User manual for op_tools ver 0.1

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1 What is this?

python module for order parameter analysis for molecular and particle simulation. this module evaluete the particle environment as the value. In molecular simulation, there are often cases where you want to mechanically determine the structure of a particle. For example, when melting simulating of solid metal, you may want to visualize how it melts. You can use such a module at such a time.

2 How to install

$ cd order_tools
$ pip install -e .

3 How to use

3.1 required data

- coord : coordinate of each particles like [[0,0,0], [0,0,1], …]
- direct : director of each particles (3d unit vector or quaternion) like [[1,0,0], …] or [[0,0,0,0] ,….]
- box_length : the length of simulation box like [3, 3, 3]
- order_parameter_parameter : parameter for calculating the order parameter

3.1.1 parameter for calculating the order parameter

ordinary, order_parameter_parameter is like follows.

```
  order_parameter_parameter = {
    'ave_times'      : 2, # averaging times with neighbor particles
    'neighbor'       : [6], # num of neighbor particle
    'radius'         : [2.75], # threshold of neighbor particle
    'oi_oj'          : [0], # position of point of director, mass point => [0], line => [1,-
1],  ellipsoid => [0, 1, -1] (center, head, tail)
    'o_factor'       : [1.00], # strength of director. if 'oi_oj' is [1,-
1] and o_factor is 2.0, actual position is [2,-2].
    'b_in_Q'         : 2, # averaging times of spheriacal harmonics with neighbor partiels
    'l_in_Q'         : [2, 4, 6], # num of spherical harmonis
    'P_in_Q'         : [0], # weight for Q parameter
    'm_in_A'         : [2],
    'angle_factor_m' : [0, 1, 2, 3, 4, 6],
    'angle_phi'      : [0]],
    'sin_exponent'   : [1, 3, 5],
    'function'       : [f_1], # function pointer for D
    'hist_num'       : [12], # number of bin for Q
    'nu_in_H'        : [3], # frequency component for H
    'perform_anal': ['A', 'B', 'C', 'D', 'H', 'Q', 'S']} # performing analysis
```

3.2 sample

- Steinhardt order parameter [1], num of neighbor particles is 6.

```
  order_parameter_parameter = {
  'ave_times'      : 1,
  'neighbor'       : [6],
  'radius'         : [],
  'oi_oj'          : [0],
  'o_factor'       : [1.00],
  'b_in_Q'         : 1,
  'l_in_Q'         : [2, 4, 6],
  'P_in_Q'         : [0],
  'm_in_A'         : [2],
  'perform_anal': ['Q']}
```

- Lechner order parameter [2], neighbor distance is 1.75.

```
  order_parameter_parameter = {
  'ave_times'      : 1,
  'neighbor'       : [],
  'radius'         : [1.75],
  'oi_oj'          : [0],
  'o_factor'       : [1.00],
  'b_in_Q'         : 2,
  'l_in_Q'         : [2, 4, 6],
```

```
'P_in_Q'         : [0],
'm_in_A'         : [2],
'perform_anal': ['Q']}
```

3.3 Format of output data

```
order_param_datas = op_analyze_without_neighbor_list(coord, direct, box_length, order_para
```

- now you can get access as follows.

  `order_param_datas['Q_N6']['a=1_b_1_of_1.00_oi=0_oj=0'].`

- Q : types of order parameter
- N6 : num of neighbor particles, if you used the neighbor distance, this string changes "R1.75"
- a=1 : ave_times
- b_1 : b_in_Q
- of : o_factor

Reference

[1] P.J. Steinhardt, D.R. Nelson, M. Ronchetti, Bond-orientational order in liquids and glasses, Physical Review B. 28 (1983) 784–805. doi:10.1103/PhysRevB.28.784.

[2] W. Lechner, C. Dellago, Accurate determination of crystal structures based on averaged local bond order parameters, Journal of Chemical Physics. 129 (2008) 114707. doi:10.1063/1.2977970.