biobb$_{m}dDocumentation$

Release 0.0.1

Bioexcel Project

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Contents

CHAPTER 1

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1.1 biobb_md

1.1.1 Introduction

Biobb_md is the Biobb module collection to perform molecular dynamics simulations. Biobb (BioExcel building blocks) packages are Python building blocks that create new layer of compatibility and interoperability over popular bioinformatics tools. The latest documentation of this package can be found in our readthedocs site: latest API documentation.

1.1.2 Version

v1.1.7 May 2019 Release

1.1.3 Copyright & Licensing

1.2 biobb_md

1.2.1 gromacs package

Submodules

gromacs.editconf module

Module containing the Editconf class and the command line interface.

class gromacs.editconf.**Editconf**(*input_gro_path*, *output_gro_path*, *properties=None*, ***kwargs*)

Bases: object

Wrapper class for the GROMACS editconf (http://manual.gromacs.org/current/onlinehelp/gmx-editconf.html) module.

Parameters

- **input_gro_path** (*str*) – Path to the input GRO file.
- **output_gro_path** (*str*) – Path to the output GRO file.
- **properties** (*dic*) –

  - **distance_to_molecule** (*float*) - (1.0) Distance of the box from the outermost atom in nm. ie 1.0nm = 10 Angstroms.
  - **box_type** (*str*) - ("cubic") Geometrical shape of the solvent box. Available box types: (http://manual.gromacs.org/current/onlinehelp/gmx-editconf.html) -bt option.
  - **center_molecule** (*bool*) - (True) Center molecule in the box.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()

Launches the execution of the GROMACS editconf module.

gromacs.editconf.**main**()

gromacs.genion module

Module containing the Genion class and the command line interface.

class gromacs.genion.**Genion**(*input_tpr_path*, *output_gro_path*, *input_top_zip_path*, *output_top_zip_path*, *properties=None*, ***kwargs*)

Bases: object

Wrapper class for the GROMACS genion (http://manual.gromacs.org/current/onlinehelp/gmx-genion.html) module.

Parameters

- **input_tpr_path** (*str*) – Path to the input portable run input TPR file.
- **output_gro_path** (*str*) – Path to the input structure GRO file.
- **input_top_zip_path** (*str*) – Path the input TOP topology in zip format.
- **output_top_zip_path** (*str*) – Path the output topology TOP and ITP files zipball.
- **properties** (*dic*) –

  - **output_top_path** (*str*) - ("gio.top") Path the output topology TOP file.
  - **replaced_group** (*str*) - ("SOL") Group of molecules that will be replaced by the solvent.
  - **neutral** (*bool*) - (False) Neutralize the charge of the system.
  - **concentration** (*float*) - (0.05) Concentration of the ions in (mol/liter).
  - **seed** (*int*) - (1993) Seed for random number generator.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()

Launches the execution of the GROMACS genion module.

gromacs.genion.**main**()

gromacs.genrestr module

Module containing the Genrestr class and the command line interface.

class gromacs.genrestr.**Genrestr**(*input_structure_path*, *input_ndx_path*, *input_top_zip_path*, *output_top_zip_path*, *properties*, ***kwargs*)

Bases: object

Wrapper class for the GROMACS genrestr (http://manual.gromacs.org/current/onlinehelp/gmx-genrestr.html) module.

Parameters

- **input_structure_path** (*str*) – Path to the input structure PDB, GRO or TPR format.
- **input_ndx_path** (*str*) – Path to the input GROMACS index file, NDX format.
- **input_top_zip_path** (*str*) – Path the input TOP topology in zip format.
- **output_top_zip_path** (*str*) – Path the output TOP topology in zip format.
- **properties** (*dic*) –

  - **output_itp_path** (*str*) - ("restrain.itp") Path to the output include for topology ITP file.
  - **force_constants** (*str*) - ("500 500 500") Array of three floats defining the force constants
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()
Launches the execution of the GROMACS genrestr module.

gromacs.genrestr.**main**()

gromacs.grompp module

Module containing the Grompp class and the command line interface.

class gromacs.grompp.**Grompp**(*input_gro_path*, *input_top_zip_path*, *output_tpr_path*, *input_cpt_path=None*, *input_ndx_path=None*, *properties=None*, ***kwargs*)

Bases: object

Wrapper of the GROMACS grompp module. The GROMACS preprocessor module needs to be feeded with the input system and the dynamics parameters to create a portable binary run input file TPR. The dynamics parameters are specified in the mdp section of the configuration YAML file. The parameter names and defaults are the same as the ones in the official MDP specification: http://manual.gromacs.org/current/online/mdp_opt.html

Parameters

- **input_gro_path** (*str*) – Path to the input GROMACS structure GRO file.
- **input_top_zip_path** (*str*) – Path the input GROMACS topology TOP and ITP files in zip format.
- **output_tpr_path** (*str*) – Path to the output portable binary run file TPR.
- **input_cpt_path** (*str*) – Path to the input GROMACS checkpoint file CPT.
- **input_ndx_path** (*str*) – Path to the input GROMACS index files NDX.
- **properties** (*dic*) –

  - **input_mdp_path** (*str*) - (None) Path of the input MDP file.
  - **mdp** (*dict*) - (defaults dict) MDP options specification. (Used if *input_mdp_path* is None) | - **type** (*str*) - ("minimization") Default options for the mdp file. Valid values: minimization, nvt, npt, free, index
  - **output_mdp_path** (*str*) - ("grompp.mdp") Path of the output MDP file.
  - **output_top_path** (*str*) - ("grompp.top") Path the output topology TOP file.
  - **maxwarn** (*int*) - (10) Maximum number of allowed warnings.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

create_mdp()
Creates an MDP file using the properties file settings

launch()
Launches the execution of the GROMACS grompp module.

gromacs.grompp.**main**()

gromacs.make_ndx module

Module containing the MakeNdx class and the command line interface.

class gromacs.make_ndx.**MakeNdx**(*input_structure_path*, *output_ndx_path*, *input_ndx_path=None*, *properties=None*, ***kwargs*)

Bases: object

Wrapper of the GROMACS make_ndx (http://manual.gromacs.org/current/onlinehelp/gmx-make_ndx.html) module.

Parameters

- **input_structure_path** (*str*) – Path to the input GRO/PDB/TPR file.
- **output_ndx_path** (*str*) – Path to the output index NDX file.
- **properties** (*dic*) –

  - **selection** (*str*) - ("a CA C N O") Heavy atoms. Atom selection string.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()
Launches the execution of the GROMACS make_ndx module.

gromacs.make_ndx.**main**()

gromacs.mdrun module

Module containing the MDrun class and the command line interface.

class gromacs.mdrun.**Mdrun**(*input_tpr_path*, *output_trr_path*, *output_gro_path*, *output_edr_path*, *output_log_path*, *output_xtc_path=None*, *output_cpt_path=None*, *output_dhdl_path=None*, *properties=None*, ***kwargs*)
Bases: object

Wrapper of the GROMACS of the mdrun module.

Parameters

- **input_tpr_path** (*str*) – Path to the portable binary run input file TPR.
- **output_trr_path** (*str*) – Path to the GROMACS uncompressed raw trajectory file TRR.
- **output_gro_path** (*str*) – Path to the output GROMACS structure GRO file.
- **output_edr_path** (*str*) – Path to the output GROMACS portable energy file EDR.
- **output_log_path** (*str*) – Path to the output GROMACS trajectory log file LOG.
- **output_xtc_path** (*str*) – Path to the GROMACS compressed trajectory file XTC.
- **output_cpt_path** (*str*) – Path to the output GROMACS checkpoint file CPT.
- **output_dhdl_path** (*str*) – Path to the output dhdl.xvg file only used when free energy calculation is turned on.
- **properties** (*dic*) –

  - **num_threads** (*int*) - (0) Let GROMACS guess. The number of threads that are going to be used.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.
  - **mpi_bin** (*str*) - (None) Path to the MPI runner. Usually "mpirun" or "srun".
  - **mpi_np** (*str*) - (None) Number of MPI processes. Usually an integer bigger than 1.
  - **mpi_hostlist** (*str*) - (None) Path to the MPI hostlist file.

launch()
Launches the execution of the GROMACS mdrun module.

gromacs.mdrun.**main**()

gromacs.pdb2gmx module

Module containing the Pdb2gmx class and the command line interface.

class gromacs.pdb2gmx.**Pdb2gmx**(*input_pdb_path*, *output_gro_path*, *output_top_zip_path*, *properties=None*, ***kwargs*)

Bases: object

Wrapper class for the GROMACS pdb2gmx (http://manual.gromacs.org/current/onlinehelp/gmx-pdb2gmx.html) module.

Parameters

- **input_pdb_path** (*str*) – Path to the input PDB file.
- **output_gro_path** (*str*) – Path to the output GRO file.
- **output_top_zip_path** (*str*) – Path the output TOP topology in zip format.
- **properties** (*dic*) –

  - **output_top_path** (*str*) - ("p2g.top") Path of the output TOP file.
  - **output_itp_path** (*str*) - ("p2g.itp") Path of the output itp file.
  - **water_type** (*str*) - ("spce") Water molecule type. Valid values: tip3p, spce, etc.
  - **force_field** (*str*) - ("amber99sb-ildn") Force field to be used during the conversion. Valid values: amber99sb-ildn, oplsaa, etc.
  - **ignh** (*bool*) - (False) Should pdb2gmx ignore the hidrogens in the original structure.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()
Launches the execution of the GROMACS pdb2gmx module.

gromacs.pdb2gmx.**main**()

gromacs.solvate module

Module containing the Editconf class and the command line interface.

class gromacs.solvate.**Solvate**(*input_solute_gro_path*, *output_gro_path*, *input_top_zip_path*, *output_top_zip_path*, *properties=None*, ***kwargs*)

Bases: object

Wrapper of the GROMACS solvate (http://manual.gromacs.org/current/onlinehelp/gmx-editconf.html) module.

Parameters

- **input_solute_gro_path** (*str*) – Path to the input GRO file.
- **output_gro_path** (*str*) – Path to the output GRO file.
- **input_top_zip_path** (*str*) – Path the input TOP topology in zip format.
- **output_top_zip_path** (*str*) – Path the output topology in zip format.
- **properties** (*dic*) –

  - **output_top_path** (*str*) - ("solvate.top") Path the output TOP file.
  - **intput_solvent_gro_path** (*str*) - ("spc216.gro") Path to the GRO file contanining the structure of the solvent.
  - **gmx_path** (*str*) - ("gmx") Path to the GROMACS executable binary.

launch()
Launches the execution of the GROMACS solvate module.

gromacs.solvate.**main**()

1.2.2 gromacs_extra package

Submodules

gromacs_extra.ndx2resttop module

Module containing the Ndx2resttop class and the command line interface.

class gromacs_extra.ndx2resttop.**Ndx2resttop**(*input_ndx_path*, *input_top_zip_path*, *output_top_zip_path*, *properties*, ***kwargs*)

Bases: object

Generate a restrained topology from an index NDX file.

Parameters

- **input_ndx_path** (*str*) – Path to the input NDX index file.
- **input_top_zip_path** (*str*) – Path the input TOP topology in zip format.
- **output_top_zip_path** (*str*) – Path the output TOP topology in zip format.
- **properties** (*dic*) –

  - **force_constants** (*float[3]*): (“500 500 500”) Array of three floats defining the force constants.
  - **ref_rest_chain_triplet_list** (*str*): (None) Triplet list composed by (reference group, restrain group, chain) list.

launch()

Launch the topology generation.

gromacs_extra.ndx2resttop.**main**()

CHAPTER 2

Indices and tables

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CHAPTER 3

Github repository.

Python Module Index

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