Gaussian Hands-On

Welcome to this *Hands-on Gaussian!*

The objective is to learn some SLURM basic commands and be able to execute Gaussian jobs through the scheduling system.

It's divided in 4 independent exercises, ordered by difficulty. Each of them is based on different scientific papers that involves Gaussian calculations.

The solutions for every exercise are located in the final page.

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Gaussian is a general purpose computational chemistry software which implementing a variety of computational chemistry methods. It was initially released by by John Pople and his research group at Carn egie Mellon University in 1970.

The range of computational methods includes molecular mechanics, semi-empirical methods, Hartree-Fock SCF, Møller-Plesset perturbation theory, DFT methods, QM/MM calculations, CI methods and CC calculations. Calculations employing these methods can be carried out in order to optimise molecular geometry, electronic structure and derived chemical properties.

For more information about Gaussian, check our ***Gaussian page***.

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SLURM is a free and open-source job scheduler for Linux, used by many of the world's supercomputers and large and small computer clusters.

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