Welcome to asmd2

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1 Quickstart

You are now using Gummi 0.6.5. Many new exciting features have been added to the 0.6 series. The document editor is now a tabbed instance, allowing multiple documents to be worked on simultaneously. Using the new projects menu, you can group files together for easy access.

Support for two high-level LaTeX building systems, *rubber*[1] & *latexmk*[2] has been added to this release as well. Your preferred typesetter can be configured through the Compilation tab in the Preferences menu. Typesetters that are not installed on your system will not be selectable.

Added for your viewing convenience is a continuous preview mode for the PDF. This mode is enabled by default, but can also be disabled through the *(View → Page layout in preview)* menu. Complementary to this feature is SyncTeX integration, which allows you to synchronize the position in your editor with the PDF preview.

2 Description

We hope you will enjoy using this release as much as we enjoyed creating it. If you have comments, suggestions or wish to report an issue you are experiencing - contact us at: *http://gummi.midnightcoding.org*.

3 Setup for NAMD

Downloaded a new molecule from the PDB(Protein Data Bank), generated a protein structure file with psfgen, run an equilibration in the desired force

[1] https://launchpad.net/rubber/
[2] http://www.phys.psu.edu/~collins/software/latexmk-jcc/

field? Now you're ready to configure that molecule for use in asmd2.

3.1 General Control Templates

Generally, only two of the following sections, mol.conf and struc, require added templates for the continued use of asmd2 to perform full-scale adaptive or simple steered molecular dynamics on new molecules. The rest of the templates, python scripts, and bash scripts are general enough to require no further adjustments. A short description is provided for each in case further development in the algorithm is required.

3.1.1 continue

The continue.py script packs the smdforces.out/tef.dat(time,extension,force) files into 1 pickle per stage. It also carries out the selection and copying of the daOut.coor and daOut.vel files for use in the following stage using the Jarzynski averaging criterion. asmd2/00.maindir/namd/continue/continue.py

3.1.2 go

The go.py script runs steered molecular dynamics any number of times.
asmd2/00.maindir/namd/go/go-ggatecpu2.py
asmd2/00.maindir/namd/go/go-ggategpu2.py
asmd2/00.maindir/namd/go/go-fgatecpu2.py

3.1.3 hb

The hb.py script generates the pickle describing the bonding in a trajectory.
asmd2/00.maindir/namd/hb/hb.py

3.1.4 hb_pkl

The hb_pkl directory contains the hb_pkl.py script. This script pickles all the hydrogen bonding trajectory pickles into 1 pickle for that stage.
asmd2/00.maindir/namd/hb_pkl/hb_pkl.py

3.1.5 job

The job directory contains the bash scripts submitted to the pbs resource manager for controlling the go.py scripts, which run steered molecular dynamics in any given stage. asmd2/00.maindir/namd/job/job-ggatecpu2.py
asmd2/00.maindir/namd/job/job-ggategpu2.py
asmd2/00.maindir/namd/job/job-fgatecpu2.py

3.1.6 jobc

The jobc directory contains the bash scripts that are submitted to a pbs resource manager for job control of the continue.py scripts. asmd2/00.maindir/namd/jobc/job-ggatecpu2.py
asmd2/00.maindir/namd/jobc/job-ggategpu2.py
asmd2/00.maindir/namd/jobc/job-fgatecpu2.py

3.1.7 jobhb

The jobhb directory contains the bash scripts that are submitted to a pbs resource manager, specific to the cluster to be used, that controls the pickling of the hydrogen bonding pickles obtained per trajectory into 1 pickle associated with the stage in which they were obtained. asmd2/00.maindir/namd/jobhb/job-ggatecpu2.py
asmd2/00.maindir/namd/jobhb/job-ggategpu2.py
asmd2/00.maindir/namd/jobhb/job-fgatecpu2.py

3.1.8 mol.conf

The mol.conf directory is where solvent configuration files by molecule first and solvent second are stored. asmd2/00.maindir/namd/mol.conf/da/01.vac
asmd2/00.maindir/namd/mol.conf/ee/03.exp
asmd2/00.maindir/namd/mol.conf/danvt/02.imp

3.1.9 plotbond

Deprecated. Useful examples still. asmd2/00.maindir/namd/continue/continue.py

3.1.10 plotpmf

Deprecated. Useful examples. asmd2/00.maindir/namd/continue/continue.py

3.1.11 psfgen

Not too significant. Potentially useful examples. asmd2/00.maindir/namd/continue/continue.py

3.1.12 restart

Not too significant. Potentially useful examples. asmd2/00.maindir/namd/continue/continue.py

3.1.13 struc

The struc directory houses the structure files by molecule first and solvent second. asmd2/00.maindir/namd/mol.conf/da/01.vac
asmd2/00.maindir/namd/mol.conf/ee/03.exp
asmd2/00.maindir/namd/mol.conf/danvt/02.imp

3.1.14 toppar

The toppar directory is for the most commonly used topology and parameter files. asmd2/00.maindir/namd/toppar/par_all27_prot_lipid.prm
asmd2/00.maindir/namd/toppar/top_all27_prot_lipid.inp

3.1.15 toppar.all

The toppar.all directory is for the least commonly used but all known topology and parameter files. asmd2/00.maindir/namd/toppar/par_all27_prot_lipid.prm
asmd2/00.maindir/namd/toppar/top_all27_prot_lipid.inp

3.2 Adding a new molecule

A few key template files must be put into place!

3.2.1 Starting Structure

The same starting coordinates are used for every steered molecular dynamics' trajectory.

Example: To study decaalanine, assigned a label "da", in three solvents, the following "equilibrated structure" files are required:

asmd2/00.maindir/namd/struc/da/01.vac/00.pdb
asmd2/00.maindir/namd/struc/da/01.vac/00.psf

asmd2/00.maindir/namd/struc/da/02.imp/00.pdb
asmd2/00.maindir/namd/struc/da/02.imp/00.psf

asmd2/00.maindir/namd/struc/da/03.exp/00.pdb
asmd2/00.maindir/namd/struc/da/03.exp/00.psf

3.2.2 Configuration files

An "initial" and "restart" configuration file is needed per solvent per molecule. As an example, in the case of running ASMD (any case with more than 1 stage of SMD), the following template files would be required in the following locations:

Example: To study decaalanine, assigned a label "da", in three solvents, the following configuration files are required:

asmd2/00.maindir/namd/mol.conf/da/01.vac/smd_initial.namd
asmd2/00.maindir/namd/mol.conf/da/01.vac/smd_continue.namd

asmd2/00.maindir/namd/mol.conf/da/02.imp/smd_initial.namd
asmd2/00.maindir/namd/mol.conf/da/02.imp/smd_continue.namd

asmd2/00.maindir/namd/mol.conf/da/03.exp/smd_initial.namd
asmd2/00.maindir/namd/mol.conf/da/03.exp/smd_continue.namd

3.2.3 Steering control

The control file, where the velocity of the pseudoatom and force constant of the harmonic potential are set, is placed in the following location.

asmd2/00.maindir/namd/mol.conf/da/01.vac/smd_force.tcl

asmd2/00.maindir/namd/mol.conf/da/02.imp/smd_force.tcl

asmd2/00.maindir/namd/mol.conf/da/03.exp/smd_force.tcl