1 Intertial Brownian motion simulation

One can write the Langevin equation as:

$$m\ddot{x} = -\gamma\dot{x} + \sqrt{2k_\mathrm{B}T\gamma}\mathrm{d}B_t \tag{1}$$

By replacing with the Euler method $\dot{x}$ by:

$$\dot{x} \simeq \frac{x_i - x_{i-1}}{\tau} , \tag{2}$$

$\ddot{x}$ by:

$$\begin{aligned} \ddot{x} &\simeq \frac{\frac{x_i - x_{i-1}}{\tau} - \frac{x_{i-1}-x_{i-2}}{\tau}}{\tau} \\ &= \frac{x_i - 2x_{i-1} + x_{i-2}}{\tau^2} . \end{aligned} \tag{3}$$

and finally, $\mathrm{d}B_t$ by a Gaussian random number w_i with a zero mean value and a τ variance, on can write x_i as:

$$x_i = \frac{2+\tau/\tau_\mathrm{B}}{1+\tau/\tau_\mathrm{B}}x_{i-1} - \frac{1}{1+\tau/\tau_\mathrm{B}}x_{i-2} + \frac{\sqrt{2k_\mathrm{B}T\gamma}}{m(1+\tau/\tau_\mathrm{B})}\tau w_i , \tag{4}$$

We will in the following use Python to simulate such a movement and check the properties of the mean squared displacement. In the end I will propose a Cython implementation that permits a 1000x speed improvement on the simulation.

[1]:
```python
# Import important libraries
import numpy as np
import matplotlib.pyplot as plt
```

[2]:
```python
# Just some matplotlib tweaks
import matplotlib as mpl

mpl.rcParams["xtick.direction"] = "in"
mpl.rcParams["ytick.direction"] = "in"
mpl.rcParams["lines.markeredgecolor"] = "k"
mpl.rcParams["lines.markeredgewidth"] = 1.5
mpl.rcParams["figure.dpi"] = 200
from matplotlib import rc

rc("font", family="serif")
rc("text", usetex=True)
rc("xtick", labelsize="medium")
rc("ytick", labelsize="medium")
rc("axes", labelsize="large")
```

```python
def cm2inch(value):
    return value / 2.54
```

[3]:
```python
N = 1000000  # length of the simulation
tau = 0.01  # simulation time step
m = 1e-8  # particle mass
a = 1e-6  # radius of the particle
eta = 0.001  # viscosity (here water)
gamma = 6 * np.pi * eta * a
kbT = 4e-21
tauB = m / gamma
```

[4]:
```python
print(
    "With such properties we have a characteristic diffusion time of {:.2f} s".
 ↪format(
        tauB
    )
)
```

```
With such properties we have a characteristic diffusion time of 0.53 s
```

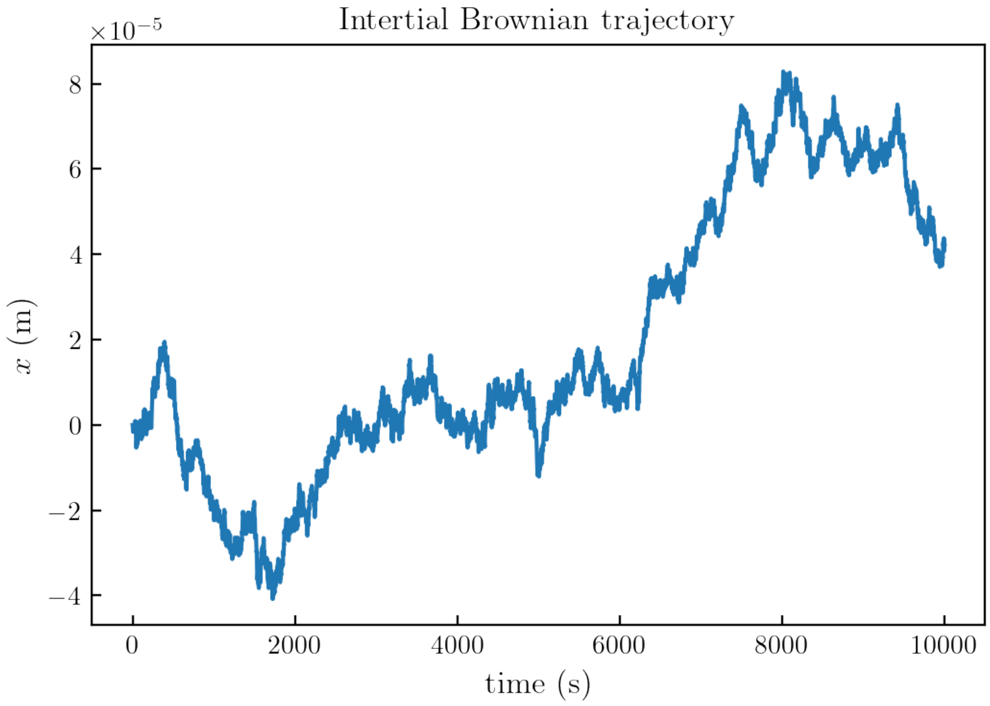
[5]:
```python
def xi(xi1, xi2):
    """
    Function that compute the position of a particle using the full Langevin␣
 ↪Equation
    """
    t = tau / tauB
    wi = np.random.normal(0, np.sqrt(tau))
    return (
        (2 + t) / (1 + t) * xi1
        - 1 / (1 + t) * xi2
        + np.sqrt(2 * kbT * gamma) / (m * (1 + t)) * np.power(tau,1) * wi
    )
```

[6]:
```python
def trajectory(N):
    x = np.zeros(N)
    for i in range(2, len(x)):
        x[i] = xi(x[i - 1], x[i - 2])
    return x
```

Now that the functions are setup one can simply generate a trajectory of length N by simply calling the the function `trajectory()`

[7]:
```python
# Generate a trajectory of 10e6 points.
x = trajectory(1000000)
```

[8]:
```
plt.plot(np.arange(len(x))*tau, x)
plt.title("Intertial Brownian trajectory")
plt.ylabel("$x$ (m)")
plt.xlabel("time (s)")
plt.show()
```



1.1 Cross checking

As we are dealing with intertial Brownian motion, the later is characterize by a characteristic time $\tau_\mathrm{B} = m/\gamma$. We will check that the simulated trajectory gives us the correct MSD properties to ensure the simulation si done properly. The MSD given by:

$$\mathrm{MSD}(\tau) = \langle (x(t) - x(t+\tau)^2 \rangle \Big|_t \,, \tag{5}$$

with Δt a lag time. The MSD, can be computed using the function defined in the cell below. For times $\tau << \tau_B$ we should have:

$$\mathrm{MSD}(\tau) = \frac{k_\mathrm{B} T}{m} \tau^2 \,, \tag{6}$$

and for $\tau >> \tau_B$:

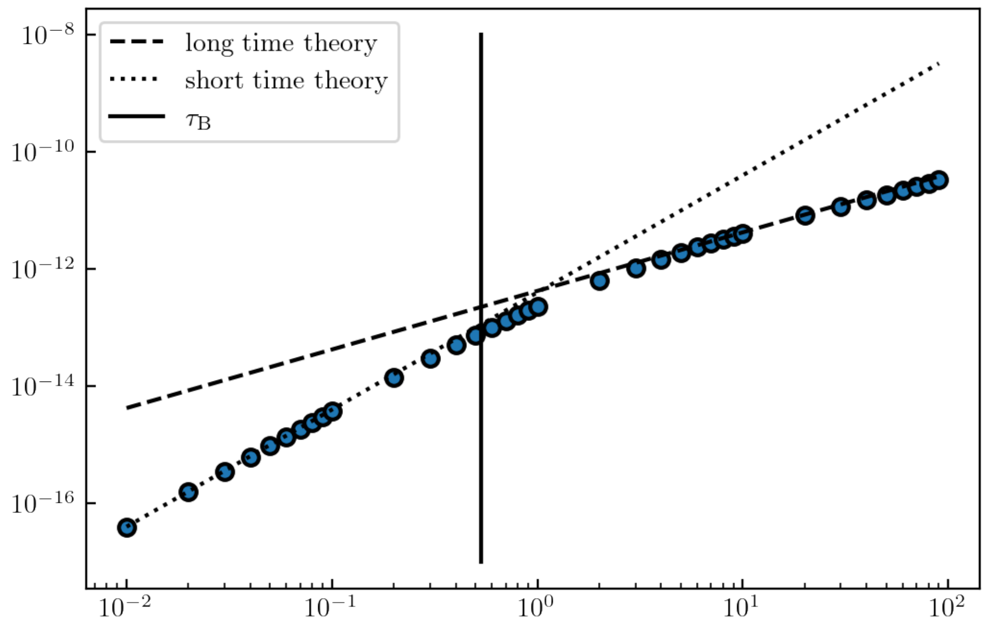
$$\mathrm{MSD}(\tau) = 2D\tau \,, \tag{7}$$

with $D = k_\mathrm{B}T/(6\pi\eta a)$.

[9]:
```
t = np.array([*np.arange(1,10,1), *np.arange(10,100,10), *np.
↪arange(100,1000,100), *np.arange(1000,10000,1000)])
def msd(x,t):
    _msd = lambda x, t : np.mean((x[:-t] - x[t:])**2)
    return [_msd(x,i) for i in t]
MSD = msd(x,t)
```

[10]:
```
D = kbT/(6*np.pi*eta*a)
t_plot = t*tau
plt.loglog(t*tau,MSD, "o")
plt.plot(t*tau, (2*D*t_plot), "--", color = "k", label="long time theory")
plt.plot(t*tau, kbT/m * t_plot**2, ":", color = "k", label="short time theory")

horiz_data = [1e-8, 1e-17]
t_horiz = [tauB, tauB]
plt.plot(t_horiz, horiz_data, "k", label="$\\tau_\mathrm{B}$")
plt.legend()
plt.show()
```



Our simulation is giving the expeted results but how much time do we need to generate this trajectory of 1000000 points

[11]:
```
%timeit trajectory(1000000)
```

```
6.32 s ± 101 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

So we need about 6 seconds to generate this trajectory, which is in the cases of someone who want to look at fine effects and need to generate millions of trajectories is too much, in order to fasten the process i will in the following use Cython to generate the trajectory using C.

1.2 Cython acceleration

[12]:
```
%load_ext Cython
```

[13]:
```
%%cython
import cython
cimport numpy as np
import numpy as np
from libc.math cimport sqrt
ctypedef np.float64_t dtype_t

cdef int N = 1000000 # length of the simulation

cdef dtype_t tau = 0.01 # simulation time step
cdef dtype_t m = 1e-8 # particle mass
cdef dtype_t a = 1e-6 # radius of the particle
cdef dtype_t eta = 0.001 # viscosity (here water)
cdef dtype_t gamma = 6 * 3.14 * eta * a
cdef dtype_t kbT = 4e-21
cdef dtype_t tauB = m/gamma
cdef dtype_t[:] x = np.zeros(N)

@cython.boundscheck(False)
@cython.wraparound(False)
@cython.nonecheck(False)
@cython.cdivision(True)
cdef dtype_t xi_cython( dtype_t xi1, dtype_t xi2, dtype_t wi):
    cdef dtype_t t = tau / tauB
    return (
        (2 + t) / (1 + t) * xi1
        - 1 / (1 + t) * xi2
        + sqrt(2 * kbT * gamma) / (m * (1 + t)) * tau * wi
    )

@cython.boundscheck(False)
@cython.wraparound(False)
@cython.nonecheck(False)
cdef dtype_t[:] _traj(dtype_t[:] x, dtype_t[:] wi):
    cdef int i
    for i in range(2, N):

        x[i] = xi_cython(x[i-1], x[i-2], wi[i])
    return x
```

```


def trajectory_cython():


    cdef dtype_t[:] wi = np.random.normal(0, np.sqrt(tau), N).astype('float64')


    return _traj(x, wi)
```

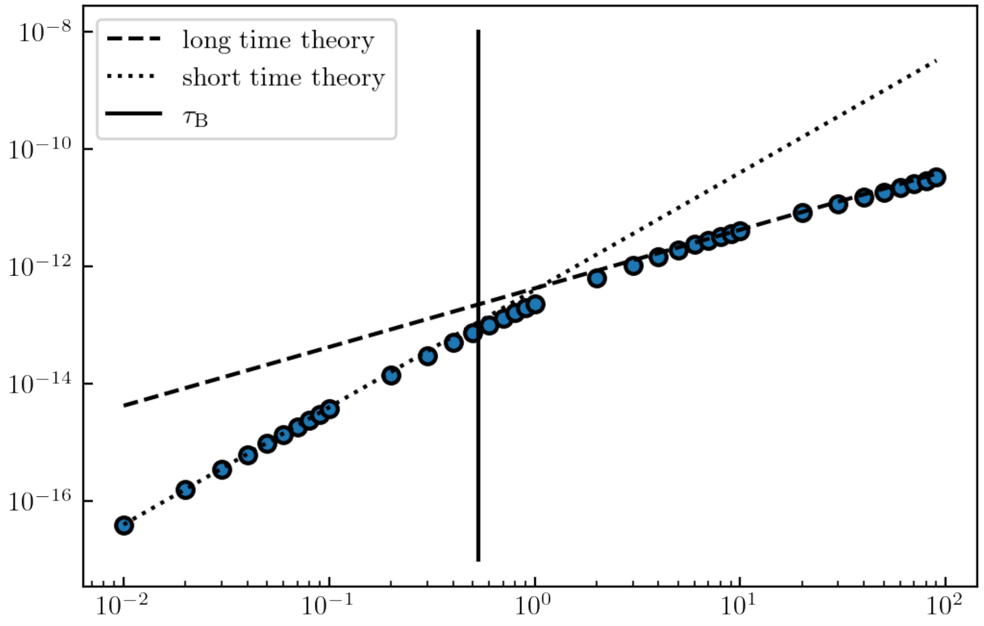
[14]:
```
%timeit trajectory_cython()
```

```
28.9 ms ± 416 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

Rapid check if the Cython code properly works.

[15]:
```
x=np.asarray(trajectory_cython())
D = kbT/(6*np.pi*eta*a)
t_plot = t*tau
plt.loglog(t*tau,MSD, "o")
plt.plot(t*tau, (2*D*t_plot), "--", color = "k", label="long time theory")
plt.plot(t*tau, kbT/m * t_plot**2, ":", color = "k", label="short time theory")

horiz_data = [1e-8, 1e-17]
t_horiz = [tauB, tauB]
plt.plot(t_horiz, horiz_data, "k", label="$\\tau_\mathrm{B}$")
plt.legend()
plt.show()
```



1.2.1 Conclusion

We finally only need $\simeq 6$ ms to generate the trajectory instead of $\simeq 6s$ which is a $\simeq 1000\times$ improvement speed. The simulation si here bound to the time needed to generate the array of random numbers which is still done using numpy function. After further checking, Numpy random generation si as optimize as one could do so there is no benefit on cythonizing the random generation. For the sake of completness one could fine a Cython version to generate random numbers. Found thanks to Senderle: https://stackoverflow.com/questions/42767816/what-is-the-most-efficient-and-portable-way-to-generate-gaussian-random-numbers

[16]:
```
%%cython
from libc.stdlib cimport rand, RAND_MAX
from libc.math cimport log, sqrt
import numpy as np
import cython

cdef double random_uniform():
    cdef double r = rand()
    return r / RAND_MAX

cdef double random_gaussian():
    cdef double x1, x2, w

    w = 2.0
    while (w >= 1.0):
        x1 = 2.0 * random_uniform() - 1.0
        x2 = 2.0 * random_uniform() - 1.0
        w = x1 * x1 + x2 * x2

    w = ((-2.0 * log(w)) / w) ** 0.5
    return x1 * w

@cython.boundscheck(False)
cdef void assign_random_gaussian_pair(double[:] out, int assign_ix):
    cdef double x1, x2, w

    w = 2.0
    while (w >= 1.0):
        x1 = 2.0 * random_uniform() - 1.0
        x2 = 2.0 * random_uniform() - 1.0
        w = x1 * x1 + x2 * x2

    w = sqrt((-2.0 * log(w)) / w)
    out[assign_ix] = x1 * w
    out[assign_ix + 1] = x2 * w
```

```
@cython.boundscheck(False)
def my_uniform(int n):
    cdef int i
    cdef double[:] result = np.zeros(n, dtype='f8', order='C')
    for i in range(n):
        result[i] = random_uniform()
    return result

@cython.boundscheck(False)
def my_gaussian(int n):
    cdef int i
    cdef double[:] result = np.zeros(n, dtype='f8', order='C')
    for i in range(n):
        result[i] = random_gaussian()
    return result

@cython.boundscheck(False)
def my_gaussian_fast(int n):
    cdef int i
    cdef double[:] result = np.zeros(n, dtype='f8', order='C')
    for i in range(n // 2):  # Int division ensures trailing index if n is odd.
        assign_random_gaussian_pair(result, i * 2)
    if n % 2 == 1:
        result[n - 1] = random_gaussian()

    return result
```

[17]:
```
%timeit my_gaussian_fast(1000000)
```

```
28.7 ms ± 963 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[18]:
```
%timeit np.random.normal(0,1,1000000)
```

```
24 ms ± 768 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

One can thus see, that even a pure C implementation can be slower than the Numpy one, thanks to impressive optimization.

[ ]:
```
```