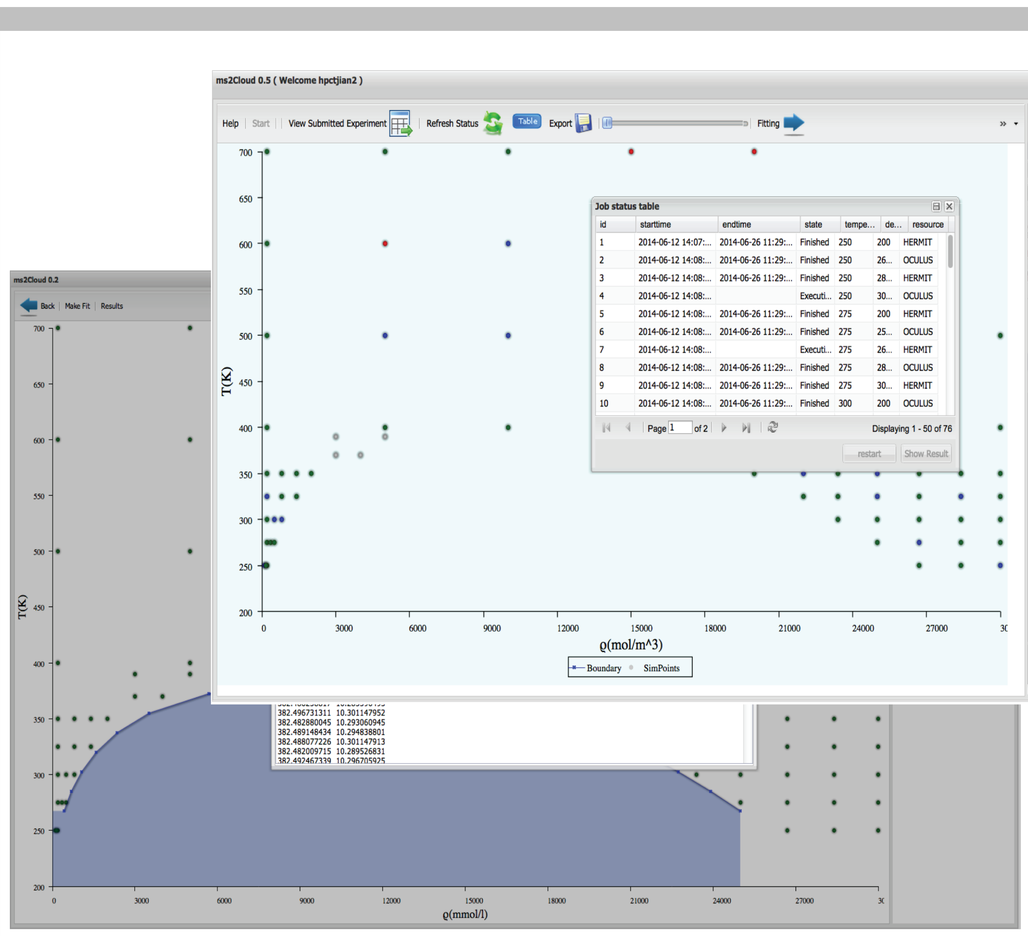
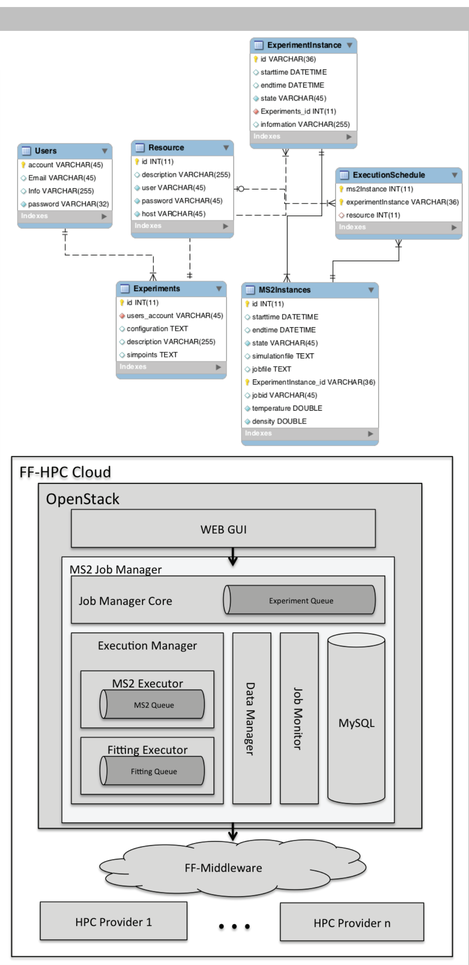
HPC-Cloud-based simulation of hazardous chemicals

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. Access to an HPC system through a Cloud-based approach would **enable simulations to be made in a reasonable length of time**.





Organisations Involved

End User:

Lonza

Domain Expert:

UNIVERSITÄT PADERBORN
Die Universität der Informationsgesellschaft

HPC Centre and HPC Expert:

HLRS

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**.

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, the cost of cycles is much less than that of owning and maintaining a large HPC system in-house.
- 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.

FORTISSIMO

European Commission

The Fortissimo project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No 609029. The Fortissimo 2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 680481.

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SEVENTH FRAMEWORK PROGRAMME