Testing MC Notebook

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In this notebook different aspects of the Monte Carlo program will be tested separatedly to secure all works well and is as optimized as possible.

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import scipy as sp
%matplotlib inline
```

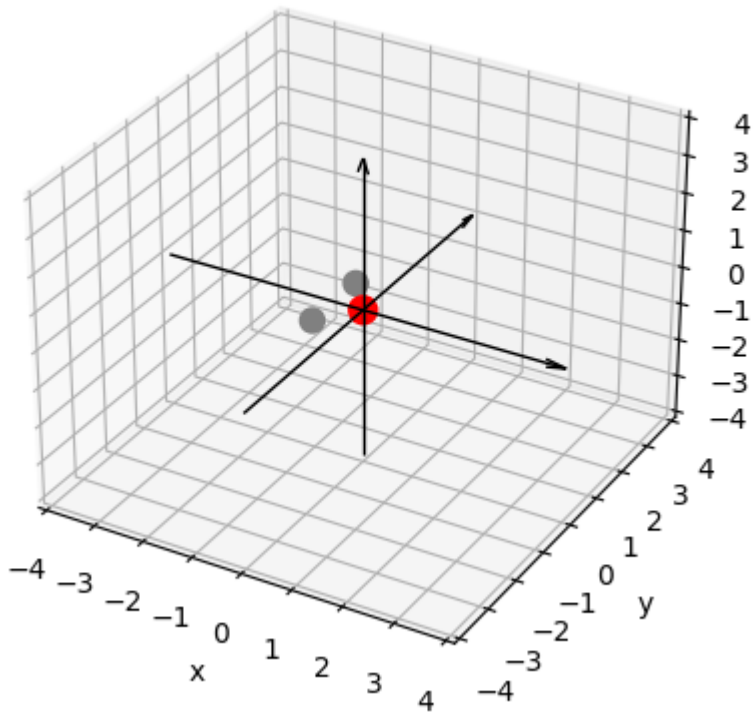
Testing the rotation matrices and visualization of coordinates

In [2]:
```
def rotate(Ax,Ay,Az,testCoord,atype="deg"):
        """Rotates the molecule a specified angle (in degrees) for each main axis."
        atype = atype.lower()
        if atype == "deg" or atype == "d": Ax,Ay,Az = np.radians(Ax),np.radians(Ay)
        elif atype == "rad" or atype == "r": pass
        else: raise TypeError("Angle type not detected. Choose deg for degrees or r

        # Rotation matrices
        Rx = np.array([[1,0,0],[0,np.cos(Ax),-np.sin(Ax)],[0,np.sin(Ax),np.cos(Ax)]
        Ry = np.array([[np.cos(Ay),0,np.sin(Ay)],[0,1,0],[-np.sin(Ay),0,np.cos(Ay)]
        Rz = np.array([[np.cos(Az),-np.sin(Az),0],[np.sin(Az),np.cos(Az),0],[0,0,1]

        # Rotates the molecule the specified angles
        for i in range(3):
            for _,R in enumerate([Rx,Ry,Rz]):
                ctemp = testCoord[i].copy()
                testCoord[i] = np.dot(R,ctemp)

def draw(coord,ax):
        ax.scatter(coord.T[0],coord.T[1],coord.T[2], sizes=(100,75,75), c=("red","g
```

In [3]:
```
# Testing Rotation
axes = np.array([[1,0,0],[0,1,0],[0,0,1]])
water = np.array([[0.,0.,0.],[0.75669,0.58589,0.],[-0.75669,0.58589,0.]])
coord = water

rotate(0,0,90,coord)
print(coord)

# Testing Visualization
fig = plt.figure()
ax = plt.axes(projection="3d")
draw(coord,ax)

lim = 4 #box limit
ax.quiver(-lim, 0, 0, 2*lim, 0, 0, color='k',lw=1, arrow_length_ratio=0.05)      # x
ax.quiver(0, -lim, 0, 0, 2*lim, 0, color='k',lw=1, arrow_length_ratio=0.05)      # y
ax.quiver(0, 0, -lim, 0, 0, 2*lim, color='k',lw=1, arrow_length_ratio=0.05)      # z
ax.set_xlim(-lim,lim);ax.set_ylim(-lim,lim);ax.set_zlim(-lim,lim)                 # B
ax.set_xlabel("x");ax.set_ylabel("y");ax.set_zlabel("z")                          # A
```

```
[[ 0.       0.       0.     ]
 [-0.58589  0.75669  0.     ]
 [-0.58589 -0.75669  0.     ]]
```

Out[3]: Text(0.5, 0, 'z')



In [4]:
```
#Energies parameters (VdW A and B, and coulomb charges)
A = np.array([[581935.563838,328.317371,328.317371],
              [328.317371,9.715859e-6,9.715859e-6],
              [328.317371,9.715859e-6,9.715859e-6]])
B = np.array([[594.825035,10.478040,10.478040],
              [10.478040,0.001337,0.001337],
              [10.478040,0.001337,0.001337]])
q = np.array([-0.834,+0.417,+0.417])
Q = np.dot(q[:,None],q[:,None].T)

coord1 = np.array([[-3.843,  -4.381,   2.479],
                   [-2.987,  -4.032,   2.783],
                   [-4.475,  -3.954,   3.055]])
coord2 = np.array([[-1.523,  -3.299,   3.460],
                   [-1.041,  -2.606,   3.024],
                   [-0.912,  -3.781,   4.007]])
```

In [5]:
```
def coulomb(qi,qj,r):
    """Returns coulomb energy between i-j pair."""
    kcal = 332.0 #To return the results in kcal/mol
    return kcal*qi*qj/r

def vdW(A,B,r):
    """Returns Van der Waals energy between i-j pair."""
    return A/r**12 - B/r**6


def looping(coord1,coord2):
        """Gets energy by looping each molecule coordinates"""
        n1 = len(coord1)
        n2 = len(coord2)

        E,Eelec,Evdw = 0,0,0
        for i in range(n1):      # For each atom in molecule 1
            for j in range(n2):  # For each atom in molecule 2
                r = np.linalg.norm(coord2[j]-coord1[i])
                # Calculadas a pares de c[1]-c[2] (no energias interas)
                Evdw += vdW(A[i][j],B[i][j],r)
                Eelec += coulomb(q[i],q[j],r)
        E = Eelec+Evdw
        return E,Eelec,Evdw

def numpyHand(coord1,coord2):
    """Gets energy using numpy arrays broadcasting and matrix operations"""

    diff = coord1-coord2[:,None]
    distances = np.sqrt((diff**2).sum(axis=-1)).T

    Evdw = (A/distances**12 - B/distances**6).sum()
    Eelec = (332.0*Q/distances).sum()
    E = Evdw + Eelec

    return E,Eelec,Evdw

def numpyLinalg(coord1,coord2):
    """Same as NumpyHand but using linalg.norm"""

    diff = coord1-coord2[:,None]
    distances = np.linalg.norm(diff, axis=-1).T

    Evdw = (A/distances**12 - B/distances**6).sum()
    Eelec = (332.0*Q/distances).sum()
    E = Evdw + Eelec

    return E,Eelec,Evdw

def scipycdist(coord1,coord2):
    """Gets energies with SciPy cdist"""
    distances = sp.spatial.distance.cdist(coord1,coord2)

    Evdw = (A/distances**12 - B/distances**6).sum()
    Eelec = (332.0*Q/distances).sum()
    E = Evdw + Eelec
```

```
    return E,Eelec,Evdw
```

In [6]:
```
#Comprobamos que los diferentes métodos den la misma energia
for method in [looping,numpyHand,numpyLinalg,scipycdist]:
    print(method.__name__)
    E,Eelec,Evdw = method(coord1,coord2)
    print(E,Eelec,Evdw)

# Todo OK
```

```
looping
-6.7650294301612615 -8.57096741359117 1.8059379834299079
numpyHand
-6.765029430161267 -8.570967413591175 1.805937983429908
numpyLinalg
-6.765029430161267 -8.570967413591175 1.805937983429908
scipycdist
-6.765029430161267 -8.570967413591175 1.805937983429908
```

Here will be tested the scaling and time consumption of the diferent energy calculation functions. Since with the Monte Carlo program a lots of steps and calculations are performed, it is important to optimize the code as much as possible to bring faster results. As we know, Python by itself is pretty slow and libraries such as `NumPy` or `SciPy` do a better job when dealing with array/matrix calculations.

For that reason, a method using matrices to calculate the pair-distances and energies is chosed to get faster results. Below are tested diferent implementations of this new method using NumPy `arrays` and `broadcasting` and the `cdist()` SciPy function.

In [123…
```
#Miramos cuanto tardan y escalado segun el numero de coordenadas
nPoints = np.logspace(1,4,10)
times = [[] for _ in range(4)]
for n in nPoints:
    coord1 = np.random.uniform(1,2,size=(int(n),3))
    coord2 = np.random.uniform(1,2,size=(int(n),3))
    A = np.random.uniform(1,2,size=(int(n),int(n)))
    B = np.random.uniform(1,2,size=(int(n),int(n)))
    q = np.random.uniform(-1,1,size=(int(n)))
    Q = np.dot(q[:,None],q[:,None].T)

    for i,method in enumerate([looping,numpyHand,numpyLinalg,scipycdist]):
        print(method.__name__)
        t = %timeit -o method(coord1,coord2)
        times[i].append(t.average)
times = np.array(times)
# Ojo al correr esta celda que tarda ~1h en evaluar todos los tiempos
```

```
looping
471 µs ± 392 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyHand
31.1 µs ± 84.8 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
numpyLinalg
32.8 µs ± 37.3 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
scipycdist
19.7 µs ± 17.9 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
looping
2.08 ms ± 8.53 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyHand
49.5 µs ± 33.7 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
numpyLinalg
51.5 µs ± 57.6 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
scipycdist
36.8 µs ± 22.8 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
looping
9.92 ms ± 12.3 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyHand
164 µs ± 532 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
numpyLinalg
169 µs ± 3.22 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
scipycdist
121 µs ± 800 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
looping
46.6 ms ± 97.9 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyHand
684 µs ± 542 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyLinalg
697 µs ± 8.2 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
scipycdist
500 µs ± 1.28 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
looping
215 ms ± 1.03 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
4.36 ms ± 273 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyLinalg
4.17 ms ± 129 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
scipycdist
2.29 ms ± 10.9 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
looping
1.01 s ± 3.86 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
21.8 ms ± 116 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyLinalg
21.9 ms ± 87.8 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
scipycdist
14.8 ms ± 199 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
looping
4.67 s ± 14.3 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
144 ms ± 90.7 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyLinalg
107 ms ± 586 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
scipycdist
68.3 ms ± 1.04 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

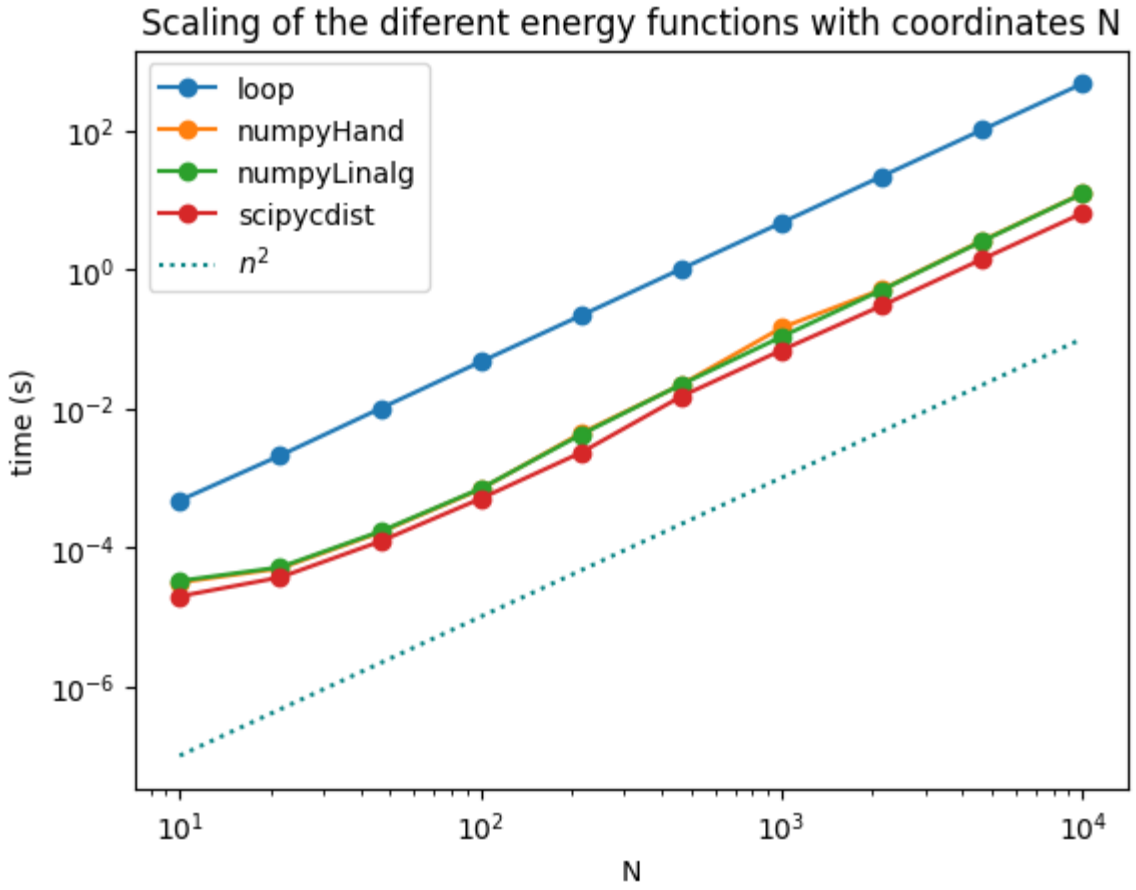
```
looping
21.7 s ± 114 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
510 ms ± 9.14 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyLinalg
501 ms ± 4.28 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
scipycdist
299 ms ± 3.09 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
looping
1min 41s ± 770 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
2.57 s ± 37.8 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyLinalg
2.53 s ± 13 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
scipycdist
1.39 s ± 14.9 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
looping
7min 48s ± 817 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
12.3 s ± 102 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyLinalg
12.2 s ± 144 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
scipycdist
6.4 s ± 19.2 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

As you can see in the plot below, each method scales with N^2 (N = number of coordinates in molecule), as expected, but the time used by the simple looping method using native Python is much higher than the ones using numpy arrays and matrix calculations. For that reason, in order to make the program as faster and optimized as posible, the arrays/matrices method will be used in the Monte Carlo program.

In [132…

```python
# Ploting df columns (timepoints)
for time in times:
    plt.loglog(nPoints,time, "o-")

# Ploting n**2 dependencies (adjusted to fit plot)
plt.plot(nPoints,nPoints**2*1e-9,":", c="teal")

# Plot settings
plt.xlabel("N"); plt.ylabel("time (s)")
plt.title("Scaling of the diferent energy functions with coordinates N")
plt.legend(["loop","numpyHand","numpyLinalg","scipycdist",r"$n^2$"])
```

Out[132]: <matplotlib.legend.Legend at 0x24b58a1a560>



In [136…

```
# Miramos cuanto tardan y escalado segun el numero de steps
nPoints2 = np.logspace(1,5,8)
times2 = [[] for _ in range(4)]

coord1 = np.random.uniform(1,2,size=(3,3))
coord2 = np.random.uniform(1,2,size=(3,3))
A = np.random.uniform(1,2,size=(3,3))
B = np.random.uniform(1,2,size=(3,3))
q = np.random.uniform(-1,1,size=(3))
Q = np.dot(q[:,None],q[:,None].T)

for n in nPoints2:
    for i,method in enumerate([looping,numpyHand,numpyLinalg,scipycdist]):
        print(method.__name__)
        t = %timeit -o for _ in range(int(n)): method(coord1,coord2)
        times2[i].append(t.average)
times2 = np.array(times2)
```

```
looping
737 µs ± 3.29 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyHand
331 µs ± 2.17 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyLinalg
227 µs ± 21.6 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
scipycdist
153 µs ± 1.67 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
looping
1.6 ms ± 10.5 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyHand
741 µs ± 11.4 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
numpyLinalg
812 µs ± 11.4 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
scipycdist
559 µs ± 1.59 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
looping
6.02 ms ± 93.5 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyHand
2.71 ms ± 8.91 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyLinalg
2.94 ms ± 22.3 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
scipycdist
2.11 ms ± 57.3 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
looping
22.8 ms ± 627 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyHand
10.2 ms ± 18.9 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
numpyLinalg
11.2 ms ± 225 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
scipycdist
7.8 ms ± 19.5 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
looping
83.4 ms ± 408 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyHand
38.2 ms ± 335 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyLinalg
42.3 ms ± 1.25 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
scipycdist
29.6 ms ± 470 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
looping
309 ms ± 1.45 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
145 ms ± 2.23 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
numpyLinalg
156 ms ± 2.39 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
scipycdist
109 ms ± 566 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
looping
1.17 s ± 8.13 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
527 ms ± 3.04 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyLinalg
575 ms ± 5.59 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
scipycdist
414 ms ± 5.77 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

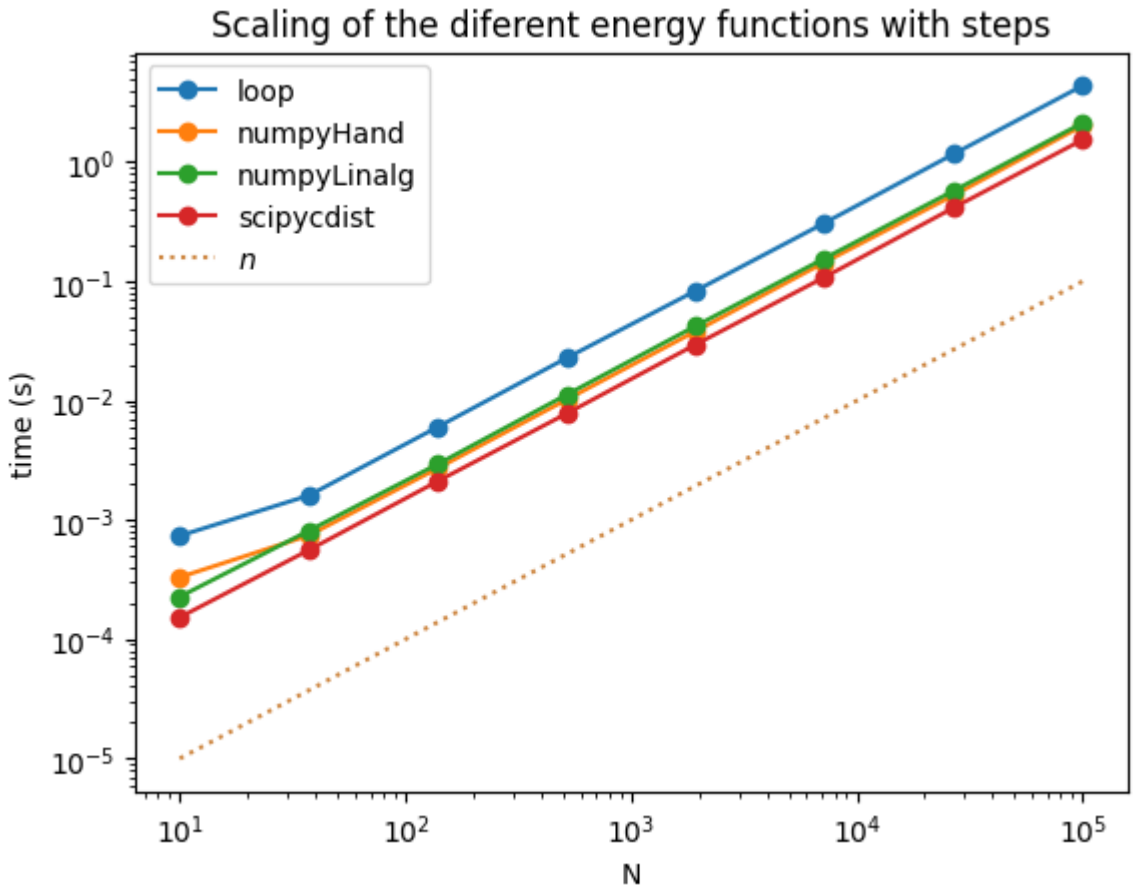
```
looping
4.37 s ± 39.3 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyHand
2.02 s ± 26.2 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
numpyLinalg
2.13 s ± 18.7 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
scipycdist
1.54 s ± 26 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Here, you can also see the scaling and time with the number of steps. As expected all scale linearly with N. Again, using the normal loop method gives slower results than using NumPy or SciPy.

In [137…

```
# Ploting df columns (timepoints)
for time in times2:
    plt.loglog(nPoints2,time, "o-")

# Ploting n dependencies (adjusted to fit plot)
plt.plot(nPoints2,(nPoints2)*1e-6,":", c="peru")

# Plot settings
plt.xlabel("N"); plt.ylabel("time (s)")
plt.title("Scaling of the diferent energy functions with steps")
plt.legend(["loop","numpyHand","numpyLinalg","scipycdist",r"$n$"])
```

Out[137]: `<matplotlib.legend.Legend at 0x24b5657d3f0>`



Instead of double looping over the coordinates to calculate the energies pair by pair (very slow), you can use arrays and broadcasting to work with matrices and faster. Below are a few examples.

In [27]:
```
#Para poder haver vector x vector.T = matrix hay que añadir nueva dimensión (vector
Qij = np.dot(q[:,None],q[:,None].T)
print(Qij)
#Lo mismo pasa con sumas/restas
Qijr =(q[:,None]-q[:,None].T)
print(Qijr)
```

```
[[ 0.695556 -0.347778 -0.347778]
 [-0.347778  0.173889  0.173889]
 [-0.347778  0.173889  0.173889]]
[[ 0.    -1.251 -1.251]
 [ 1.251  0.     0.   ]
 [ 1.251  0.     0.   ]]
```

In [10]:
```
#Se puede calcular la matriz de distancias con arrays y broadcasting
diff1 = coord1-coord2[:,None]
diff1 = diff1**2
diff1 = diff1.sum(axis=-1)
diff1 = np.sqrt(diff1)
print(diff1.T)
```

```
[[2.74143849 3.3613768  3.35939652]
 [1.77169806 2.42455625 2.42214822]
 [3.05079563 3.68923041 3.69204577]]
```

In [92]:
```
#Lo mismo pero mas resumido
diff = coord1-coord2[:,None]
distances = np.sqrt((diff**2).sum(axis=-1)).T
print(distances)
```

```
[[2.74143849 3.3613768  3.35939652]
 [1.77169806 2.42455625 2.42214822]
 [3.05079563 3.68923041 3.69204577]]
```

In [88]:
```
#Lo mismo pero utilizando np.linalg.norm
diff = coord1-coord2[:,None]
distances = np.linalg.norm(diff, axis=-1).T
print(distances)
```

```
[[2.74143849 3.3613768  3.35939652]
 [1.77169806 2.42455625 2.42214822]
 [3.05079563 3.68923041 3.69204577]]
```

In [93]:
```
#SciPy tiene cdist que pinta bien
distances = sp.spatial.distance.cdist(coord1,coord2)
print(distances)
print(A/distances)
```

```
[[2.74143849 3.3613768  3.35939652]
 [1.77169806 2.42455625 2.42214822]
 [3.05079563 3.68923041 3.69204577]]
[[2.12273799e+05 9.76734804e+01 9.77310564e+01]
 [1.85312260e+02 4.00727309e-06 4.01125700e-06]
 [1.07616966e+02 2.63357338e-06 2.63156515e-06]]
```