Task 1

P1

In [67]:
```python
import math
import numpy as np

def replicas(x, y, L):
    """
    Function to generate replicas of a single particle.

    Parameters
    ==========
    x, y : Position.
    L : Side of the squared arena.
    """
    xr = np.zeros(9)
    yr = np.zeros(9)

    for i in range(3):
        for j in range(3):
            xr[3 * i + j] = x + (j - 1) * L
            yr[3 * i + j] = y + (i - 1) * L

    return xr, yr
```

In [68]:
```python
def pbc(x, y, L):
    """
    Function to enforce periodic boundary conditions on the positions.

    Parameters
    ==========
    x, y : Position.
    L : Side of the squared arena.
    """

    outside_left = np.where(x < - L / 2)[0]
    x[outside_left] = x[outside_left] + L

    outside_right = np.where(x > L / 2)[0]
    x[outside_right] = x[outside_right] - L

    outside_up = np.where(y > L / 2)[0]
    y[outside_up] = y[outside_up] - L

    outside_down = np.where(y < - L / 2)[0]
    y[outside_down] = y[outside_down] + L

    return x, y
```

In [69]:
```python
from functools import reduce

def interaction(x, y, theta, Rf, L):
    """
```

```
    Function to calculate the orientation at the next time step.

    Parameters
    ==========
    x, y : Positions.
    theta : Orientations.
    Rf : Flocking radius.
    L : Dimension of the squared arena.
    s : Discrete steps.
    """

    N = np.size(x)

    theta_next = np.zeros(N)

    # Preselect what particles are closer than Rf to the boundaries.
    replicas_needed = reduce(
        np.union1d, (
            np.where(y + Rf > L / 2)[0],
            np.where(y - Rf < - L / 2)[0],
            np.where(x + Rf > L / 2)[0],
            np.where(x - Rf > - L / 2)[0]
        )
    )

    for j in range(N):
        # Check if replicas are needed to find the nearest neighbours.
        if np.size(np.where(replicas_needed == j)[0]):
            # Use replicas.
            xr, yr = replicas(x[j], y[j], L)
            nn = []
            for nr in range(9):
                dist2 = (x - xr[nr]) ** 2 + (y - yr[nr]) ** 2
                nn = np.union1d(nn, np.where(dist2 <= Rf ** 2)[0])
        else:
            dist2 = (x - x[j]) ** 2 + (y - y[j]) ** 2
            nn = np.where(dist2 <= Rf ** 2)[0]

        # The list of nearest neighbours is set.
        nn = nn.astype(int)

        # Circular average.
        av_sin_theta = np.mean(np.sin(theta[nn]))
        av_cos_theta = np.mean(np.cos(theta[nn]))

        theta_next[j] = np.arctan2(av_sin_theta, av_cos_theta)

    return theta_next
```

In [70]:

```
from scipy.spatial import Voronoi, voronoi_plot_2d

def area_polygon(vertices):
    """
    Function to calculate the area of a Voronoi region given its vertices.

    Parameters
    ==========
    vertices : Coordinates (array, 2 dimensional).
    """
```

```
    N, dim = vertices.shape

    # dim is 2.
    # Vertices are listed consecutively.

    A = 0

    for i in range(N-1):
        # Below is the formula of the area of a triangle given the vertices.
        A += np.abs(
            vertices[- 1, 0] * (vertices[i, 1] - vertices[i + 1, 1]) +
            vertices[i, 0] * (vertices[i + 1, 1] - vertices[- 1, 1]) +
            vertices[i + 1, 0] * (vertices[- 1, 1] - vertices[i, 1])
        )

    A *= 0.5

    return A


def global_clustering(x, y, Rf, L):
    """
    Function to calculate the global alignment coefficient.

    Parameters
    ==========
    x, y : Positions.
    Rf : Flocking radius.
    L : Dimension of the squared arena.
    """

    N = np.size(x)

    # Use the replicas of all points to calculate Voronoi for
    # a more precise estimate.
    points = np.zeros([9 * N, 2])

    for i in range(3):
        for j in range(3):
            s = 3 * i + j
            points[s * N:(s + 1) * N, 0] = x + (j - 1) * L
            points[s * N:(s + 1) * N, 1] = y + (i - 1) * L

    # The format of points is the one needed by Voronoi.
    # points[:, 0] contains the x coordinates
    # points[:, 1] contains the y coordinates

    vor = Voronoi(points)
    '''
    vertices = vor.vertices  # Voronoi vertices.
    regions = vor.regions  # Region list.
    # regions[i]: list of the vertices indices for region i.
    # If -1 is listed: the region is open (includes point at infinity).
    point_region = vor.point_region  # Region associated to input point.
    '''

    # Consider only regions of original set of points (no replicas).
    list_regions = vor.point_region[4 * N:5 * N]

    c = 0
```

```
    for i in list_regions:
        indices = vor.regions[i]
        # print(f'indices = {indices}')
        if len(indices) > 0:
            if np.size(np.where(np.array(indices) == -1)[0]) == 0:
                # Region is finite.
                # Calculate area.
                A = area_polygon(vor.vertices[indices,:])
                if A < np.pi * Rf ** 2:
                    c += 1

    c = c / N

    return c
```

In [71]:
```
def global_alignment(theta):
    """
    Function to calculate the global alignment coefficient.

    Parameters
    ==========
    theta : Orientations.
    """

    N = np.size(theta)

    global_direction_x = np.sum(np.sin(theta))
    global_direction_y = np.sum(np.cos(theta))

    psi = np.sqrt(global_direction_x ** 2 + global_direction_y ** 2) / N


    return psi
```

In [72]:
```
N_part = 200
L = 100
v = 1
Rf = 2
eta = 0.01
dt = 1

x = (np.random.rand(N_part) - 0.5) * L  # in [-L/2, L/2]
y = (np.random.rand(N_part) - 0.5) * L  # in [-L/2, L/2]

theta = 2 * (np.random.rand(N_part) - 0.5) * np.pi  # in [-pi, pi]
```

In [ ]:
```
import time
from scipy.constants import Boltzmann as kB
from tkinter import *


step = 0
t_tot = 6000

config_x1 = []
config_y1 = []
config_theta1 = []
```

```
psi = np.zeros(t_tot+1)
c = np.zeros(t_tot+1)

while step <= t_tot:
    psi[step] = global_alignment(theta)
    c[step] = global_clustering(x, y, Rf, L)

    # Calculate next theta from the rule.
    dtheta = eta * (np.random.rand(N_part) - 0.5) * dt
    ntheta = interaction(x, y, theta, Rf, L) + dtheta
    nx = x + v * np.cos(ntheta)
    ny = y + v * np.sin(ntheta)

    # Reflecting boundary conditions.
    nx, ny = pbc(nx, ny, L)

    if(step == 0 or step == 2000 or step == 4000 or step == 6000):
        config_x1.append(nx[:])
        config_y1.append(ny[:])
        config_theta1.append(ntheta[:])

    step += 1
    if step % 100 == 0:
        print(step)

    x[:] = nx[:]
    y[:] = ny[:]
    theta[:] = ntheta[:]
```

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4600
4700
4800
4900
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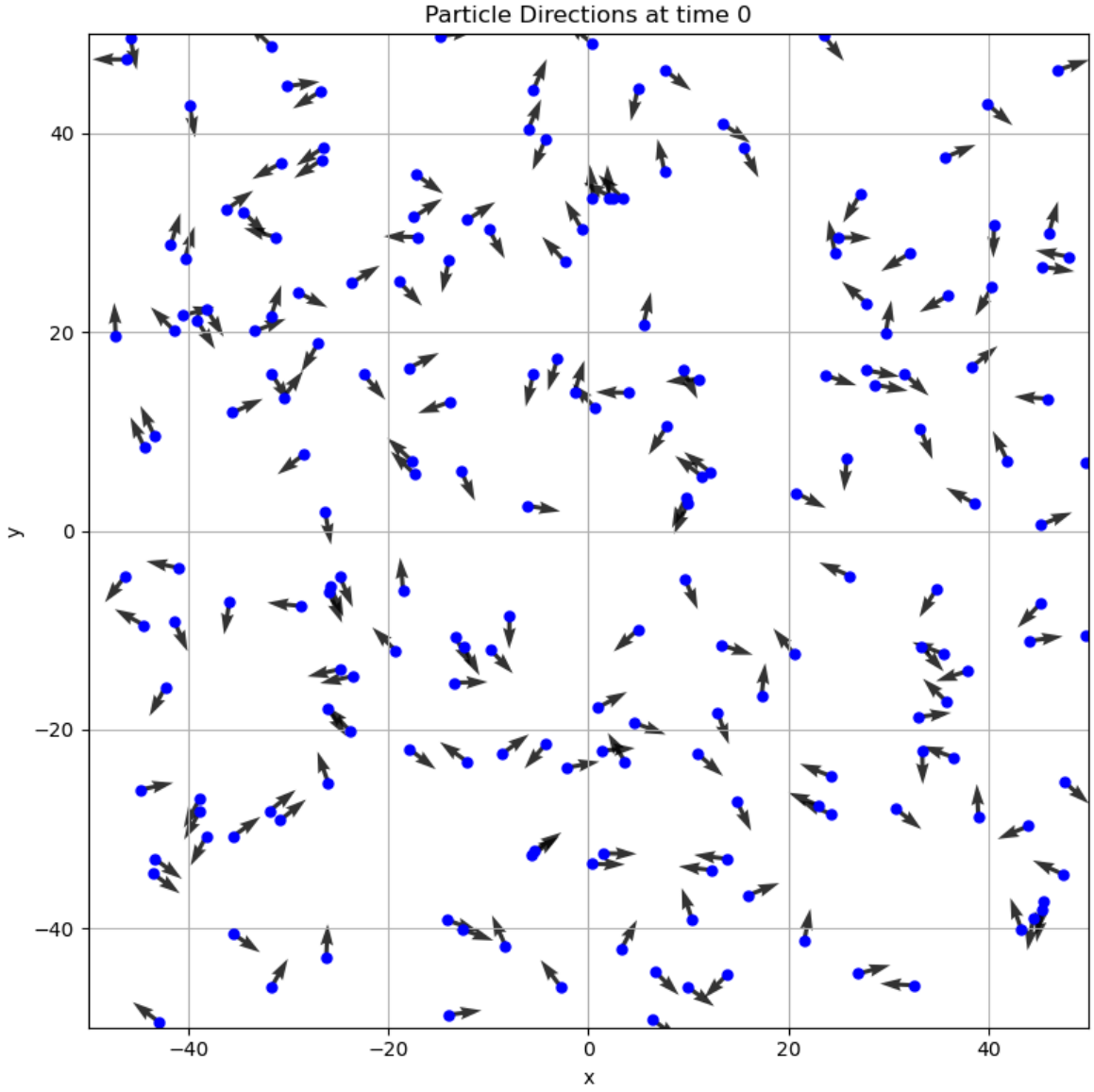
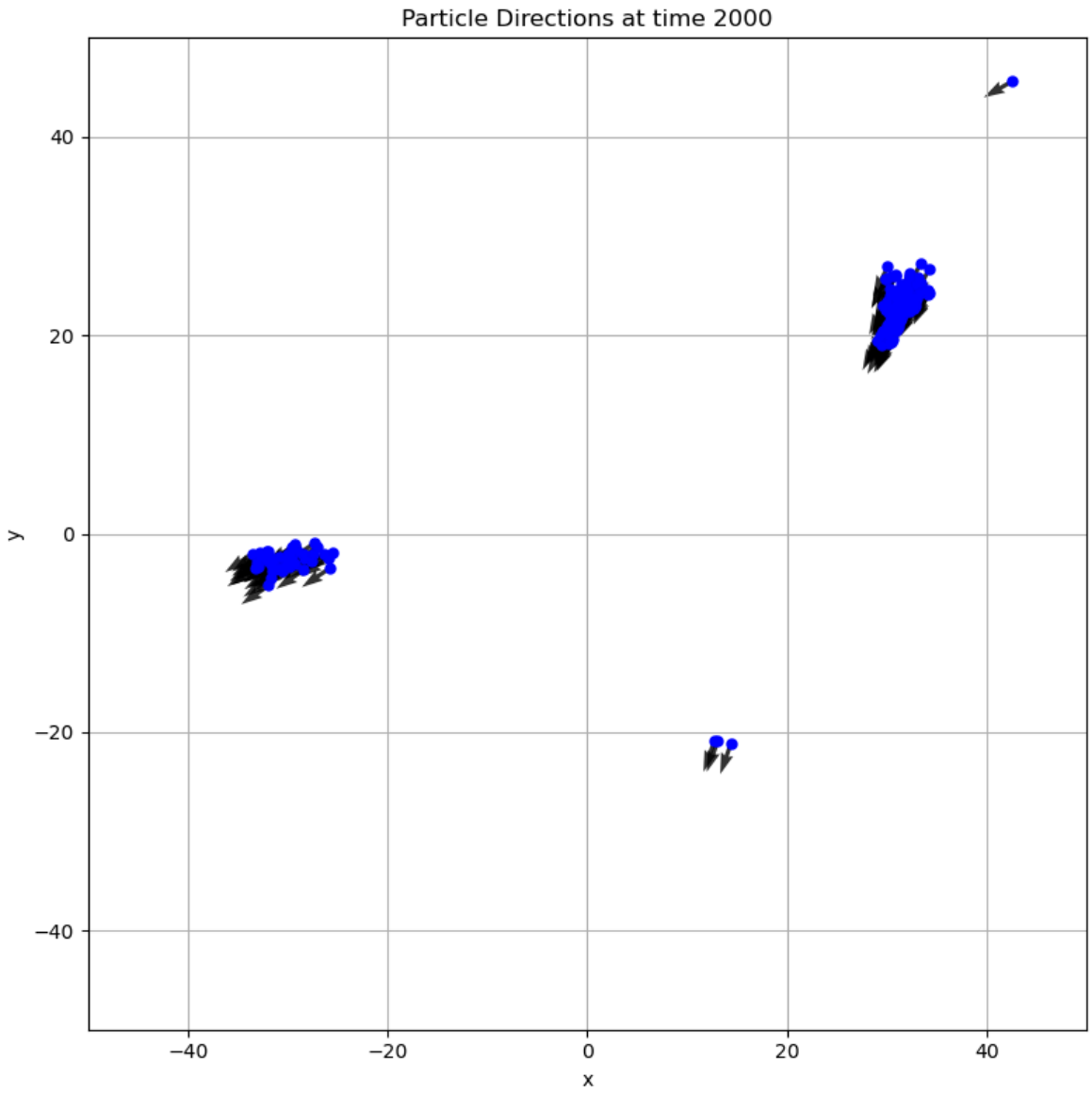
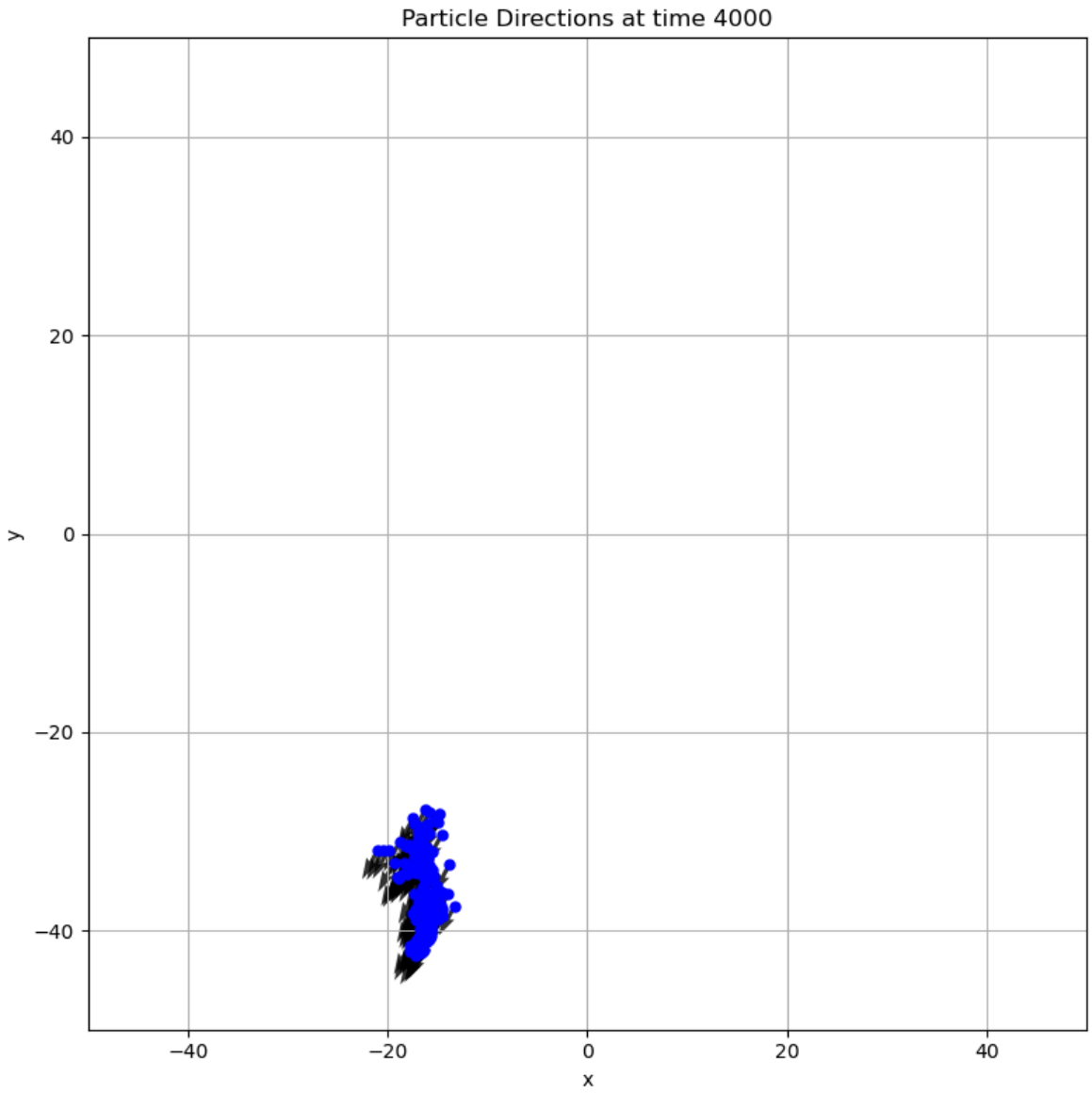
5900
6000

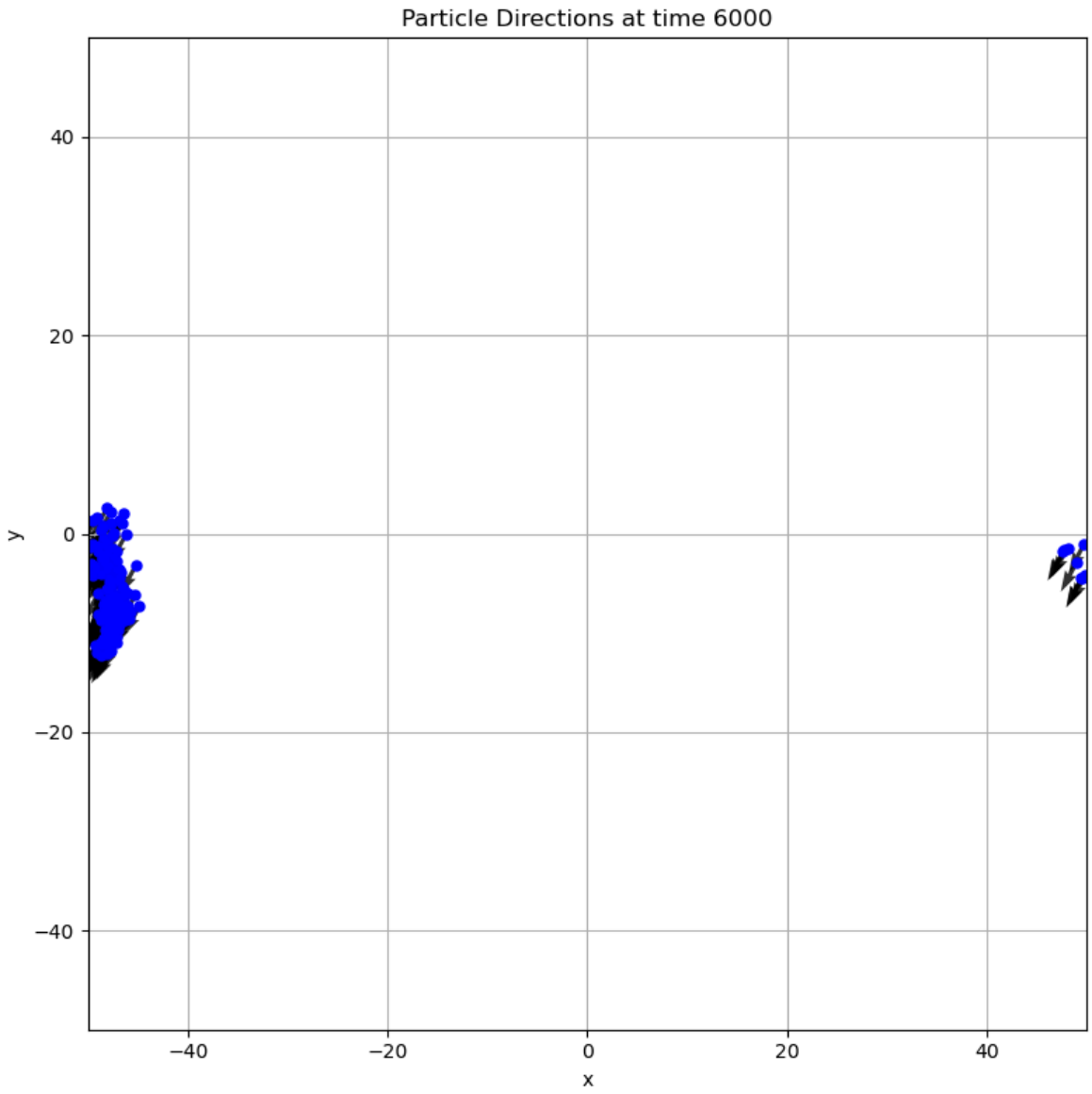
In [ ]:

```
import numpy as np
import matplotlib.pyplot as plt


# Prepare time steps corresponding to snapshots
time_steps = [0, 2000, 4000, 6000]

# Plot arrows representing particle directions at each snapshot
for i, time in enumerate(time_steps):
    plt.figure(figsize=(8, 8))
    x_positions_p1 = config_x1[i]
    y_positions_p1 = config_y1[i]
    angles = config_theta1[i]

    u_p1 = np.cos(angles)
    v_p1 = np.sin(angles)

    plt.plot(x_positions_p1, y_positions_p1, '.', color='blue', markersize=10)
    plt.quiver(x_positions_p1, y_positions_p1, u_p1, v_p1, color='black', angles
    """plt.scatter(x_positions_p1, y_positions_p1 )
    for j in range(len(x_positions_p1)):
        plt.arrow(x_positions_p1[j], y_positions_p1[j], u[j], v[j])"""
    plt.title(f'Particle Directions at time {time}')
    plt.xlabel('x')
    plt.ylabel('y')
    plt.grid()
    plt.xlim([-L/2,L/2])
    plt.ylim([-L/2,L/2])
    plt.tight_layout()
    plt.show()
```


Particle Directions at time 0
40
20
0
−20
−40
y
−40
−20
0
20
40
x

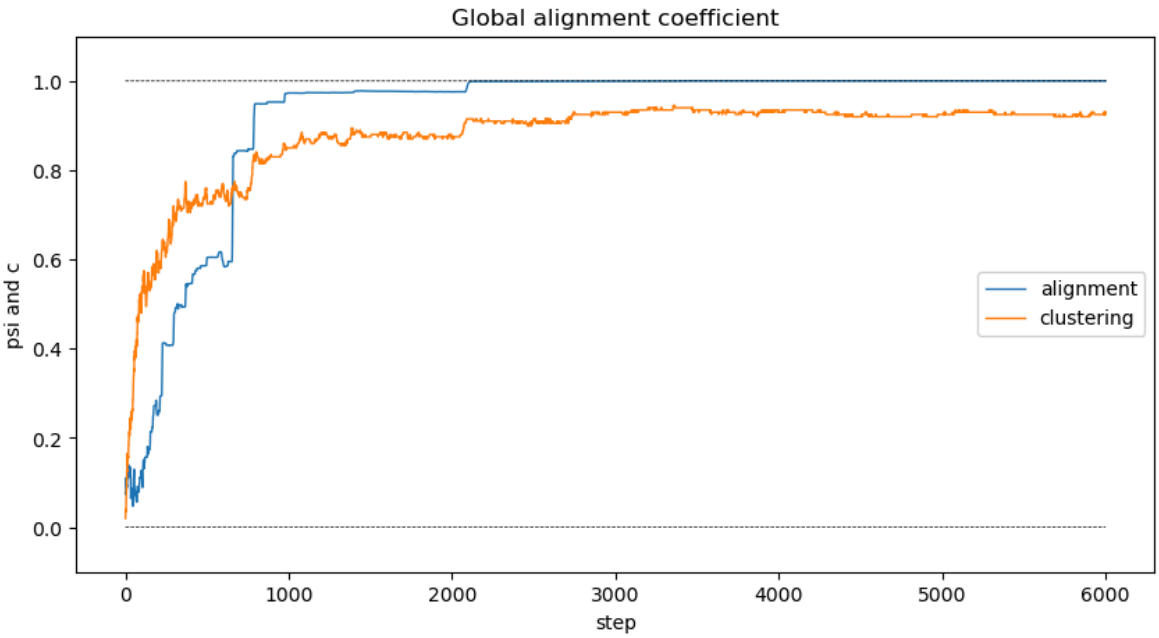

Particle Directions at time 2000
40
20
0
−20
−40
y
−40
−20
0
20
40
x


Particle Directions at time 4000
40
20
0
−20
−40
y
−40
−20
0
20
40
x



P2

In [75]:
```
from matplotlib import pyplot as plt
plt.figure(figsize=(10, 5))
plt.plot(psi, '-', linewidth=1, label='alignment')
plt.plot(c, '-', linewidth=1, label='clustering')
plt.plot(0 * psi, '--', color='k', linewidth=0.5)
plt.plot(0 * psi + 1, '--', color='k', linewidth=0.5)
plt.title('Global alignment coefficient')
plt.legend()
plt.xlabel('step')
plt.ylabel('psi and c')
plt.ylim([-0.1, 1.1])
plt.show()
```



Task 2

P3

In [76]:
```
N_part = 200
L = 100
v = 1
Rf = 2
eta1 = 0.01
eta2 = 0.3
dt = 1

x = (np.random.rand(N_part) - 0.5) * L
y = (np.random.rand(N_part) - 0.5) * L

# Random orientation.
theta = 2 * (np.random.rand(N_part) - 0.5) * np.pi
```

In [77]:
```
from IPython.display import clear_output
from matplotlib import pyplot as plt
import time

step = 0
t_tot = 6000
half_N = N_part // 2

config_x = []
config_y = []
config_theta = []

psi2 = np.zeros(t_tot+1)
c2 = np.zeros(t_tot+1)
fig, ax = plt.subplots(figsize=(10, 10))

while step <= t_tot:
```

```
    """ if step % 1 == 0:
        ax.clear()  # Clear previous plot.

        # Plot first subpopulation
        ax.plot(x[:half_N], y[:half_N], '.', markersize=10, color='blue', label=
        ax.quiver(x[:half_N], y[:half_N], np.cos(theta[:half_N]), np.sin(theta[:

        # Plot second subpopulation
        ax.plot(x[half_N:], y[half_N:], '.', markersize=10, color='red', label='
        ax.quiver(x[half_N:], y[half_N:], np.cos(theta[half_N:]), np.sin(theta[h

        # Plot boundary (if needed)
        ax.plot(Rf * np.cos(2 * np.pi * np.arange(360) / 360),
                Rf * np.sin(2 * np.pi * np.arange(360) / 360),
                '-', color='#FFA0FF', linewidth=3)

        ax.set_xlim([-L / 2, L / 2])
        ax.set_ylim([-L / 2, L / 2])
        ax.set_title(f'Step {step}')
        ax.legend(loc='upper right')  # Add legend to distinguish subpopulations

        display(fig)  # Display updated plot.
        clear_output(wait=True)  # Clear previous output."""

    psi2[step] = global_alignment(theta)
    c2[step] = global_clustering(x, y, Rf, L)

    dtheta = np.zeros(N_part)

    dtheta[:half_N] = eta1 * (np.random.rand(half_N) - 0.5) * dt
    dtheta[half_N:] = eta2 * (np.random.rand(N_part-half_N) - 0.5) * dt

    ntheta = interaction(x, y, theta, Rf, L) + dtheta
    nx = x + v * np.cos(ntheta)
    ny = y + v * np.sin(ntheta)

    # Reflecting boundary conditions.
    nx, ny = pbc(nx, ny, L)

    if(step == 0 or step == 2000 or step == 4000 or step == 6000):
        config_x.append(nx[:])
        config_y.append(ny[:])
        config_theta.append(ntheta[:])

    step += 1
    if step % 100 == 0:
        print(step)

    x[:] = nx[:]
    y[:] = ny[:]
    theta[:] = ntheta[:]
```

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4500
4600
4700
4800
4900
5000
5100
5200
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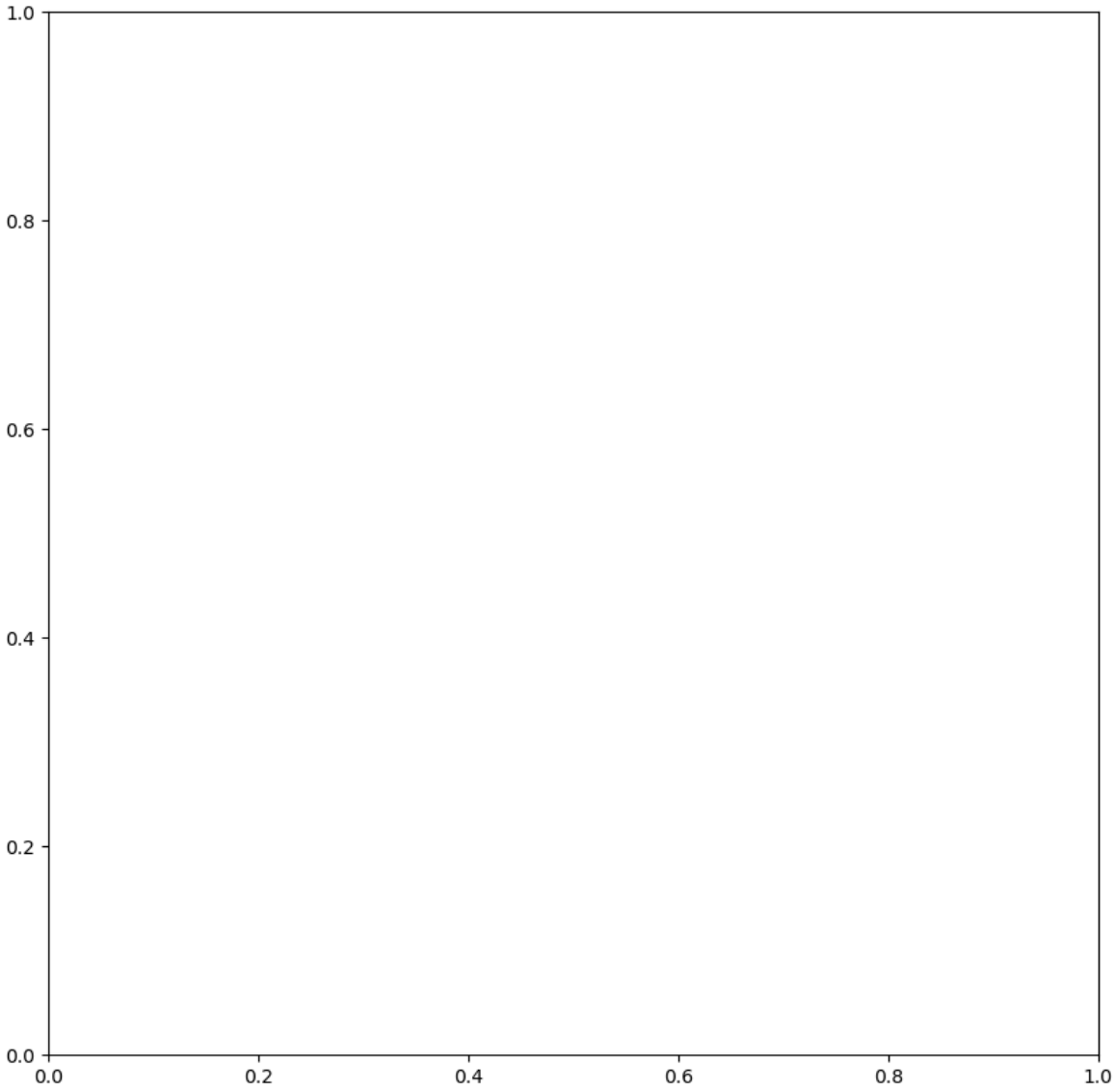
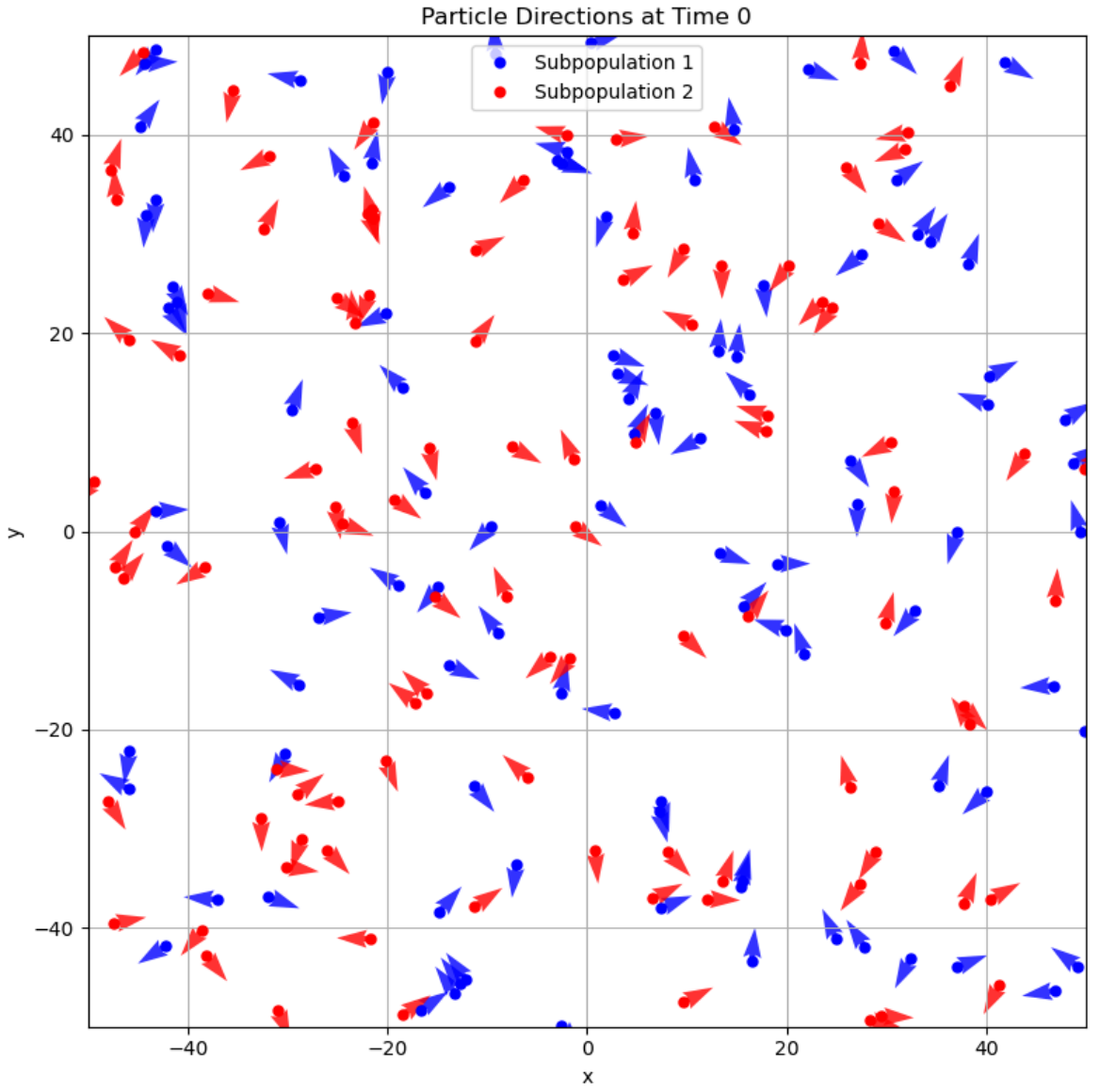
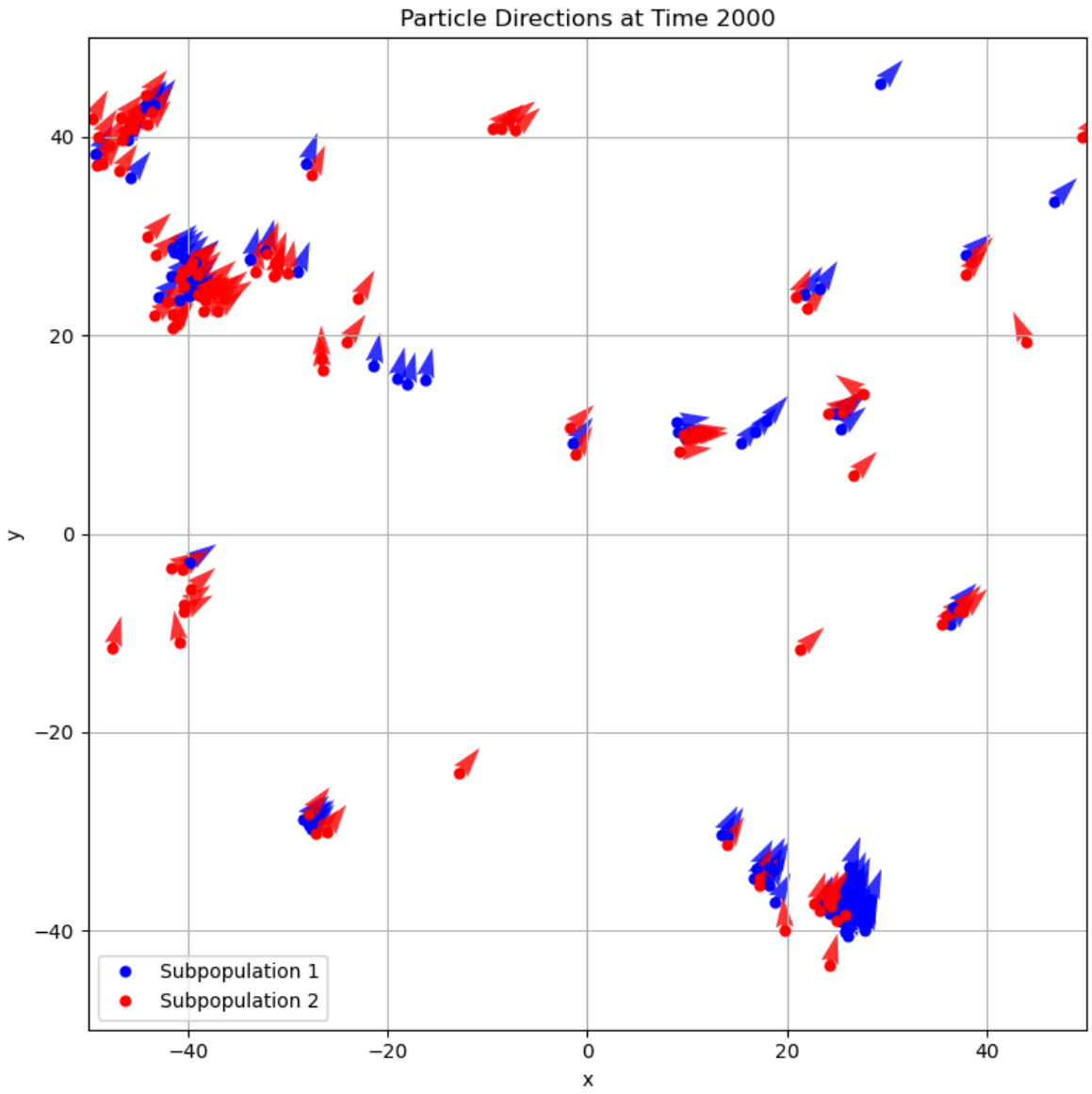
6000

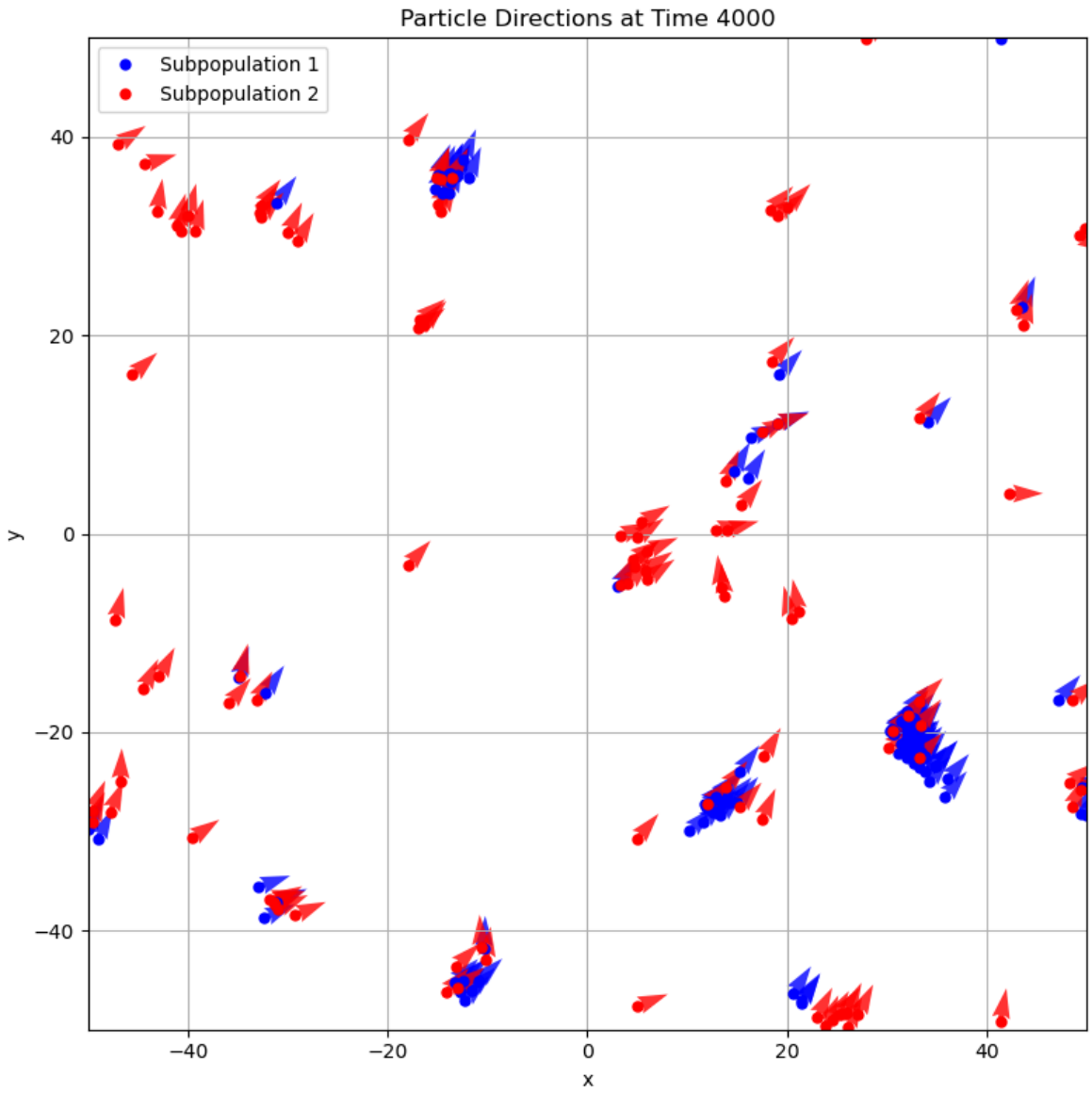


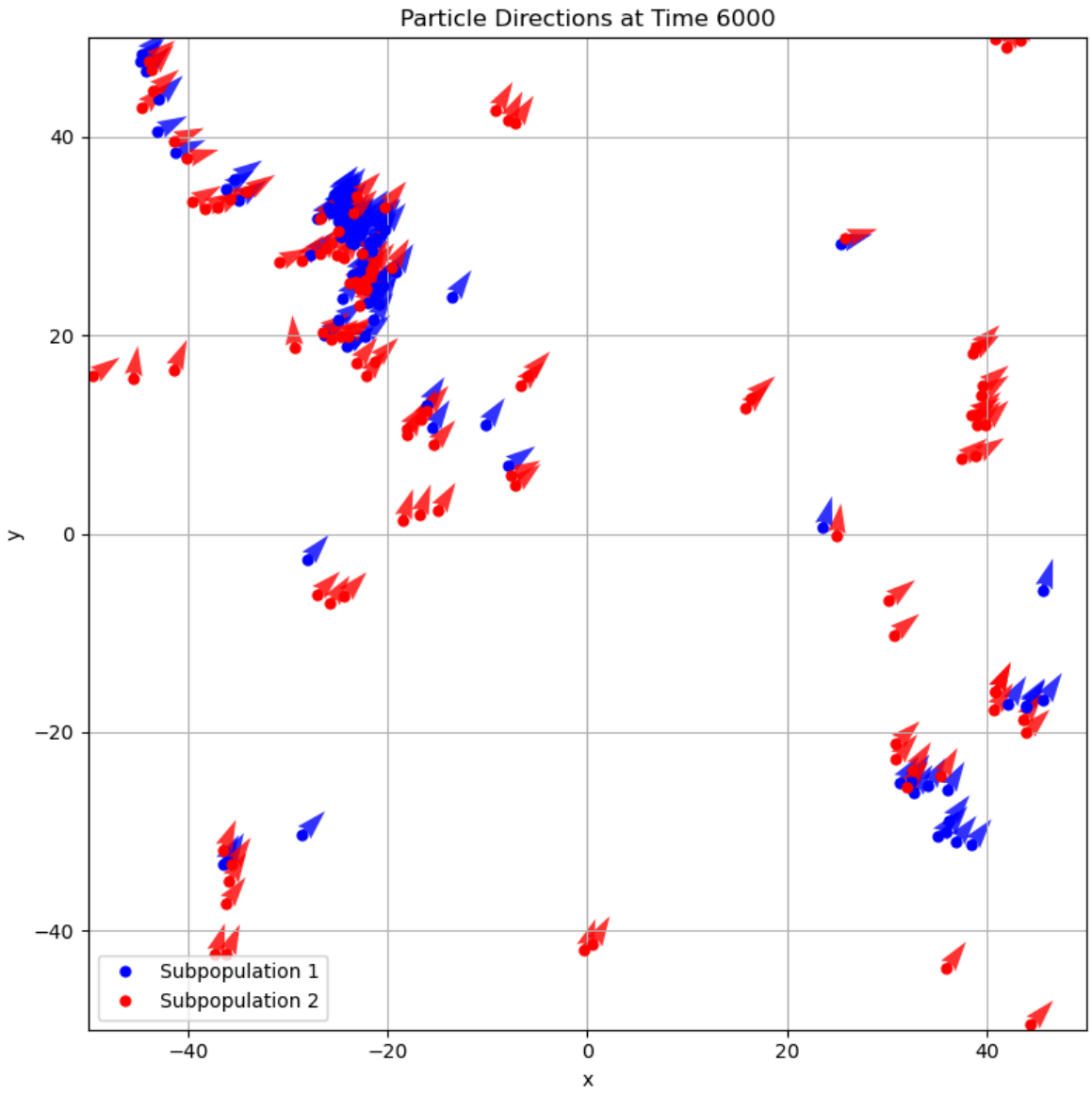
In [78]:
```
time_steps = [0, 2000, 4000, 6000]
N_half = N_part // 2

for i, time in enumerate(time_steps):
    plt.figure(figsize=(8, 8))

    x_positions = config_x[i]
    y_positions = config_y[i]
    angles = config_theta[i]

    x_positions_1, x_positions_2 = x_positions[:N_half], x_positions[N_half:]
    y_positions_1, y_positions_2 = y_positions[:N_half], y_positions[N_half:]
    angles_1, angles_2 = angles[:N_half], angles[N_half:]

    u1, v1 = np.cos(angles_1), np.sin(angles_1)
    u2, v2 = np.cos(angles_2), np.sin(angles_2)

    plt.plot(x_positions_1, y_positions_1, '.', color='blue', markersize=10, lab
    plt.plot(x_positions_2, y_positions_2, '.', color='red', markersize=10, labe

    plt.quiver(x_positions_1, y_positions_1, u1, v1, color='blue', angles='xy',
    plt.quiver(x_positions_2, y_positions_2, u2, v2, color='red', angles='xy', s

    plt.title(f'Particle Directions at Time {time}')
    plt.xlabel('x')
```

```
    plt.ylabel('y')
    plt.grid()
    plt.xlim([-L / 2, L / 2])
    plt.ylim([-L / 2, L / 2])
    plt.legend()
    plt.tight_layout()
    plt.show()
```




Particle Directions at Time 2000
40
20
0
−20
−40
y
−40
−20
0
20
40
x
Subpopulation 1
Subpopulation 2

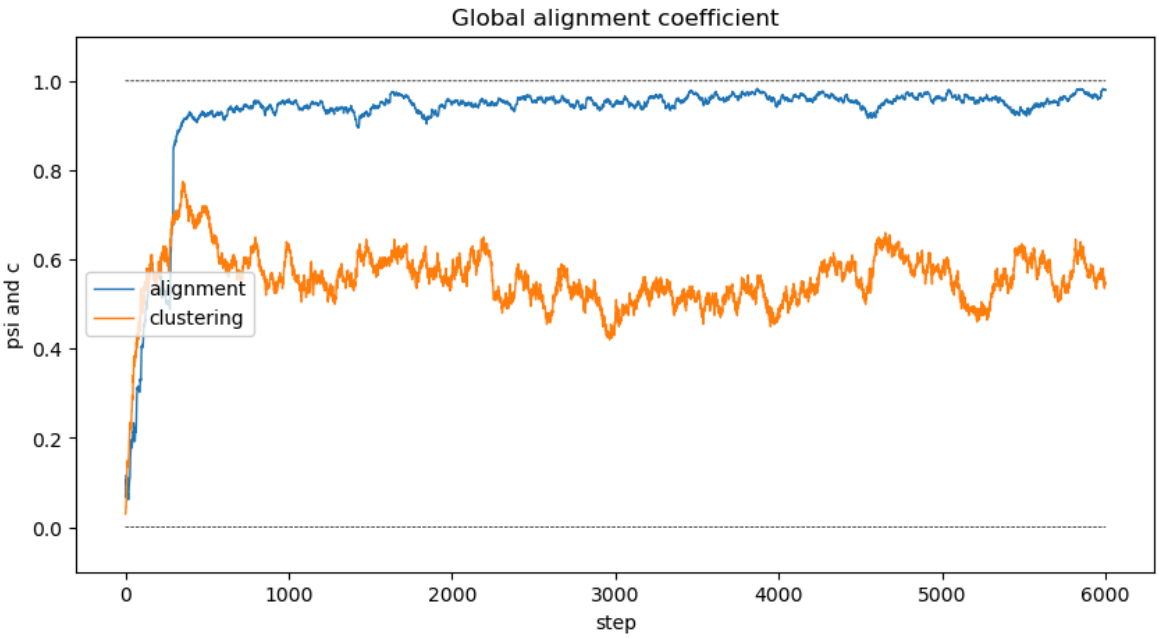

Particle Directions at Time 4000
Subpopulation 1
Subpopulation 2
40
20
0
−20
−40
y
−40
−20
0
20
40
x



P4

In [79]:

```
from matplotlib import pyplot as plt
plt.figure(figsize=(10, 5))
plt.plot(psi2, '-', linewidth=1, label='alignment')
plt.plot(c2, '-', linewidth=1, label='clustering')
plt.plot(0 * psi2, '--', color='k', linewidth=0.5)
plt.plot(0 * psi2 + 1, '--', color='k', linewidth=0.5)
plt.title('Global alignment coefficient')
plt.legend()
plt.xlabel('step')
plt.ylabel('psi and c')
plt.ylim([-0.1, 1.1])
plt.show()
```



Q1

Studying the simulation, i can see that when clusters are formed, the low-noise particles remain aligned whereas the high-noise particles tend to defer from the alignment of the cluster. That is, the high-noise particles tend to move more randomly, disrupting the overall order and clustering of the system.

The low-noise particles try to form clusters, but the presence of the high-noise particles makes it harder for the entire system to achieve a coherent structure.