



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

Agnès-Elisabeth Petit, Jean-Stéphane Venisse, Philippe Label, Nadia Goué

► To cite this version:

Agnès-Elisabeth Petit, Jean-Stéphane Venisse, Philippe Label, Nadia Goué. Creation of an integrated molecular dynamics workflow on the Galaxy platform: Characterization of aquaporin pores. JOBIM, Jul 2022, Rennes, France. . hal-03716631

HAL Id: hal-03716631

<https://uca.hal.science/hal-03716631>

Submitted on 7 Jul 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

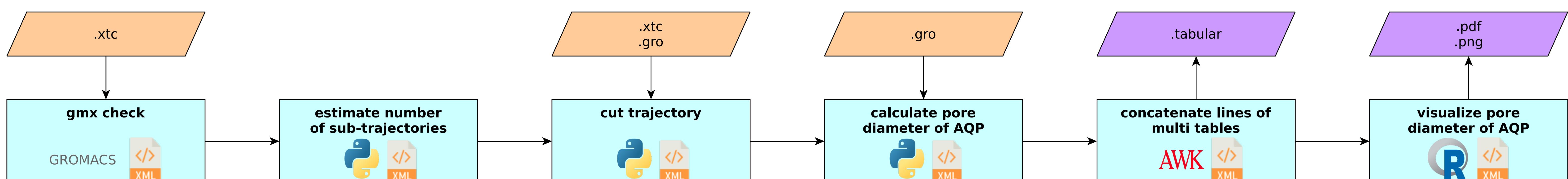
Agnès-Elisabeth PETIT¹, Jean-Stéphane VENISSE², Philippe LABEL² and Nadia GOUÉ^{1*}

¹ AuBi Platform, Clermont Auvergne Mesocenter, UCA, 7 avenue Blaise Pascal, 63 178 Aubière, France. ² UMR PIAF, Université Clermont Auvergne, INRAE, PIAF, 63000 Clermont-Ferrand, France

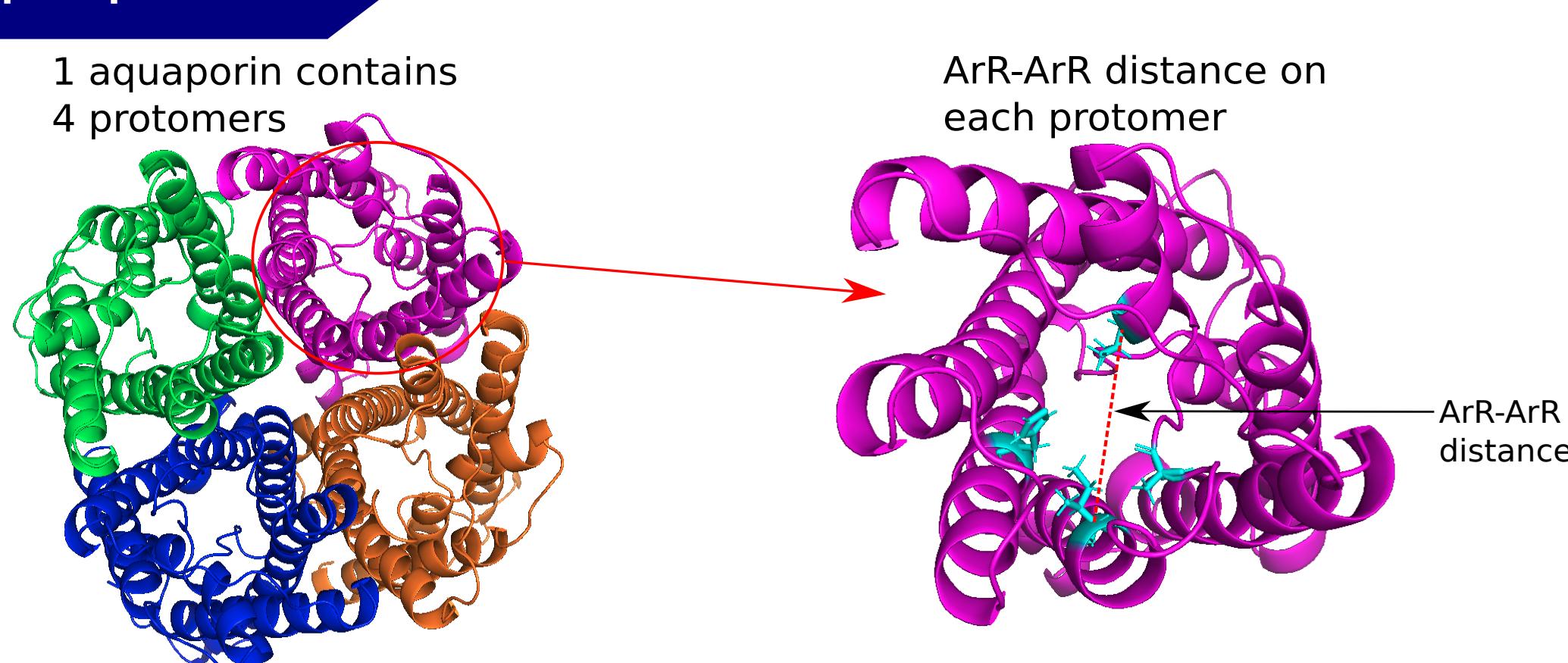
* corresponding author : nadia.goue@uca.fr

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

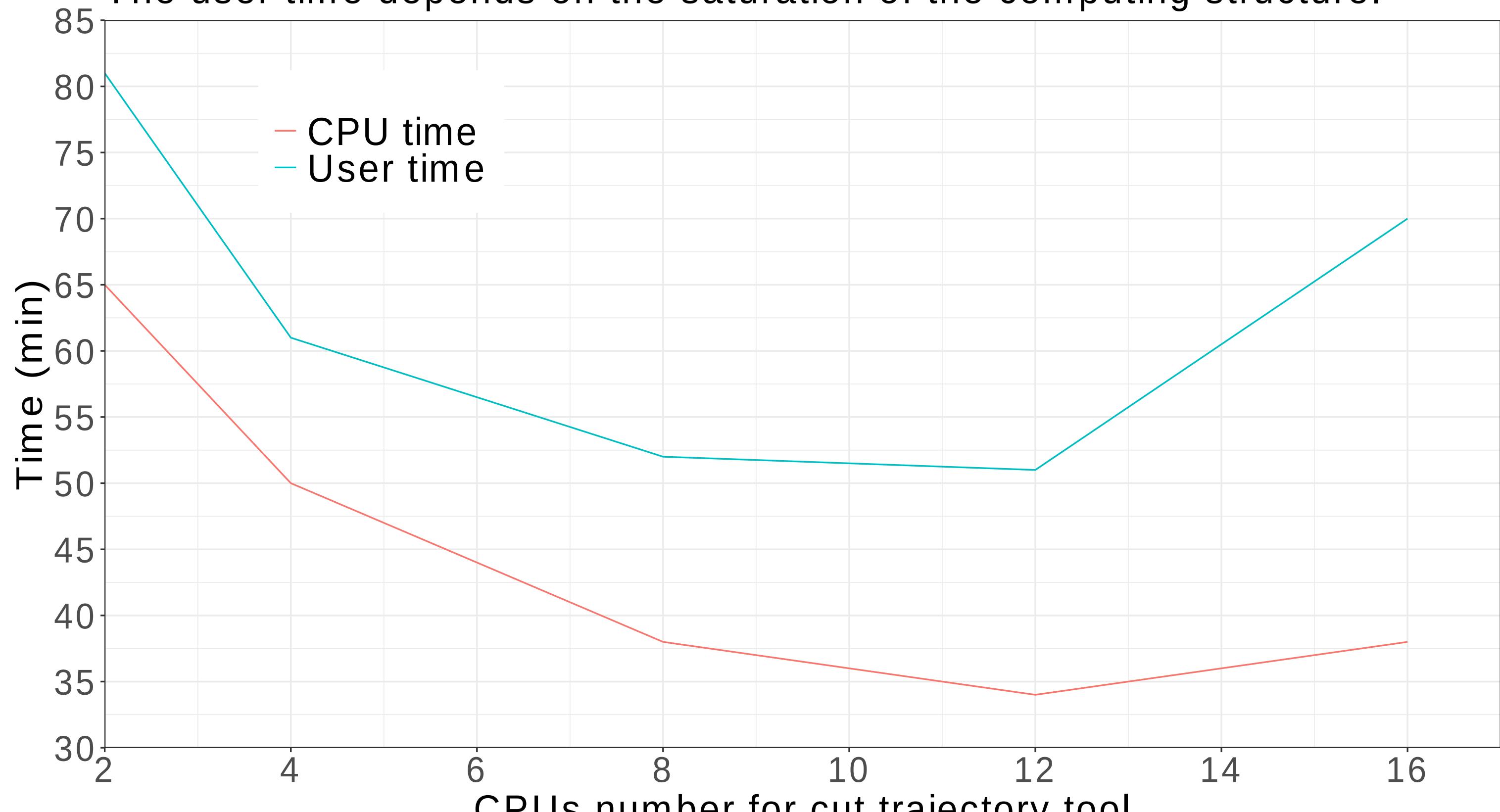


Aquaporins



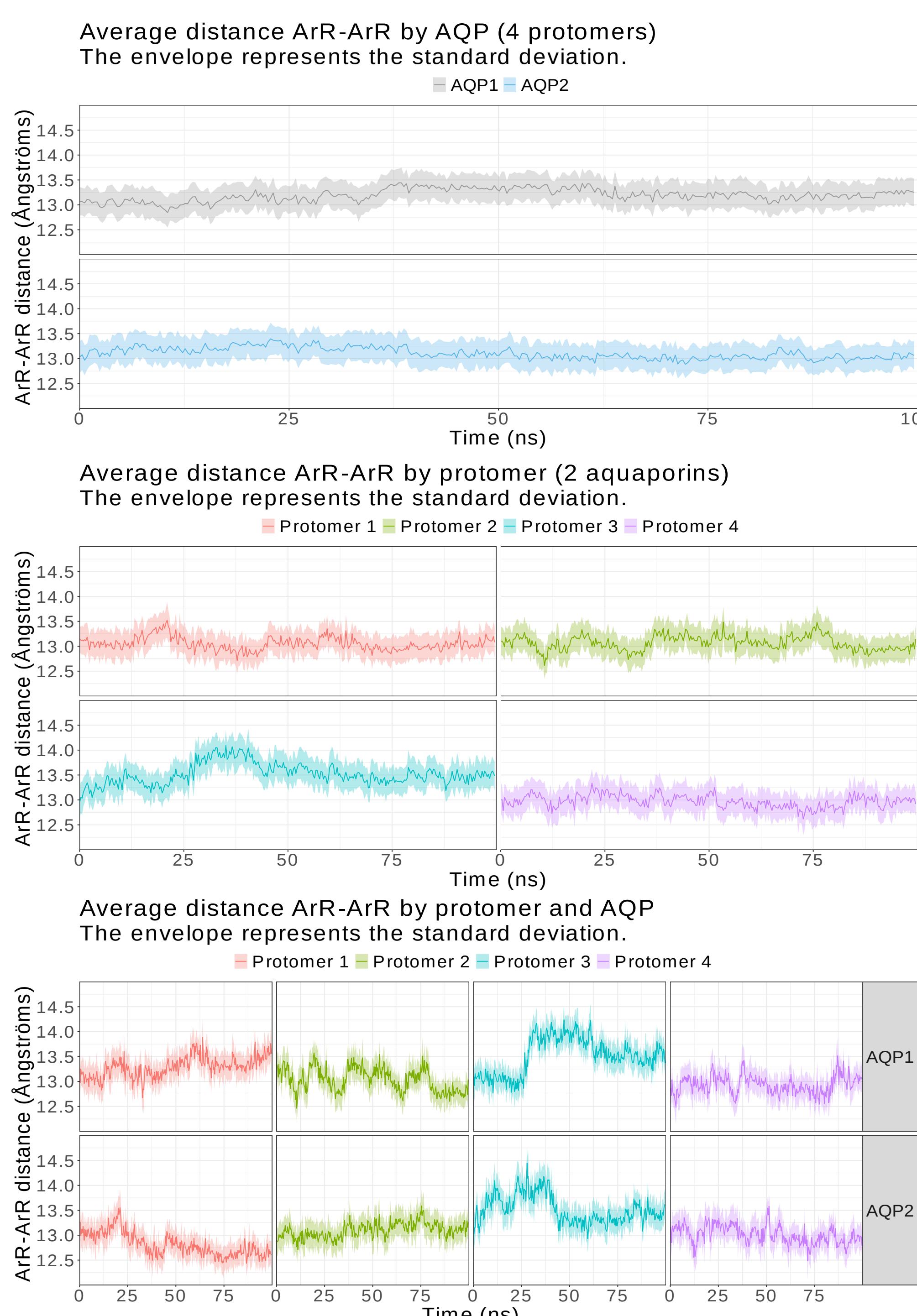
Benchmark

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



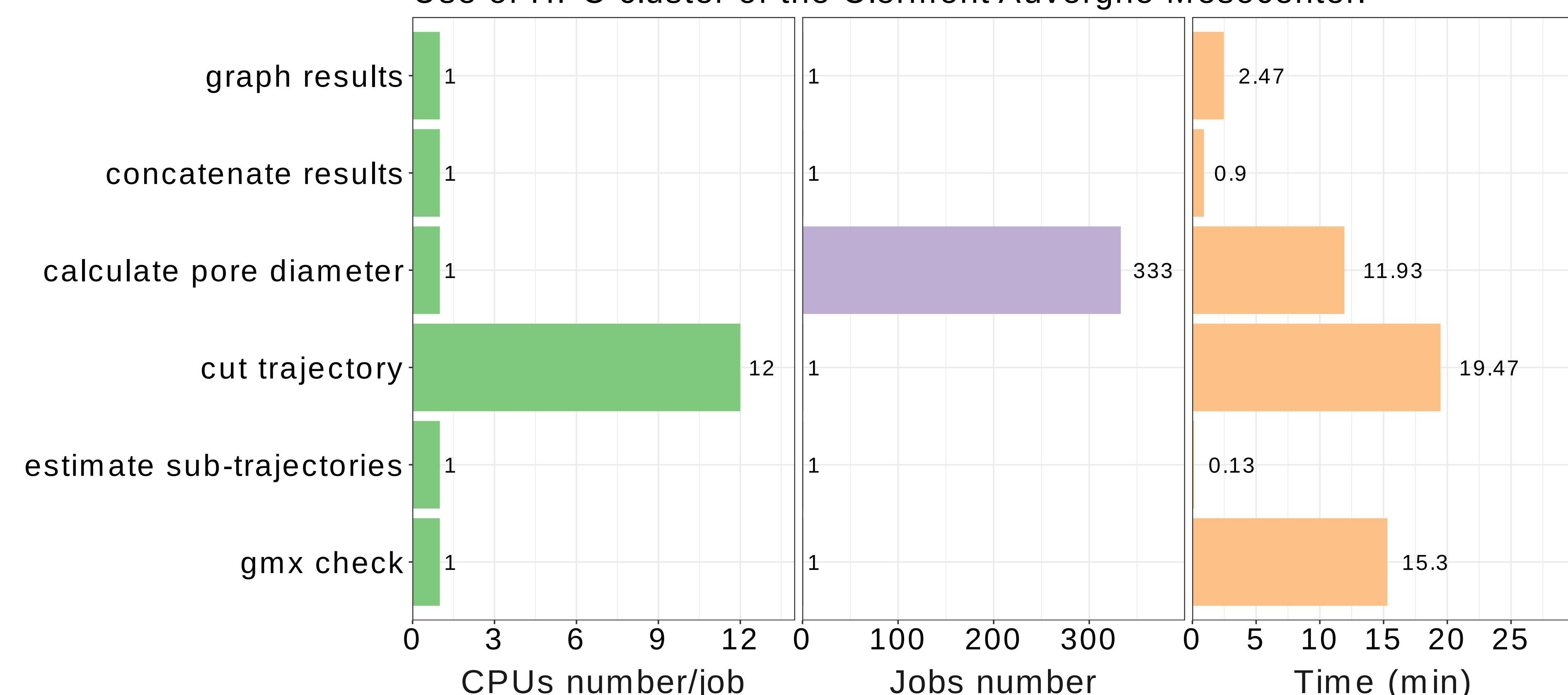
Results

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



Workflow execution on a computing cluster

Use of HPC cluster of the Clermont Auvergne Mesocenter.



Acknowledgements

This work was supported by a travel grant from the Société Française de Bioinformatique. This internship was supported by a grant from DOSI, Clermont Auvergne University. Trajectory calculations were performed on IDRIS HPC cluster under the GENCI allocation 2019-A0060710751. I-SITE CAP 20-25 (ANR grant 16-IDEX-0001) Emergence 2017 from the Clermont Auvergne University. SCUSI 2019 (grant P010003) from the Clermont Auvergne University and the AURA Region.