OMMProtocol: A command line application to launch molecular dynamics simulations with OpenMM

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ABSTRACT

OpenMM is a free and GPU-accelerated Molecular Dynamics (MD) engine written as a layered and reusable library. This approach allows maximum flexibility to configure MD simulations and develop new molecular mechanics (MM) methods. However, this powerful versatility comes at a cost: the user is expected to write Python scripts to run a simulation. OMMProtocol aims to fill this gap by stitching OpenMM and additional third-party modules together, providing an easy way to create an input file to configure a full multi-stage simulation protocol, from minimization