1: for(int i=0;i < atomnum;i++)

2: for(int j=0;j < atomnum;j++)

**3: if( atoms[i].id >= atoms[j].id )**

4: continue;

5: r = ( atoms[i].pos- atoms[j].pos ) \* ( atoms[i].pos - atoms[j].pos );

6: r = sqrt(r);

**7: if( r > r0 )** //距离大于截断半径

8: continue;

9: u = calu(r); //计算势能

10: f = calforce(r); //由势函数的梯度函数求得

11: atoms[i].force -= f;

12: atoms[j].force += f;

13: atoms[i].u += 1/2\*u;

14: atoms[j].u += 1/2\*u;