

Supporting Information for:

A Sidekick for Membrane Simulations: Automated Ensemble Molecular Dynamics Simulations of Transmembrane Helices

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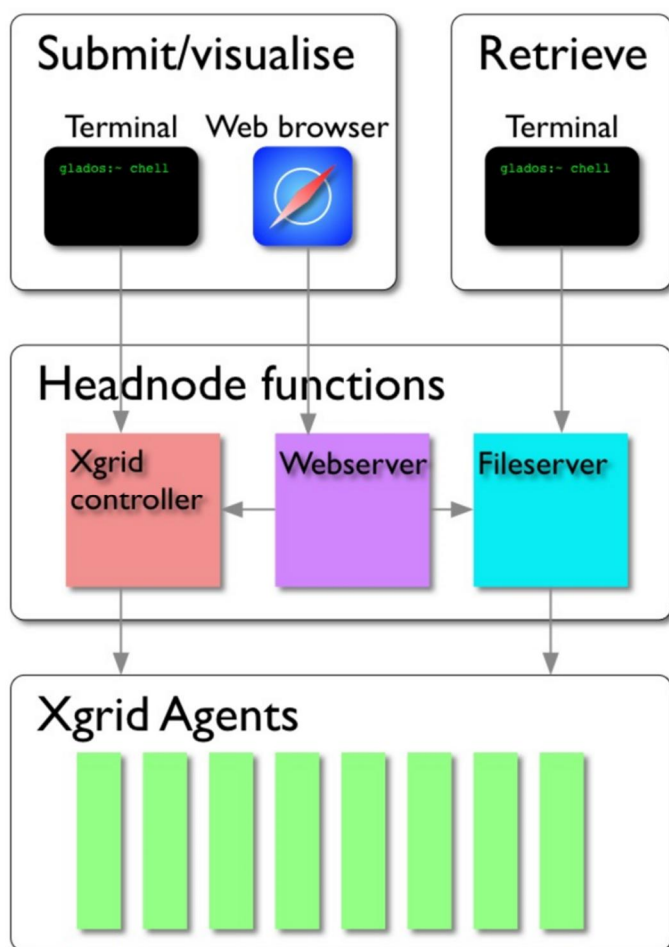


Figure S1: Description of the Sidekick hardware architecture. Users submit jobs either from the command line (direct to the Xgrid controller), or through the web browser (where the webserver communicates job information to the controller). Xgrid agents receive commands from the controller and files from a fileserver. Raw simulation data can be retrieved directly from the fileserver, or automatically visualised on the webserver.