# Statistics_of_Polymer_Models

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# 1 Statistics of Polymer Models

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Here explore some statistical properties of two simples polymer models. We use the freely jointed and the freely rotating chain and simulate both using random walk models. In all cases $N$ denotes the number of chain segments and $a$ is the segment length. For the freely rotating chain model $\theta$ is the rotation angle. In this exercise we work in two dimensions exclusively.

```
In [1]: import numpy as np
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        from scipy import stats
```

```
In [2]: # define measurement functions here

        def get_msd(X, Y, sampleLengths):
            '''
            Calculates the msd of two-dimensional trajectories.
            '''
            msd = np.zeros((len(sampleLengths),))

            for i in range(len(sampleLengths)):

                msd[i] = np.mean(np.square(X[i, :]) + np.square(Y[i, :]))

            return msd

        def FloryC(theta):
            '''
            Flory's characterictic ratio $C_{\infty}$
            '''
            return (1.0 + np.cos(theta)) / (1.0 - np.cos(theta))
```

```
In [3]: def FJC(sampleLengths, m, a = 1.0e-3, x0 = 0.0, y0 = 0.0):
            '''
            Random walk model for the freely jointed chain (FJC) in two dimensions (d = 2).
            '''
```

```
    nSamples = len(sampleLengths)
    iterations = (sampleLengths).astype(int)
    iterations[1:] = iterations[1:] - iterations[0:-1]
    totalIterations = np.cumsum(iterations)[-1]
    print("totalIterations = ",totalIterations)

    LOW, HIGH = 0.0, 2.0 * np.pi

    outx = np.zeros((nSamples, m))
    outy = np.zeros((nSamples, m))

    for k in range(m):

        x, y = x0, y0 # set initial position

        for j in range(nSamples):

            for i in range(iterations[j]):

                phi = np.random.uniform(low = LOW, high = HIGH)

                x += a * np.cos(phi)
                y += a * np.sin(phi)

            outx[j, k] = x
            outy[j, k] = y

    return outx, outy
```

```
In [4]: def FJC_vec(sampleLengths, m, a = 1.0e-3, x0 = 0.0, y0 = 0.0):
            '''
            Random walk model for the freely jointed chain (FJC) in two dimensions (d = 2).
            Vectorized version of the FJC algorithm.
            '''
            nSamples = len(sampleLengths)
            iterations = (sampleLengths).astype(int)
            iterations[1:] = iterations[1:] - iterations[0:-1]
            totalIterations = np.cumsum(iterations)[-1]
            print("totalIterations = ",totalIterations)

            LOW, HIGH = 0.0, 2.0 * np.pi

            outx = np.zeros((nSamples, m))
            outy = np.zeros((nSamples, m))

            x = np.ones((1, m)) * x0
            y = np.ones((1, m)) * y0
```

```
    outx[0, :] = x
    outy[0, :] = y

    for j in range(nSamples):

        for i in range(iterations[j]):

            phis = np.random.uniform(low = LOW, high = HIGH, size = m)

            x += a * np.cos(phis)
            y += a * np.sin(phis)

            outx[j, :] = x
            outy[j, :] = y

    return outx, outy
```

To understand the implementation for the FRC algorithm below recall that in two dimensions the standard rotation matrix $R(\theta)$ reads

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} . \tag{1}$$

The binary coin flip choice at each iteration then simply decides whether the current orientation is either rotated by $R_+ := R(+\theta)$ or by $R_- := R(-\theta)$. Given a starting orientation vector $\boldsymbol{f}$ we update the orientation by invoking

$$\boldsymbol{f}_{i+1} = \begin{cases} R_+ \cdot \boldsymbol{f}_i & \text{for} \quad p_{\text{coin}} > 0.5 \\ R_- \cdot \boldsymbol{f}_i & \text{else} \end{cases} \tag{2}$$

Then the position update follows immediately as

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + a \cdot \boldsymbol{f}_{i+1} . \tag{3}$$

Here $\boldsymbol{x}$ and $\boldsymbol{f}$ are both two-dimensional position and orientation vectors, respectively.

```
In [5]: def FRC(sampleLengths, m, a = 1.0e-3, theta = 0.2 * np.pi, x0 = 0.0, y0 = 0.0):
            '''
            Random walk model for the freely rotating chain (FRC) in two dimensions (d = 2).
            '''
            nSamples = len(sampleLengths)
            iterations = (sampleLengths).astype(int)
            iterations[1:] = iterations[1:] - iterations[0:-1]
            totalIterations = np.cumsum(iterations)[-1]
            print("totalIterations = ",totalIterations)

            LOW, HIGH = 0.0, 2.0 * np.pi

            outx = np.zeros((nSamples, m))
```

```
    outy = np.zeros((nSamples, m))

    # make sure to precalculate R0 and R1 outside of all the loops below!
    R0 = np.matrix([[np.cos(theta), -np.sin(theta)],\
                    [np.sin(theta), np.cos(theta)]])
    R1 = np.matrix([[np.cos(-theta), -np.sin(-theta)],\
                    [np.sin(-theta), np.cos(-theta)]])

    for k in range(m):

        x = np.array([[x0], [y0]]) # set initial position
        phi = np.random.uniform(LOW, HIGH)
        ori = np.array([[np.cos(phi)],[np.sin(phi)]])

        for j in range(nSamples):

            for i in range(iterations[j]):

                flip = np.random.choice([0, 1])

                if (flip == 1):
                    ori = np.dot(R1, ori)
                else:
                    ori = np.dot(R0, ori)

                x += a * ori

            outx[j, k] = x[0]
            outy[j, k] = x[1]

    return outx, outy
```

The implementation of the FRC function above is a very literal and explicit implementation. It is a straight forward implementation of the described formulaes and very literally implements the algorithm. This makes it clear to understand what is going on, at the expense of computational speed. Below I show you a vectorized version for the FRC model, which is much faster and hence recommended for more extensive statistical analysis of the model.

```
In [6]: def FRC_vecSingle(N, a = 1.0e-3, theta = 0.2 * np.pi, x0 = 0.0, y0 = 0.0):
            '''
            Random walk model for the freely rotating chain (FRC) in two dimensions (d = 2).
            Vectorized version for a single trajectory (polymer).
            '''
            outx = np.zeros((N + 1,))
            outy = np.zeros((N + 1,))

            # initialize the random walker at the origin
            outx[0], outy[0] = x0, y0
```

```
    angles = np.zeros((N))
    # initial orientation uniformly sampled in [0, 2 * Pi)
    angles[0] = np.random.uniform(0.0, 2.0 * np.pi)
    angles[1:] = theta * np.random.choice([-1.0, 1.0], N - 1)

    angles = np.cumsum(angles)
    outx[1:] = np.cumsum(a * np.cos(angles))
    outy[1:] = np.cumsum(a * np.sin(angles))

    return outx, outy

def FRC_wrapper(sampleIndices, m, a = 1.0e-3,\
                theta = 0.2 * np.pi, x0 = 0.0, y0 = 0.0):
    '''
    Wrapper function which creates m statistically
    independent realizations of the FRC model.
    '''
    xVals = np.zeros((len(sampleIndices), m))
    yVals = np.zeros((len(sampleIndices), m))

    N = sampleIndices[-1]

    for i in range(m):
        tmpX, tmpY = FRC_vecSingle(N, a, theta, x0, y0)
        xVals[:, i] = tmpX[sampleIndices]
        yVals[:, i] = tmpY[sampleIndices]

    return xVals, yVals
```

```
In [7]: def plot_trajectories(X, Y, m = 10):

            f, ax = plt.subplots(1)
            f.set_size_inches(5.5, 5.5)

            ax.set_xlabel('$x$ coordinate', fontsize = 18)
            ax.set_ylabel('$y$ coordinate', fontsize = 18)
            labelfontsize = 15.0
            for tick in ax.xaxis.get_major_ticks():
                tick.label.set_fontsize(labelfontsize)
            for tick in ax.yaxis.get_major_ticks():
                tick.label.set_fontsize(labelfontsize)

            for i in range(m):
                ax.plot(X[:, i], Y[:, i], lw = 1.0, alpha = 0.80)

            rx = np.max(X)
            ry = np.max(Y)
```

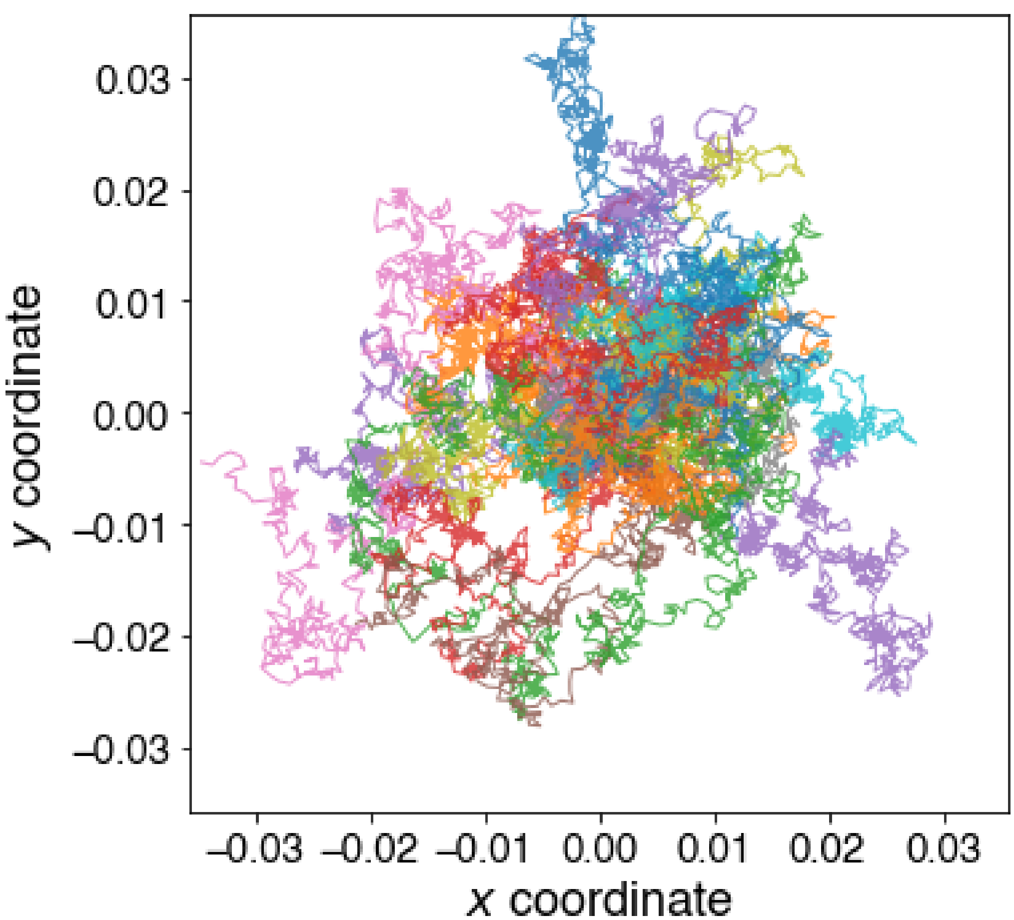
```
    r = np.max([rx, ry])
    ax.set_xlim(-r, r)
    ax.set_ylim(-r, r)

    return None
```

### 1.2 Assay 1 - Random walk model for the FJC

In [8]:
```
%%time
np.random.seed(123456789)
# create m = 25 FJC polymer configurations
m = 25
sampleLengths = np.arange(0.0, 501.0, 1)
X1, Y1 = FJC(sampleLengths, m)
```

```
totalIterations =  500
CPU times: user 92.2 ms, sys: 4.81 ms, total: 97 ms
Wall time: 108 ms
```

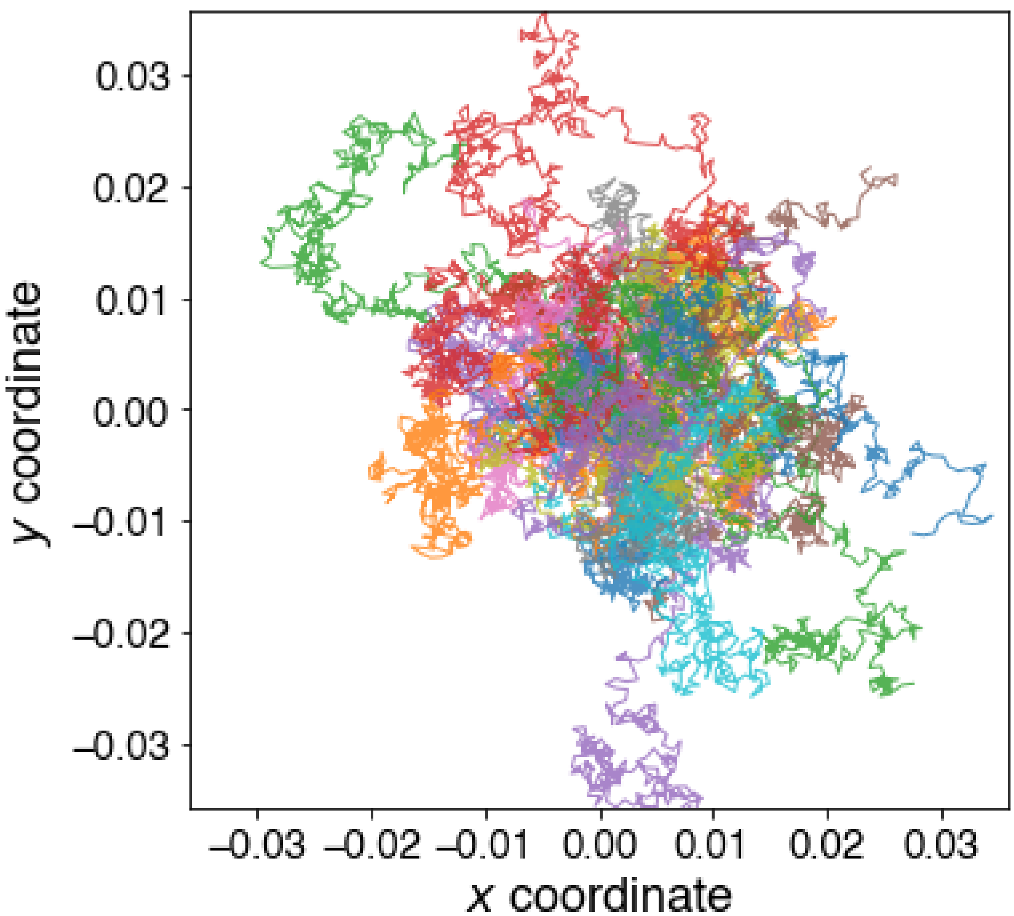
In [9]:
```
m = 25
plot_trajectories(X1, Y1, m)
```



```
In [10]: %%time
         np.random.seed(923456789)
         # create m = 25 FJC polymer configurations
         m = 25
         sampleLengths = np.arange(0.0, 501.0, 1)
         X1vec, Y1vec = FJC_vec(sampleLengths, m)
```

```
totalIterations =  500
CPU times: user 16.8 ms, sys: 1.94 ms, total: 18.7 ms
Wall time: 18.4 ms
```

```
In [11]: m = 25
         plot_trajectories(X1vec, Y1vec, m)
```



### 1.3 Random walk model for the FRC

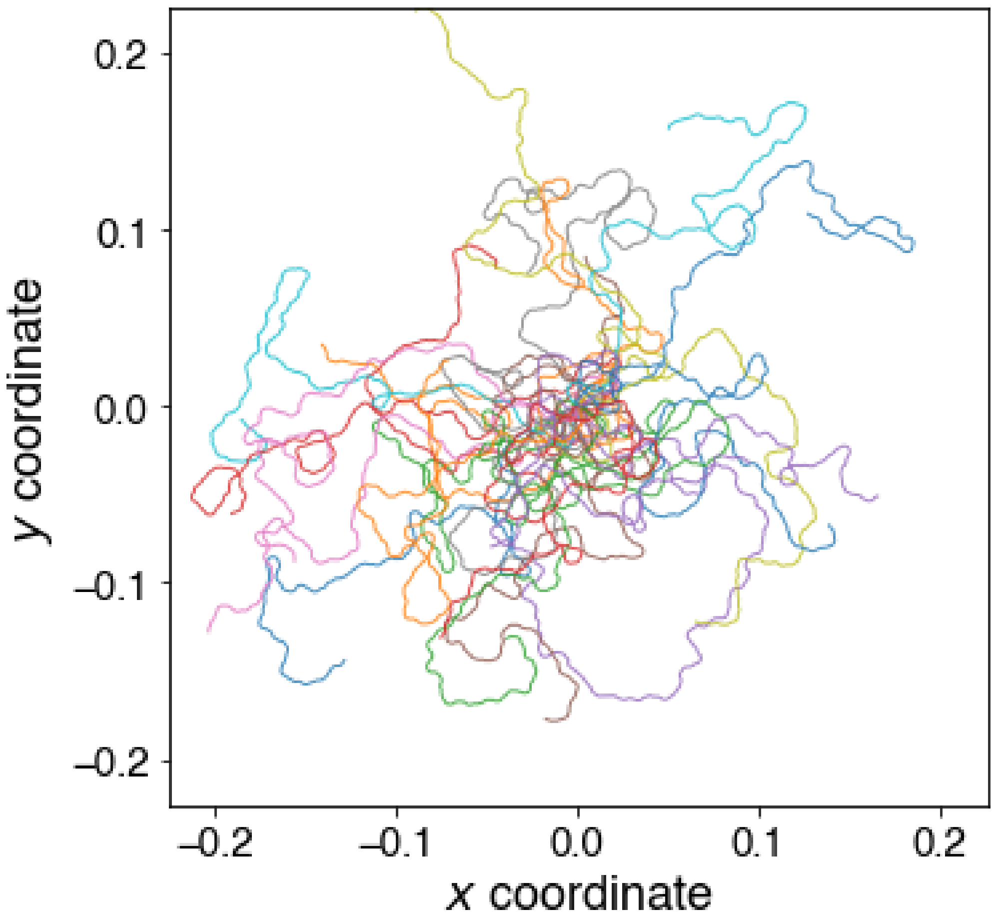
In [12]:
```
%%time
np.random.seed(123456789)
# create m = 25 FRC polymer configurations
m = 25
sampleLengths = np.arange(0.0, 501.0, 1)
X2, Y2 = FRC(sampleLengths, m, theta = 0.1 * np.pi)
```

```
totalIterations =  500
CPU times: user 325 ms, sys: 32.1 ms, total: 357 ms
Wall time: 337 ms
```

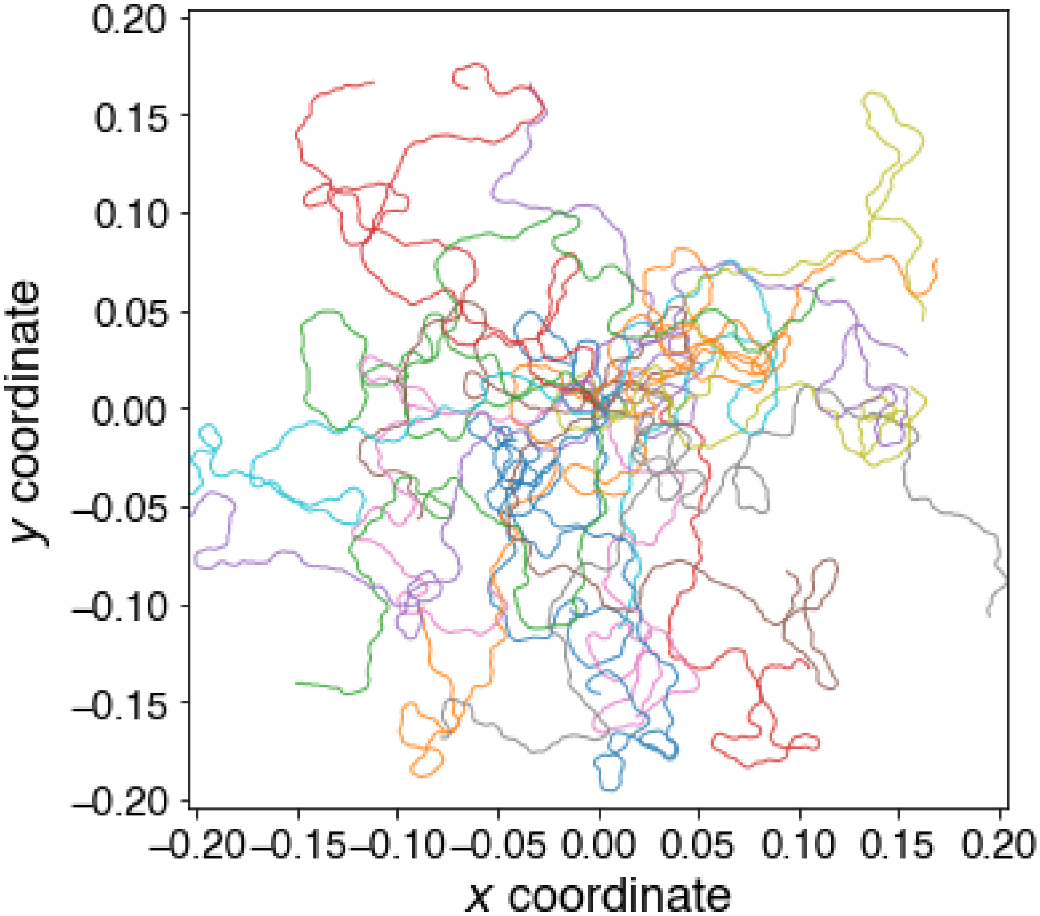
In [13]:
```
%%time
# We repeat the same, using the vectorized version of the FRC algorithm.
np.random.seed(223456789)
# create m = 25 FJC polymer configurations
m = 25
sampleIndices = np.arange(0.0, 501.0, 1).astype(int)
X2_vec, Y2_vec = FRC_wrapper(sampleIndices, m, a = 1.0e-3, theta = 0.1 * np.pi)
```

```
CPU times: user 4.88 ms, sys: 1.02 ms, total: 5.9 ms
Wall time: 5.18 ms
```

In [14]:
```
m = 25
plot_trajectories(X2, Y2, m)
```

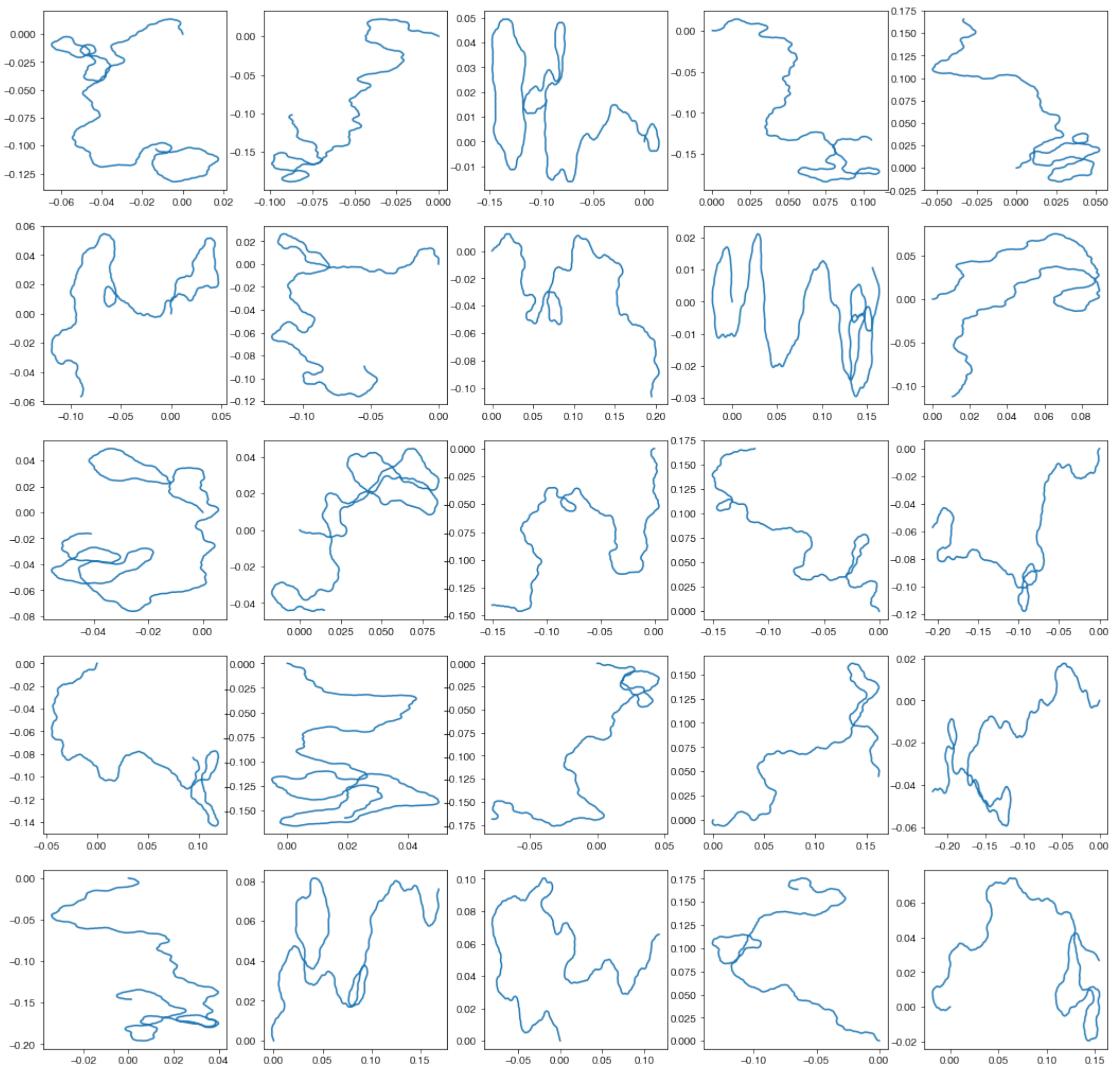



```
In [15]: m = 25
         plot_trajectories(X2_vec, Y2_vec, m)
```




```
In [16]: # separate plotting for m = 25 polymer chains
         print(X2_vec.shape)
         print(Y2_vec.shape)
         f, ax = plt.subplots(5, 5, figsize = (18.0, 18.0))
         for i in range(25):
             plt.subplot(5, 5, i + 1)
             plt.plot(X2_vec[:, i], Y2_vec[:, i])
```

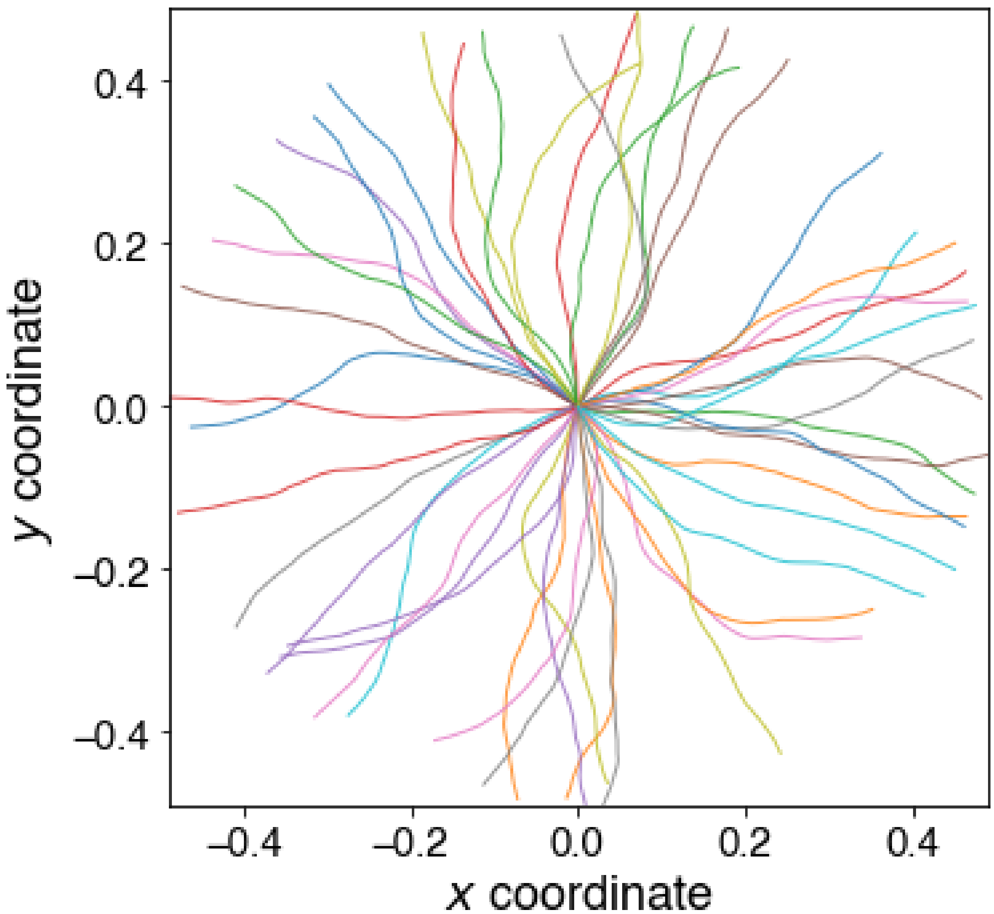
```
(501, 25)
(501, 25)
```



```
In [17]: %%time
         np.random.seed(923456789)
         # create m = 50 FRC polymer configurations
         m = 50
         sampleIndices = np.arange(0.0, 501.0, 1).astype(int)
         X3_vec, Y3_vec = FRC_wrapper(sampleIndices, m, theta = 0.01 * np.pi)
```

```
CPU times: user 7.86 ms, sys: 1.11 ms, total: 8.98 ms
Wall time: 8.14 ms
```

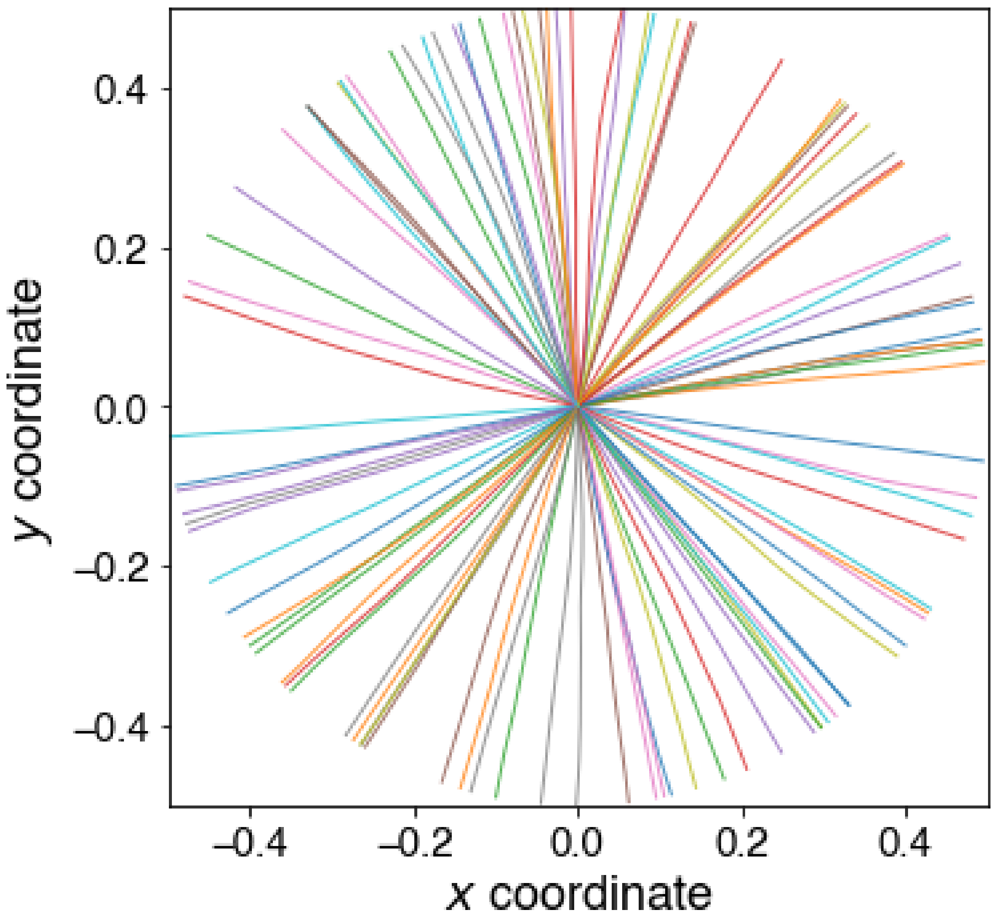
```
In [18]: m = 50
         plot_trajectories(X3_vec, Y3_vec, m)
```




```
In [19]: %%time
         np.random.seed(123456789)
         # create m = 100 FRC polymer configurations
         m = 100
         sampleIndices = np.arange(0.0, 501.0, 1).astype(int)
         X3_vec, Y3_vec = FRC_wrapper(sampleIndices, m, theta = 0.001
                                      * np.pi)
```

```
CPU times: user 12 ms, sys: 1.31 ms, total: 13.4 ms
Wall time: 12.3 ms
```

```
In [23]: m = 100
         plot_trajectories(X3_vec, Y3_vec, m)
```



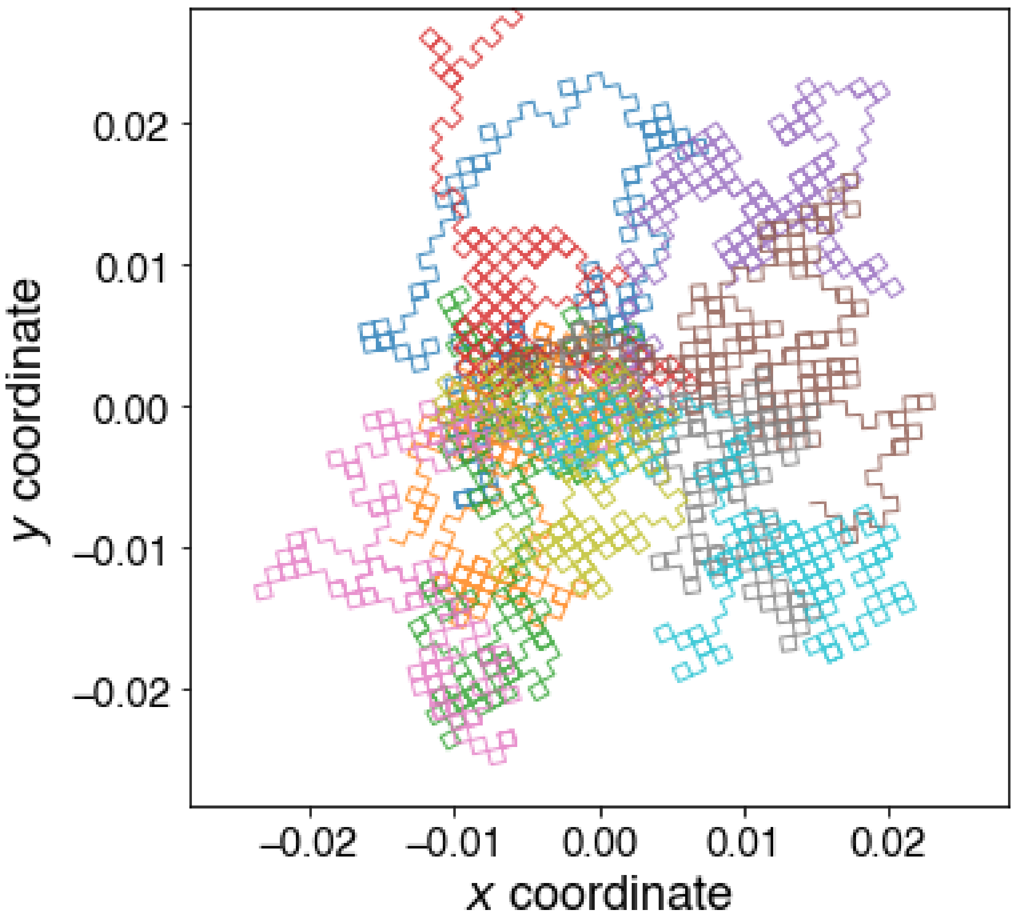

Changing the rotation angle $\theta$ we can change the polymers persitence lenght $l_P$. The well established relation for the freely rotating chain model reads

$$l_P = -\frac{a}{\ln(\cos\theta)}\,. \tag{4}$$

```
In [20]: %%time
         np.random.seed(123456789)
         # create m = 25 FRC polymer configurations
         m = 10
         sampleIndices = np.arange(0.0, 501.0, 1).astype(int)
         X3_vec, Y3_vec = FRC_wrapper(sampleIndices, m, theta = 0.5 * np.pi)
```

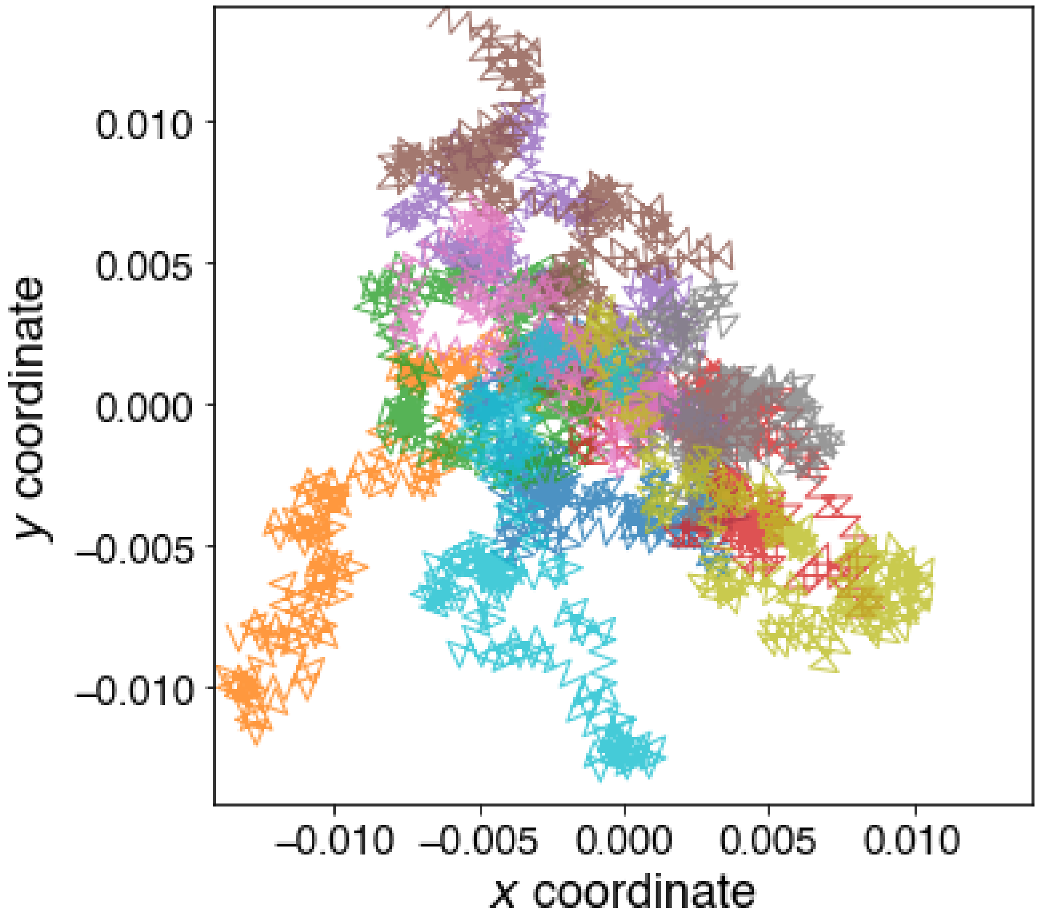
```
CPU times: user 2.48 ms, sys: 654 ţs, total: 3.13 ms
Wall time: 2.7 ms
```

```
In [21]: m = 10
         plot_trajectories(X3_vec, Y3_vec, m)
```




```
In [22]: %%time
         np.random.seed(123456789)
         # create m = 25 FRC polymer configurations
         m = 10
         sampleIndices = np.arange(0.0, 501.0, 1).astype(int)
         X3_vec, Y3_vec = FRC_wrapper(sampleIndices, m, theta = 0.75 * np.pi)

CPU times: user 2.57 ms, sys: 691 ţs, total: 3.26 ms
Wall time: 2.86 ms
```

```
In [23]: m = 10
         plot_trajectories(X3_vec, Y3_vec, m)
```




### 1.4 Assay 2 - FJC mean-squared-end-to-end vector as a function of chain length $N$

Next, we analyze the mean-squared end-to-end vector as a function of segment length. The goal is of course to verify, that the well known relation

$$\langle \boldsymbol{R}^2 \rangle = Na^2 \tag{5}$$

holds for the freely jointed chain (FJC). This is of course equivalent to

$$R = \sqrt{\langle \boldsymbol{R}^2 \rangle} = \sqrt{N}a\,. \tag{6}$$

In the first part of this section on the FJC model we will show the $\sim N$ scaling and in the second part we verify the $\sim a^2$ scaling of the MSD.

```
In [24]: %%time
         np.random.seed(123456789)
         m = 1000 # number of statistically independent configurations
         sampleLengths = np.array([10, 500, 1000, 2500, 5000])
```

```
X_ex2, Y_ex2 = FJC(sampleLengths, m)

print(X_ex2.shape)
print(Y_ex2.shape)
```

```
totalIterations =  5000
(5, 1000)
(5, 1000)
CPU times: user 23.4 s, sys: 294 ms, total: 23.7 s
Wall time: 24.8 s
```

In [25]:
```
%%time
np.random.seed(123456789)
m = 1000 # number of statistically independent configurations
sampleLengths = np.array([10, 500, 1000, 2500, 5000])

X_ex2_vec, Y_ex2_vec = FJC_vec(sampleLengths, m)

print(X_ex2_vec.shape)
print(Y_ex2_vec.shape)
```

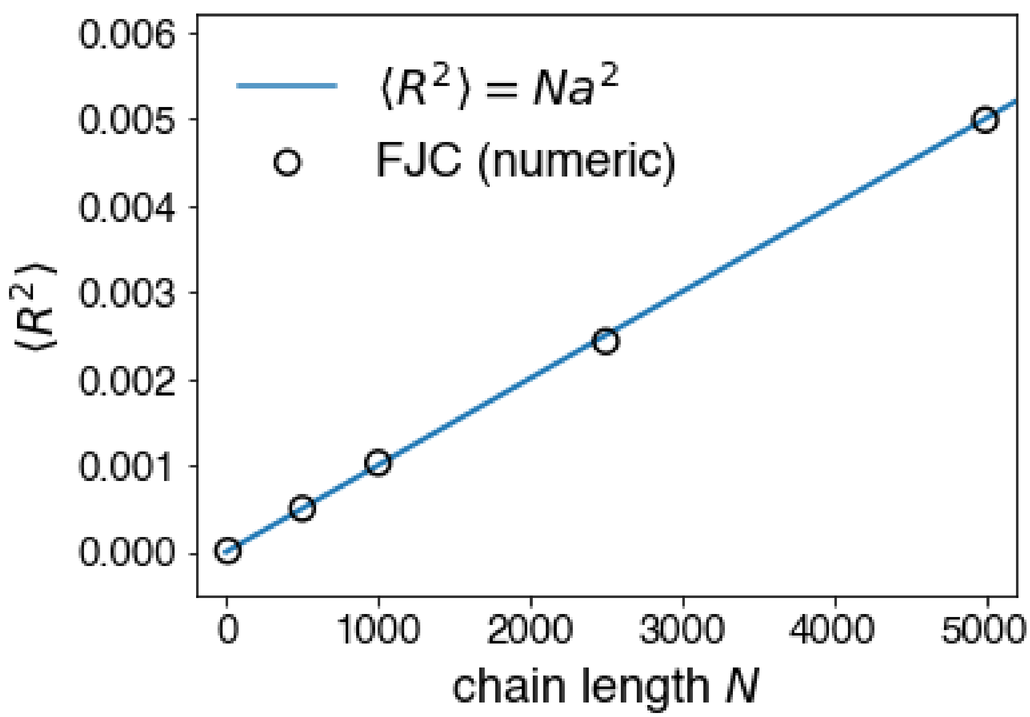
```
totalIterations =  5000
(5, 1000)
(5, 1000)
CPU times: user 420 ms, sys: 3.91 ms, total: 423 ms
Wall time: 427 ms
```

Here you can compare the execution time of the vectorized version against the execution time of the naive implementation of the FJC model. One gets a speed up of roughly 50 times faster code.

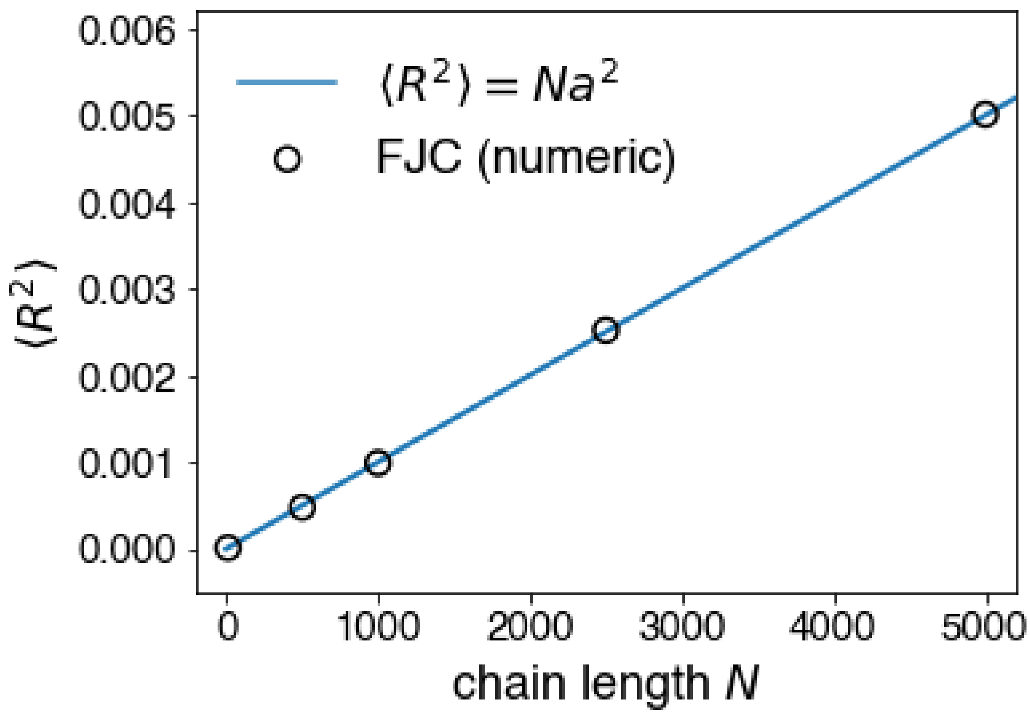
In [26]:
```
def plot_msd_FJC(X, Y, a = 1.0e-3):

    f, ax = plt.subplots(1)
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('chain length $N$', fontsize = 18)
    ax.set_ylabel(r'$\langle R^2\rangle$', fontsize = 18)
    labelfontsize = 15.0
    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    ax.plot([-2.0, 6000.0], [a ** 2 * (-2.0), a ** 2 * (6000.0)],
            lw = 2.0,
```

```
                color = 'C0',
                label = r'$\langle R^2\rangle = Na^2$',
                zorder = 1)
        ax.scatter(X, Y, color = 'k',
                   s = 80,
                   marker = 'o',
                   facecolors = 'None',
                   edgecolors = 'k',
                   linewidth = 1.5,
                   label = r'FJC (numeric)', zorder = 2)

        ax.set_xlim(-200.0, 5200.0)
        ax.set_ylim(-0.0005, 0.0062)

        leg = ax.legend(scatterpoints = 1,
                        markerscale = 1.0,
                        ncol = 1,
                        fontsize = 18)
        for i, legobj in enumerate(leg.legendHandles):
            legobj.set_linewidth(1.5)
        leg.draw_frame(False)
        return None
```

```
In [27]: sampleLengths_ex2 = np.array([10, 500, 1000, 2500, 5000])
         msd_ex2 = get_msd(X_ex2, Y_ex2, sampleLengths_ex2)
         plot_msd_FJC(sampleLengths_ex2, msd_ex2, a = 1.0e-3)
```



```
In [28]: sampleLengths_ex2 = np.array([10, 500, 1000, 2500, 5000])
         msd_ex2_vec = get_msd(X_ex2_vec, Y_ex2_vec, sampleLengths_ex2)
         plot_msd_FJC(sampleLengths_ex2, msd_ex2_vec, a = 1.0e-3)
```




### 1.5 Assay 3 FJC mean-squared-end-to-end vector as a function of the segment length $a$

```
In [29]: %%time
         np.random.seed(123456789)
         m = 1000
         N = 2000
         sampleLengths_ex3 = np.array([N])
         stepSizes_ex3 = np.array([1.0e-3, 2.0e-3, 3.0e-3, 5.0e-3, 7.5e-3, 1.0e-2])
         res_ex3 = np.zeros((len(stepSizes_ex3)))
         for i, a in enumerate(stepSizes_ex3):
             print("segment length", a)
             tmpX, tmpY = FJC(sampleLengths_ex3, m, a)
             msd = get_msd(tmpX, tmpY, sampleLengths_ex3)
             res_ex3[i] = msd[0]
```

```
segment length 0.001
totalIterations =  2000
segment length 0.002
totalIterations =  2000
segment length 0.003
totalIterations =  2000
segment length 0.005
totalIterations =  2000
segment length 0.0075
totalIterations =  2000
segment length 0.01
totalIterations =  2000
CPU times: user 53.1 s, sys: 390 ms, total: 53.5 s
Wall time: 54.1 s
```

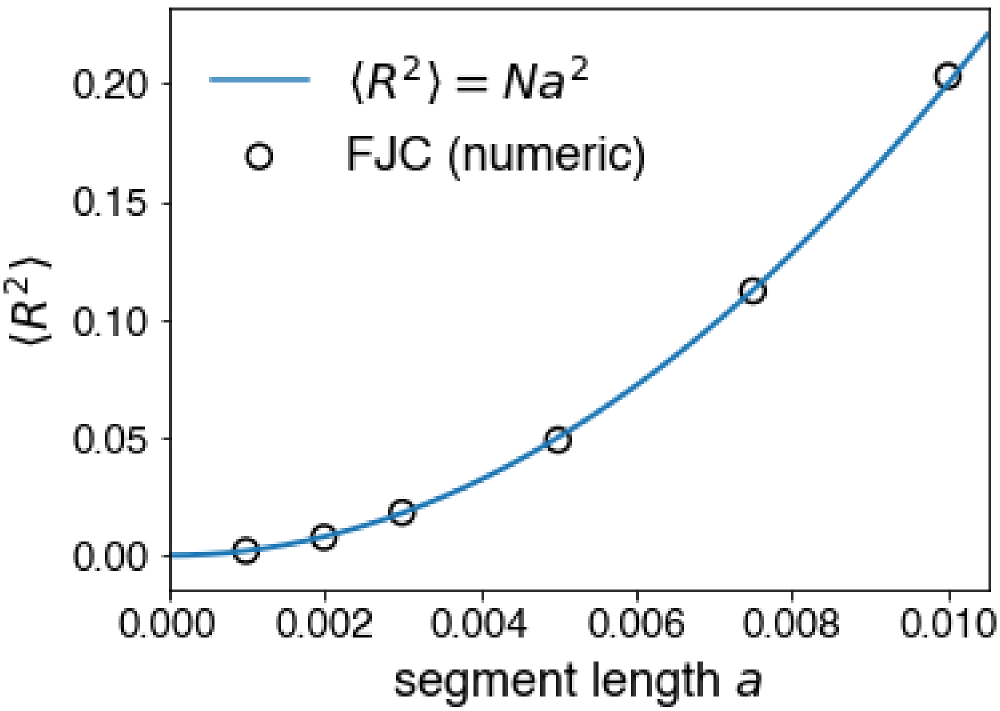
```
In [30]: %%time
         np.random.seed(123456789)
         m = 10000 # we can afford 10000 here
         N = 2000
         sampleLengths_ex3 = np.array([N])
         stepSizes_ex3 = np.array([1.0e-3, 2.0e-3, 3.0e-3, 5.0e-3, 7.5e-3, 1.0e-2])
         res_ex3_vec = np.zeros((len(stepSizes_ex3)))
         for i, a in enumerate(stepSizes_ex3):
             print("segment length", a)
             tmpX, tmpY = FJC_vec(sampleLengths_ex3, m, a)
             msd = get_msd(tmpX, tmpY, sampleLengths_ex3)
             res_ex3_vec[i] = msd[0]
```

```
segment length 0.001
totalIterations =  2000
segment length 0.002
totalIterations =  2000
segment length 0.003
totalIterations =  2000
segment length 0.005
totalIterations =  2000
segment length 0.0075
totalIterations =  2000
segment length 0.01
totalIterations =  2000
CPU times: user 8.57 s, sys: 157 ms, total: 8.72 s
Wall time: 9.74 s
```

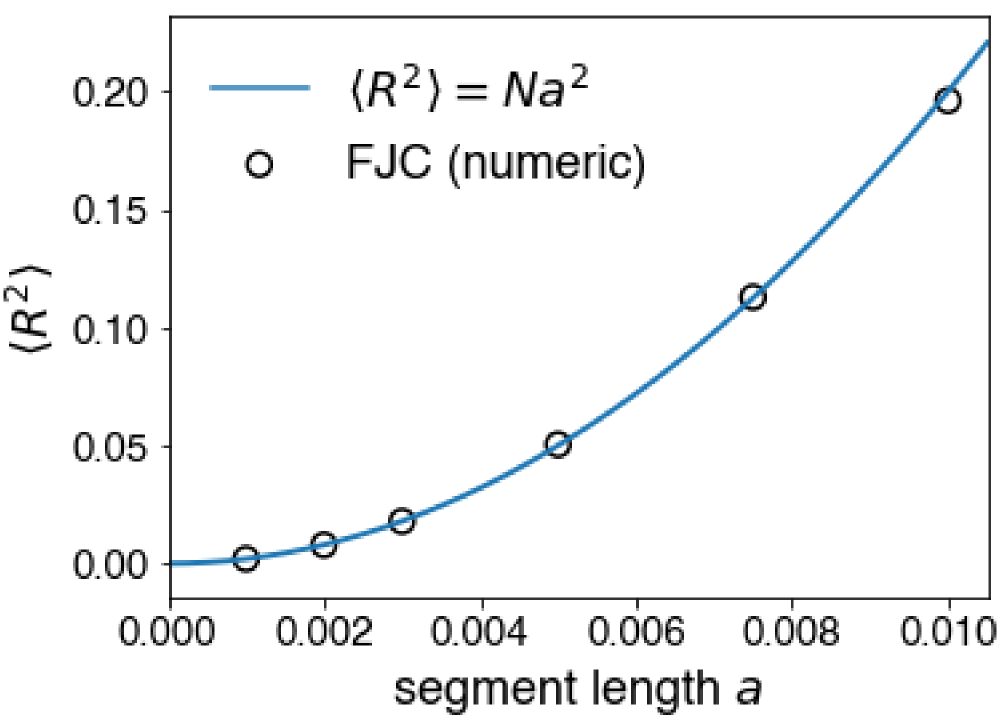
```
In [31]: def plot_msd_FJC_a(X, Y, N = 2000.0):

             f, ax = plt.subplots(1)
```

```
    f.set_size_inches(5.5, 4.0)

    ax.set_xlabel('segment length $a$', fontsize = 18)
    ax.set_ylabel(r'$\langle R^2\rangle$', fontsize = 18)
    labelfontsize = 15.0

    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(labelfontsize)

    xVals = np.linspace(0.0, 1.05e-2, 500)
    yVals = np.array([N * a ** 2 for a in xVals])
    ax.plot(xVals, yVals,
            lw = 2.0, color = 'C0', label = r'$\langle R^2\rangle = Na^2$')

    ax.scatter(X, Y, color = 'k',
               s = 80,
               marker = 'o',
               facecolors = 'None',
               edgecolors = 'k',
               linewidth = 1.5,
               label = r'FJC (numeric)', zorder = 2)

    ax.set_xlim(0.0, 1.05e-2)
    #ax.set_ylim(-0.0005, 0.0062)

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None
```

```
In [32]: stepSizes_ex3 = np.array([1.0e-3, 2.0e-3, 3.0e-3, 5.0e-3, 7.5e-3, 1.0e-2])
         plot_msd_FJC_a(stepSizes_ex3, res_ex3, N = 2000.0)
```




```
In [33]: stepSizes_ex3 = np.array([1.0e-3, 2.0e-3, 3.0e-3, 5.0e-3, 7.5e-3, 1.0e-2])
         plot_msd_FJC_a(stepSizes_ex3, res_ex3_vec, N = 2000.0)
```



### 1.6 Assay 4 FRC mean-squared-end-to-end vector as a function of N

```
In [34]: %%time
         np.random.seed(923456789) # fix random seed
         m = 2000 # number of independent configurations
         sampleLengths_ex4 = np.array([10, 500, 1000, 2500, 5000])
         X_ex4, Y_ex4 = FRC(sampleLengths_ex4, m)

         np.savetxt('./assay_4_xdata.txt', X_ex4, fmt = '%.8f')
         np.savetxt('./assay_4_ydata.txt', Y_ex4, fmt = '%.8f')
```

```
totalIterations =  5000
CPU times: user 3min 6s, sys: 1.77 s, total: 3min 7s
Wall time: 3min 10s
```

```
In [36]: %%time
         # vectorized version
         np.random.seed(923456789) # fix random seed
         m = 2000 # number of independent configurations
         sampleLengths_ex4 = np.array([10, 500, 1000, 2500, 5000])
         X_ex4_vec, Y_ex4_vec = FRC_wrapper(sampleLengths_ex4, m)
```

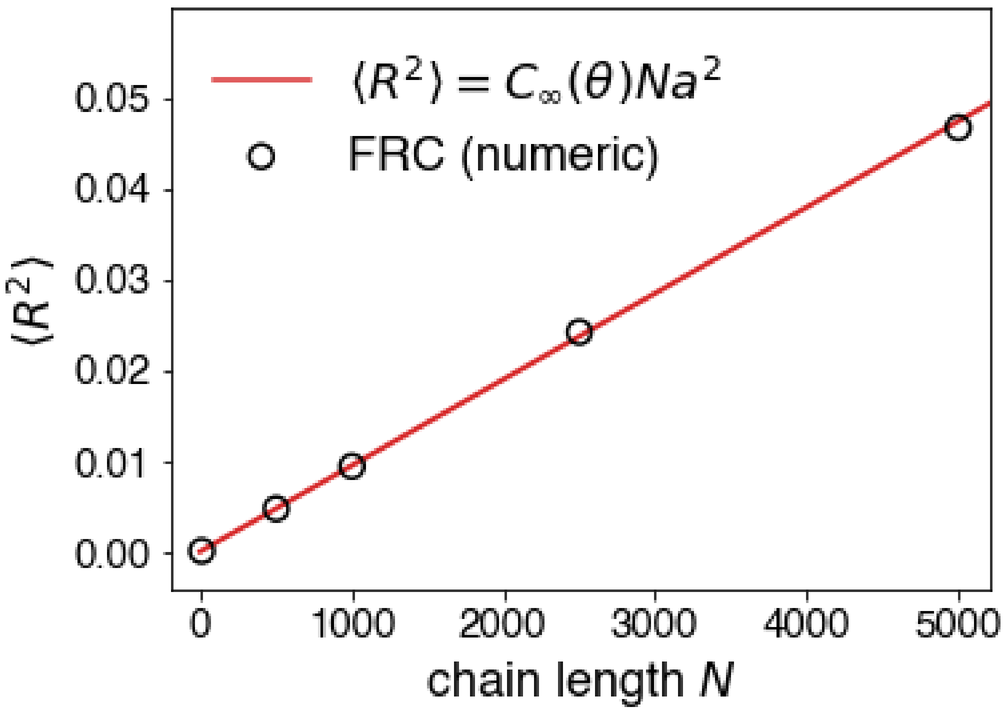
```
CPU times: user 811 ms, sys: 10.1 ms, total: 821 ms
Wall time: 839 ms
```

```
In [37]: def plot_msd_FRC(X, Y, a = 1.0e-3, theta = 0.2 * np.pi):

             f, ax = plt.subplots(1)
             f.set_size_inches(5.5, 4.0)

             ax.set_xlabel('chain length $N$', fontsize = 18)
             ax.set_ylabel(r'$\langle R^2\rangle$', fontsize = 18)
             labelfontsize = 15.0
             for tick in ax.xaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)
             for tick in ax.yaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)

             xVals = np.linspace(0.0, 6000.0, 500)
             yVals = np.array([N * a ** 2 * FloryC(theta) for N in xVals])
             ax.plot(xVals, yVals,
                     lw = 2.0,
                     color = 'C3',
                     label = r'$\langle R^2\rangle = C_{\infty}(\theta)Na^2$',
```

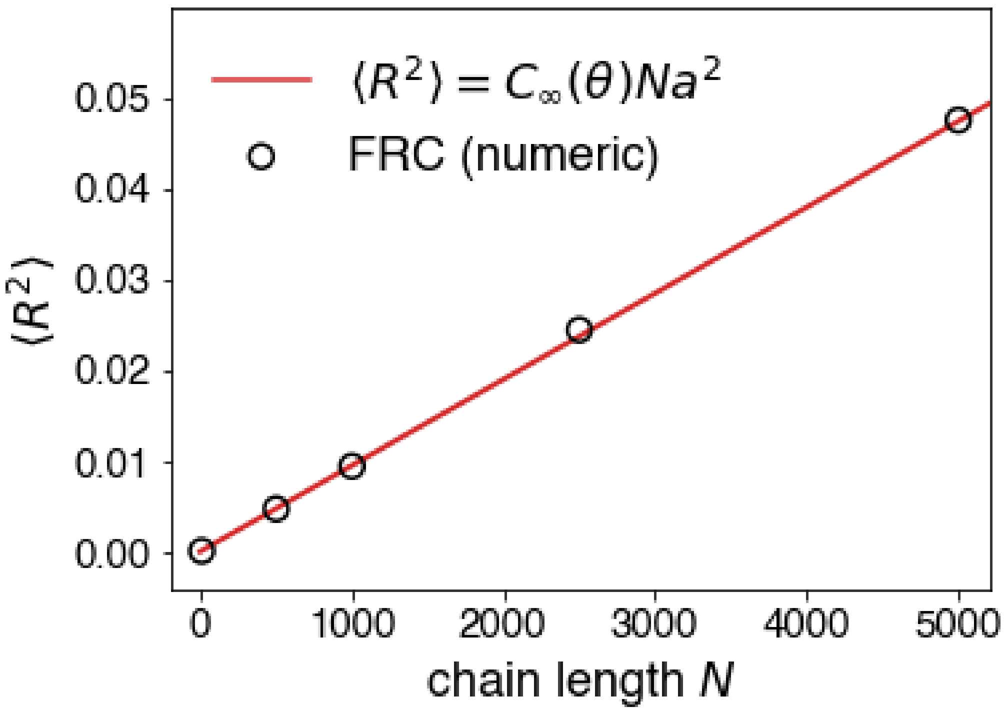
```
                 zorder = 1)

        ax.scatter(X, Y, color = 'k',
                   s = 80,
                   marker = 'o',
                   facecolors = 'None',
                   edgecolors = 'k',
                   linewidth = 1.5,
                   zorder = 2,
                   label = r'FRC (numeric)')

        ax.set_xlim(-200.0, 5200.0)
        #ax.set_ylim(-0.0005, 0.0062)

        leg = ax.legend(scatterpoints = 1,
                        markerscale = 1.0,
                        ncol = 1,
                        fontsize = 18)
        for i, legobj in enumerate(leg.legendHandles):
            legobj.set_linewidth(1.5)
        leg.draw_frame(False)
        return None
```

```
In [38]: file = './assay_4_xdata.txt'
         X_ex4 = np.genfromtxt(file)
         file = './assay_4_ydata.txt'
         Y_ex4 = np.genfromtxt(file)
```

```
In [39]: sampleLengths_ex4 = np.array([10, 500, 1000, 2500, 5000])
         msd_ex4 = get_msd(X_ex4, Y_ex4, sampleLengths_ex4)
         plot_msd_FRC(sampleLengths_ex4, msd_ex4)
```




In [40]:
```
# visualization of the same result, using the vectorized FRC code
sampleLengths_ex4 = np.array([10, 500, 1000, 2500, 5000])
msd_ex4_vec = get_msd(X_ex4_vec, Y_ex4_vec, sampleLengths_ex4)
plot_msd_FRC(sampleLengths_ex4, msd_ex4_vec)
```




The proportionalty factor here is Flory's characteristic ratio $C_\infty$, which for the freely rotating chain model is

$$C_\infty(\theta) = \frac{1+\cos(\theta)}{1-\cos(\theta)} \,. \tag{7}$$

With this, the MSD for the FRC model is of course

$$\langle \boldsymbol{R}^2 \rangle = C_\infty(\theta)Na^2 = \frac{1+\cos(\theta)}{1-\cos(\theta)}\, Na^2 \,. \tag{8}$$

### 1.7 Assay 5 FRC mean-squared-end-to-end vector as a function of the rotation angle $\theta$

In [41]:
```
%%time
np.random.seed(123456789)
m = 1000 # number of independent configurations
N = 2000

sampleLengths_ex5 = np.array([N])

thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                   0.1 * np.pi, 0.3 * np.pi, 0.6 * np.pi, np.pi])

res_ex5 = np.zeros((len(thetas)))
```

```
for i, theta in enumerate(thetas):
    print("theta", theta)
    tmpX, tmpY = FRC(sampleLengths_ex5, m, a = 1.0e-3, theta = theta)
    tmpMSD = get_msd(tmpX, tmpY, sampleLengths_ex5)
    res_ex5[i] = tmpMSD[0]

np.savetxt('./assay_5_msd.txt', res_ex5, fmt = '%.8f')
```

```
theta 0.06283185307179587
totalIterations =  2000
theta 0.15707963267948966
totalIterations =  2000
theta 0.3141592653589793
totalIterations =  2000
theta 0.9424777960769379
totalIterations =  2000
theta 1.8849555921538759
totalIterations =  2000
theta 3.141592653589793
totalIterations =  2000
CPU times: user 3min 47s, sys: 2.35 s, total: 3min 49s
Wall time: 3min 54s
```

```
In [43]: file = './assay_5_msd.txt'
         res_ex5 = np.genfromtxt(file)
         print(res_ex5.shape)
```

```
(6,)
```

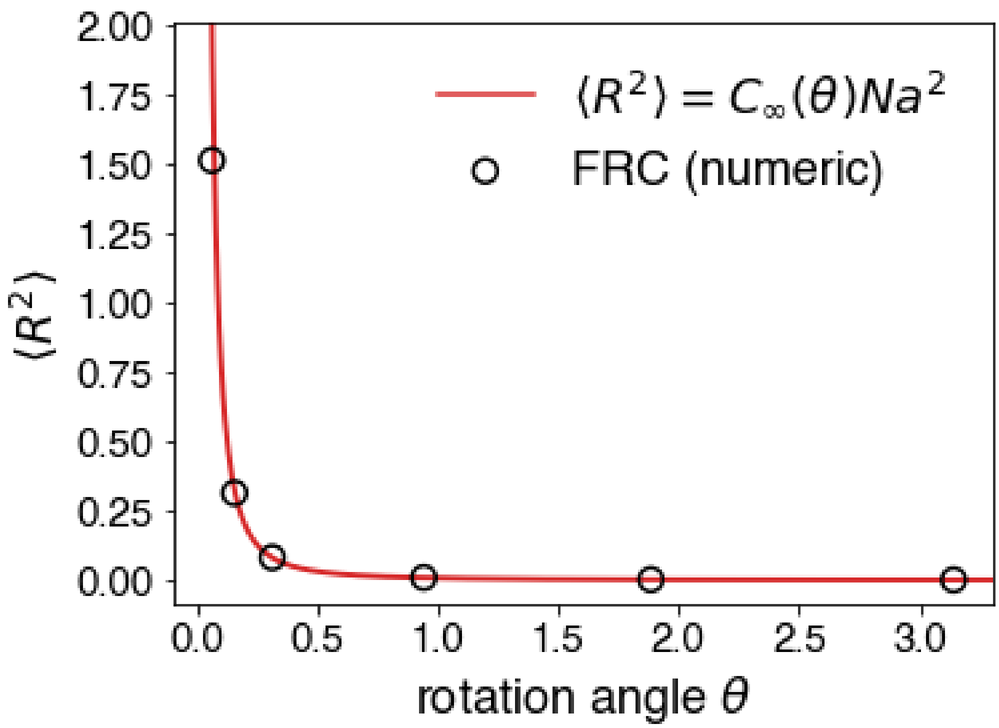
```
In [44]: %%time
         np.random.seed(123456789)
         m = 1000 # number of independent configurations
         N = 2000

         sampleLengths_ex5 = np.array([N])

         thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                            0.1 * np.pi, 0.3 * np.pi, 0.6 * np.pi, np.pi])

         res_ex5_vec = np.zeros((len(thetas)))

         for i, theta in enumerate(thetas):
             print("theta", theta)
             tmpX, tmpY = FRC_wrapper(sampleLengths_ex5, m, a = 1.0e-3, theta = theta)
             tmpMSD = get_msd(tmpX, tmpY, sampleLengths_ex5)
             res_ex5_vec[i] = tmpMSD[0]
```

```
theta 0.06283185307179587
theta 0.15707963267948966
theta 0.3141592653589793
theta 0.9424777960769379
theta 1.8849555921538759
theta 3.141592653589793
CPU times: user 1.2 s, sys: 16.4 ms, total: 1.22 s
Wall time: 1.24 s
```

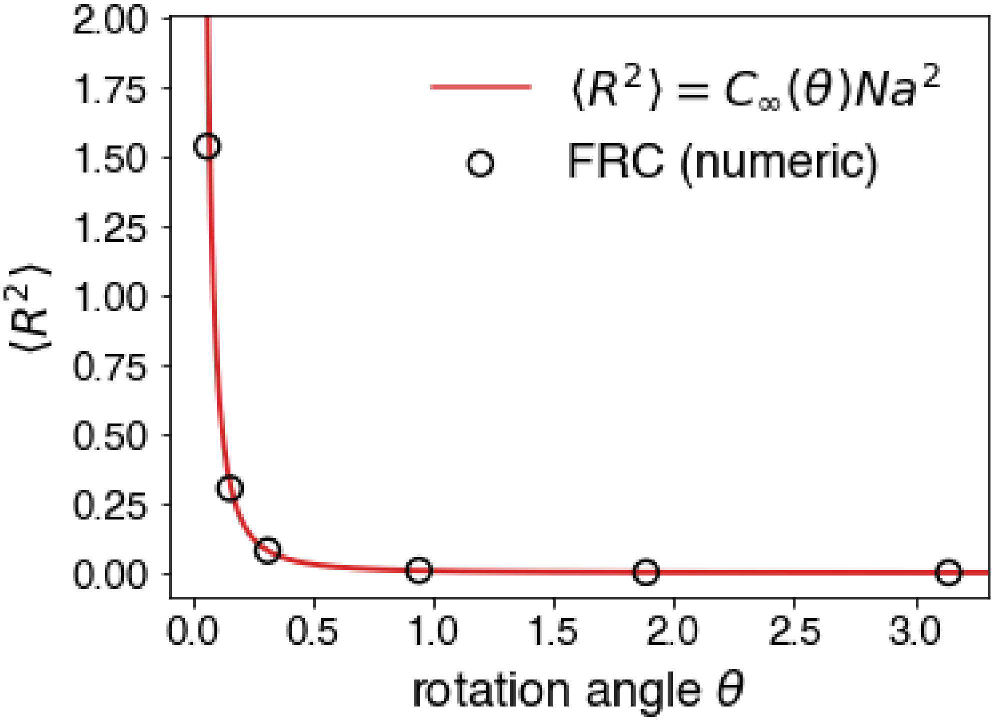
```
In [45]: def plot_msd_FRC_theta(X, Y, N = 2000.0, a = 1.0e-3):

             f, ax = plt.subplots(1)
             f.set_size_inches(5.5, 4.0)

             ax.set_xlabel(r'rotation angle $\theta$', fontsize = 18)
             ax.set_ylabel(r'$\langle R^2\rangle$', fontsize = 18)
             labelfontsize = 15.0
             for tick in ax.xaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)
             for tick in ax.yaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)

             xVals = np.linspace(0.05, 1.2 * np.pi, 500)
             yVals = np.array([N * a ** 2 * FloryC(theta) for theta in xVals])
             ax.plot(xVals, yVals,
                     lw = 2.0,
                     color = 'C3',
                     label = r'$\langle R^2\rangle = C_{\infty}(\theta)Na^2$',
                     zorder = 1)
             ax.scatter(X, Y, color = 'k',
                        s = 80,
                        marker = 'o',
                        facecolors = 'None',
                        edgecolors = 'k',
                        linewidth = 1.5,
                        zorder = 2,
                        label = r'FRC (numeric)')

             ax.set_xlim(-0.1, 1.05 * np.pi)
             ax.set_ylim(-0.085, 2.0062)

             leg = ax.legend(scatterpoints = 1,
                             markerscale = 1.0,
                             ncol = 1,
                             fontsize = 18)
             for i, legobj in enumerate(leg.legendHandles):
                 legobj.set_linewidth(1.5)
```

```
            leg.draw_frame(False)
            return None
```

In [46]:
```
thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                   0.1 * np.pi, 0.3 * np.pi, 0.6 * np.pi, np.pi])
plot_msd_FRC_theta(thetas, res_ex5, N = 2000.0)
```




In [47]:
```
# visualization of the same result using the vectorized version of the FRC model
thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                   0.1 * np.pi, 0.3 * np.pi, 0.6 * np.pi, np.pi])
plot_msd_FRC_theta(thetas, res_ex5_vec, N = 2000.0)
```




```
In [48]: def plot_msd_FRC_theta_LOG(X, Y, N = 2000.0, a = 1.0e-3):

             f, ax = plt.subplots(1)
             f.set_size_inches(5.5, 4.0)

             ax.set_xlabel(r'rotation angle $\theta$', fontsize = 18)
             ax.set_ylabel(r'$\langle R^2\rangle$', fontsize = 18)
             labelfontsize = 15.0
             for tick in ax.xaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)
             for tick in ax.yaxis.get_major_ticks():
                 tick.label.set_fontsize(labelfontsize)

             xVals = np.linspace(0.01, 1.2 * np.pi, 500)
             yVals = np.array([N * a ** 2 * FloryC(theta) for theta in xVals])
             ax.plot(xVals, yVals,
                     lw = 2.0,
                     color = 'C3',
                     label = r'$\langle R^2\rangle = C_{\infty}(\theta)Na^2$',
                     zorder = 1)
             ax.scatter(X, Y, color = 'k',
                        s = 80,
                        marker = 'o',
```

```
                 facecolors = 'None',
                 edgecolors = 'k',
                 linewidth = 1.5,
                 zorder = 2,
                 label = r'FRC (numeric)')

    ax.set_xlim(-0.1, 1.05 * np.pi)
    ax.set_ylim(1.0e-9, 5.1)

    ax.set_yscale('log')

    leg = ax.legend(scatterpoints = 1,
                    markerscale = 1.0,
                    ncol = 1,
                    fontsize = 18)
    for i, legobj in enumerate(leg.legendHandles):
        legobj.set_linewidth(1.5)
    leg.draw_frame(False)
    return None
```

In [49]:
```
%%time
np.random.seed(123456789)
m = 10000 # number of independent configurations
N = 2000

sampleLengths_ex6 = np.array([N])

thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                   0.1 * np.pi, 0.2 * np.pi, 0.3 * np.pi, 0.4 * np.pi,\
                   0.5 * np.pi, 0.6 * np.pi, 0.7 * np.pi, 0.8 * np.pi,\
                   0.9 * np.pi, 0.95 * np.pi, 0.98 * np.pi, 0.99 * np.pi])

res_ex6_vec = np.zeros((len(thetas)))

for i, theta in enumerate(thetas):
    print("theta", theta)
    tmpX, tmpY = FRC_wrapper(sampleLengths_ex6, m, a = 1.0e-3, theta = theta)
    tmpMSD = get_msd(tmpX, tmpY, sampleLengths_ex6)
    res_ex6_vec[i] = tmpMSD[0]
```

```
theta 0.06283185307179587
theta 0.15707963267948966
theta 0.3141592653589793
theta 0.6283185307179586
theta 0.9424777960769379
theta 1.2566370614359172
theta 1.5707963267948966
theta 1.8849555921538759
```

```
theta 2.199114857512855
theta 2.5132741228718345
theta 2.827433388230814
theta 2.9845130209103035
theta 3.078760800517997
theta 3.1101767270538954
CPU times: user 26.6 s, sys: 191 ms, total: 26.7 s
Wall time: 27.1 s
```

In [50]:
```
# visualization of the same result using the vectorized version of the FRC model
thetas = np.array([0.02 * np.pi, 0.05 * np.pi,\
                   0.1 * np.pi, 0.2 * np.pi, 0.3 * np.pi, 0.4 * np.pi,\
                   0.5 * np.pi, 0.6 * np.pi, 0.7 * np.pi, 0.8 * np.pi,\
                   0.9 * np.pi, 0.95 * np.pi, 0.98 * np.pi, 0.99 * np.pi])
plot_msd_FRC_theta_LOG(thetas, res_ex6_vec, N = 2000.0)
# print(res_ex6_vec)
```