Coarse-grained OpenMM Documentation

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This documentation is generated automatically using Sphinx, which reads all docstring-formatted comments from Python functions in the 'cg_openmm' repository. (See cg_openmm/doc for Sphinx source files.)

CHAPTER

ONE

OPENMM SIMULATION() PROTOCOLS FOR COARSE GRAINED MODELING

This page details the functions in cg_openmm/src/build/cg_build.py.

build.cg_build.**add_new_elements**(*cgmodel*, *list_of_masses*)

Adds new coarse grained particle types to OpenMM

cgmodel: CGModel() class object

list_of_masses: List of masses for the particles we want to add to OpenMM

build.cg_build.**build_mm_force**(*sigma*, *epsilon*, *charge*, *num_beads*, *cutoff=Quantity(value=1*, *unit=nanometer)*)

Build an OpenMM 'Force' for the non-bonded interactions in our model.

sigma: Non-bonded bead Lennard-Jones interaction distances, (float * simtk.unit.distance)

epsilon: Non-bonded bead Lennard-Jones interaction strength, (float * simtk.unit.energy)

charge: Charge for all beads (float * simtk.unit.charge)

cutoff: Cutoff distance for nonbonded interactions (float * simtk.unit.distance)

num_beads: Total number of beads in our coarse grained model (integer)

build.cg_build.**build_mm_simulation**(*topology*, *system*, *positions*, *temperature=Quantity(value=300.0*, *unit=kelvin)*, *simulation_time_step=None*, *total_simulation_time=Quantity(value=1.0*, *unit=picosecond)*, *output_pdb='output.pdb'*, *output_data='output.dat'*, *print_frequency=100*)

Construct an OpenMM simulation object for our coarse grained model.

topology: OpenMM topology object

system: OpenMM system object

positions: Array containing the positions of all beads in the coarse grained model (np.array('num_beads' x 3 , (float * simtk.unit.distance))

temperature: Simulation temperature (float * simtk.unit.temperature)

simulation_time_step: Simulation integration time step (float * simtk.unit.time)

total_simulation_time: Total simulation time (float * simtk.unit.time)

output_data: Name of output file where we will write the data from this simulation (string)

print_frequency: Number of simulation steps to skip when writing data to 'output_data' (integer)

build.cg_build.**build_system**(*cgmodel*)

Builds an OpenMM System() class object, given a CGModel() class object as input.

cgmodel: CGModel() class object

system: OpenMM System() class object

build.cg_build.**build_topology**(*cgmodel*)

Construct an OpenMM topology for our coarse grained model

polymer_length: Number of monomers in our coarse grained model (integer)

backbone_length: Number of backbone beads on individual monomers in our coarse grained model, (integer)

sidechain_length: Number of sidechain beads on individual monomers in our coarse grained model, (integer)

CHAPTER

TWO

OPENMM SIMULATION TOOLS FOR COARSE GRAINED MODELING

This page details the functions in cg_openmm/src/simulation/.

2.1 Replica exchange simulation tools for coarse grained modeling

2.2 General simulation tools for coarse grained modeling

simulation.tools.**get_simulation_time_step**(*topology*, *system*, *positions*, *temperature*, *time_step_list*, *total_simulation_time*)

Determine a valid simulation time step for our coarse grained model.

simulation: OpenMM simulation object

time_step_list: List of time steps for which to attempt a simulation in OpenMM.

time_step: A time step that was successful for our simulation object.

simulation.tools.**minimize_structure**(*topology*, *system*, *positions*, *temperature=Quantity(value=0.0, unit=kelvin)*, *simulation_time_step=None*, *total_simulation_time=Quantity(value=1.0, unit=picosecond)*, *output_pdb='minimum.pdb'*, *output_data='minimization.dat'*, *print_frequency=10*)

Construct an OpenMM simulation object for our coarse grained model.

topology: OpenMM topology object

system: OpenMM system object

positions: Array containing the positions of all beads in the coarse grained model (np.array('num_beads' x 3 , (float * simtk.unit.distance))

temperature: Simulation temperature (float * simtk.unit.temperature)

simulation_time_step: Simulation integration time step (float * simtk.unit.time)

output_data: Name of output file where we will write the data from this simulation (string)

print_frequency: Number of simulation steps to skip when writing data to 'output_data' (integer)

CHAPTER

THREE

UTILITIES FOR COARSE GRAINED MODELING IN OPENMM

This page details the functionality of utilities in cg_openmm/src/utilities/util.py.

`utilities.util.`**`distance`**(*positions_1*, *positions_2*)

Construct a matrix of the distances between all particles.

positions_1: Positions for a particle (np.array(length = 3))

positions_2: Positions for a particle (np.array(length = 3))

distance (float * unit)

`utilities.util.`**`get_box_vectors`**(*box_size*)

Assign all side lengths for simulation box.

box_size: Simulation box length (float * simtk.unit.length)

`utilities.util.`**`set_box_vectors`**(*system*, *box_size*)

Build a simulation box.

system: OpenMM system object

box_size: Simulation box length (float * simtk.unit.length)

CHAPTER

FOUR

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