2.1 Flow Models

---

1. Fundamental Definition

Flow models 是由 ODEs (Ordinary Differential Equations) 所建構而成的模型，其中有三個重要的元素:

- Trajectory
- Vector Filed (VF)
- Flow

Trajectory 是在描述 ODE 的空間中的路徑，可以想像成一顆粒子在空間中隨時間移動的路徑。它有以下形式:

$$X : [0,1] \to \mathbb{R}^d, \quad t \mapsto X_t$$

VF 是粒子在空間中隨時間移動的方向 (或者可以想像成是方向向量)，我們會假設粒子皆遵循VF的方向在移動。它有以下形式:

$$u : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d, \quad (x,t) \mapsto u_t(x)$$

透過定義 **Trajectory** 和 **VF**，我們可以定義以下 ODE 問題: 給定初始條件 $X_0 = x_0$，則

$$\frac{d}{dt} X_t = u_t(X_t)$$

Flow 則是上述 ODE 問題的解。Flow ψ 是一個 function

$$\psi : \mathbb{R}^d \times [0,1] \mapsto \mathbb{R}^d, \quad (x_0, t) \mapsto \psi_t(x_0)$$

該解有以下形式，給定初始條件為 $\psi_0(x_0) = x_0$，則

$$\frac{d}{dt} \psi_t(X_t) = u_t(\psi_t(x_0))$$

Keypoint: ***Vector fileds define ODEs whose solutions are flows.***

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2. Simulating an ODE

數值微分方程中有提供一個基本的模擬方法，**Euler method**。

給定初始條件 $X_0 = x_0$，Euler method 有以下迭代公式，

$$X_{t+h} = X_t + h u_t(X_t), \quad t = 0, h, 2h, \ldots, 1-h$$

其中，$h = 1/n$ 為 step size。

Note: 此處可以直接放 $u_t(X_t)$ 是因為 $\frac{d}{dt}X_t = u_t(X_t)$。

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3. Flow Models

Flow models 是由 ODEs 所描述，也就是

$$X_0 \sim p_{\text{init}}$$
$$\frac{d}{dt}X_t = u_t^{\theta}(X_t)$$

其中 p_{init} 為一個任意分佈，以及 $u_t^{\theta}(X_t)$ 為由類神經網路搭配參數 θ 所建構的 VF。

Flow models 的目標在透過上述的 learning process 使得最後得到的 X_1 和 p_{data} 夠相似，也就是我們相信 X_1 是來自 p_{data}。

Algorithm 1 Sampling from a Flow Model with Euler method

```
Require: Neural network vector field $u_t^\theta$, number of steps $n$
1: Set $t = 0$
2: Set step size $h = \frac{1}{n}$
3: Draw a sample $X_0 \sim p_{\text{init}}$
4: for $i = 1, \dots, n$ do
5:     $X_{t+h} = X_t + h u_t^\theta(X_t)$
6:     Update $t \leftarrow t + h$
7: end for
8: return $X_1$
```

---

4. Simulation

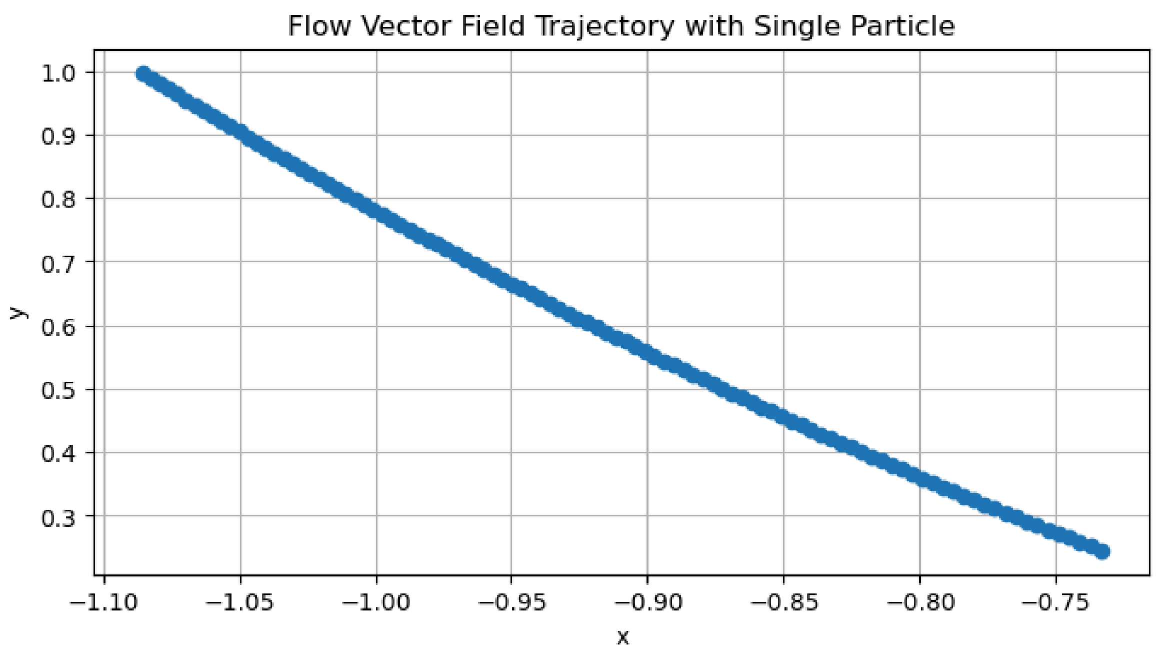
以下模擬展示，在 flow model 作用下單個粒子的 trajectory 和多個粒子的 trajectories

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

from typing import Optional

import torch
import torch.nn as nn
import torch.nn.functional as F

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

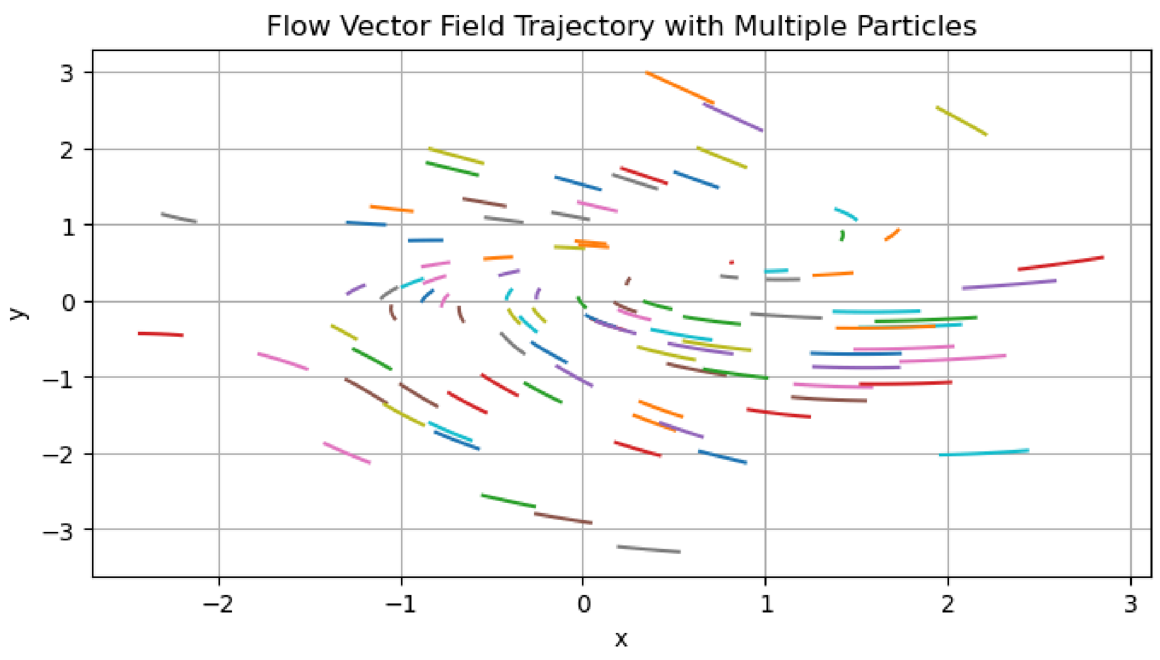
In [2]:
```python
# set up an arbitrary neural network for flow step
class VF_step_flow(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super(VF_step_flow, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.fc2 = nn.Linear(hidden_size, output_size)

    def forward(self, x):
        x = F.relu(self.fc1(x))
        x = self.fc2(x)

        return x
```

In [3]:
```
def flow_model(num_particle: int, step_size: int, random_seed: Optional[i

    """
    Simulate the flow field of particles using a neural network model.
    Args:
        num_particle (int): Number of particles to simulate.
        step_size (int): Number of steps for the simulation.
        random_seed (int, optional): Random seed for initial positions. D
    Returns:
        list: A list of numpy arrays representing the history of particle
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    # generate initial positions of particles
    X = np.random.normal(0, 1, size=(num_particle, 2))
    X_input = torch.tensor(X, dtype=torch.float32, requires_grad=False).t
    X_history = [X]

    model = VF_step_flow(input_size=2, hidden_size=10, output_size=2).to(

    t = 0   # time step
    h = 1 / step_size

    # main
    while t < 1:
        for _ in range(step_size):
            with torch.no_grad():
                X_input = X_input + h * model(X_input)
            X_history.append(X_input.cpu().detach().numpy())
            t = t + h

    return X_history
```

In [4]:
```
# simulate the trajectory of a single particle in the flow model
single_particle_flow = flow_model(num_particle=1, step_size=100, random_s

x = [single_particle_flow[i][0][0] for i in range(len(single_particle_flo
y = [single_particle_flow[i][0][1] for i in range(len(single_particle_flo

plt.figure(figsize=(8, 4))
plt.plot(x, y, marker="o")
plt.grid()
plt.xlabel("x")
plt.ylabel("y")
plt.title("Flow Vector Field Trajectory with Single Particle")
plt.show()
```



In [5]:
```
# simulate the trajectory of multiple particles in the flow model
multiple_particle_flow = flow_model(num_particle=100, step_size=100, rand

particle = {
    f"particle_{j}": [multiple_particle_flow[i][j] for i in range(len(mul
    for j in range(len(multiple_particle_flow[0]))
}

plt.figure(figsize=(8, 4))
for key in particle.keys():
    plt.plot(
        [particle[key][i][0] for i in range(len(particle[key]))],
        [particle[key][i][1] for i in range(len(particle[key]))]
    )
plt.grid()
plt.xlabel("x")
plt.ylabel("y")
plt.title("Flow Vector Field Trajectory with Multiple Particles")
plt.show()
```



2.2 Diffusion Models

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1. Fundamental Definition

Diffusion models 是由 SDEs (Stochastic Differential Equations) 所建構而成的模型，其元素與 flow models 類似，差別在於 diffusion models 中的 trajectory 具有隨機性。

對於這樣有隨機性的 trajectory 我們可以將其視為一個隨機過程 (stochastic process) $(X_t)_{0\leq t\leq 1}$，也就是

$$X_t \text{ is a random variable for every } 0 \leq t \leq 1$$

$$X : [0,1] \to \mathbb{R}^d, \quad t \mapsto X_t \text{ is a random trajectory for every draw of } X$$

Brownian Motion

在 SDEs 中，**Brownian motion** 常被用於描述隨機項 (stochastic term)。對於一個隨機過程，$(W_t)_{0\leq t\leq 1}$，我們有以下性質:

1. $W_0 = 0$.
2. **normal increments**: $W_t - W_s \sim N(0, t-s)$ for all $0 < s < t$.
3. **independent increments**: For any $0 \leq t_0 \leq t_1 \leq \ldots \leq t_n = 1$, the increments $W_{t_1} - W_{t_0}, \ldots, W_{t_n} - W_{t_{n-1}}$ are independent random variables.

滿足這三個性質的隨機過程就稱為 Brownian motion 或是 Wiener process。

Brownian motion 可以由以下迭代式進行模擬，給定初始條件 $W_0 = 0$，則

$$W_{t+h} = W_t + \sqrt{h}\varepsilon, \quad \varepsilon \sim N(0,1)$$

From ODEs to SDEs

由於 SDEs 中包含了隨機項，因此無法像 ODEs 一樣可以對其進行微分，因此我們需要做一些適當的處理。

首先，我們需要對 ODEs 做**離散化**：

$$
\begin{aligned}
&\frac{d}{dt}X_t = u_t(X_t) \\
\Leftrightarrow\ &\frac{1}{h}(X_{t+h} - X_t) = u_t(X_t) + R_t(h) \\
\Leftrightarrow\ &X_{t+h} = X_t + hu_t(X_t) + hR_t(h)
\end{aligned}
$$

其中 $R_t(h)$ 為誤差項，滿足 $\lim\limits_{h\to 0} R_t(h) = 0$。

接著，我們在上述離散化後的 ODEs 中加入隨機項，也就是 Brownian motion，

$$X_{t+h} = X_t + hu_t(X_t) + \sigma_t(W_{t+h} - W_t)$$

其中 $hu_t(X_t)$ 為固定項 (deterministic term)、$W_{t+h} - W_t$ 為隨機項，以及σ_t 為擴散係數 (diffusion coefficient)。從 Brownian motion 的性質中，我們可以得到 $W_{t+h} - W_t \sim N(0, h)$。

最後，我們就可以得到 SDEs 問題，給定初始條件為 $X_0 = x_0$ 以及 $W_0 = 0$，則

$$dX_t = u_t(X_t)dt + \sigma_t dW_t$$

Note: 此處並沒有 flows 這個解，僅能依賴於數值解。

---

2. Simulation an SDE

數值微分方程中有提供一個基本的模擬方法，**Euler-Maruyama method**。

給定初始條件 $X_0 = x_0$，Euler-Maruyama method 有以下迭代公式，

$$X_{t+h} = X_t + hu_t(X_t) + \sqrt{h}\sigma_t\varepsilon, \quad \varepsilon \sim N(0,1) \text{ and } t = 0, h, 2h, \ldots, 1-h$$

其中，$h = 1/n$ 為 step size。

---

3. Diffusion Models

Diffusion models 是由 SDEs 所描述，也就是

$$
\begin{aligned}
X_0 &\sim p_{\text{init}} \\
dX_t &= u_t^\theta(X_t)dt + \sigma_t dW_t
\end{aligned}
$$

其中 p_{init} 為一個任意分佈，以及 $u_t^\theta(X_t)$ 為由類神經網路搭配參數 θ 所建構的 VF。

Diffusion models 的目標同樣是透過上述的 learning process 使得最後得到的 X_1 和 p_{data} 夠相似。

Algorithm 2 Sampling from a Diffusion Model (Euler-Maruyama method)

```
Require: Neural network $u_t^\theta$, number of steps $n$, diffusion coefficient $\sigma_t$
1: Set $t = 0$
2: Set step size $h = \frac{1}{n}$
3: Draw a sample $X_0 \sim p_{\text{init}}$
4: for $i = 1, \dots, n$ do
5:     Draw a sample $\epsilon \sim \mathcal{N}(0, I_d)$
6:     $X_{t+h} = X_t + h u_t^\theta(X_t) + \sigma_t \sqrt{h}\epsilon$
7:     Update $t \leftarrow t + h$
8: end for
9: return $X_1$
```

---

4. Simulation

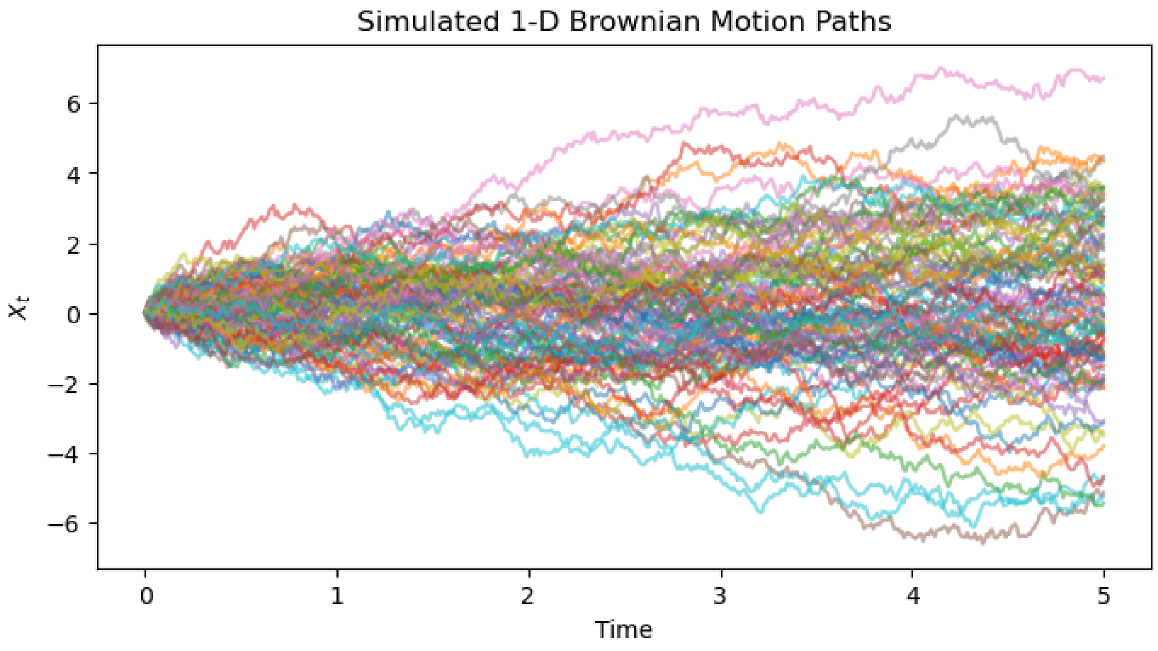
以下模擬展示:

1. 1-D Brownian motion 路徑過程
2. 在 diffusion model 作用下，單個粒子的 trajectory 和多個粒子的 trajectories
3. 在 diffusion model 作用下，考慮不同擴散係數對於 trajectory 的影響

In [6]:
```python
# import necessary libraries
import numpy as np
import matplotlib.pyplot as plt

from typing import Optional

import torch
import torch.nn as nn
import torch.nn.functional as F

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

In [7]:
```python
def brownian_motion(num_path: int, num_period: float, step_size: int, ran

    """
    Simulate the 1-D Brownian motion.
    Args:
        num_path (int): Number of paths to simulate.
        num_period (float): Total time duration.
        step_size (int): Number of discrete time steps.
        random_seed (int, optional): Random seed for reproducibility. Def
    Returns:
        np.ndarray: A 1D array of shape (num_path, step_size) representin
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    dt = num_period / step_size
    dW = np.sqrt(dt) * np.random.randn(num_path, step_size)
    X = np.cumsum(dW, axis=1)
    X = np.hstack((np.zeros((num_path, 1)), X))  # add initial position a
    return X
```

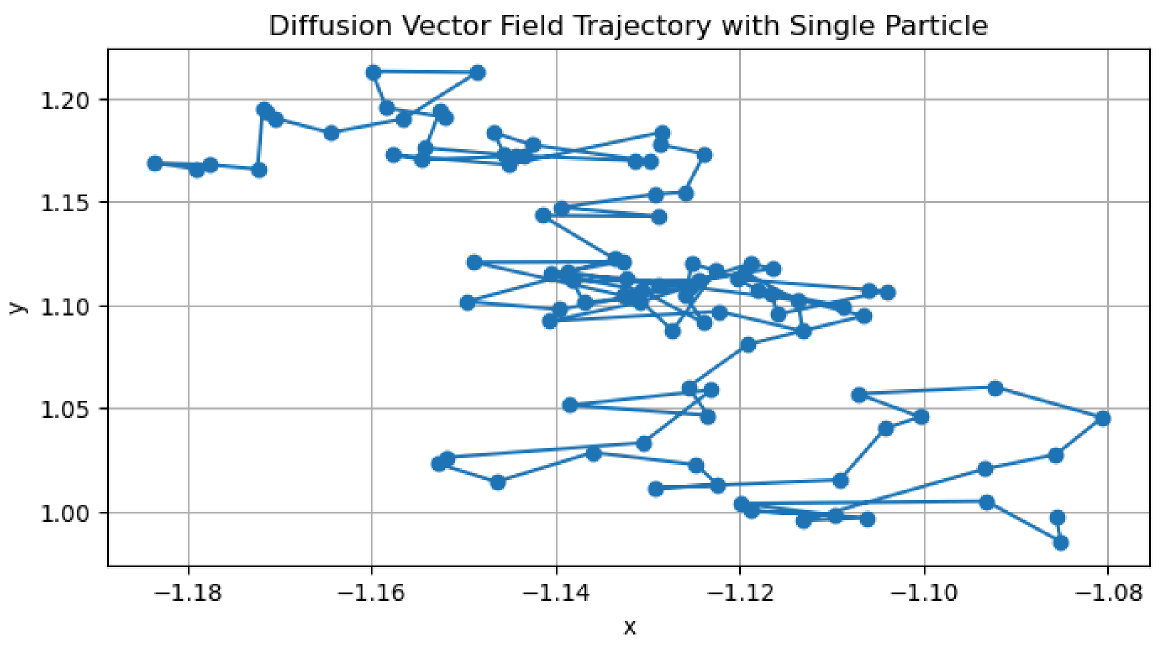
In [8]:
```
# simulate the 1-D Brownian motion
num_path = 100
num_period = 5
step_size = 500
BM = brownian_motion(num_path, num_period, step_size, random_seed=123)

time_points = np.linspace(0, num_period, step_size + 1)

plt.figure(figsize=(8, 4))
for path in range(BM.shape[0]):
    plt.plot(time_points, BM[path], alpha=0.5)
plt.xlabel("Time")
plt.ylabel("$X_t$")
plt.title("Simulated 1-D Brownian Motion Paths")
plt.show()
```



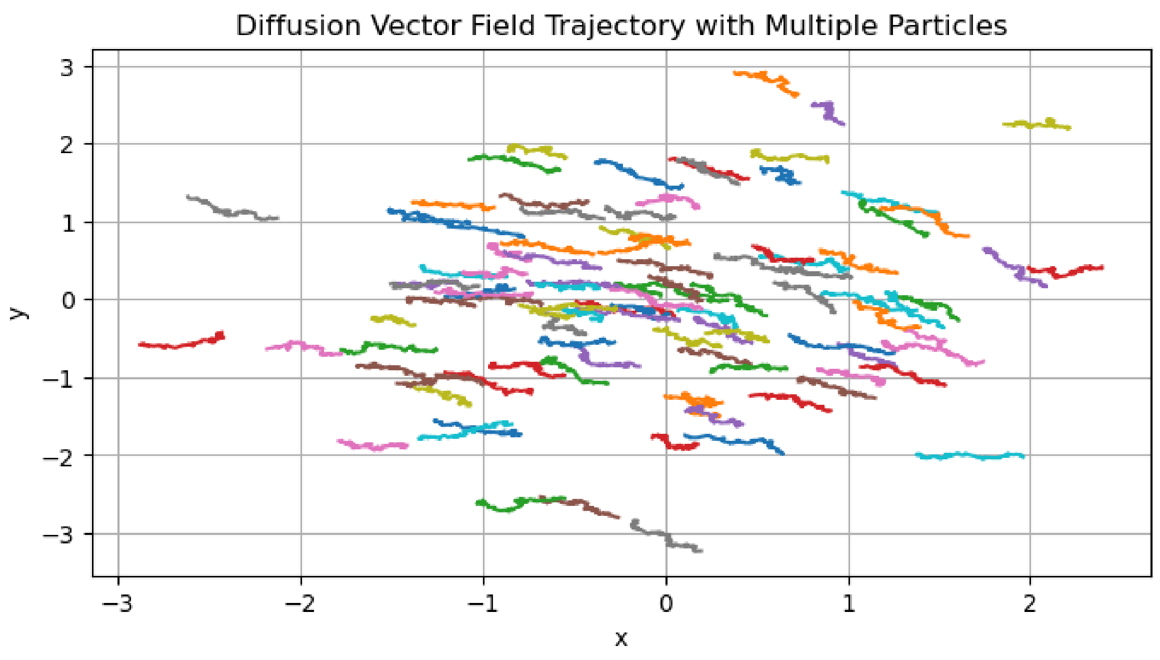
In [9]:
```
# set up an arbitrary neural network for diffusion step
class VF_step_diffusion(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super(VF_step_diffusion, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.fc2 = nn.Linear(hidden_size, output_size)

    def forward(self, x):
        x = F.relu(self.fc1(x))
        x = self.fc2(x)

        return x
```

In [10]:
```
def diffusion_model(num_particle: int, step_size: int, sigma: float, rand

    """
    Simulate the diffusion field of particles using a neural network mode
    Args:
        num_particle (int): Number of particles to simulate.
        step_size (int): Number of steps for the simulation.
        sigma (float): Standard deviation for the diffusion term.
        random_seed (int, optional): Random seed for initial positions. D
    Returns:
        list: A list of numpy arrays representing the history of particle
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    # generate initial positions of particles
    X = np.random.normal(0, 1, size=(num_particle, 2))
    X_input = torch.tensor(X, dtype=torch.float32, requires_grad=False).t
    X_history = [X]

    model = VF_step_diffusion(input_size=2, hidden_size=10, output_size=2

    t = 0  # time step

    # main
    while t < 1:
        for _ in range(step_size):
            h = 1 / step_size
            with torch.no_grad():
                epsilon = np.random.normal(0, 1, size=(num_particle, 2))
                diffusion_term = torch.tensor(sigma * np.sqrt(h) * epsilo
                X_input = X_input + h * model(X_input) + diffusion_term
            X_history.append(X_input.cpu().detach().numpy())
            t = t + h

    return X_history
```

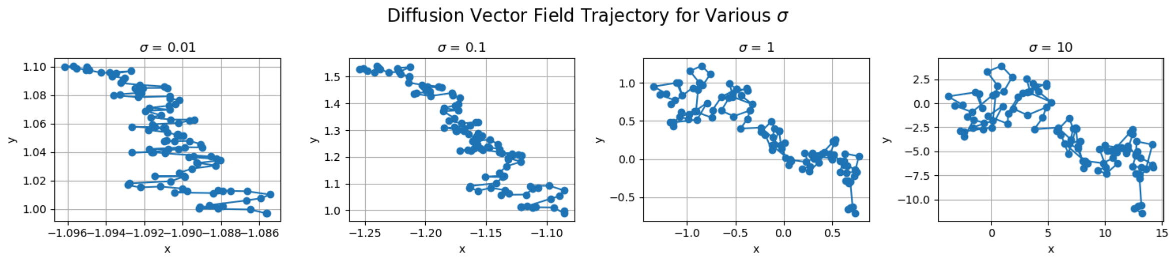
In [11]:
```
# simulate the trajectory of a single particle in the diffusion model
single_particle_diffusion = diffusion_model(num_particle=1, step_size=100

x = [single_particle_diffusion[i][0][0] for i in range(len(single_particl
y = [single_particle_diffusion[i][0][1] for i in range(len(single_particl

plt.figure(figsize=(8, 4))
plt.plot(x, y, marker="o")
plt.grid()
plt.xlabel("x")
plt.ylabel("y")
plt.title("Diffusion Vector Field Trajectory with Single Particle")
plt.show()
```



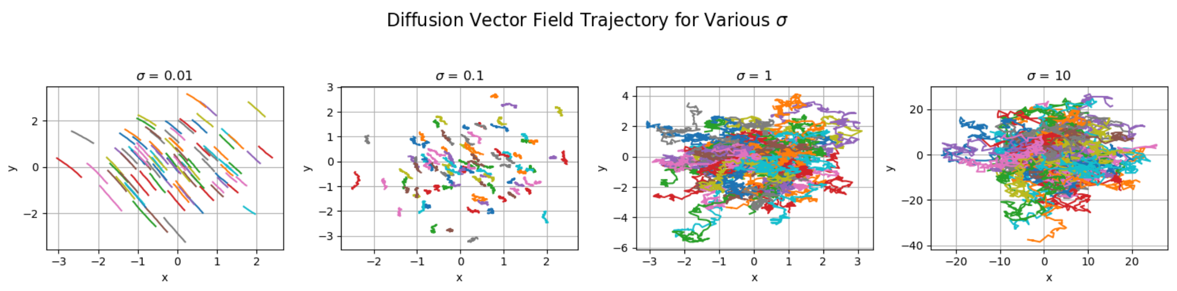
In [12]:
```
# simulate the trajectory of multiple particles in the diffusion model
multiple_particle_diffusion = diffusion_model(num_particle=100, step_size

particle = {
    f"particle_{j}": [multiple_particle_diffusion[i][j] for i in range(le
    for j in range(len(multiple_particle_diffusion[0]))
}

plt.figure(figsize=(8, 4))
for key in particle.keys():
    plt.plot(
        [particle[key][i][0] for i in range(len(particle[key]))],
        [particle[key][i][1] for i in range(len(particle[key]))]
    )
plt.grid()
plt.xlabel("x")
plt.ylabel("y")
plt.title("Diffusion Vector Field Trajectory with Multiple Particles")
plt.show()
```



In [13]:
```python
# simulate the trajectory of a single particle in the diffusion model for
sigma_list = [0.01, 0.1, 1, 10]
fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, sigma in enumerate(sigma_list):
    single_particle_diffusion = diffusion_model(num_particle=1, step_size

    x = [single_particle_diffusion[i][0][0] for i in range(len(single_par
    y = [single_particle_diffusion[i][0][1] for i in range(len(single_par

    axs[idx].plot(x, y, marker="o")
    axs[idx].grid()
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
    axs[idx].set_title(rf"$\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Diffusion Vector Field Trajectory for Various $\sigma$", f
plt.show()
```



In [14]:
```python
# simulate the trajectory of multiple particles in the diffusion model fo
sigma_list = [0.01, 0.1, 1, 10]
fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, sigma in enumerate(sigma_list):
    multiple_particle_diffusion = diffusion_model(num_particle=100, step_

    particle = {
        f"particle_{j}": [multiple_particle_diffusion[i][j] for i in rang
        for j in range(len(multiple_particle_diffusion[0]))
    }
    for key in particle.keys():
        axs[idx].plot(
            [particle[key][i][0] for i in range(len(particle[key]))],
            [particle[key][i][1] for i in range(len(particle[key]))]
        )
    axs[idx].grid()
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
    axs[idx].set_title(rf"$\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Diffusion Vector Field Trajectory for Various $\sigma$", f
plt.show()
```



2.3 More Example, Simulation, and Discussion

In [15]:
```
# import necessary libraries
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from typing import Optional

import torch
import torch.nn as nn
import torch.nn.functional as F

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

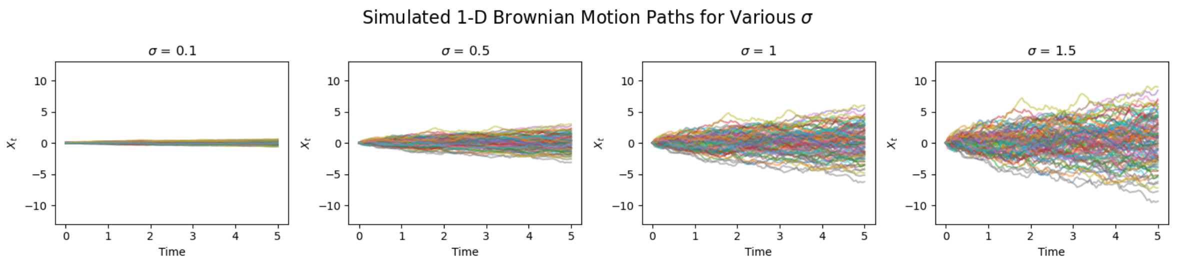
1. Implementing Brownian Motion with various sigma

給定初始條件 $X_0 = 0$，

$$dX_t = \sigma dW_t$$

In [16]:
```
def brownian_motion_2(num_path: int, num_period: float, step_size: int, s

    """
    Simulate the 1-D Brownian motion.
    Args:
        num_path (int): Number of paths to simulate.
        num_period (float): Total time duration.
        step_size (int): Number of discrete time steps.
        sigma (float): Diffusion term for the Brownian motion.
        random_seed (int, optional): Random seed for reproducibility. Def
    Returns:
        np.ndarray: A 1D array of shape (num_path, step_size) representin
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    dt = num_period / step_size
    dW = sigma * np.sqrt(dt) * np.random.randn(num_path, step_size)
    X = np.cumsum(dW, axis=1)
    X = np.hstack((np.zeros((num_path, 1)), X)) # add initial position at
    return X
```

In [17]:
```
# simulate the 1-D Brownian motion with various sigma values
sigma_list = [0.1, 0.5, 1, 1.5]
num_path = 100
num_period = 5
step_size = 100
time_points = np.linspace(0, num_period, step_size + 1)

fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, sigma in enumerate(sigma_list):
    BM_2 = brownian_motion_2(num_path, num_period, step_size, sigma, rand
    for path in range(BM_2.shape[0]):
        axs[idx].plot(time_points, BM_2[path], alpha=0.5)
    axs[idx].set_ylim([-13, 13])
    axs[idx].set_xlabel("Time")
    axs[idx].set_ylabel("$X_t$")
    axs[idx].set_title(rf"$\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Simulated 1-D Brownian Motion Paths for Various $\sigma$",
plt.show()
```



---

2. Implementing an Ornstein-Uhlenbeck Process

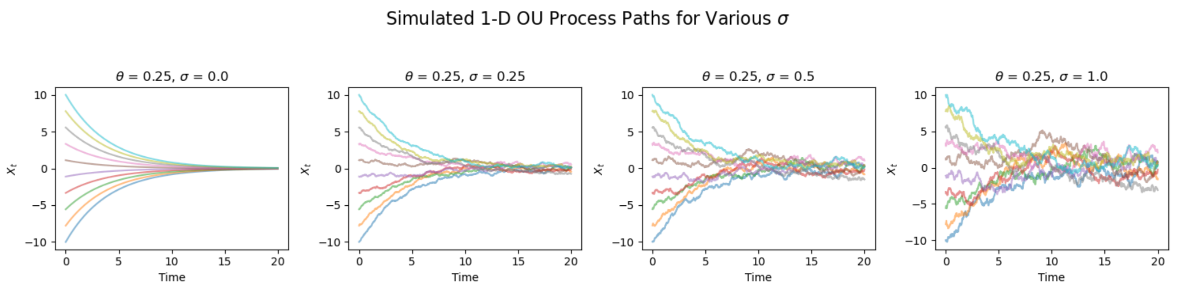
對於一個 Ornstein-Uhlenbeck 過程 (OU process)，其趨勢項 $u_t(X_t) = -\theta X_t$ 以及隨機項 $\sigma_t = \sigma$，即給定初始條件 $X_0 = x_0$，

$$dX_t = -\theta X_t dt + \sigma dW_t$$

Note: OU 過程為一種具有均數回歸性質的隨機過程，其回復速度為 θ。

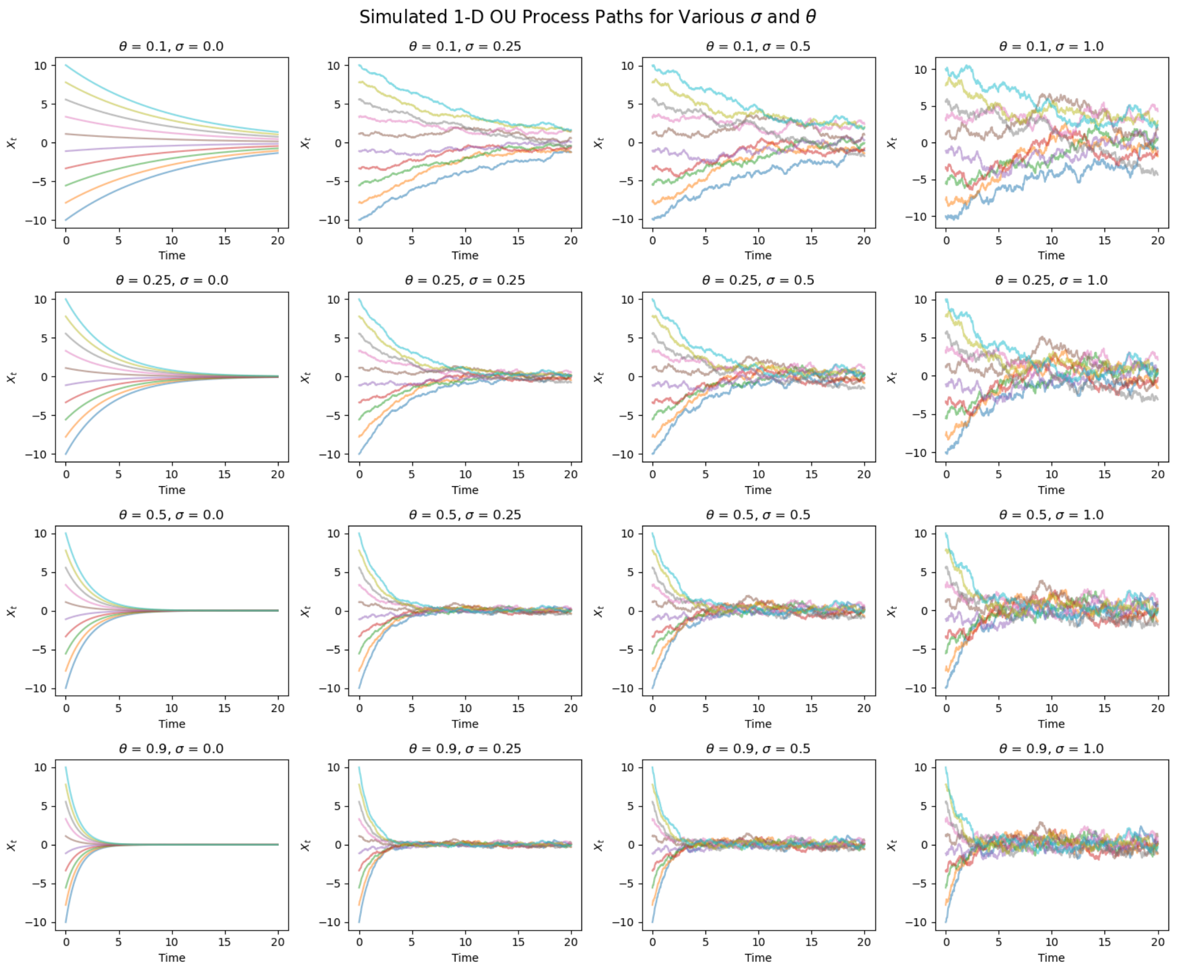
In [18]:
```
def OU_process(num_path: int, num_period: float, step_size: int,
               theta: float, sigma: float, random_seed: Optional[int]=Non

    """
    Simulate the 1-D Ornstein–Uhlenbeck (OU) process using Euler–Maruyama

    Args:
        num_path (int): Number of paths to simulate.
        num_period (float): Total time duration.
        step_size (int): Number of discrete time steps.
        theta (float): Mean-reversion rate.
        sigma (float): Volatility parameter.
        random_seed (int, optional): Random seed for reproducibility.

    Returns:
        np.ndarray: Array of shape (num_path, step_size + 1) with OU proc
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    dt = num_period / step_size

    X = np.zeros((num_path, step_size + 1))
    X[:, 0] = np.linspace(-10, 10, num_path)

    for i in range(1, step_size + 1):
        dW = np.sqrt(dt) * np.random.randn(num_path)
        X[:, i] = X[:, i - 1] - theta * X[:, i - 1] * dt + sigma * dW

    return X
```

In [19]:
```
# simulate the 1-D OU process with various sigma values
parameters = [
    (0.25, 0.0),
    (0.25, 0.25),
    (0.25, 0.5),
    (0.25, 1.0)
]
num_path = 10
num_period = 20
step_size = 1000
time_points = np.linspace(0, num_period, step_size + 1)

fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, (theta, sigma) in enumerate(parameters):
    OU = OU_process(num_path, num_period, step_size, theta, sigma, random
    for path in range(OU.shape[0]):
        axs[idx].plot(time_points, OU[path], alpha=0.5)
    axs[idx].set_xlabel("Time")
    axs[idx].set_ylabel("$X_t$")
    axs[idx].set_title(rf"$\theta$ = {theta}, $\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Simulated 1-D OU Process Paths for Various $\sigma$", font
plt.show()
```



In [20]:
```
# simulate the 1-D OU process with various sigma values and theta values
parameters = [(theta, sigma) for theta in [0.1, 0.25, 0.5, 0.9] for sigma
num_path = 10
```

```
num_period = 20
step_size = 1000
time_points = np.linspace(0, num_period, step_size + 1)

fig, axs = plt.subplots(4, 4, figsize=(15, 12))
axs = axs.flatten()

for idx, (theta, sigma) in enumerate(parameters):
    OU = OU_process(num_path, num_period, step_size, theta, sigma, random
    for path in range(OU.shape[0]):
        axs[idx].plot(time_points, OU[path], alpha=0.5)
    axs[idx].set_xlabel("Time")
    axs[idx].set_ylabel("$X_t$")
    axs[idx].set_title(rf"$\theta$ = {theta}, $\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Simulated 1-D OU Process Paths for Various $\sigma$ and $\
plt.show()
```



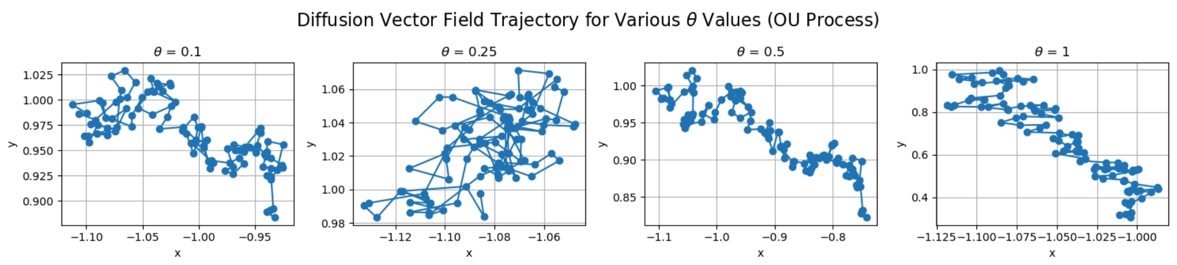
---

3. Simulating Diffusion Models with OU Process

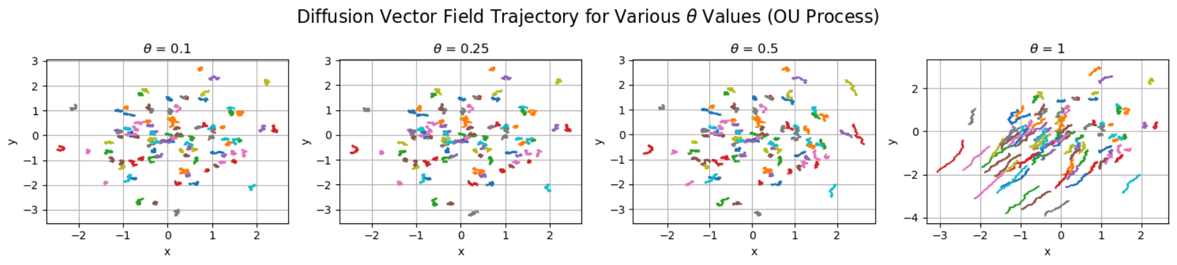
以下模擬為嘗試在 Diffusion models 中結合 OU 過程，來展示對粒子的影響。

In [21]:
```
def diffusion_model_OU(num_particle: int, step_size: int, theta: float, s

    """
    Simulate the diffusion field of particles based on OU process.
    Args:
        num_particle (int): Number of particles to simulate.
        step_size (int): Number of steps for the simulation.
        theta (float): Mean-reversion rate for the OU process.
        sigma (float): Standard deviation for the diffusion term.
        random_seed (int, optional): Random seed for initial positions. D
    Returns:
        list: A list of numpy arrays representing the history of particle
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    # generate initial positions of particles
    X = np.random.normal(0, 1, size=(num_particle, 2))
    X_input = torch.tensor(X, dtype=torch.float32, requires_grad=False).t
    X_history = [X]

    model = VF_step_diffusion(input_size=2, hidden_size=10, output_size=2

    t = 0  # time step

    # main
    while t < 1:
        for _ in range(step_size):
            h = 1 / step_size
            with torch.no_grad():
                epsilon = np.random.normal(0, 1, size=(num_particle, 2))
                diffusion_term = torch.tensor(sigma * np.sqrt(h) * epsilo
                X_input = X_input - theta * h * model(X_input) + diffusio
            X_history.append(X_input.cpu().detach().numpy())
            t = t + h

    return X_history
```

In [22]:
```
# simulate the trajectory of a single particle in the diffusion model bas
theta_list = [0.1, 0.25, 0.5, 1]
fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, theta in enumerate(theta_list):
    single_particle_OU = diffusion_model_OU(num_particle=1, step_size=100

    x = [single_particle_OU[i][0][0] for i in range(len(single_particle_O
    y = [single_particle_OU[i][0][1] for i in range(len(single_particle_O

    axs[idx].plot(x, y, marker="o")
    axs[idx].grid()
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
    axs[idx].set_title(rf"$\theta$ = {theta}")

plt.tight_layout()
plt.suptitle(r"Diffusion Vector Field Trajectory for Various $\theta$ Val
plt.show()
```



In [23]:
```
# simulate the trajectory of multiple particles in the diffusion model ba
theta_list = [0.1, 0.25, 0.5, 1]
fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, theta in enumerate(theta_list):
    multiple_particle_OU = diffusion_model_OU(num_particle=100, step_size

    particle = {
        f"particle_{j}": [multiple_particle_OU[i][j] for i in range(len(m
        for j in range(len(multiple_particle_OU[0]))
    }
    for key in particle.keys():
        axs[idx].plot(
            [particle[key][i][0] for i in range(len(particle[key]))],
            [particle[key][i][1] for i in range(len(particle[key]))]
        )
    axs[idx].grid()
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
    axs[idx].set_title(rf"$\theta$ = {theta}")

plt.tight_layout()
plt.suptitle(r"Diffusion Vector Field Trajectory for Various $\theta$ Val
plt.show()
```



4. Transforming Distribution with SDEs

上述的隨機過程都是觀察粒子如何被 SDEs 所轉換；然而，我們真正的目標是想要轉換一個分佈，也就是如何從 p_{init} 變成 p_{data}。

在文獻上有一種 SDEs 可以完成這件事，也就是 **Langvein dynamic**，其表達式如下：

$$dX_t = \frac{1}{2}\sigma^2 \nabla \log p(X_t)dt + \sigma dWt$$

對於這個分佈我們有一些限制：

1. 該分佈可以進行微分或者是說計算梯度
2. 我們可以從這個分佈進行抽樣

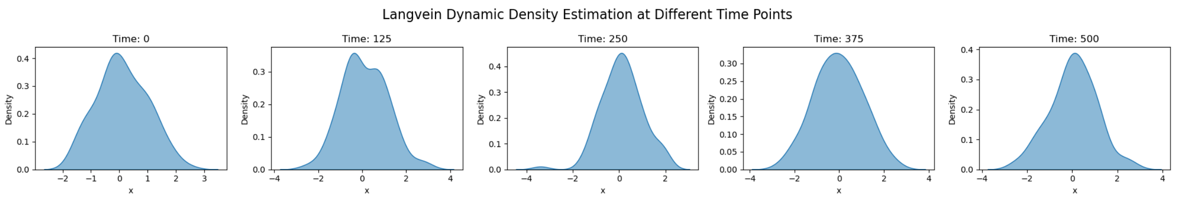
這裡我們同樣對 Langvein dynamic 進行一些簡單的模擬。

Case 1. 假設 $X \sim N(0,1)$，則 $p(x) \propto e^{-x^2/x}$ 且

$$\nabla \log p(x) = -x$$

In [24]:
```python
def Langvein_dynamic(num_path: int, num_period: float, step_size: int, si
                     random_seed: Optional[int]=None) -> np.ndarray:

    """
    Simulate the Langvein dynamic process.
    Args:
        num_path (int): Number of paths to simulate.
        num_period (float): Total time duration.
        step_size (int): Number of discrete time steps.
        sigma (float): Standard deviation for the diffusion term.
        random_seed (int, optional): Random seed for reproducibility. Def
    Returns:
        np.ndarray: A 1D array of shape (num_path, step_size + 1) represe
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    dt = num_period / step_size

    X = np.zeros((num_path, step_size + 1))
    X[:, 0] = np.random.randn(num_path) # initial positions

    for i in range(1, step_size + 1):
        score = -X[:, i - 1]
        dW = np.sqrt(dt) * np.random.randn(num_path)
        X[:, i] = X[:, i - 1] + 0.5 * sigma ** 2 * score * dt + sigma * d

    return X
```

In [25]:
```python
# simulate the Langvein dynamic density estimation at different time poin
num_path = 100
num_period = 20
step_size = 500
time_points = np.linspace(0, 500, 5)

Langvein = Langvein_dynamic(num_path, num_period, step_size, sigma=1)

particle = {f"particle_{j}": [Langvein[i][j] for i in range(len(Langvein)
            for j in range(len(Langvein[0]))}

fig, axs = plt.subplots(1, 5, figsize=(20, 3))
axs = axs.flatten()

for idx, key in enumerate(time_points):
    key = int(key)
    sns.kdeplot(particle[f"particle_{key}"], ax=axs[idx], fill=True, alph
    axs[idx].set_title(f"Time: {key}")
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("Density")
plt.tight_layout()
plt.suptitle("Langvein Dynamic Density Estimation at Different Time Point
plt.show()
```

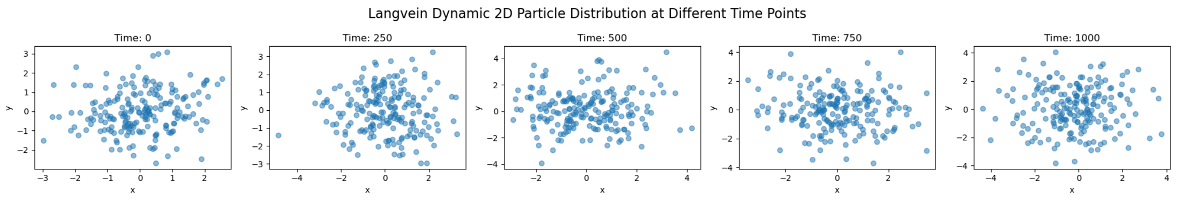


Case 2. 假設 $\mathbf{X} \sim \mathcal{N}_2(\mu, \Sigma)$，則

$$\nabla \log p(x) \propto -\Sigma^{-1}(\mathbf{x} - \mu)$$

In [26]:
```
def Langvein_dynamic_2D(num_path: int, num_period: float, step_size: int,
                        mu: np.ndarray, cov: np.ndarray, random_seed: Opt

    """
    Simulate the 2-D Langvein dynamic process.
    Args:
        num_path (int): Number of paths to simulate.
        num_period (float): Total time duration.
        step_size (int): Number of discrete time steps.
        sigma (float): Standard deviation for the diffusion term.
        mu (np.ndarray): Mean vector for the multivariate normal distribu
        cov (np.ndarray): Covariance matrix for the multivariate normal d
        random_seed (int, optional): Random seed for reproducibility. Def
    Returns:
        np.ndarray: A 2D array of shape (num_path, step_size + 1, 2) repr
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    dt = num_period / step_size
    dim = 2
    inv_cov = np.linalg.inv(cov)

    X = np.zeros((num_path, step_size + 1, dim))
    X[:, 0, :] = np.random.multivariate_normal(mean=mu, cov=cov, size=num

    for i in range(1, step_size + 1):
        score = -((X[:, i - 1, :] - mu) @ inv_cov.T)  # score function
        dW = np.sqrt(dt) * np.random.randn(num_path, dim)
        X[:, i, :] = X[:, i - 1, :] + 0.5 * sigma ** 2 * score * dt + sig

    return X
```

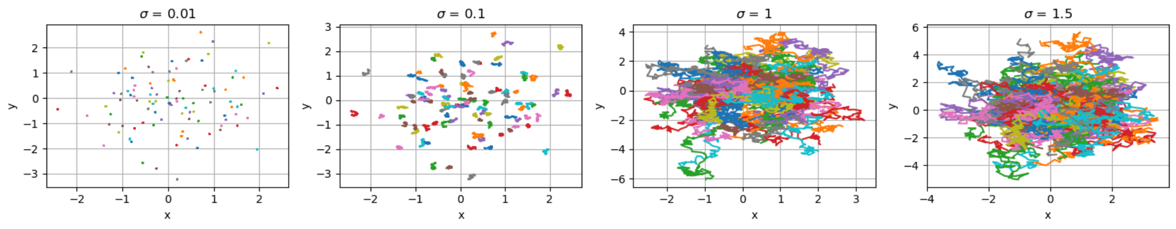
In [27]:
```
# simulate the Langvein dynamic distribution estimation at different time
num_path = 200
num_period = 20
step_size = 1000
time_points = np.linspace(0, step_size, 5)

Langvein_2D = Langvein_dynamic_2D(num_path, num_period, step_size, sigma=

particle_2D = {f"particle_{j}": [Langvein_2D[i][j] for i in range(len(Lan
fig, axs = plt.subplots(1, 5, figsize=(20, 3))
axs = axs.flatten()

for idx, key in enumerate(time_points):
    key = int(key)
    x = [particle_2D[f"particle_{key}"][i][0] for i in range(len(particle
    y = [particle_2D[f"particle_{key}"][i][1] for i in range(len(particle
    axs[idx].scatter(x, y, alpha=0.5)
    axs[idx].set_title(f"Time: {key}")
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
plt.tight_layout()
plt.suptitle("Langvein Dynamic 2D Particle Distribution at Different Time
plt.show()
```



In [28]:
```
def diffusion_model_Langvein(num_particle: int, step_size: int, sigma: fl

    """
    Simulate the diffusion field of particles based on Langvein dynamic a
    Args:
        num_particle (int): Number of particles to simulate.
        step_size (int): Number of steps for the simulation.
        sigma (float): Standard deviation for the diffusion term.
        random_seed (int, optional): Random seed for initial positions. D
    Returns:
        list: A list of numpy arrays representing the history of particle
    """

    if random_seed is not None:
        np.random.seed(random_seed)

    # generate initial positions of particles
    X = np.random.normal(0, 1, size=(num_particle, 2))
    X_input = torch.tensor(X, dtype=torch.float32, requires_grad=False).t
    X_history = [X]

    model = VF_step_diffusion(input_size=2, hidden_size=10, output_size=2

    t = 0  # time step

    # main
    while t < 1:
        for _ in range(step_size):
            h = 1 / step_size
            with torch.no_grad():
                score = -X_input
                epsilon = np.random.normal(0, 1, size=(num_particle, 2))
                diffusion_term = torch.tensor(sigma * np.sqrt(h) * epsilo
                X_input = X_input + 0.5 * sigma ** 2 * score * h * model(
            X_history.append(X_input.cpu().detach().numpy())
            t = t + h
    return X_history
```

In [29]:
```
# simulate the trajectory of multiple particles in the diffusion model fo
sigma_list = [0.01, 0.1, 1, 1.5]
fig, axs = plt.subplots(1, 4, figsize=(15, 3))
axs = axs.flatten()

for idx, sigma in enumerate(sigma_list):
    multiple_particle_diffusion = diffusion_model_Langvein(num_particle=1

    particle = {
        f"particle_{j}": [multiple_particle_diffusion[i][j] for i in rang
        for j in range(len(multiple_particle_diffusion[0]))
    }
    for key in particle.keys():
        axs[idx].plot(
            [particle[key][i][0] for i in range(len(particle[key]))],
            [particle[key][i][1] for i in range(len(particle[key]))]
        )
    axs[idx].grid()
    axs[idx].set_xlabel("x")
    axs[idx].set_ylabel("y")
    axs[idx].set_title(rf"$\sigma$ = {sigma}")

plt.tight_layout()
plt.suptitle(r"Diffusion Vector Field Trajectory for Various $\sigma$ (La
plt.show()
```

Diffusion Vector Field Trajectory for Various $\sigma$ (Langvein Dynamic)



σ = 0.01
σ = 0.1
σ = 1
σ = 1.5
x
y