

#Author: Jingwen Qian ID:108660470

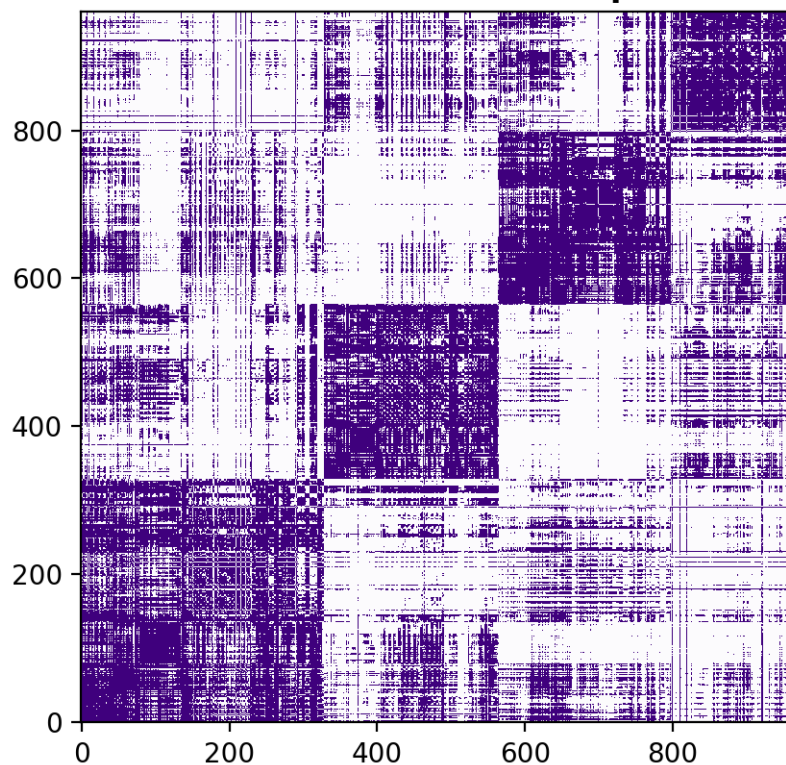
Output

To plot an interaction map, please enter the file name: hamreal1-C.dat

This is what the first 10 by 10 matrix looks like:

```
[[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  0.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]  
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]
```

Atom Interaction Map



Map is generated.

The dimension is: (961, 961)

The two partial matrices associated with the first two interaction info:

```
[[ -0.4955  0.    0.    0.   ]
 [  0.   -0.1939  0.    0.   ]
 [  0.    0.   -0.1939  0.   ]
 [  0.    0.    0.   -0.1939]]
[[-0.22332459 -0.06446747  0.03992473 -0.22968922]
 [ 0.06446747 -0.06602348 -0.01421713  0.08179194]
 [-0.03992473 -0.01421713 -0.08017556 -0.05065379]
 [ 0.22968922  0.08179194 -0.05065379  0.20243385]]
The dimension of M is: (3844, 3844)
```