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The MoSGrid - e-science gateway: molecular simulations in a distributed computing environment

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Modern tools for computational chemistry allow the calculation of a wide range of properties of all sorts of molecules applying various levels of theory. But to perform convincing and significant calculations with these tools not only requires insight into the scientific theory itself, but also knowledge and experience on how to operate the simulation tools.

In addition to the general challenge of gaining access to a powerful computing environment, very often a high level of technical competence is necessary to set up and run calculations efficiently. These prerequisites often hamper scientists to routinely use computational tools to support or confirm their perceptions.

To overcome some of these problems, the MoSGrid consortium develops an open source e-science portal for grid based environments with respect to computational chemistry. At present residing in the German Grid Initiative (D-Grid), MoSGrid enables users to set up, run and evaluate calculations using tools from the domains of Quantum Chemistry, Molecular Dynamics and Docking [1].

This talk underlines the basic motivation, layout, development, properties and available tools of MoSGrid as well as the procedure of gaining access to the grid environment.

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