Manual:
Molecular Dynamics Analysis with Matlab

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This manual contains an explanation on how to use the Matlab code to analyse Molecular Dynamics simulations, publicly available at: `https://bitbucket.org/niekdeklerk/md-analysis-with-matlab`. This manual only tells how the code should be used, the accompanying paper contains a thorough explanation on how all the properties are calculated. When you use the code in academic work please cite the paper:
Analysis of diffusion in solid state electrolytes through MD-simulations, improvement of the Li-ion conductivity in $\beta-Li_3PS_4$ as an example; ***Niek J.J. de Klerk, Eveline van der Maas and Marnix Wagemaker (submitted)***

If you find bugs, make additions that could be useful to others, or have questions about the code, you can contact me at: njjdeklerk AT gmail.com

1 How to use the code

After performing an MD simulation the Matlab code can be used for analysis via the following steps:

1. Put the OUTCAR-file from VASP [1] in a folder which is accessible to Matlab.
2. Put the settings to the required values in analyse_md.m, for more information on the settings see section 2.
3. Make sure that the crystallographic positions of the diffusing element in your material are in 'known_materials.m', see section 3 for more information on how to add a material to this file.
4. In Matlab type the command: analyse_md('folder', 'diffusing element', 'material')
   For example: to analyse the Li-diffusion in a MD simulation of β-Li_3PS_4 in the folder 'Li3PS4/24Li/600K', the command would be: analyse_md('Li3PS4/24Li/600K', 'Li', 'li3ps4_beta')
   The time it takes to analyse the MD simulation depends on the number of atoms and time steps in the simulation, for small systems/short simulations it can be done in minutes, but for large simulations it can take hours.
5. Analyse the plots and output files, for more information on the information contained in the output files see section 4.
6. (Optionally) Compare several different MD simulations on the same material using compare_sims.m, see section 5 for more information.

[1] At this moment only the output files from VASP are supported, but other MD programs can be added quite easily; from an output file created by your favourite MD software read in the same data as is read in read_vasp.m.

2 Settings

The settings controlling the analysis of the MD simulation are shown at the top of the file analyse_md.m:

- equil_time: Equilibration time in seconds (1 picosecond = 1E-12 seconds).
- diffusion_dimensions: Number of diffusion dimensions.
- z_ion: Ionic charge of the diffusing ion.
- nr_parts: In how many parts to divide the MD simulation for calculating the standard deviation of certain properties.
- dist_collective: Maximum distance allowed for collective motions (in Ångstrom).
- show_pics: Show plots with the results of the analysis (*true* or *false*).
- density_resolution: Resolution for the density plot of the diffusing atom (in Ångstrom).
- jump_res: Resolution for the plot showing the number of jumps vs. distance (in Ångstrom).
- rdfs: Show the Radial Distribution Functions (RDF's), and calculate if rdfs.mat does not exist yet (*true* or *false*).
- rdf_res: Resolution of the RDF's (in Ångstrom).
- rdf_max_dist: Maximum distance taken into account for the RDF's (in Ångstrom).
- movie: Make a movie showing the jumps between sites (*true* or *false*).
- nr_steps_frame: How many time steps are used per frame of the movie, by increasing this the movie becomes quicker, but some details might be lost.
- start_end: The time-steps for which to make a movie ([start at step; end at step]).

3 How to add a material

To analyse the jump diffusion in a material knowledge about the (possible) crystallographic positions of the diffusing element is required. For each material the crystallographic positions are saved in the file known_materials.m, to add a material open the file known_materials.m and follow the steps below:

1. Obtain the space-group of the material and the crystallographic (Wyckoff) positions of the diffusing element. Information about Wyckoff positions and the symmetries of a space-group can be obtained from the Bilbao Crystallographic Server at `http://www.cryst.ehu.es/cryst/get_wp.html`, or from the International Tables for Crystallography (Volume A: Space-group symmetry).
2. In the function 'known_materials' add the material by adding an elseif-statement containing the name of the material, the supercell used for the MD simulations, and the function containing the crystallographic positions.
3. Create a function for the material with [names, pos] as output and the supercell as input. This function must contain:
   - sym: the symmetry operations applicable to all the Wyckoff sites in the space-group, including the identity operator ([0 0 0]).
   - pos_sym: the fractional coordinates of the Wyckoff sites which the diffusing element can occupy.
   - names_sym: the names given to the Wyckoff sites which the diffusing element can occupy.

   Using the symmetries, coordinates and names given the function 'construct' determines all the positions in the (super)cell and their corresponding names. Have a look at the materials already present in known_materials.m for examples.

4 Output-files

The code can make four output files:

- simulation_data.mat: Contains information about the MD-simulation, the settings used, and properties determined from the raw data (e.g. displacements and the vibration amplitude).
- sites.mat: Contains all the information related to the sites and jumps between sites (jump rates, activation energies, etc.).
- rdfs.mat (optional): Contains the Radial Distribution Functions for the diffusing element.
- jumps_movie.mp4 (optional): Movie showing the jumps between different sites.

4.1 simulation_data.mat

The file simulation_data.mat contains all the data from the output file of the MD simulation which is necessary for the analysis, properties which are derived from this data, and the settings which were used for the analysis. Table 1 contains a short description of the information in simulation_data.mat and which units are used.

4.2 sites.mat

In sites.mat all the information related to the sites of the diffusing element and jumps between sites can be found. A short description of the information in sites.mat and which units are used can be found in Table 2.

4.3 rdfs.mat

The Radial Distribution Functions of the diffusing element are stored in rdfs.mat, Table 3 contains a description of this file.

5 Compare MD simulations

To compare properties obtained from different MD simulations on the same material, e.g. with different vacancy concentrations or doping, the file compare_sims.m can be used. This file reads in the simulation_data.mat and sites.mat files in all the folders given by combining the names given in 'folder', 'subfolder' and 'temps' (e.g. [folder]/[subfolders]/[temps]). Then all the information in the function 'read_sim_info' is read in and saved in the file: [folder]/sims_compare.mat.
After making, or reading in this file if it already exists, for each property a plot will be shown with the values from all the simulations.

Name	**Description**	**Units**
e_charge	Elementary charge	Coulomb
k_boltzmann	Boltzmann's constant	Joule/Kelvin
avogadro	Avogadro's number	-
diffusion_dim	Number of diffusion dimensions	-
ion_charge	Ionic charge of the diffusing element	-
lattice	Crystal lattice of the MD simulation, represented as a 3x3 matrix	Ångstrom
diff_elem	Diffusing element	-
equilibration_time	Equilibration time used	Seconds
elements	Elements present in the MD simulation	-
nr_elements	Number of elements	-
nr_per_element	Number of atoms per element	-
nr_atoms	Total number of atoms	-
time_step	Time step used in the MD simulation	Seconds
temperature	Temperature of the MD simulation	Kelvin
element_mass	Atomic mass of the elements	u
volume	Volume of the simulated system	m^3
equilibration_steps	Number of steps in the equilibration time	-
nr_steps	Number of time steps used for the analysis	-
cart_pos	Cartesian positions of all atoms at all time steps	Ångstrom
atom_element	Element per atom	-
nr_diffusing	Number of atoms which are the diffusing element	-
start_diff_elem	Where in the atom list the diffusing element starts	-
end_diff_elem	Where in the atom list the diffusing element ends	-
total_time	Total time analysed	Seconds
frac_pos	Fractional positions of all atoms at all time steps	-
displacement	Displacement of all atoms at each time step	Ångstrom
attempt_freq	Attempt frequency	Hz
std_attempt_freq	Standard deviation of the attempt frequency	Hz
vibration_amp	Vibration amplitude	Ångstrom
tracer_diffusion	Tracer diffusivity of diffusing element based on the displacement	m^2/sec
tracer_conductivity	Tracer conductivity of diffusing element based on the displacement	Siemens/m
particle_density	Particle density of the diffusing element	Atoms/m^3
mol_per_liter	Concentration of the diffusing element	mol/liter

Table 1: Name, description and units of the information in simulation_data.mat.

Name	Description	Units
sites.correlation_factor	Correlation factor	-
sites.jump_diffusivity	Diffusivity based on the jump rates and jump distances	m^2/sec
sites.solo_frac	Fraction of solo jumps, i.e. which is NOT collective	-
sites.solo_jumps	Number of solo jumps	-
sites.multi_coll	Which jumps show collective behaviour with multiple other jumps	
sites.coll_matrix	Matrix showing which combinations of sites show collective jumps	
sites.coll_jumps	Names of jumps which are collective	
sites.collective	Combinations of jumps which are collective	
sites.e_act	Activation energy per jump type	eV
sites.rates	Average jump rate (1^{st} column) and standard deviation (2^{nd} column)	Hz
sites.nr_jumps	Total number of jumps in the MD simulation	-
sites.jump_names	Names of jumps	
sites.atom_locations	Fraction of their time the diffusing element spends at a type of site	
sites.sites_occup	Fraction of time that sites are occupied	
sites.stable_names	Names of the sites given in known_materials.mat	
sites.material	Material used for the sites analysis	-
sites.nr_parts	Number of parts the simulation is divided in for determining standard deviations	-
sites.succes	Matrix of how many jumps occur between combinations of sites divided in nr_parts	
sites.all_trans	For all jumps the information on which atom, between which sites, and between which time steps. The different columns contain: 1 = atom, 2 = start site, 3 = end site, 4 = starting time step, 5 = ending time step	
sites.transitions	Matrix of how many jumps occur between combinations of sites	
sites.atoms	At which site each diffusing atom is at each time step	-
sites.occupancy	Number of time steps each site is occupied	
sites.site_names	Name of each site	
sites.cart_pos	Cartesian coordinates of the sites	Ångstrom
sites.frac_pos	Fractional coordinates of the sites	-
sites.site_radius	Site radius which was used to determine at which site the atoms are	Ångstrom
sites.nr_per_name	Number of sites with the same name	-
sites.supercell	Supercell used	-
sites.names	Unique site names	-

Table 2: Name, description and units of the information in sites.mat.

Name	Description	Units
distributions	Radial Distribution Functions (RDF's) of the diffusing element	-
integrated	Integrated RDF's	-
rdf_names	Names describing the RDF's. When the element is at a certain site the rdf_name is: 'site_name', when atoms are moving from one site to another site (i.e. during jumps): 'Transition:site_name - site_name', when an atom leaves a site but then returns (i.e. failed jumps): 'Transition:site_name'	-
elements	Elements in the RDF's	-
max_dist	Maximum distance of the RDF	Ångstrom
resolution	Resolution of the RDF	Ångstrom
total	RDF of the diffusing element for the entire MD simulation	-

Table 3: Name, description and units of the information in rdfs.mat.