Implementing Workflow for Biophysical Simulations in openDIEL
Background
About BD simulation

Brownian Dynamics simulation (BDS) is 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 pre-calculated intermolecular physical potentials.
Fig. 1 shows the organisational structure for preliminary molecular structure computations.
About openDIEL

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

Fig. 2, simple mechanism of openDIEL
Abstract/Objectives

• 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.
Objectives
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.

- Configure file for openDIEL
- Input files for Running BD simulation
GUI V1—configure file & input files (cont’d)

GUI V1 (for implementing workflow of BMSIF)

Fig. 3, the user interface of GUI V1
GUI V1—configure file & input files (cont’d)

Fig. 4, the user interface of GUI V1
GUI V1—configure file & input files (cont’d)

About configure file:

size of tuple space / executable path / running size for each module, execution order / dependencies of each group / etc.

Fig. 4, details of the configure file
GUI V1—configure file & input files (cont’d)

About Setting files:

Fig. 5, the setting files to generate input files
About Setting files:

Fig. 6, the setting file to store machine information
About input files for BD simulation:

Fig. 5, the input files to print for running BD simulation
GUI V2— supplements of GUI V1

Transfer files to server:

![Fig.5, transfer file to server](image)

Targets:

- Run simulation from GUI
- Get outputs back to GUI
- Display it for post-process
GUI V2—Parallel Version (in process)

GUI V1 focuses mainly on running BDS and configuring the pre-calculation modules to optimize models in the simulation, requiring iteration and other small changes within the workflow. So GUI V2 for running biophysical simulations in parallel is on the way.
Demonstration
Acknowledgements

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