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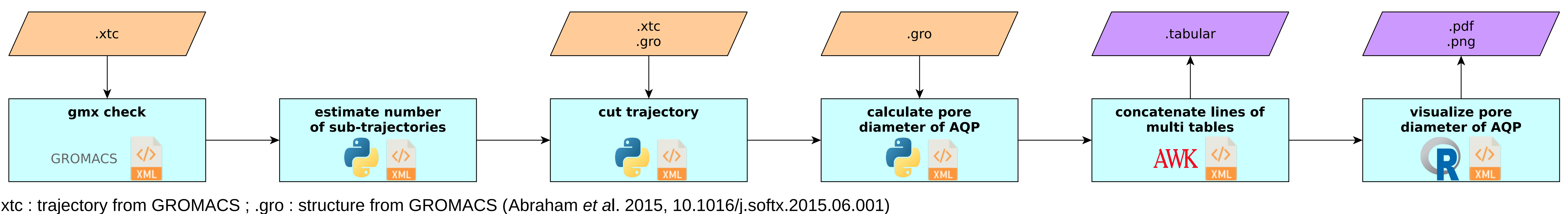
Creation of an integrated molecular dynamics workflow on the *Galaxy* platform : measure of aquaporin pores

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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.

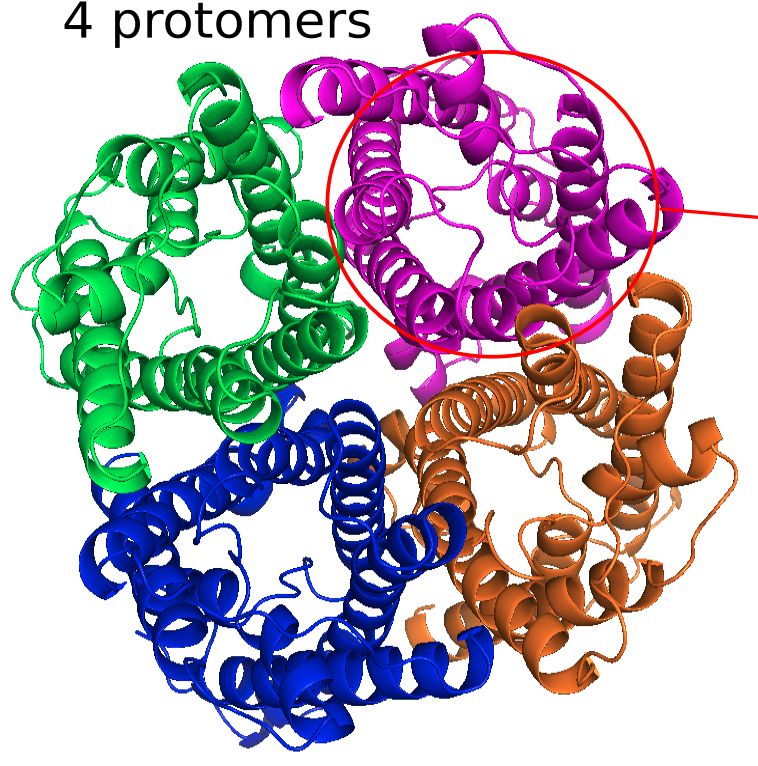
Galaxy workflow



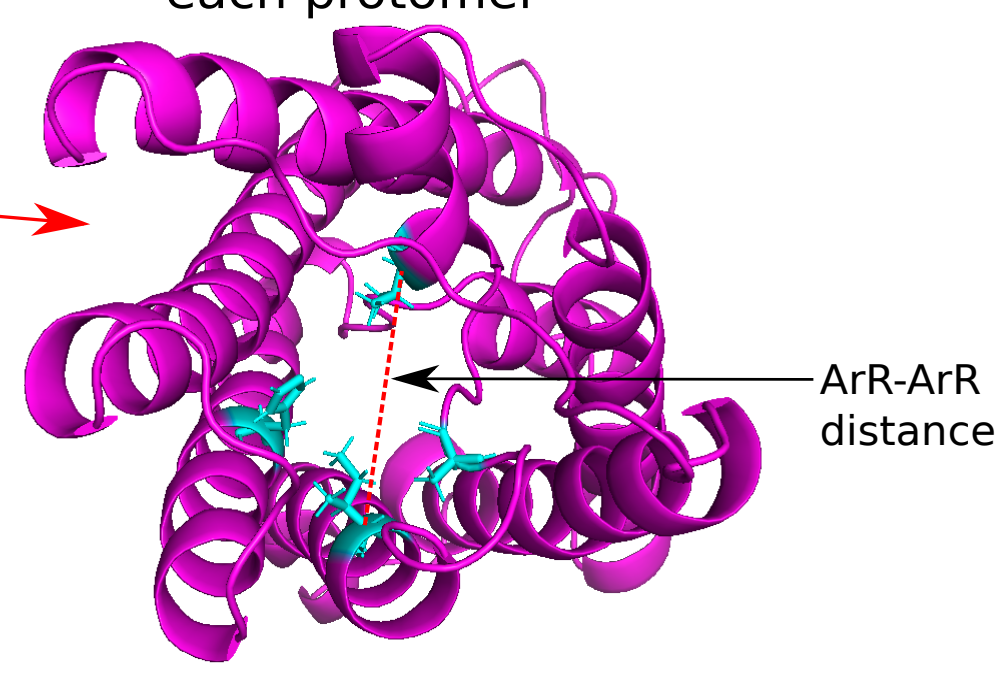
.xtc : trajectory from GROMACS ; .gro : structure from GROMACS (Abraham et al. 2015, 10.1016/j.softx.2015.06.001)

Aquaporins

1 aquaporin contains
4 protomers

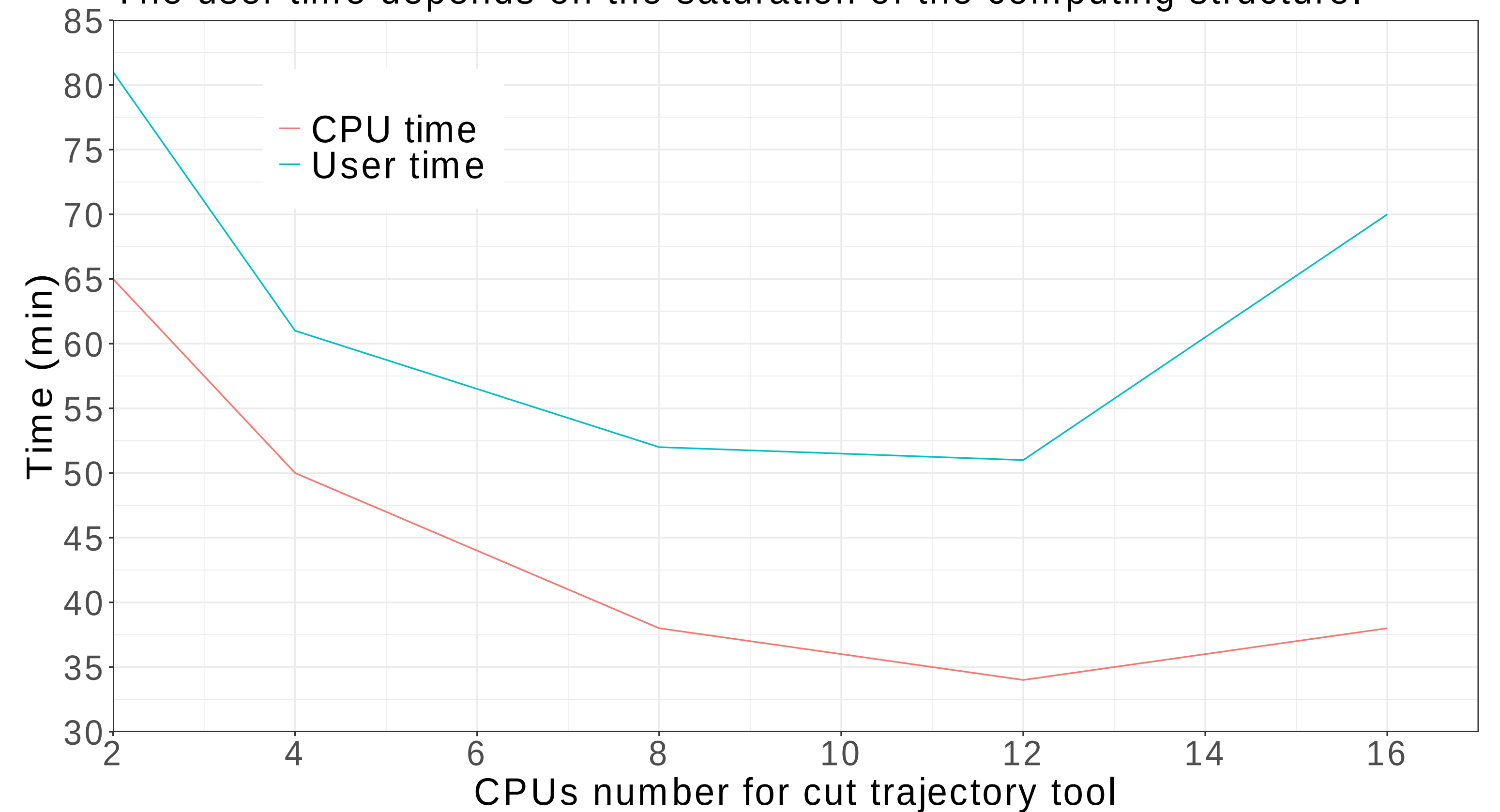


ArR-ArR distance on
each protomer



Benchmark

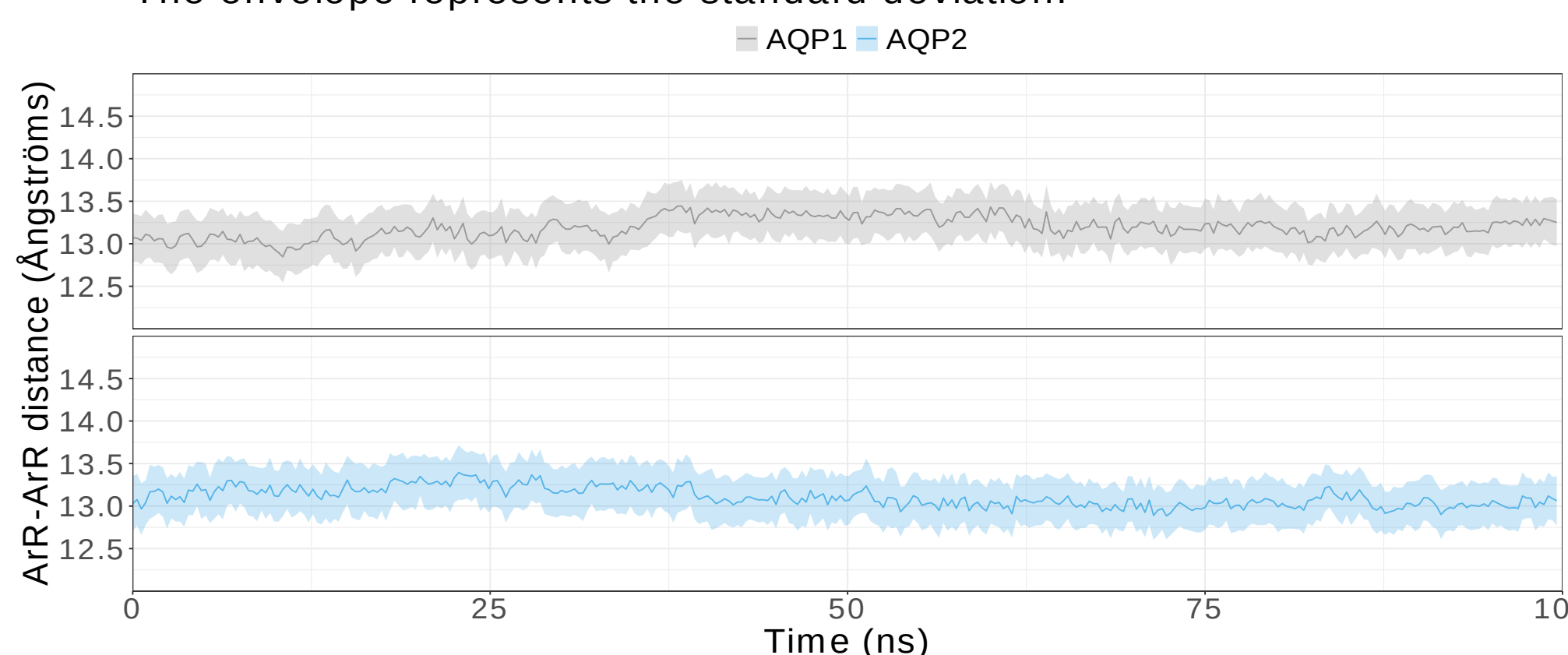
Workflow duration as a function of the CPUs number for cut trajectory
The user time depends on the saturation of the computing structure.



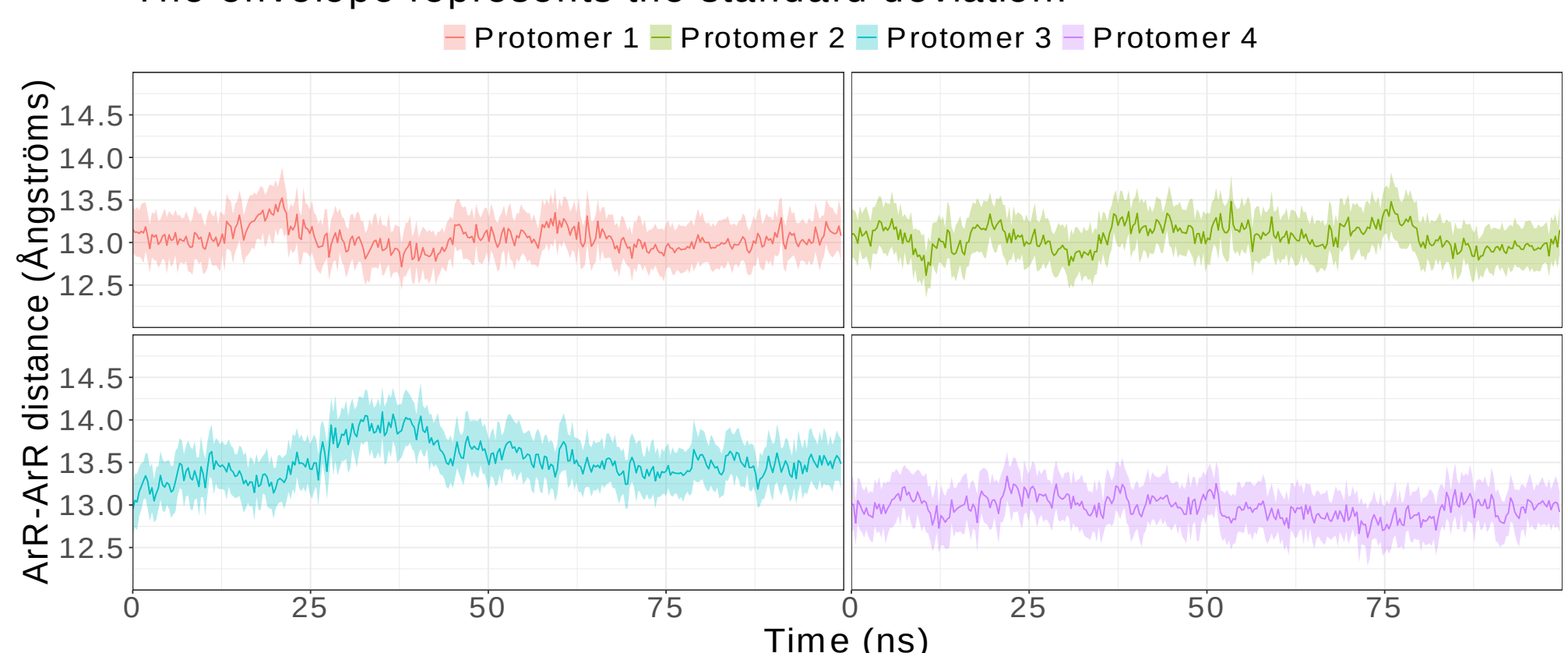
Results

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

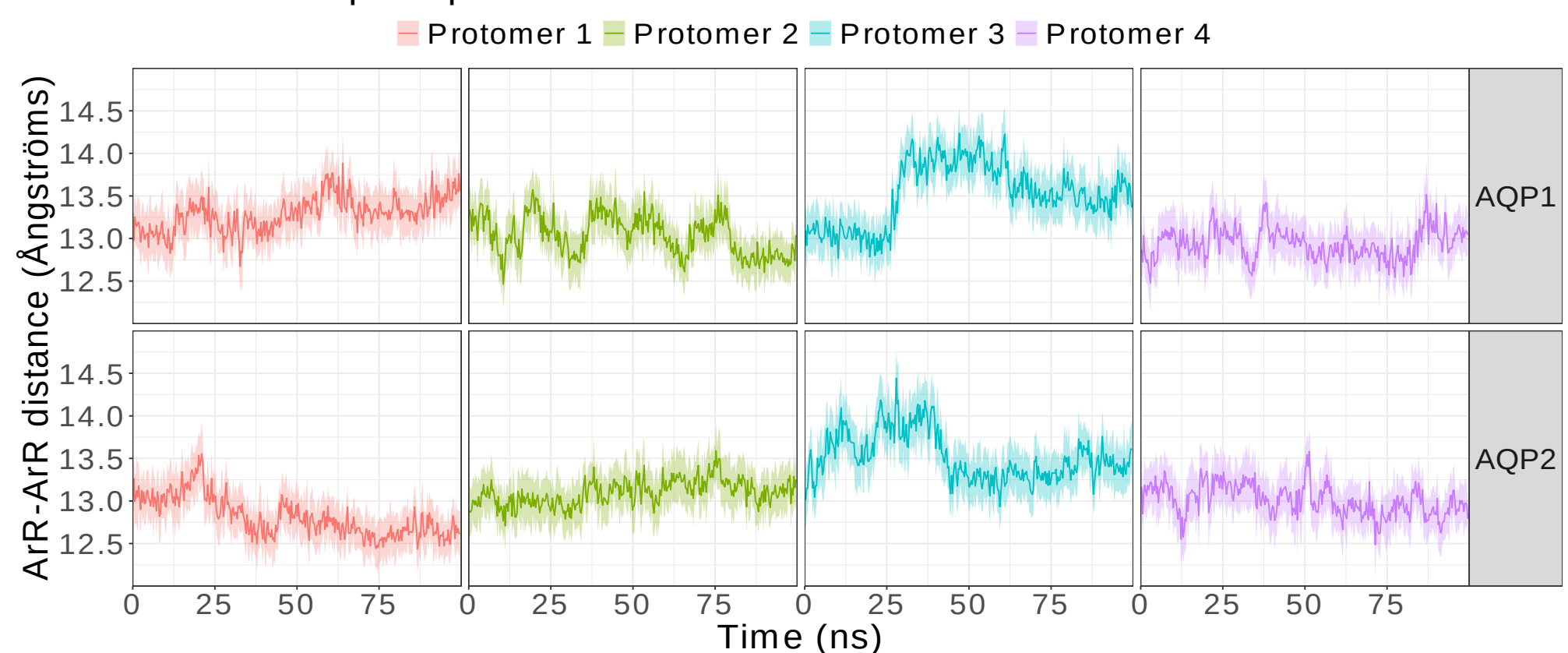
Average distance ArR-ArR by AQP (4 protomers)
The envelope represents the standard deviation.



Average distance ArR-ArR by protomer (2 aquaporins)
The envelope represents the standard deviation.

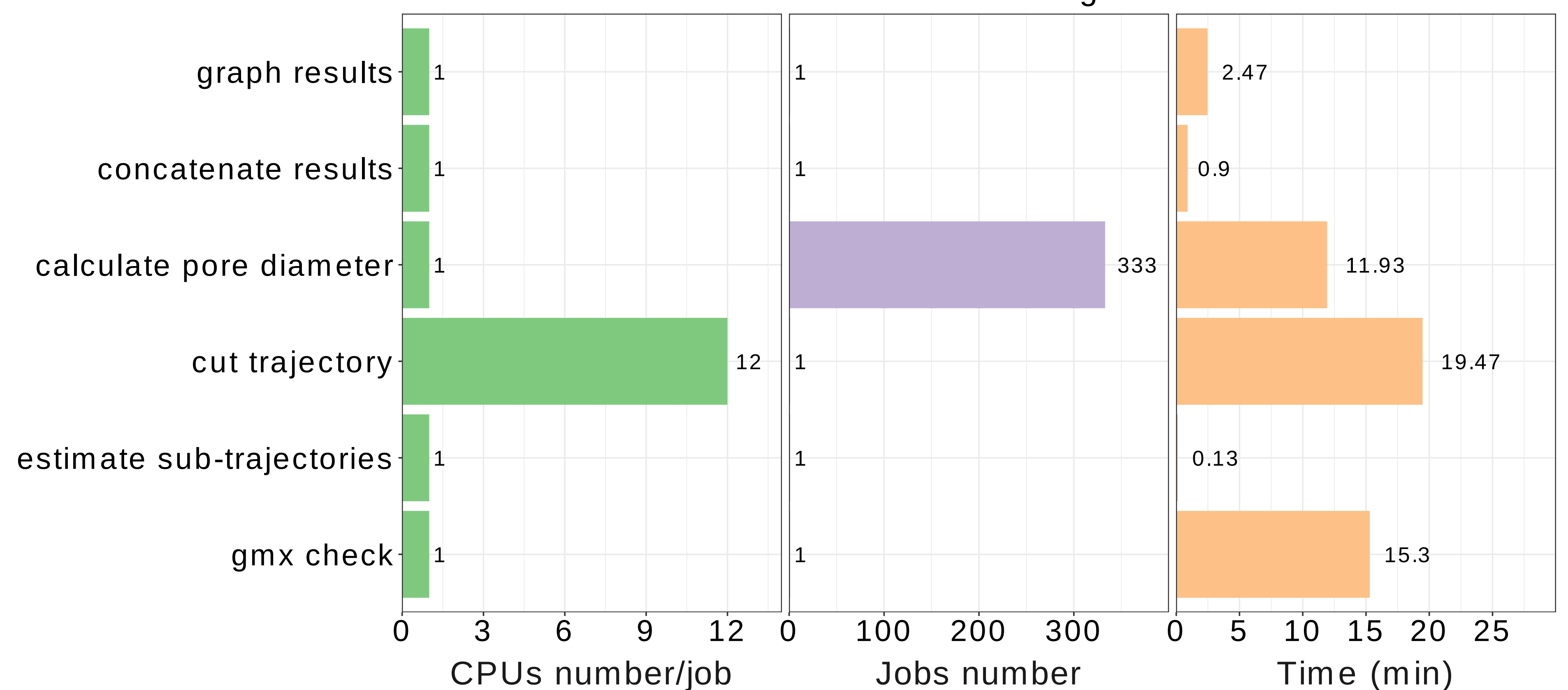


Average distance ArR-ArR by protomer and AQP
The envelope represents the standard deviation.



Workflow execution on a computing cluster

Use of HPC cluster of the Clermont Auvergne Mesocenter.



Acknowledgements

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