A brief introduction of *modGro*

Jian Zhang

jianzhang1920@gmail.com

2025-Mar-9

Main Function 1: Show residue information

- *Show all residue information on the present system*: Show all atoms and residues information on the screen

If you choose ***Show all residue information on the present system***, something like the following will be displayed on the screen

1MOL	O	1	0.256	0.435	0.333
1MOL	O	2	1.382	2.384	0.333
1MOL	O	3	0.121	1.259	0.350
1MOL	O	4	1.246	3.208	0.350
		……			
5MOL	C	1199	1.246	3.208	0.350

In fact, this information above is the information in the gro file after removing the number of atoms and the box size

Main Function 1: Show residue information

- *Show particular residue in index of the residue*: Show particular atoms and residues information on the screen

If you choose ***Show particular residue in index of the residue***, and Enter ***1***, something like the following will be displayed on the screen

You also can Enter something, just like 1,2,9-10,4

Information about residues in the system with **a residue index of 1** is displayed on the screen

1MOL	O	1	0.256	0.435	0.333
1MOL	O	2	1.382	2.384	0.333
1MOL	O	3	0.121	1.259	0.350
1MOL	O	4	1.246	3.208	0.350
		……			
1MOL	C	240	1.246	3.208	0.350

Main Function 1: Show residue information

- *Show particular atom in index of the atom*: Show particular atoms information on the screen

If you choose ***Show particular atom in index of the atom***, and Enter ***1-10***, something like the following will be displayed on the screen

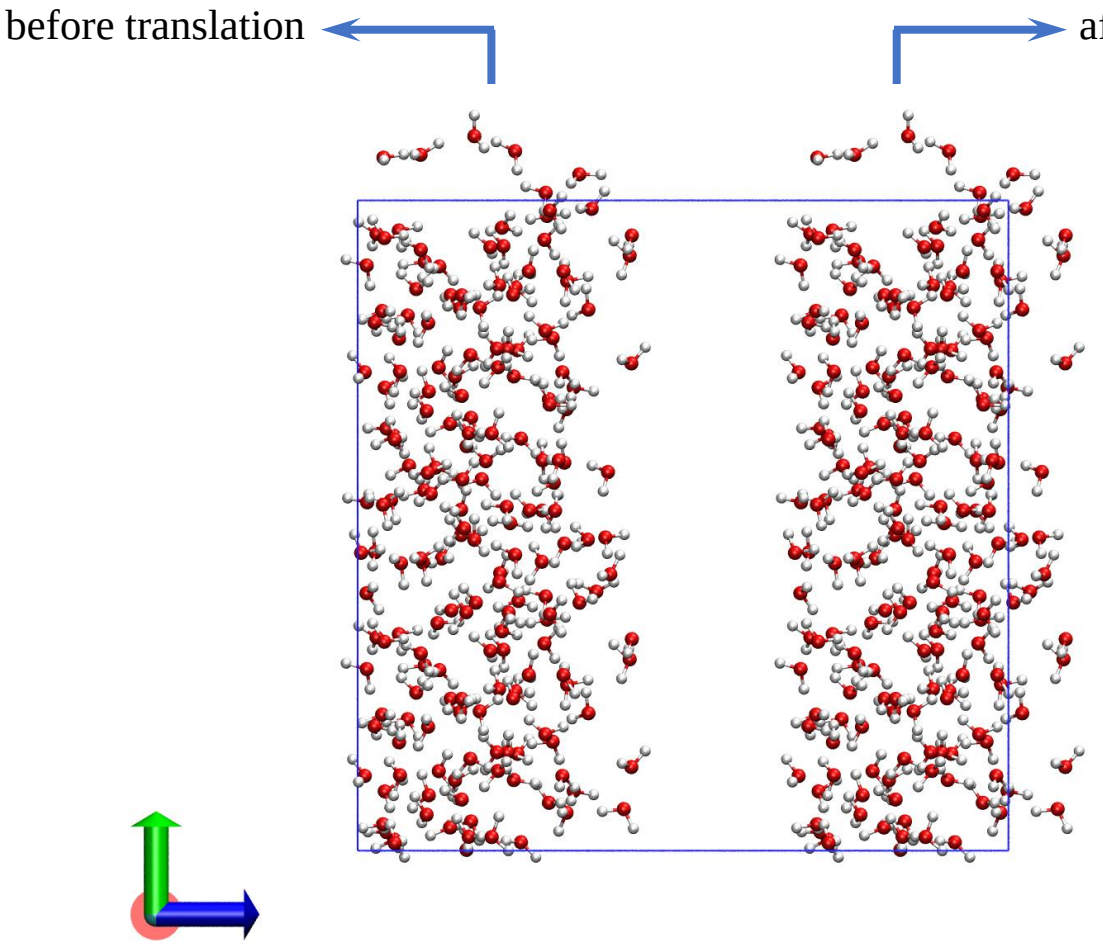
You also can Enter something, just like 1,2,9-10,4

Information about atom in the system with **a residue index of 1 to 10** is displayed on the screen

1MOL	O	1	0.256	0.435	0.333
1MOL	O	2	1.382	2.384	0.333
1MOL	O	3	0.121	1.259	0.350
1MOL	O	4	1.246	3.208	0.350
		……			
1MOL	C	10	1.246	3.208	0.350

Main Function 2: Geometry operation on the present system

- *Translate selected residues according to a translation vector*: You can input translation vector and translate selected residue



example/example-1-input.gro # Load gro file

2 # Geometry operation on the present system

1 # Translate selected residue according to a translation vector

[Enter] # Select all atoms

0,0,20 # Translation vector

0 # Return

4 # Output gro file

example/example-1-out.gro # Path for outputting gro file

Main Function 2: Geometry operation on the present system

- *Rotate selected residues around an axis*: Rotate selected residue

rotation matrix

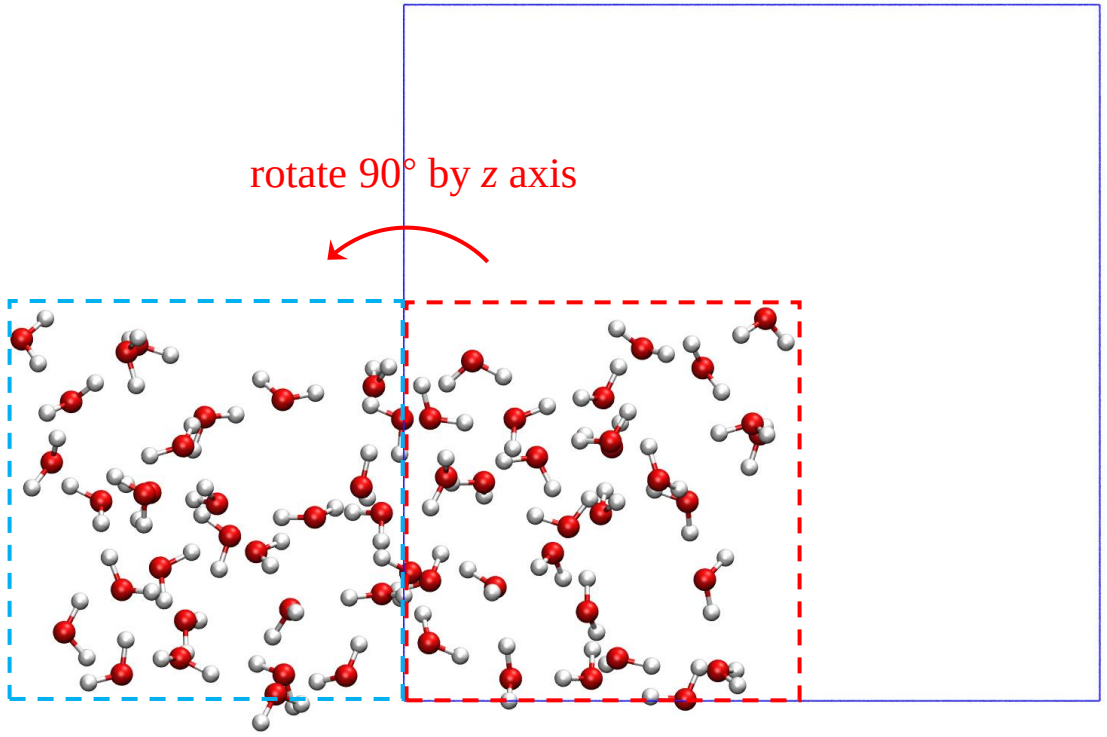
$\boldsymbol{v}_{\text{new}} = \boldsymbol{M}\boldsymbol{v}_{\text{old}}$ — column vector consisting of *x*, *y* and *z*

$\boldsymbol{w}_{\text{new}} = \boldsymbol{w}_{\text{old}}\boldsymbol{M}$ — row vector consisting of *x*, *y* and *z*

$$M = \begin{bmatrix} u_x^2(1-\cos\theta)+\cos\theta & u_x u_y(1-\cos\theta)-u_z\sin\theta & u_x u_z(1-\cos\theta)+u_y\sin\theta \\ u_x u_y(1-\cos\theta)+u_z\sin\theta & u_y^2(1-\cos\theta)+\cos\theta & u_y u_z(1-\cos\theta)-u_x\sin\theta \\ u_x u_z(1-\cos\theta)-u_y\sin\theta & u_y u_z(1-\cos\theta)+u_x\sin\theta & u_z^2(1-\cos\theta)+\cos\theta \end{bmatrix}$$

Main Function 2: Geometry operation on the present system

- *Rotate selected residues around an axis*: Rotate selected residue



example/example-2-input.gro # Load gro file

2 # Geometry operation on the present system

2 # Rotate selected residue around an axis

[Enter] # Select all atoms

0,0,1 # Rotation vector

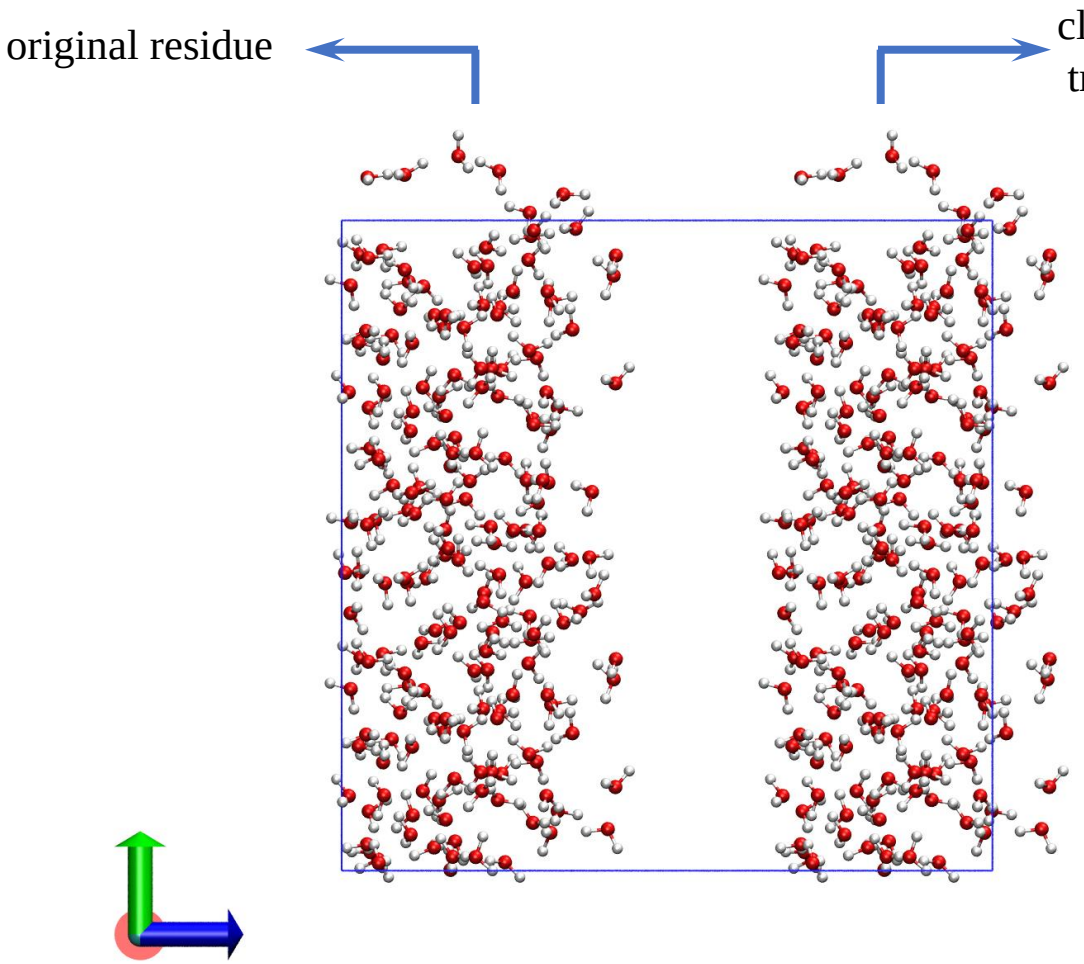
0 # Return

4 # Output gro file

example/example-2-out.gro # Path for outputting gro file

Main Function 2: Geometry operation on the present system

- *Clone residues*: Clone selected residue



example/example-1-input.gro # Load gro file

2 # Geometry operation on the present system

3 # Clone selected residue

[Enter] # Select all atoms

1 # Translate atoms

287-572 # Indices of the residue

0,0,20 # Translation vector

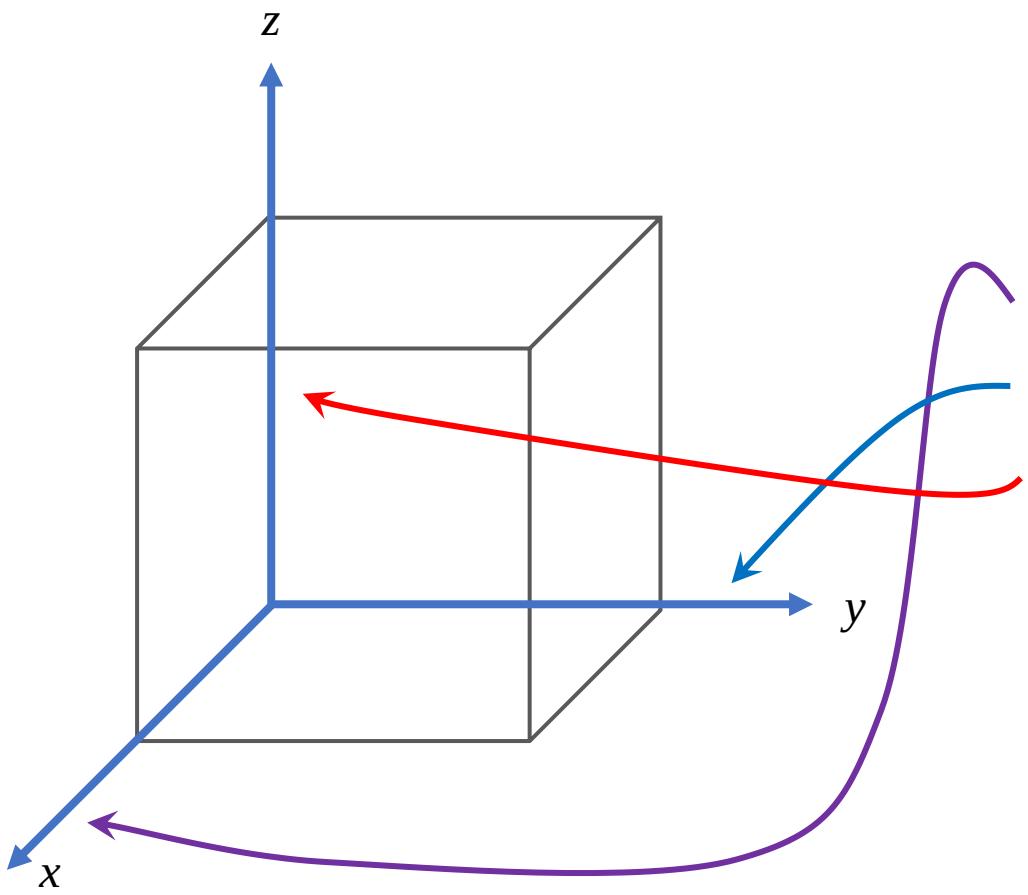
0 # Return

4 # Output gro file

example/example-2-out.gro # Path for outputting gro file

Main Function 2: Geometry operation on the present system

- *Remove residues*: Remove selected residue
- *Set cell information*: Set cell information




```
example/example-1-input.gro   # Load gro file
2    # Geometry operation on the present system
5    # Set cell information
40,0,0      # Cell vector for the first axis
0,40,0      # Cell vector for the second axis
0,0,40      # Cell vector for the third axis
0           # Return
q           # Exit program
```

Main Function 2: Geometry operation on the present system

- *Merge multiple .gro file*: Merge gro file one by one

example/example-1-input.gro # Load gro file
2 # Geometry operation on the present system
6 # Merge multiple .gro file
example/example-1-input.gro # Load gro file
0 # Return
q # Exit program

- *Check residues coordinate information*: Get the coordinate range of the selected residue

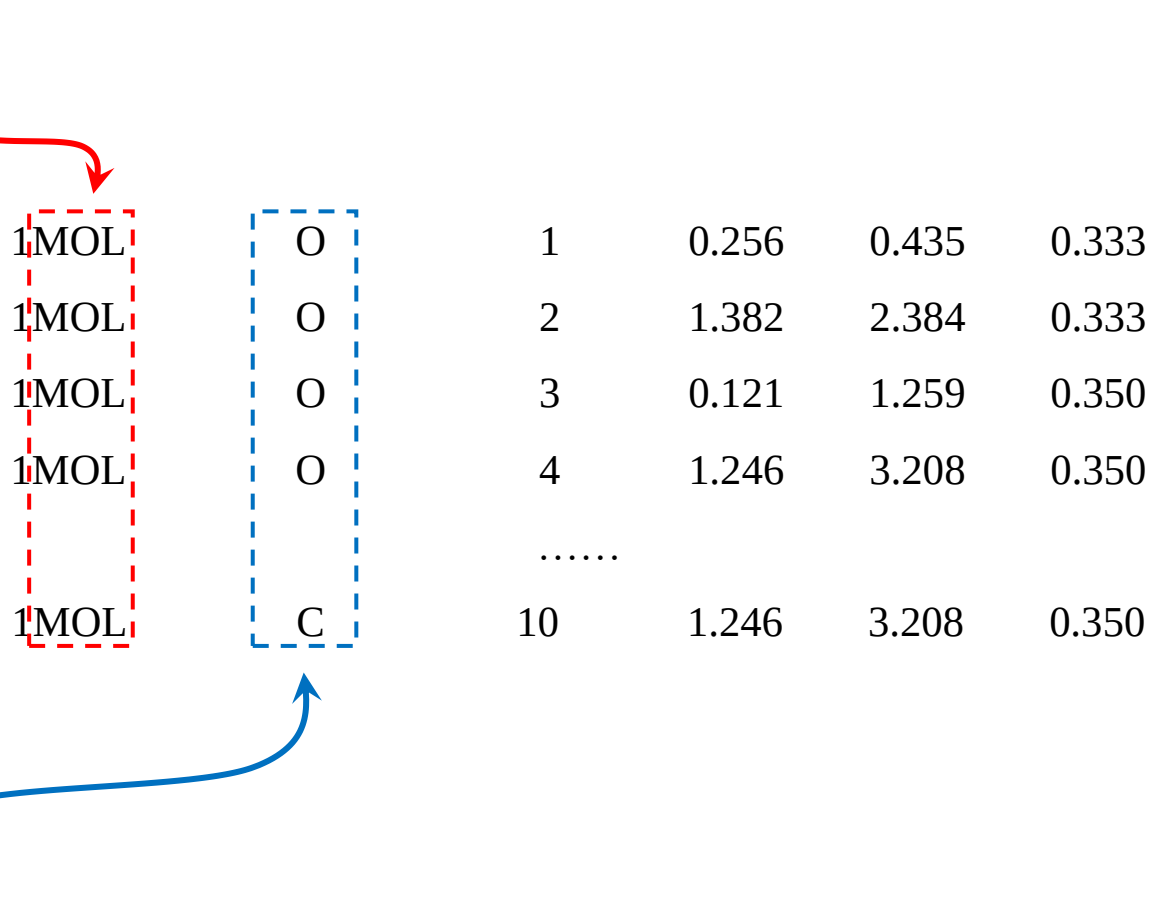
If you choose ***Check residues coordinate information***, something like the following will be displayed on the screen

Note: The unit is Angstrim

x:	Min:	-0.850	Max:	31.570
y:	Min:	-0.300	Max:	33.920
z:	Min:	-0.530	Max:	13.260

Main Function 3: Modify the residue or atom names

- *Modify the residue names*



- *Modify the atom names*

How to store information of *.gro* file? Use Map