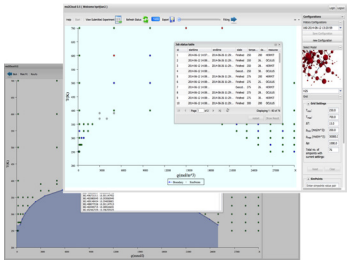
FORTISSIMO

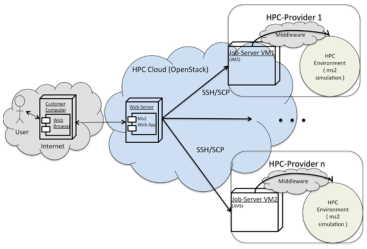
HPC-Cloud-based simulation of hazardous chemicals

Fortissimo Experiment Facts:
- Segment: Chemical Engineering
- Application Domain: Molecular Simulation
- Application: ms2









The Company

Founded in 1897 in Switzerland, Lonza is one of the world's leading and most trusted suppliers to the Pharma&Biotech and Specialty Ingredients markets. Lonza's products and services range from active pharmaceutical ingredients and stem-cell therapies to drinking water sanitizers, from industrial preservatives to microbial control solutions that combat dangerous viruses, bacteria and other pathogens, from the manufacture of vitamin B compounds and organic personal care ingredients to agricultural services and products. In particular, Lonza utilizes distillation columns, whose operation requires a detailed knowledge of the thermodynamic properties of the target compounds.

Nowadays, powerful predictive methods, using computer-based simulations, exist that calculate the thermophysical properties of compounds. These can form the basis for the design and optimization of chemical engineering processes. Nevertheless, the chemical industry typically measures the required data experimentally. However, if they are needed for hazardous substances (explosive, toxic or mutagenic), the associated costs of physical testing may be prohibitive. In such cases, computer-based simulations are a very attractive alternative. To carry out such simulations, a large number of model runs are necessary requiring a very powerful computer. Previously, Lonza had determined the physical properties of compounds experimentally. The objective of this case study was to evaluate the use of HPC-based simulation in the determination of such physical properties.

The Challenge

The challenge of this case study was to take an existing third-party code for the determination of the physical properties of compounds, port it to an HPC-system and to demonstrate the accuracy and cost-effectiveness of such an approach. An accurate calculation of thermodynamic properties at a given state point currently requires around 20 hours on a computer with 16 processing cores. In order to acquire enough data to determine the full set of physical properties, around 200 state points need to be evaluated. This means that even with exclusive access to small compute cluster, the calculation would take up to 4000 hours (close to six months). Access to an HPC system through a Cloud-based approach would therefore be very attractive because it would enable simulations to be made in a reasonable length of time.

The expertise and experience of Lonza, an HPC-Centre and the code owner were combined to tackle this challenge.

The Solution

A detailed molecular-simulation code has been implemented on an HPC system driven by a simple, web-based user interface. Multiple simulations of state points can be initiated through this interface enabling the complete thermodynamic properties of a compound to be determined in a reasonable length of time. For example, whilst the calculation of a complete set of physical properties would take ~6 months on a 16-core cluster, the calculation time can be reduced to below 20 hours on an HPC system.

Fortissimo Experiment Partners:
- Lonza (End-user and Code Owner)
- University of Paderborn (Domain Expert)
- University of Stuttgart (HPC Centre and HPC Expert)

More Information:
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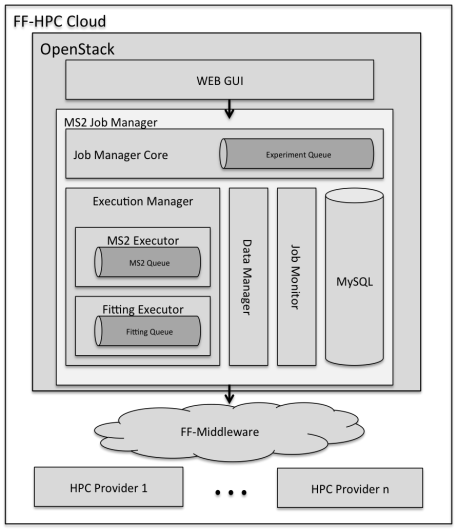

The Benefits

Lonza is a company which manufactures various chemical intermediates requiring detailed knowledge of the thermodynamic properties of target compunds, starting materials and side products. The use of simulation can bring massive savings to Lonza's production process. There are clearly benefits to the design process in being able to determine the complete thermodynamic properties of a compound in a much shorter time. It is also clear that the cost of cycles is much less than that of owning and maintaining a large HPC system in-house

Experimentally determined pure component densities cost around 2,700 € per substance for a very limited temperature and pressure range, when bought from an external supplier. Compared to that, 60 molecular simulations carried out in the entire fluid region up to arbitrary high pressures will cost around €1,600 yielding not just the density but every static thermodynamic property simultaneously.

For mixtures of compounds, the difference in costs is more extreme. 60 experimentally measured gas solubility data points of a binary mixture can cost up to €50,000, while the cost for the molecular simulation usually increases by a factor of two compared to a pure component to €3,200. It should be noted that the prices for the experimental data gathered by physical measurements only apply to moderate conditions and non-hazardous substances. Such measurements at high temperatures or pressures can be much more expensive or even impossible to conduct.

For the design of a distillation column costing €1.5 million, the following cost calculation can be made: A given system requiring €100,000 to obtain all required physical properties through experimental measurements (corresponding to 100 staff days at €1,000), would be expected to be developed by calculating the same physical properties by rigorous modelling, which would cost only approximately €13,600. This value was estimated according to a physical case study (computer cycles €6,400, 4 staff days at €550 and 5 staff days at €1,000). The overall saving in the design process would add up to approximately €86,400. Clearly HPC-based simulation has considerable benefits for Lonza. It should be noted that Lonza usually designs more than 5 distillation processes per 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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