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BRIDGE: Biomolecular Reaction & Interaction Dynamics Global Environment

biochemical processes make the discovery of drugs and biomaterials possible. A research framework common to genomics and proteomics is needed to conduct biomolecular simulations that will connect biological data to the dynamic molecular mechanisms of enzymes and proteins. Novice biomolecular modelers are faced with the daunting task of complex setups and a myriad of possible choices preventing their use of molecular simulations and their ability to conduct reliable and reproducible computations that can be shared with collaborators and verified for procedural accuracy.
We present the foundations of BRIDGE 1 developed on the Galaxy platform 2 that makes possible fundamental molecular dynamics and analysis of proteins through workflows and pipelines via commonly used packages such as NAMD, GROMACS, CHARMM and MDAnalysis. BRIDGE can be used to facilitate the set up and simulation of biological macromolecules, perform conformational analysis from trajectory data and conduct data analytics of large-scale protein motions using statistical rigor. All of these computational tasks can be connected using workflows, for repeatability and automation, and then distributed to run on cloud or HPC platforms. We illustrate the basic BRIDGE simulation and analytics capabilities on a previously reported CBH1 protein simulation.

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