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Running ECCE on EGEE clusters

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The Extensible Computational Chemistry Environment (ECCE) is a package of programs developed at the Pacific Northwest National Laboratory (PNNL). It consists of a graphical user interface for building molecular systems and submitting jobs to remote computational resources, as well as the storing and managing of the results in a database. In this presentation the main features of ECCE are discussed and recent developments for adapting it for use on grid resources are presented.

Primary author: Dr VAHTRAS, Olav

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