Creation of an integrated molecular dynamics workflow on the Galaxy platform : Characterization of aquaporin pores

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Creation of an integrated molecular dynamics workflow on the *Galaxy* platform : measure of aquaporin pores

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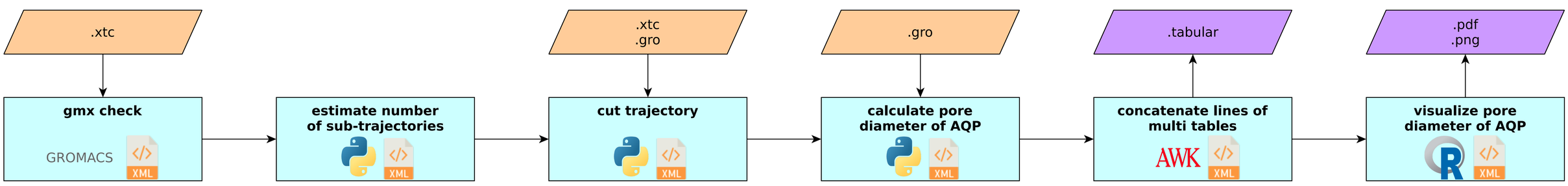
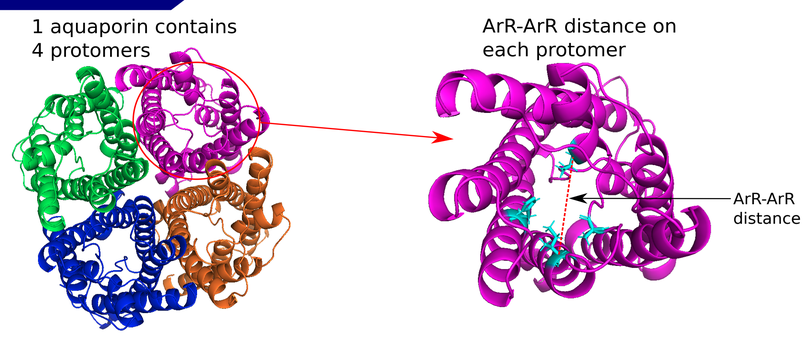
With global warming, it is vital to understand how **water** flows within plants. **Aquaporins** (AQP) are major actors in water transport and the study of the pore of these aquaporins is key to water transport across **membrane**. It is therefore necessary to characterize this **pore** and more precisely to measure the diameter in order to estimate the water flow. This is why a **Galaxy** workflow has been created to measure and visualize this **diameter** over time. The positioning information of the atoms over time is obtained by **molecular dynamics** and is available in a file called trajectory.

Galaxy workflow

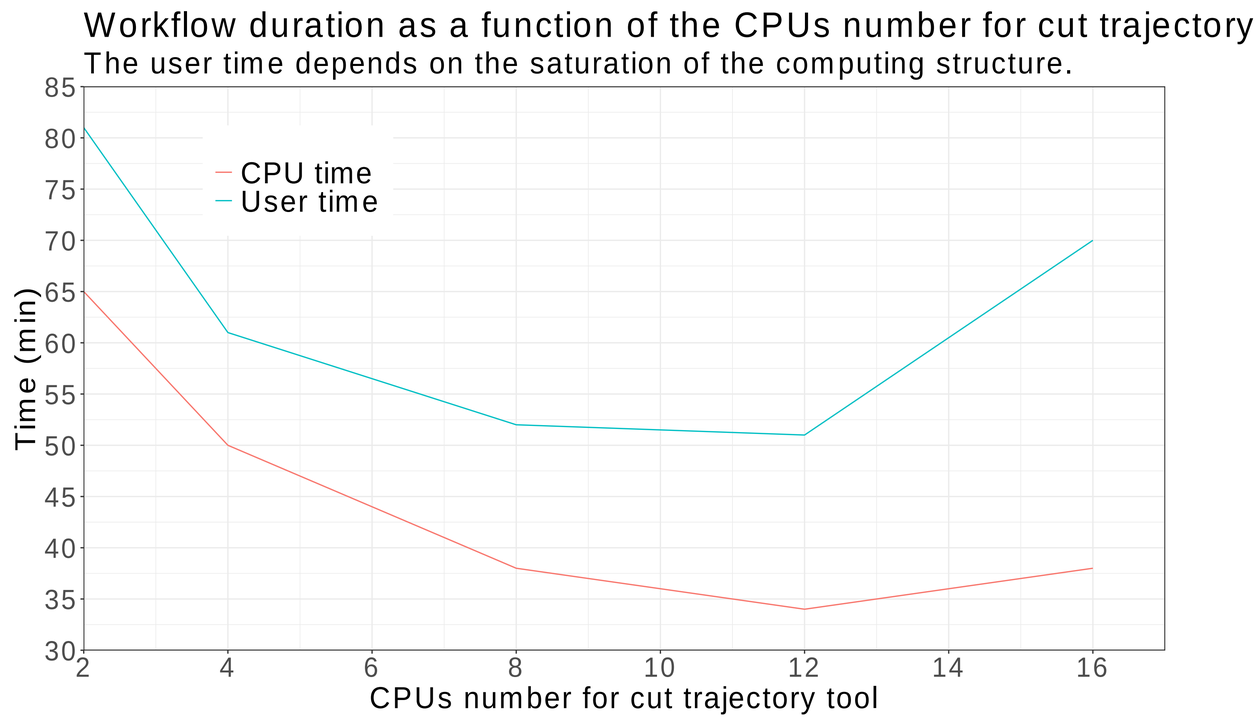


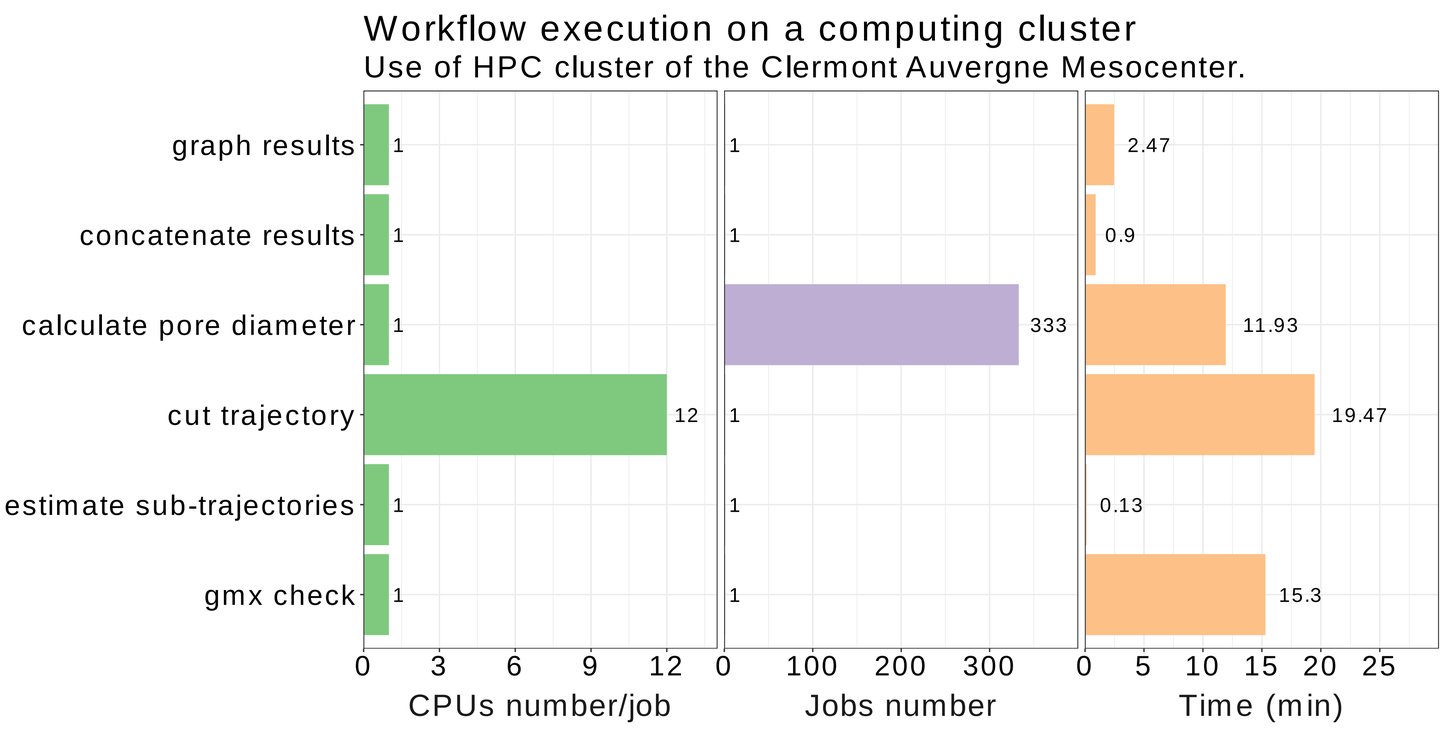
.xtc : trajectory from GROMACS ; .gro : structure from GROMACS (Abraham *et al*. 2015, 10.1016/j.softx.2015.06.001)

Aquaporins



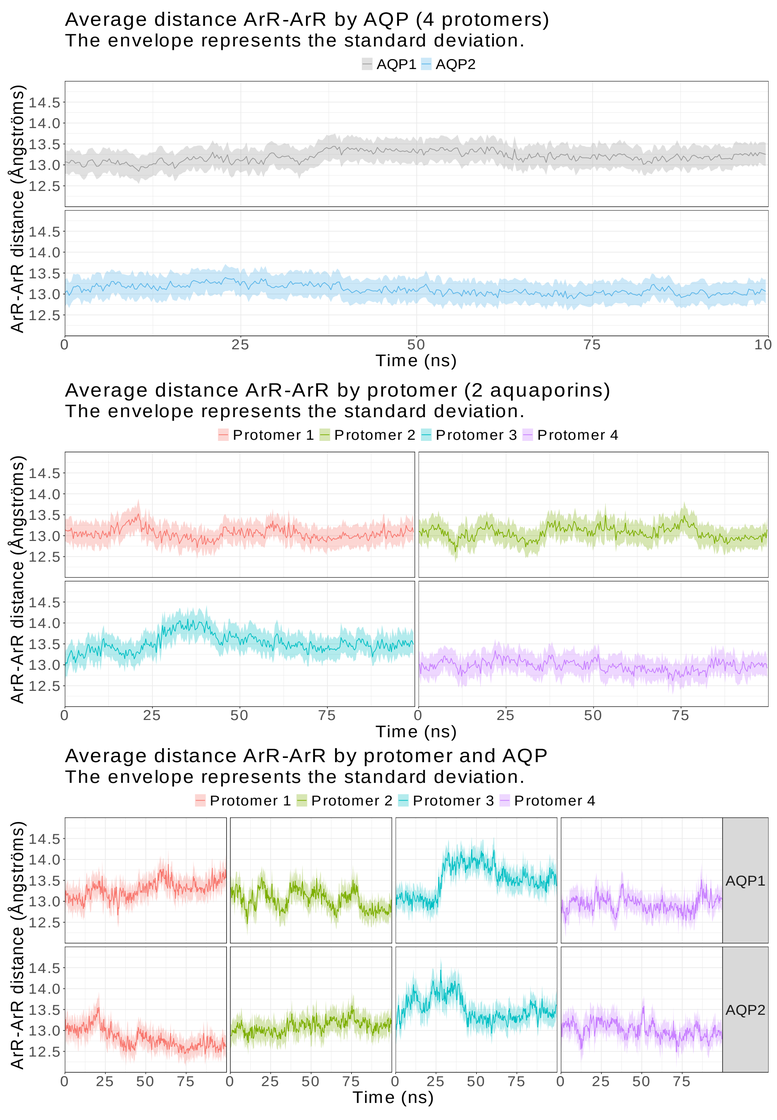
Benchmark





Results

This .gro structure contains 2 complete poplar AQPs sequenced from Tonoplast Intrinsic Protein TIP1.7



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