HARLEM: Hamiltonians to Research LargE Molecules

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A molecular modeling package HARLEM is designed to help in solving complex structure-function relation problems arising in the modern biomedical research. The package provides interoperability among different types of molecular representation and flexible interface that allows for an efficient setup and design of the complex multi-model simulations; as well as visualization of computational results. HARLEM provides a convenient interface to several popular molecular modeling programs such as AMBER, GAUSSIAN, FIRST. HARLEM is an object oriented highly extensible package; it uses flexible xml-like file formats to store and transfer internal information and has a variety of molecular structure format converters. Some computational modules are parallelized. HARLEM is a cross-platform software and currently running under Windows and Linux operating systems. Windows executables of the program can be downloaded from the HARLEM web-site http://www.harlemprog.org; A detailed description of the program, and tutorials can also be found.

The demonstration session will include an introduction to the HARLEM architecture and an organization of its computation modules. The following aspects of HARLEM functionality will be highlighted:

- **Setup and interactive manipulation of molecular structure**

Geometry editing, fragment creation and overlap, different types of molecular visualization, residue mutations

- **Molecular Mechanics calculations**

Interactive editing of atomic parameters, setup and editing of molecular mechanics model, submission of molecular dynamics jobs, analysis of MD trajectories.

- **Quantum chemical calculations**

Setup of *ab initio* and semiempirical quantum chemical calculations, graphical analysis of molecular orbitals and electron density

- **Modeling long-range electron transfer reactions**

Donor and acceptor groups setup, reorganization energy calculations using continuum electrostatics approach, PATHWAYS analysis of donor/acceptor interactions, graphical display of best coupling pathways and atom coupling maps, semiempirical quantum chemical calculations of donor/acceptor interactions. Bimolecular ET reactions between cyt b_5 and myoglobin.

- **Calculations of ionic currents through biological channels**

Setup of PNP (Poisson-Nernst-Planck) calculations of ionic currents through a channel protein and the subsequent graphical analysis of the electrostatic potential and ion density inside the channel

- **Rigid-body Monte Carlo simulations**

An assembly of alpha- helicies of a membrane-bound protein using replica-exchange rigid body Monte Carlo simulations

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