In [1]:
```
import numpy as np
import pylab as plt
nt = 1000
natom = 864
L = 10.229
Sigma = 3.4
t = np.zeros((nt))
x = np.zeros((natom, 3, nt))
v = np.zeros((natom, 3, nt))
```

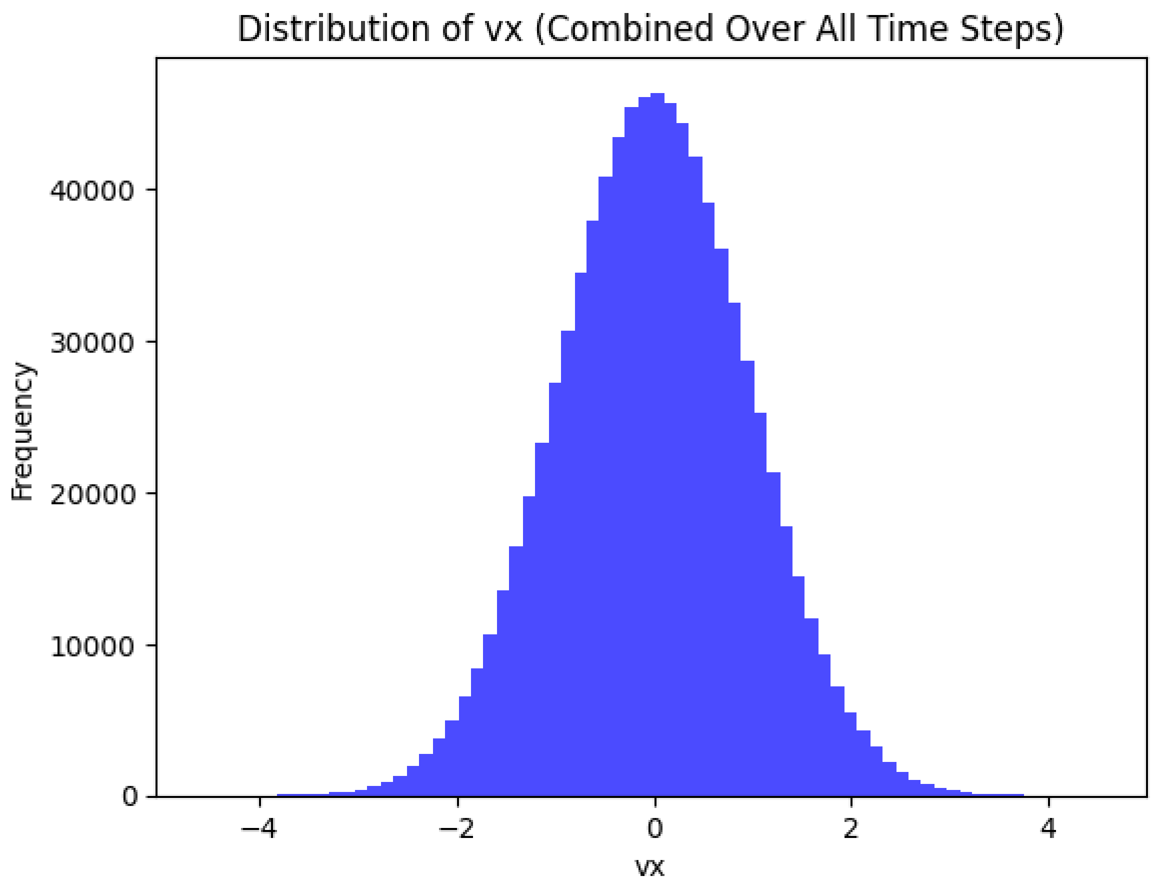
Open and read the Data file, the variable saved will be position (x) and velocity (v), the first axis is index of atom, the second is %the direction, the third is time step. Format:

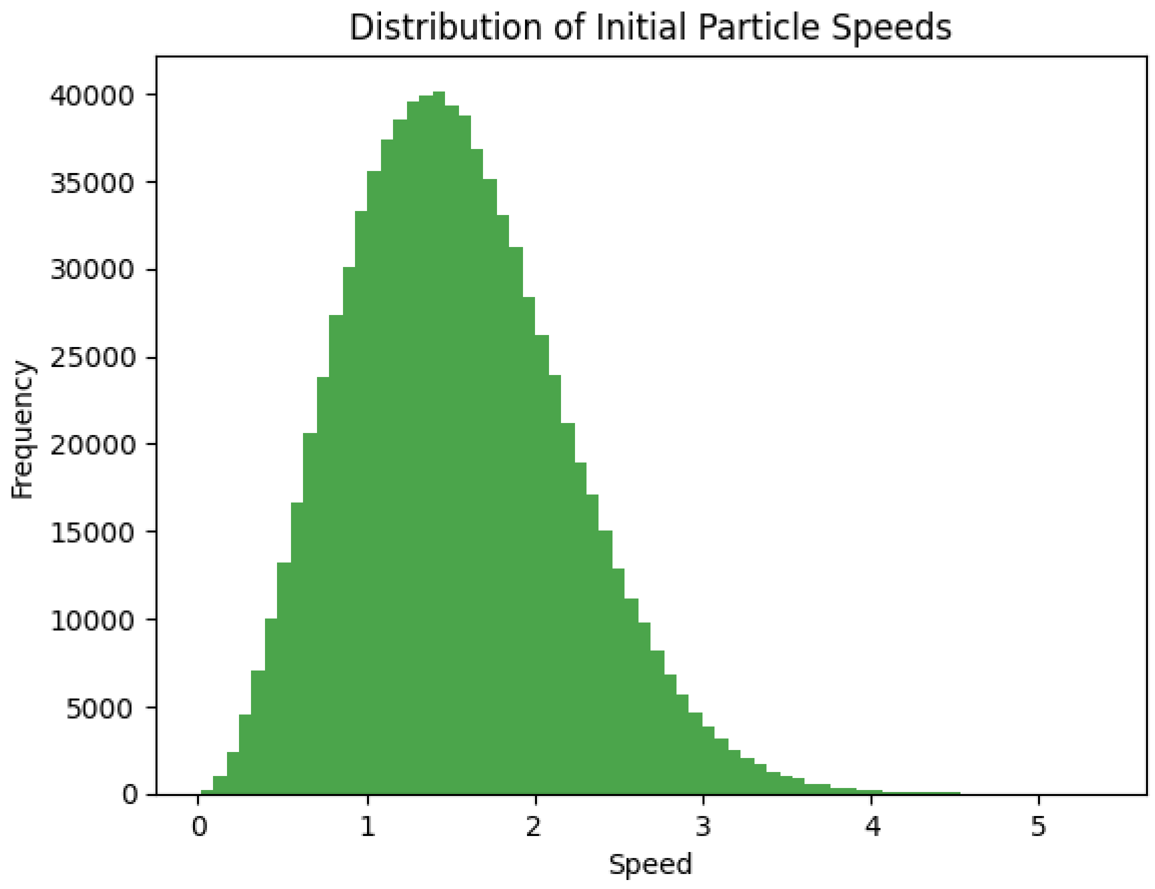
$$x[n = (0, 1, 2, \ldots), direction(x, y, z), time(ex: 0.1, 0.2)] = avlue$$

$$v[n = (0, 1, 2, \ldots), direction(x, y, z), time(ex: 0.1, 0.2)] = avlue$$

In [2]:
```
with open("Data/Output.lammpstrj") as f:
    for i in range(nt):
        dummy = f.readline()
        t[i] = f.readline()
        for d in range(7):
            dummy = f.readline()
        for j in range(natom):
            dummy = f.readline()
            line = dummy.split()
            for k in range(3):
                x[j, k, i] = float(line[k + 1])
                v[j, k, i] = float(line[k + 4])
```

In [3]:
```
#plot histogram of velocity
# Extract velocity in x direction at the first time step
# Extract velocity in x direction at the first time step
vx_combined = v[:, 0, :].flatten()
vy_combined = v[:, 1, :].flatten()
vz_combined = v[:, 2, :].flatten()
# Plot histogram of vx
plt.hist(vx_combined, bins=70, alpha=0.7, color='blue')
#plt.hist(vy_combined, bins=70, alpha=0.7, color='red')
#plt.hist(vz_combined, bins=70, alpha=0.7, color='purple')
plt.xlabel('vx')
plt.ylabel('Frequency')
plt.title('Distribution of vx (Combined Over All Time Steps)')
plt.show()
# Plot histogram of speeds
# Calculate the speed of each particle as the magnitude of the velocity v
speed = np.linalg.norm(v, axis=1).flatten()  # Flatten to combine all tim
plt.hist(speed, bins=70, alpha=0.7, color='green')
plt.xlabel('Speed')
plt.ylabel('Frequency')
plt.title('Distribution of Initial Particle Speeds')
plt.show()
```

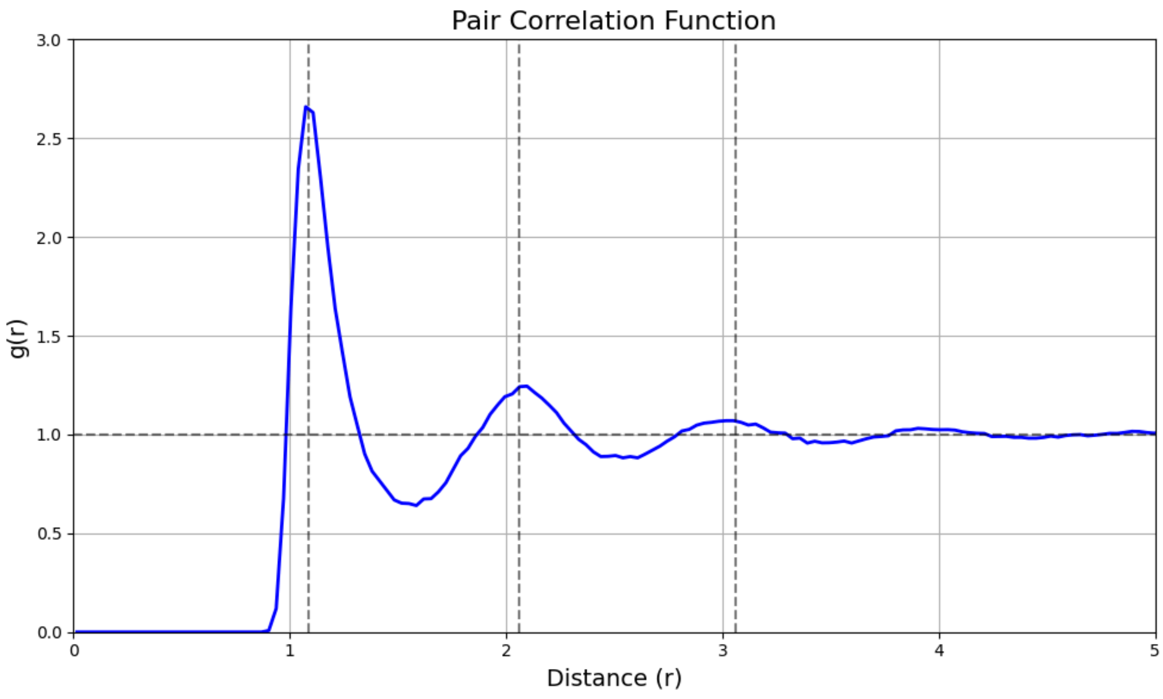


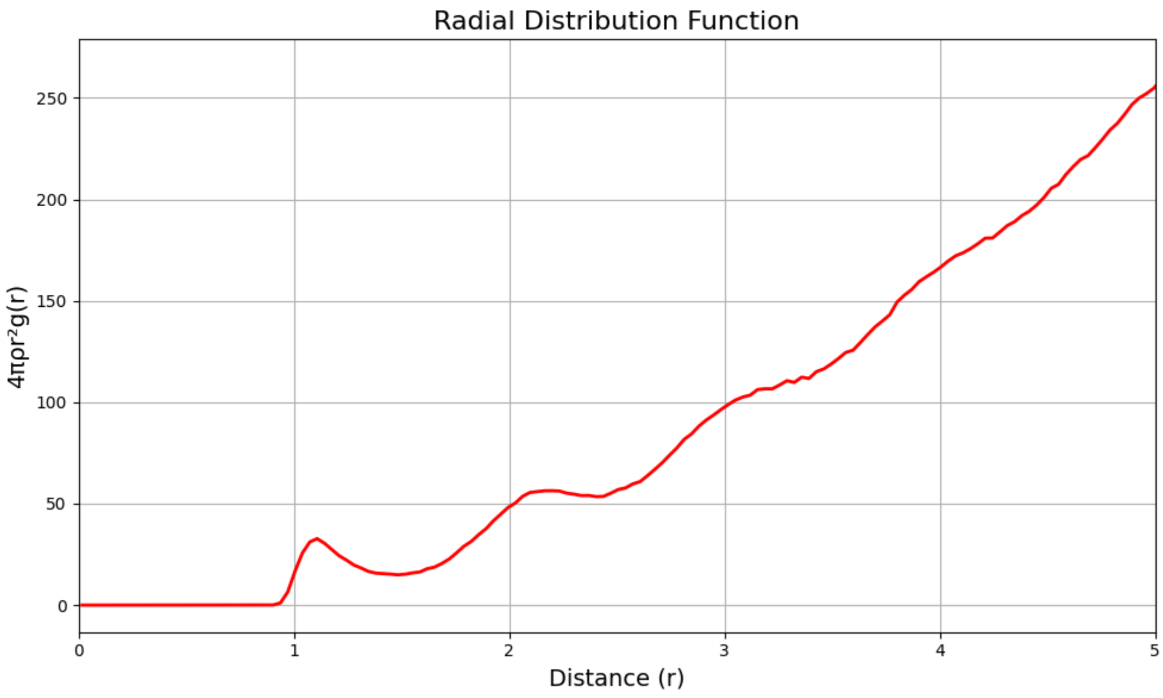


In [4]:
```
def compute_pair_correlation(positions, box_length, nbins=100, r_max=None
    """
    Compute the pair correlation function g(r) for a system of particles.

    Parameters:
```

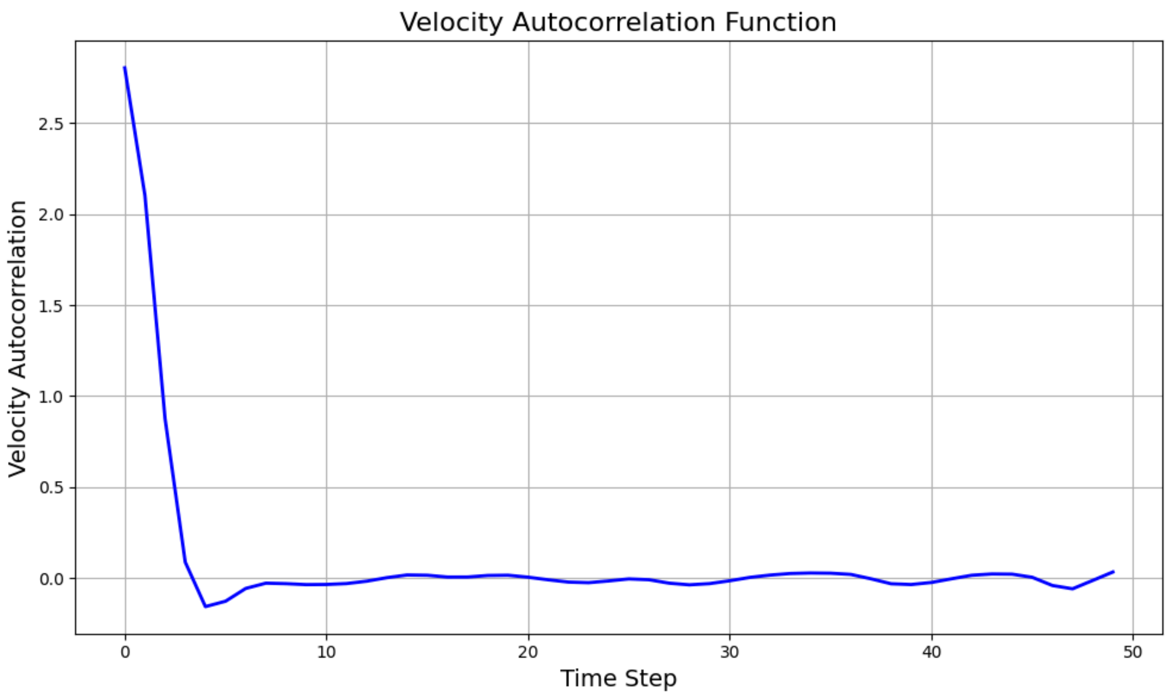
```
    positions (numpy.ndarray): Positions of atoms at a specific time step
    box_length (float): Length of the simulation box (assuming cubic)
    nbins (int): Number of bins for histogram
    r_max (float): Maximum distance to consider (defaults to half box len

    Returns:
    r (numpy.ndarray): Radial distance values
    g_r (numpy.ndarray): Pair correlation function values
    """
    natom = positions.shape[0]

    # If r_max is not specified, use half of the box length
    if r_max is None:
        r_max = box_length / 2.0

    # Create bins for the histogram
    bins = np.linspace(0, r_max, nbins + 1)
    r = 0.5 * (bins[1:] + bins[:-1])  # Centers of bins
    dr = bins[1] - bins[0]  # Bin width

    # Initialize histogram for pair distances
    hist = np.zeros(nbins)

    # Calculate all pairwise distances considering periodic boundary cond
    for i in range(natom):
        for j in range(i+1, natom):
            # Calculate distance vector, accounting for periodic boundary
            dx = positions[i, 0] - positions[j, 0]
            dy = positions[i, 1] - positions[j, 1]
            dz = positions[i, 2] - positions[j, 2]

            # Apply minimum image convention
            dx = dx - box_length * np.round(dx / box_length)
            dy = dy - box_length * np.round(dy / box_length)
            dz = dz - box_length * np.round(dz / box_length)

            # Calculate distance
            r_ij = np.sqrt(dx**2 + dy**2 + dz**2)

            # Add to histogram if within range
            if r_ij < r_max:
                bin_index = int(r_ij / dr)
                if bin_index < nbins:
                    hist[bin_index] += 2  # Count each pair twice (i->j a

    # Normalize histogram to get g(r)
    # Volume of the shell at distance r with width dr
    shell_volume = 4.0 * np.pi * r**2 * dr

    # Number density of the system
    number_density = natom / (box_length**3)

    # Expected number of particles in each shell for an ideal gas
    ideal_count = number_density * shell_volume

    # Normalize to get g(r)
    g_r = hist / (natom * ideal_count)

    return r, g_r
```

```python
# Calculate g(r) for multiple time steps and average
def average_pair_correlation(x, box_length, time_steps=10, nbins=100):
    """
    Calculate the average pair correlation function over multiple time st

    Parameters:
    x (numpy.ndarray): Positions of atoms for all time steps, shape (nato
    box_length (float): Length of the simulation box
    time_steps (int): Number of time steps to use for averaging
    nbins (int): Number of bins for histogram

    Returns:
    r (numpy.ndarray): Radial distance values
    g_r_avg (numpy.ndarray): Average pair correlation function values
    """
    natom, _, nt = x.shape

    # Use equally spaced time steps for averaging
    step = nt // time_steps
    selected_times = np.arange(0, nt, step)[:time_steps]

    # Initialize arrays
    r = None
    g_r_avg = np.zeros(nbins)

    # Calculate g(r) for each selected time step
    for t_idx in selected_times:
        positions = x[:, :, t_idx]
        r, g_r = compute_pair_correlation(positions, box_length, nbins)
        g_r_avg += g_r

    # Average over all time steps
    g_r_avg /= len(selected_times)

    return r, g_r_avg

# Calculate and plot the pair correlation function
r, g_r = average_pair_correlation(x, L, time_steps=20, nbins=150)

plt.figure(figsize=(10, 6))
plt.plot(r, g_r, 'b-', linewidth=2)
plt.xlabel('Distance (r)', fontsize=14)
plt.ylabel('g(r)', fontsize=14)
plt.title('Pair Correlation Function', fontsize=16)
plt.grid(True)
plt.vlines(x=(3.7/Sigma), color='k', linestyle='--', alpha=0.5, ymin = 0,
plt.vlines(x=(7.0/Sigma), color='k', linestyle='--', alpha=0.5, ymin = 0,
plt.vlines(x=(10.4/Sigma), color='k', linestyle='--', alpha=0.5, ymin = 0
plt.xlim(0, min(5, L/2))
plt.ylim(0, 3)
plt.axhline(y=1, color='k', linestyle='--', alpha=0.5)
plt.tight_layout()
plt.show()

# Also display the radial distribution function (RDF) which is 4πρr²g(r)
rho = natom / L**3  # Number density
rdf = 4 * np.pi * rho * r**2 * g_r

plt.figure(figsize=(10, 6))
plt.plot(r, rdf, 'r-', linewidth=2)
plt.xlabel('Distance (r)', fontsize=14)
plt.ylabel('4πρr²g(r)', fontsize=14)
plt.title('Radial Distribution Function', fontsize=16)
plt.grid(True)
plt.xlim(0, min(5, L/2))
plt.tight_layout()
plt.show()
```

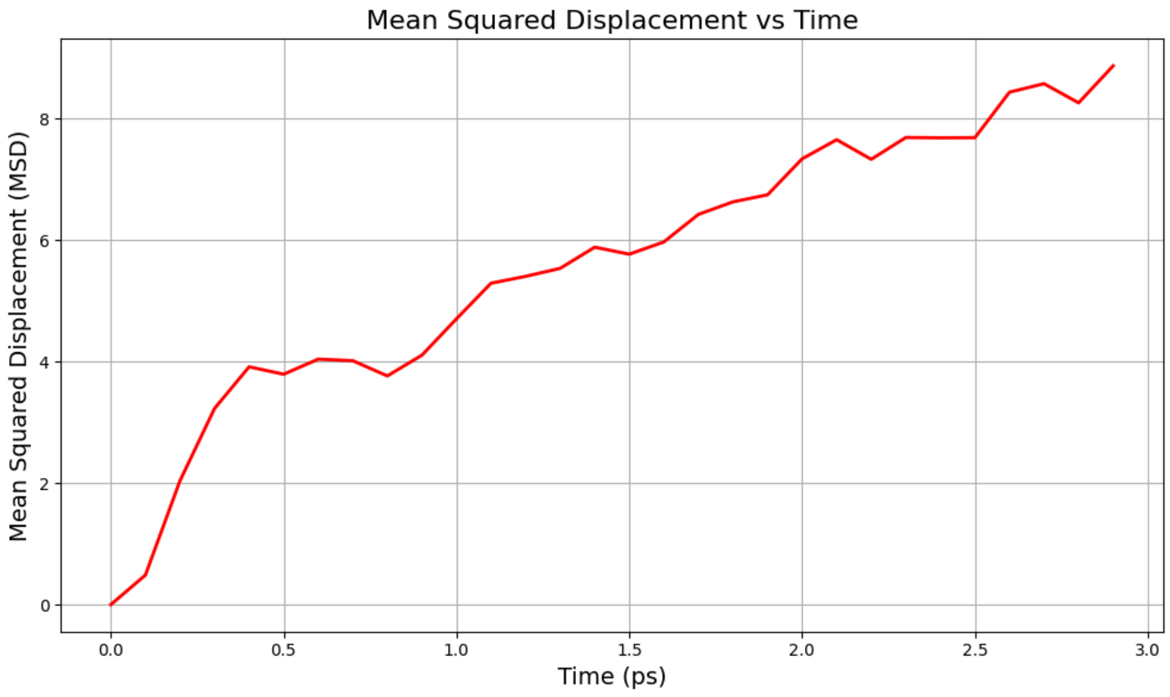




In [5]:
```
def velocity_correlation(v, nt):
    """
    Calculate the velocity autocorrelation function.

    Parameters:
    v (numpy.ndarray): Velocity array of shape (natom, 3, nt)
    nt (int): Number of time steps

    Returns:
    numpy.ndarray: Velocity autocorrelation function
    """
    natom = v.shape[0]
    vacf = np.zeros(nt)

    for t in range(nt):
        for tau in range(nt - t):
            vacf[t] += np.sum(v[:, :, tau] * v[:, :, tau + t])
        vacf[t] /= (natom * (nt - t))

    return vacf
ntpl = 50
# Calculate velocity autocorrelation function
vacf = velocity_correlation(v, ntpl)

# Plot velocity autocorrelation function
plt.figure(figsize=(10, 6))
plt.plot(np.arange(ntpl), vacf, 'b-', linewidth=2)
plt.xlabel('Time Step', fontsize=14)
plt.ylabel('Velocity Autocorrelation', fontsize=14)
plt.title('Velocity Autocorrelation Function', fontsize=16)
plt.grid(True)
plt.tight_layout()
plt.show()
```



In [6]:
```
ntpl = 30
msd = np.zeros(ntpl)
for nts in range(ntpl):
    msd[nts] = np.mean(np.sum((x[:, :, nts] - x[:, :, 0])**2, axis=1))
plt.figure(figsize=(10, 6))
plt.plot(np.arange(ntpl)/10, msd, 'r-', linewidth=2)
plt.xlabel('Time (ps)', fontsize=14)
plt.ylabel('Mean Squared Displacement (MSD)', fontsize=14)
plt.title('Mean Squared Displacement vs Time', fontsize=16)
plt.grid(True)
plt.tight_layout()
plt.show()
```


Mean Squared Displacement vs Time
Mean Squared Displacement (MSD)
Time (ps)
0
2
4
6
8
0.0
0.5
1.0
1.5
2.0
2.5
3.0