MDBuilder User's Manual

Release 1.0
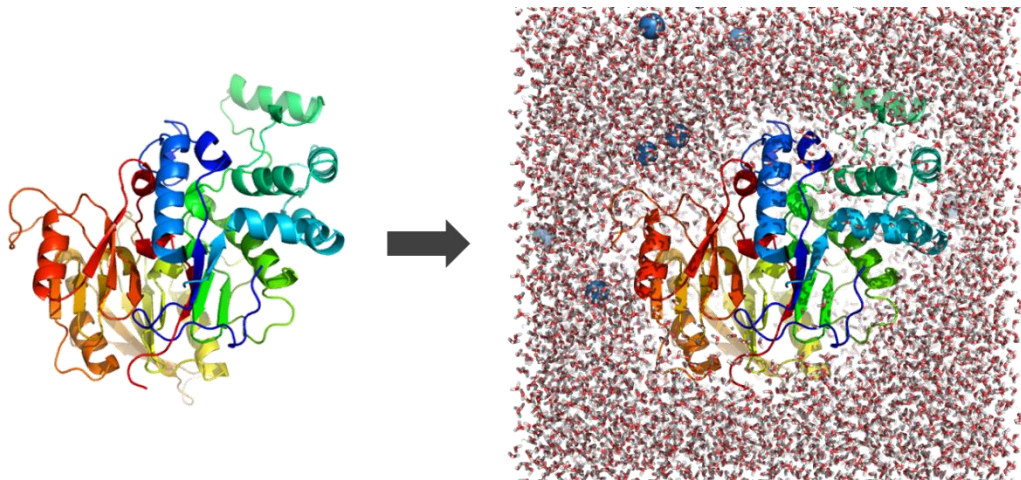
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Chapter 1

Introduction

1.1 Basics of MDBuilder

MDBuilder is a free and open-source tool that allows users to build the initial structural files feeding different popular molecular dynamics (MD) simulation packages. It is written in the Python language. NumPy, the *de facto* standard library for numerical computation in Python is also utilized to enable all of its functionality. A graphical user interface (GUI) incorporated into the popular molecular visualization software PyMOL is provided.

Supported Packages:

- AMBER (version >= 10, including CHAMBER)

- NAMD

- ACEMD

- OpenMM

The general scheme of the operation flow in MDBuilder is presented in Fig. 1. Here the primary steps are summarized from the top to bottom in the figure. First of all, information from force-field-related topology and parameter files as well as the PDB-format input file is read to fill certain internal data structures. Next, MDBuilder employs required information to construct the biomolecular structures compatible with the CHARMM force field. Then, it can build initial structures by adding hydrogen atoms, wrapping each side of the protein with a layer of water, adding counter-ions, and preparing lists of force field terms and their associated parameters. At last, the resulting data is generated in two types of files that contain information required for performing energy minimization or MD simulation.
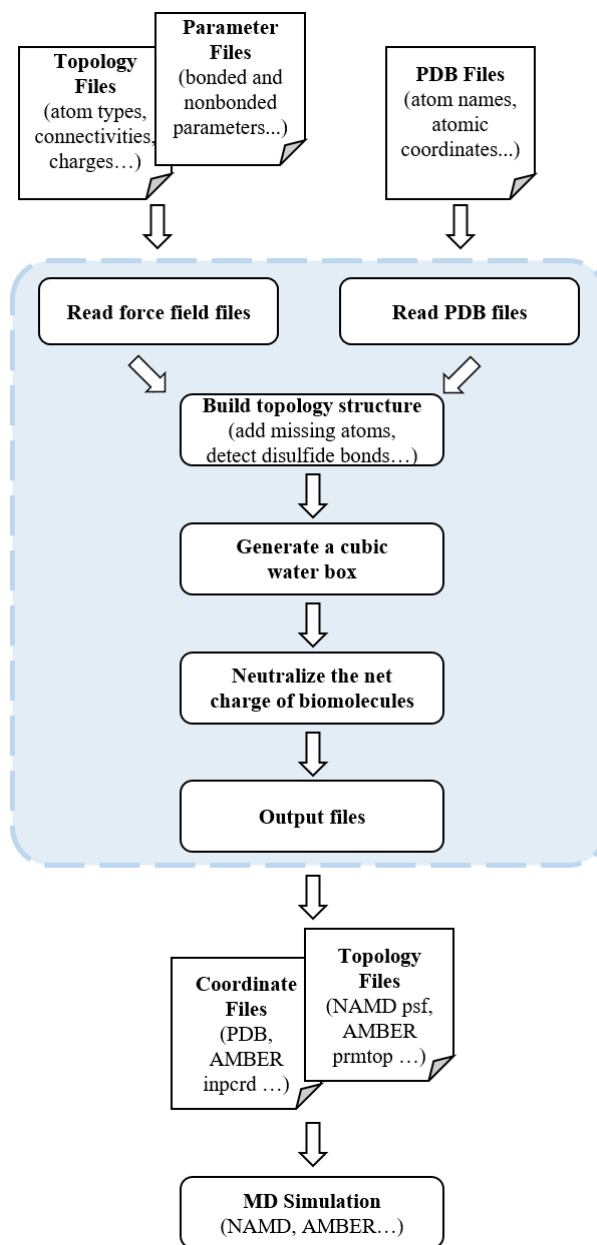
Fig. 1. The flowchart of the preparation of an initial file for a typical MD simulation. Procedures with light blue background are conducted by MDBuilder.

1.2 License

MDBuilder is freely available under the GPL License:

> *This program is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.*

Chapter 2

Installation

2.1 Prerequisites

- Python 2.7.x
- NumPy
- PyMOL 1.7.x, 1.8.x

Please download the installation files and follow the corresponding instructions on their websites.

2.2 Download and Install

After installing the above required programs, you can download the MDBuilder source code from https://github.com/HuiLiuCode/MDBuilder. To install MDBuilder, simply extract the downloaded source file to a scratch directory. PyMOL can install plugins into the correct directory automatically with the help of the built-in plugin installation tool, via "Menu Bar -> Plugin -> Plugin Manager -> Install New Plugin-> Choose file...".

Bibliography

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