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

About BD simulation(cont'd)

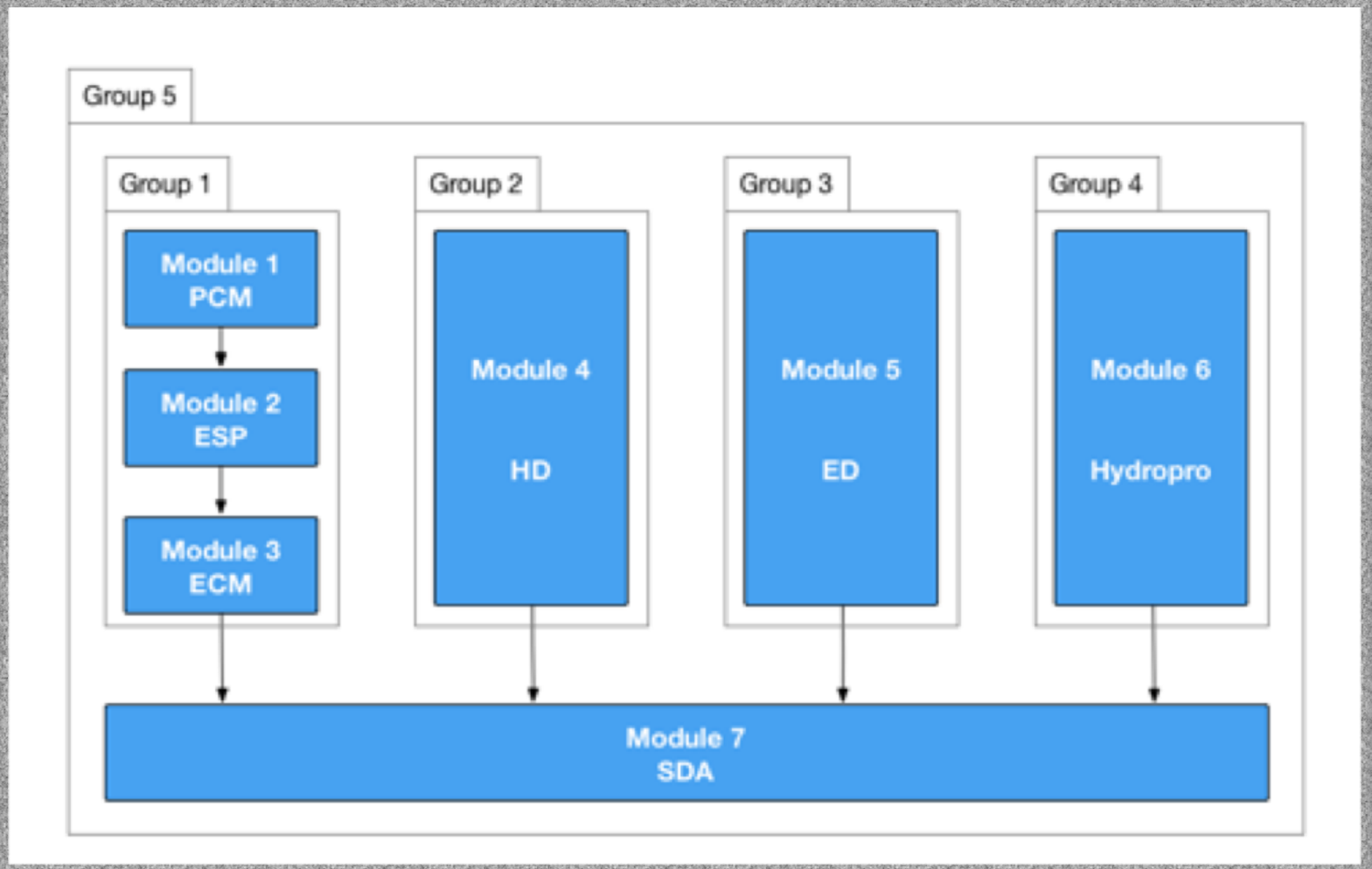


Fig. 1

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.)

About openDIEL(cont'd)

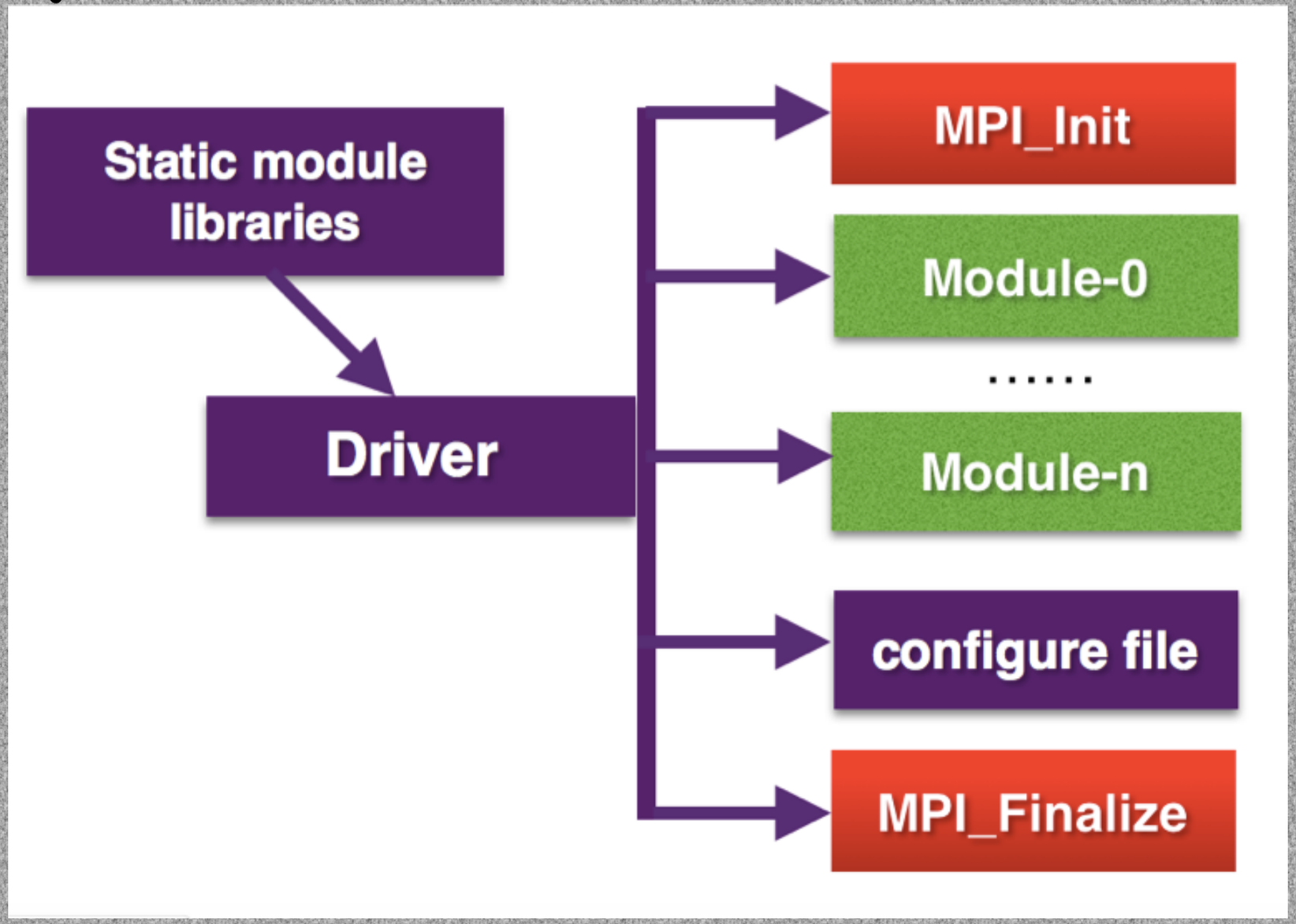


Fig. 2

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.

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

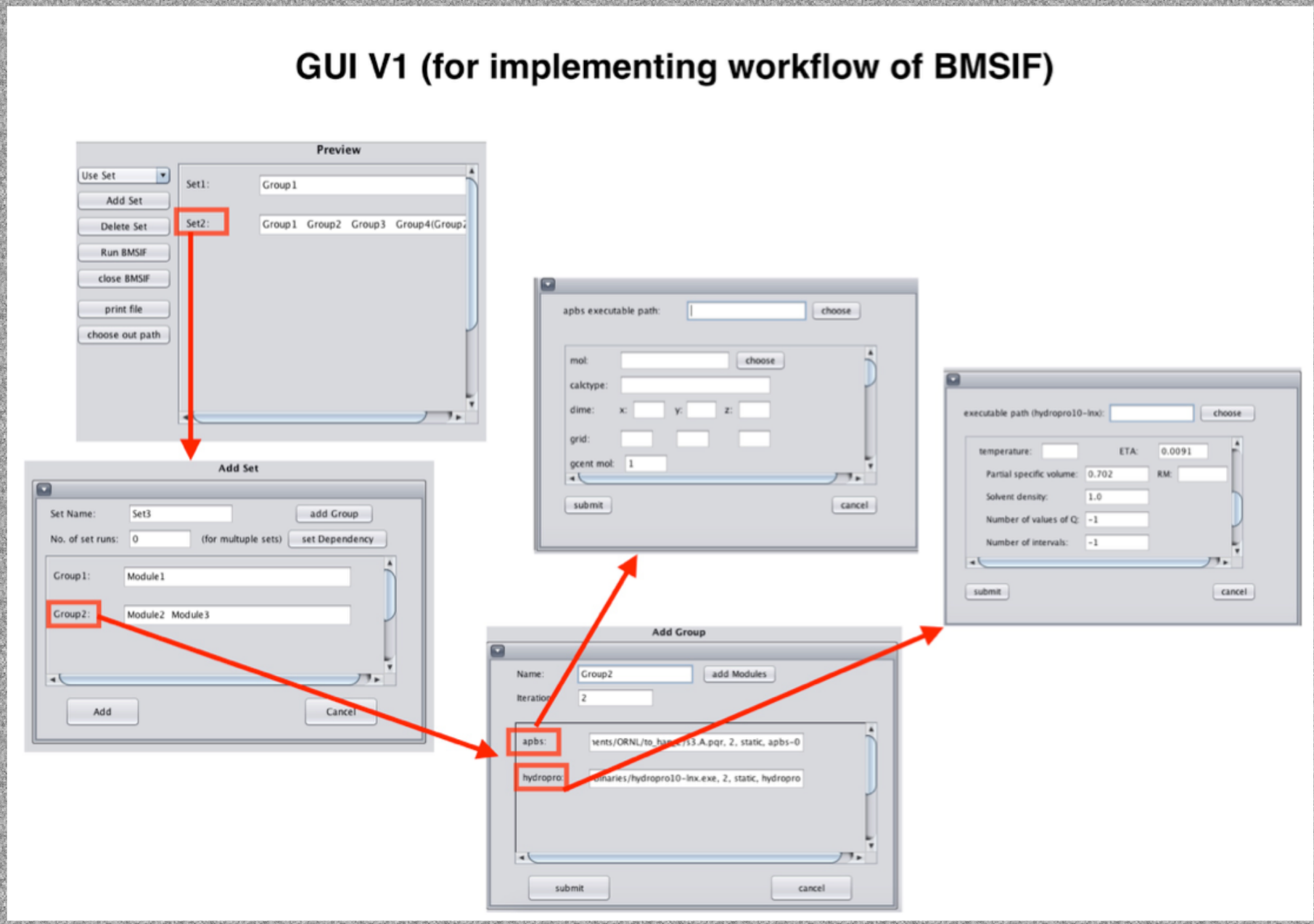


Fig.3 , the user interface of GUI V1

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.

workflow.cfg

```
shared_bc_sizes = [];
tuple_space_size = 1;
```

```
group8:
{
    order=("MODULE-11")
    iterations=1
}
group9:
{
    order=("MODULE-12")
    iterations=1
    depends=("group1","group2","group3","group4","group5",
    oup6","group7","group8")
}
```

```
modules=(
    {
        function="ielTupleServer";
        args=();
        libtype="static";
        library="libIELexec.a";
        size=1;
    }
    {
        function="MODULE-0";
        args=("../executables/s1a.sh");
        libtype="static";
        splitdir="pdb2pqr"
        size=1
        points=(
            (())
        );
```

Fig.4, details of the configure file

GUI V1—configure file & input files(cont'd

About input files for BD simulation:

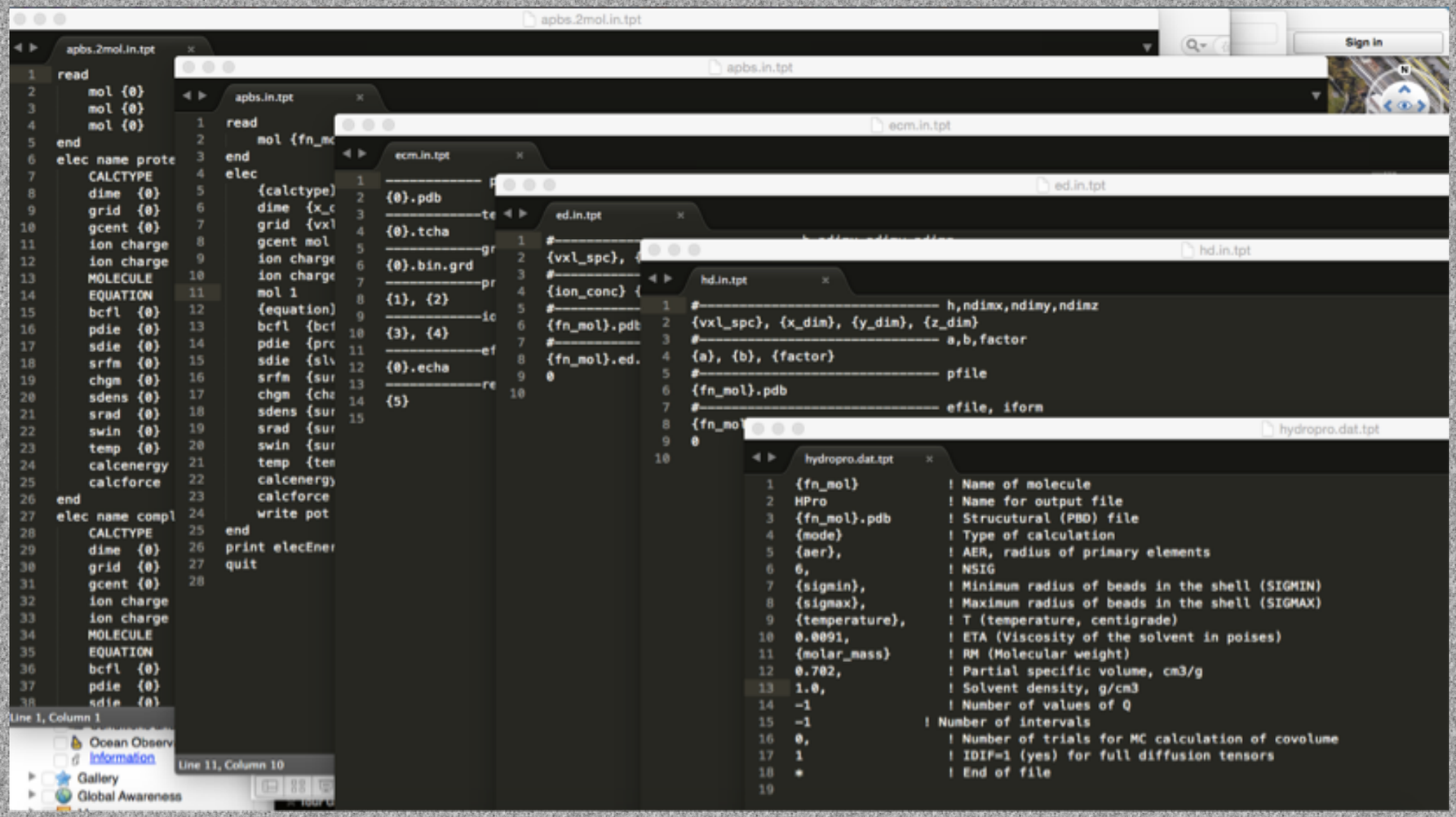
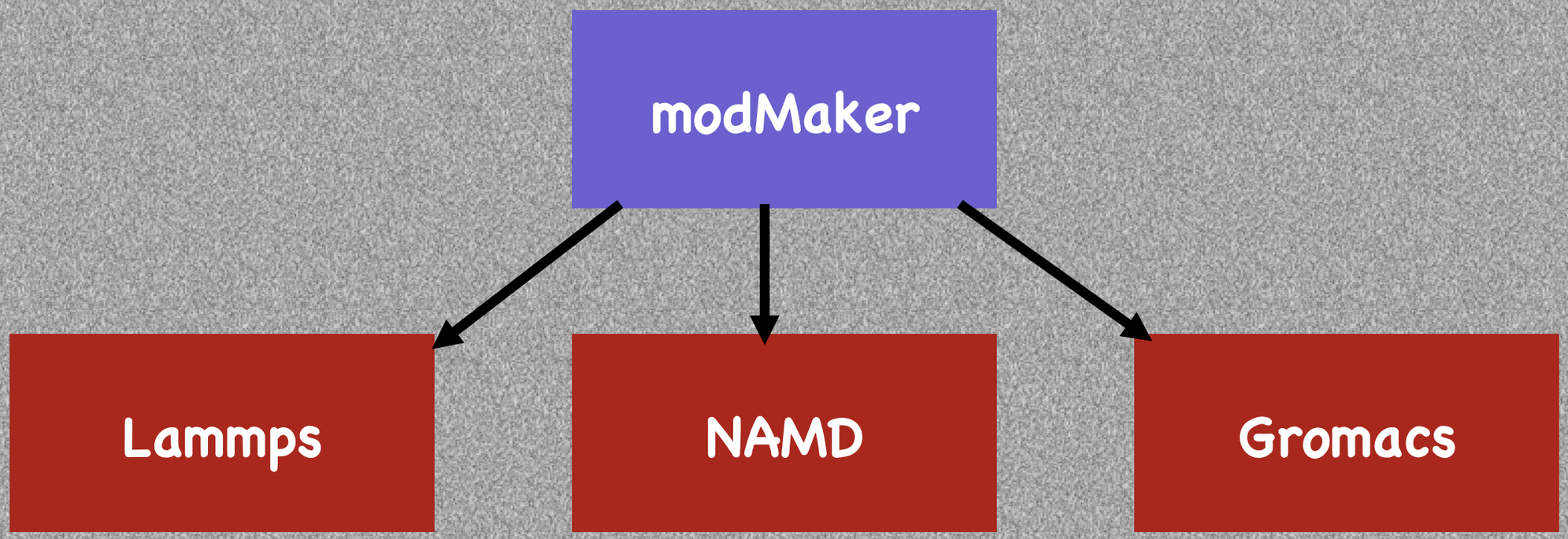


Fig.5, the input files to print for running BD simulation

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.



Acknowledgements

This project is supported by University of Tennessee, NSF, and Oak Ridge National Laboratory.