Implementing Workflow for Biophysical Simulations in openDIEL

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Background

About BD simulation:

Brownian Dynamics simulations (BDS) are a method in computational biophysics used to study protein diffusion processes such as association mechanisms, measuring binding rates. The biomolecules are regarded as rigid bodies; for each molecule, the motion is computed based on precalculated intermolecular physical potentials.

Before running a BDS, PDB (protein structure) files are used to for the various molecular potential calculations. As rigid bodies, the potential components from each molecule do not change during simulation, so precalculation increases the simulation speed.

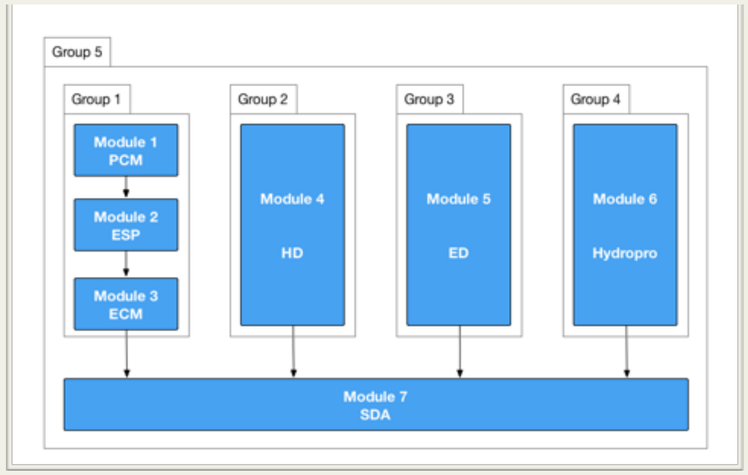

Fig. 1 shows the organizational structure for preliminary molecular structure computations and their downstream use in Brownian Dynamics Simulation (BDS).

About openDIEL:

The **openDIEL**(open Distributive Interoperable Executive Library) is workflow engine that aims to facilitate communication between loosely coupled simulations in large-scale parallel computing. openDIEL is developed by UT CFD LAB.

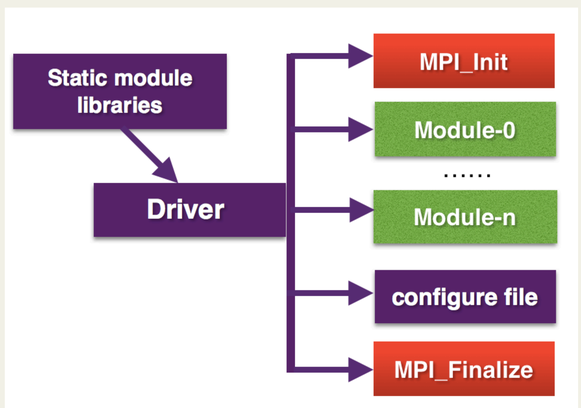

Fig.2, simple mechanism of openDIEL

Abstract/Objectives

The primary goal of this project is to use openDIEL to optimize the workflow leading to BDS.

- First stage: Integrate with BDS toolkit from Mr. John Ossyra
- Second stage: build GUI with which users can configure and run BDS in openDIEL
- Third stage: Expand the GUI for parallel computing, insert modules of commonly used biophysical packages such as NAMD, Gromacs into the workflow and build physical coupling between simulations.

GUI V1—configure file & input files

GUI V1 provides a graphical user interface to interact with users, then generate the required input files for BD simulation and a configure file for openDIEL, according to user's definitions.

As shown in Fig.3, GUI V1 is built based on the design of openDIEL. Different computations are read as modules, and which constitute the groups groups, multiple groups may also form a set when necessary.

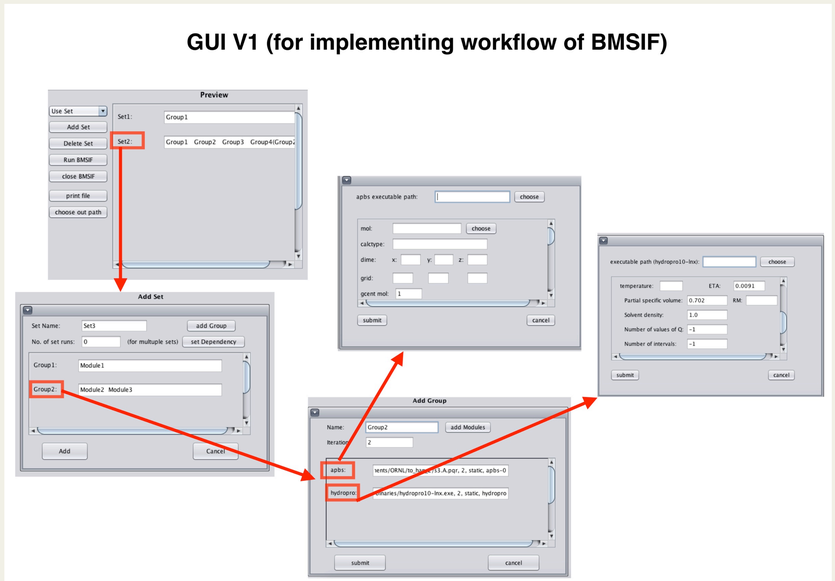

Fig.3 , the user interface of GUI V1

Fig.4 is screenshots of the configure file for openDIEL, it contains information such as the size of tuple space that used to facilitate communication between different processes, executable path and running size for each module, execution order and dependencies of each group, etc.

For GUI V1, all the work done in openDIEL is determined by the configure file, but more work will be required in GUI V2, which is still in process.

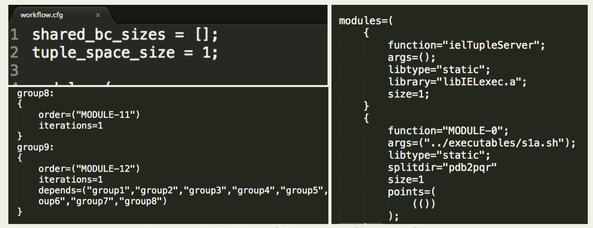

Fig.4, details of the configure file

After printing configure file, the other thing is to do pre-calculation and generate the input files for BD simulation, which are shown in Fig.5. This step will be done with the help of BDS toolkit scripts. With front end interface designed in Java using Netbeans IDE.

Some of the parameters are from user's inputs directly, while the others, such as the mass of a certain molecule, will be generated by backend code automatically from the input data, or calculated based on upstream module output.

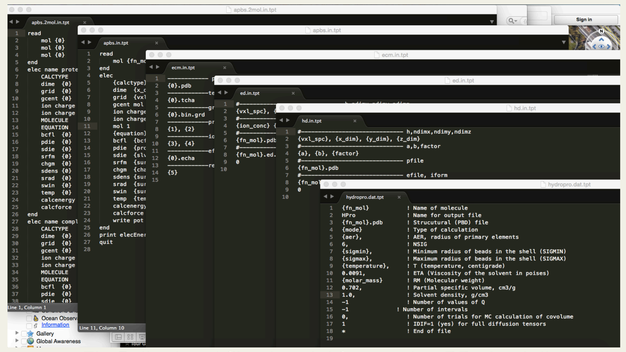

Fig.5, the input files to print for running BD simulation

GUI V2—Parallel Version(in process)

GUI V1 focuses mainly on running BDS and configuring the precalculation modules to optimize models in the simulation, requiring iteration and other small changes within the workflowso GUI V2 for running biophysical simulations in parallel is on the way.

GUI V2 will take advantage of modMaker from Mr Argens Ng Mr. Tanner Curren to achieve parallel support. In GUI V2, the source code from user will be transferred to follow the format required by openDIEL. Besides, some popular biophysical simulation packages such as NAMD, Gromacs and LAMMPS will be added, hence it would be able to support more complex biophysical simulations.

Acknowledgements

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