The Fokker-Planck Equation

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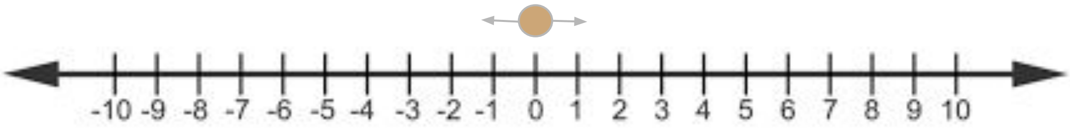
Background

- A PDE, really an SDE (stochastic differential equation), coupling advection and diffusion with a rich history
- Describes the time evolution of the probability density function of the velocity of a particle under the influence of drag forces and random forces, as in Brownian motion
- Discovered independently multiple times under varying circumstances
    - First discovered by Adriaan Fokker and Max Planck working on statistical quantum mechanics in 1914 and 1917 respectively
    - Discovered in 1931 by Andrey Kolmogorov working on continuous time markov chains

The Fokker-Planck Equation in 1D Derivation

- When dealing with stochastic variables one cannot deal with them like normal variables
  - There is a whole separate field of study for SDE's
- One of the few reasonably solvable forms of an SDE is: $\mathrm{d}X_t = \mu(X_t, t)\,\mathrm{d}t + \sigma(X_t, t)\,\mathrm{d}B_t$
  - This is called the Ito Equation, and this is the form a of first derivative in Ito Calculus
- Here, B denotes a Wiener Process (Brownian Motion)
  - This is the term that injects randomness into our system and makes it stochastic
  - In 1D a Wiener process is equivalent to a random walk on a number line



Derivation continued

- Recall: $\mu(X_t, t)$
- Define: $D(X_t, t) = \sigma^2(X_t, t)/2$
- Lastly, define $X_t \sim p(x, t)$
- Plug into Ito Equation: $\mathrm{d}X_t = \mu(X_t, t)\,\mathrm{d}t + \sigma(X_t, t)\,\mathrm{d}B_t$
- We get: $$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x}\left[\mu(x,t)p(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[D(x,t)p(x,t)\right]$$

- This the general form of the Fokker Planck Equation

Something to Note

- The FPE with no drift/advection is simply a stochastic version of the diffusion equation and is classical Brownian Motion
  - $$\frac{\partial}{\partial t}p(x,t) = D_0\frac{\partial^2}{\partial x^2}\left[p(x,t)\right]$$
  - Very similar to the PDE diffusion equation, except returns a spectrum of solutions given initial conditions
  - Constraint that: $\Delta x\,\Delta v \geq D_0$

Our case of the FPE

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\frac{\partial}{\partial x}\left(-F(x)W(x,t)\right) + D\frac{\partial^2 W}{\partial x^2} \qquad F(x) = -\frac{\partial U}{\partial x}$$

Where:

$$U(x) = a_0 kT(a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x)$$

$$a_0 = 300,\ a_1 = -0.38,\ a_2 = 1.37,\ a_3 = -2,\ a_4 = 1$$

With boundary conditions:

$$W(x=0, t=0) = 0,\ W(x=1, t=0) = 0.$$

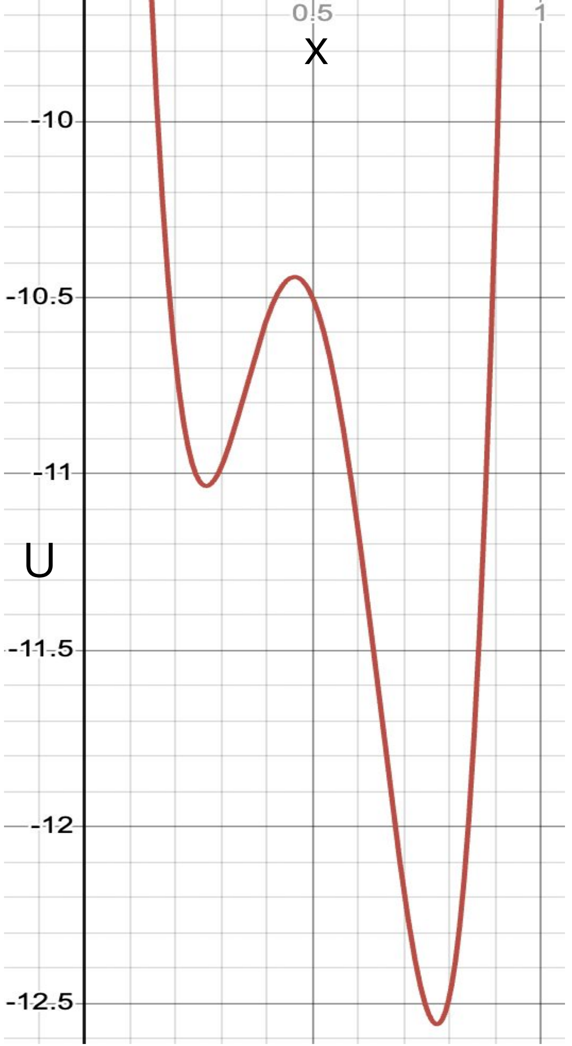
The Potential Function

$$U(x) = a_0 kT(a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x)$$

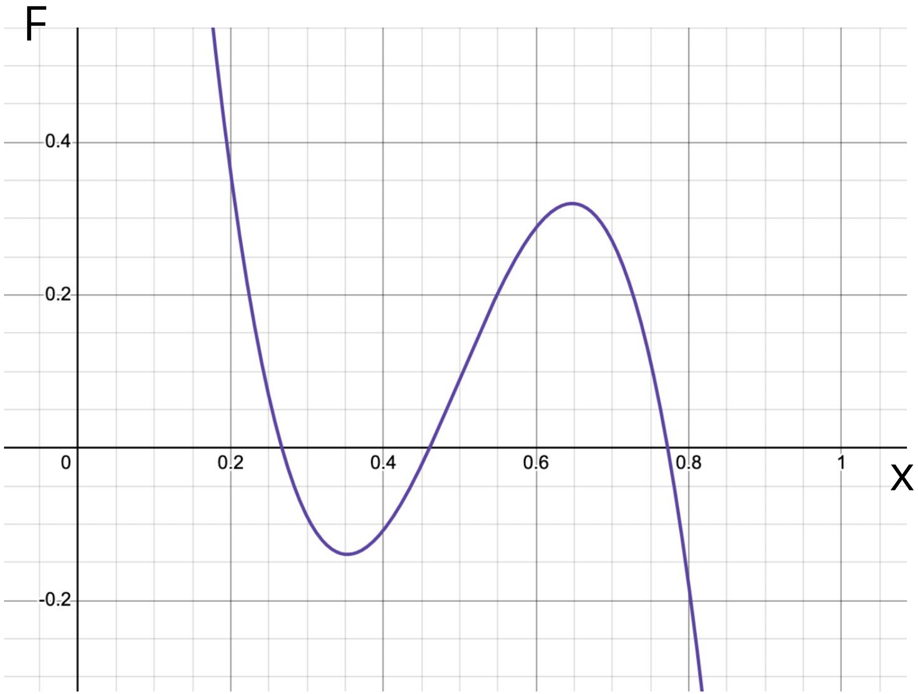
$$a_0 = 300,\ a_1 = -0.38,\ a_2 = 1.37,\ a_3 = -2,\ a_4 = 1$$

- For simplicity & visibility, we set kT = 1

- Minima at x = 0.27, 0.77
- Local maximum at x = 0.46
- U → ∞ at both ends



Equilibrium Positions with no Diffusion



$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\left[-\frac{\partial F}{\partial x}W(x,t) - F(x)\frac{\partial W(x,t)}{\partial x}\right]$$

$$x' = \{0.267, 0.461, 0.772\} \rightarrow F(x) = 0$$

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\left[-\frac{\partial F}{\partial x}W(x,t) - \cancel{F(x)\frac{\partial W(x,t)}{\partial x}}\right]$$

This allows us to analytically solve for the time-evolution of W(x,t) at these points

$$\frac{\partial W(x',t)}{\partial t} = -\frac{1}{kT} \left.\frac{\partial F}{\partial x}\right|_{x=x'} W(x',t)$$

Note that the partial of F at a specific x value is just a constant → we have a separable equation

$$\kappa \equiv \frac{1}{kT} \left.\frac{\partial F}{\partial x}\right|_{x=x'}$$

$$\frac{\partial W(x',t)}{\partial t} = -\kappa W(x',t)$$

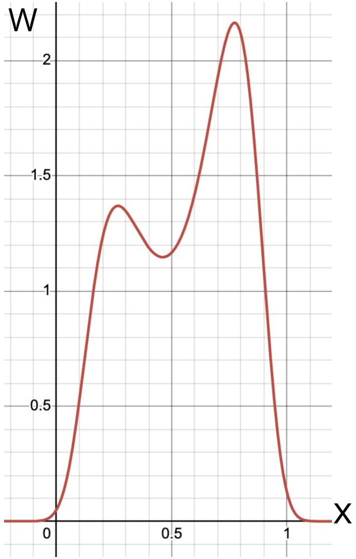
$$\frac{\partial W(x',t)}{\partial t}\frac{1}{W(x',t)} = -\kappa$$

$$W(x',t) = Ae^{-\kappa t}$$

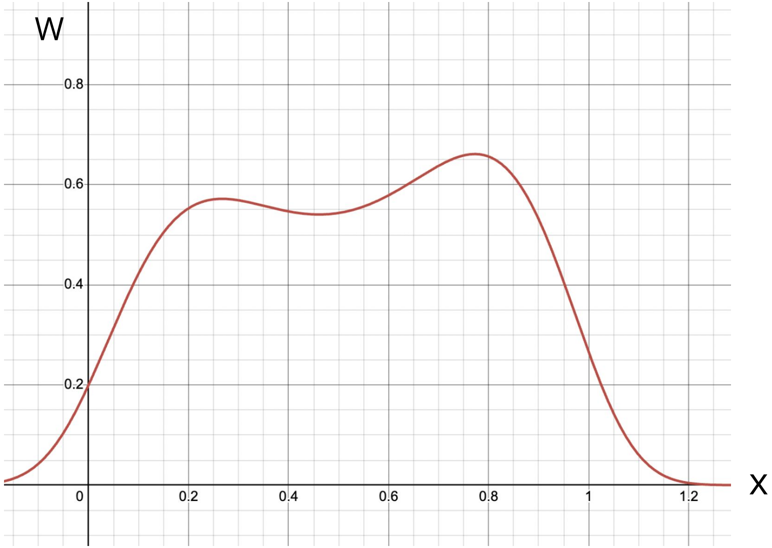
- If the derivative of F is positive, W decays exponentially. This is the case for x=0.46
- If the derivative is negative, W is a positive exponential and blows up. Thus the solution at zero diffusion converges to the two potential minima, x=0.27 and x=0.77

Equilibrium Distribution with Diffusion

$$0 = \frac{1}{kT}\left[-\frac{\partial F}{\partial x}W(x,t) - F(x)\frac{\partial W(x,t)}{\partial x}\right] + D\frac{\partial^2 W(x,t)}{\partial x^2} \longrightarrow W = Ae^{-\frac{U(x)}{D}}$$



Low Diffusion case (D<1)



High Diffusion case (D>1)

Solving 1

We aim to solve the Fokker-Planck equation (FPE):

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\frac{\partial}{\partial x}\left[-F(x)W(x,t)\right] + D\frac{\partial^2}{\partial x^2}\left[W(x,t)\right].$$

Using the relationship:

$$\frac{\partial U}{\partial x} = -F(x),$$

we substitute $F(x) = -\frac{\partial U}{\partial x}$ into the FPE to rewrite it as:

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\frac{\partial}{\partial x}\left[\frac{\partial U}{\partial x}W(x,t)\right] + D\frac{\partial^2}{\partial x^2}\left[W(x,t)\right].$$

Initial and Boundary Conditions

The initial and boundary conditions for our system are:

$$U(x) = a_0 kT(a_4x^4 + a_3x^3 + a_2x^2 + a_1x),$$

$$W(x=0, t=0) = 0, \quad W(x=1, t=0) = 0.$$

The constants in the potential $U(x)$ are:

$$a_0 = 300, \quad a_1 = -0.38, \quad a_2 = 1.37, \quad a_3 = -2, \quad a_4 = 1.$$

To simplify notation, we define b as:

$$b = \frac{1}{kT}.$$

Solving 2

Now solving:

$$\frac{\partial W(x,t)}{\partial t} = b\frac{\partial}{\partial x}\left[\frac{\partial U}{\partial x}W(x,t)\right] + D\frac{\partial^2}{\partial x^2}\left[W(x,t)\right].$$

Applying the product rule to the first term on the right-hand side, we obtain:

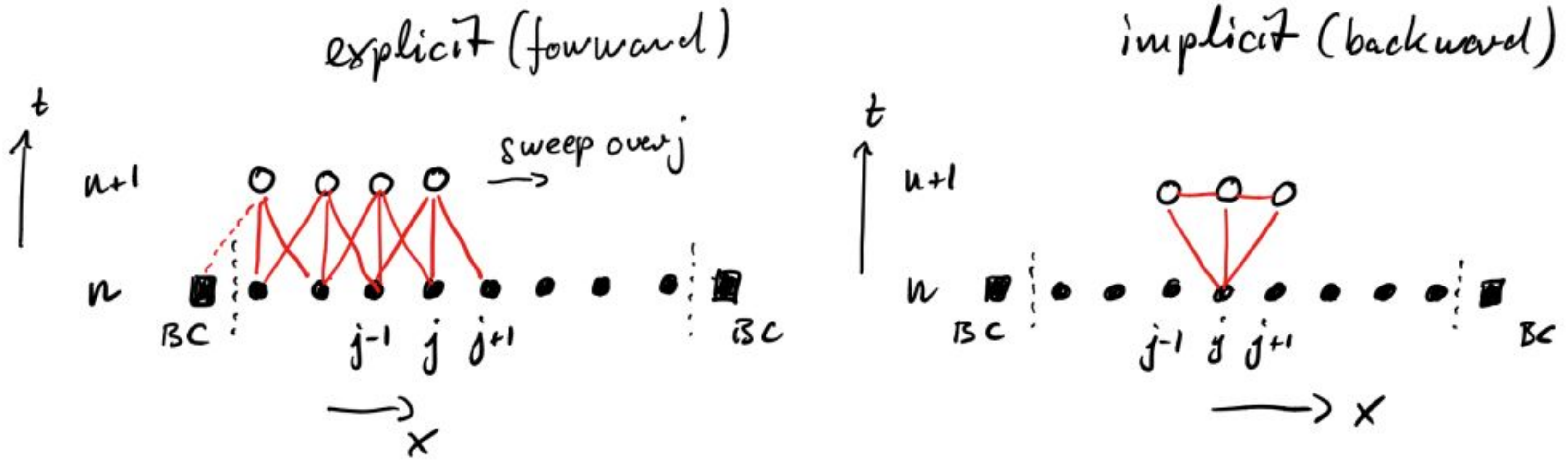
$$\frac{\partial W(x,t)}{\partial t} = b\frac{\partial^2 U}{\partial x^2}W(x,t) + b\left(\frac{\partial U}{\partial x}\right)\left(\frac{\partial W(x,t)}{\partial x}\right) + D\frac{\partial^2 W(x,t)}{\partial x^2}.$$

From here, there are analytical methods for very simple cases of W as well as other approximations techniques, but we will be discretizing our problem and using the finite differencing numerical technique.

First we recognize that our terms containing potential U should not undergo discretization because the derivative of U is known and easy to solve for. Next we break up the W terms because these terms we cannot solve for analytically, opting to use symmetric derivatives when we can.

Next, we recognize two methods to solve for W, an explicit method and an implicit method. Pursuing the explicit method first, **we notice for the explicit technique that our first time step cannot be done as a symmetric derivative (spatially we still can thanks to ghost zones) so we must develop a two stage approach**, taking one step with asymmetric derivatives and the rest with symmetric.

Explicit and Implicit Methods Visually



- Boxes are ghost zones
- Dots are discrete points on the grid
- Think Euler vs Backward Euler

Numerical Methods Boundary Conditions (Both Methods)

The boundary conditions used are Dirichlet Boundary conditions:

The boundary conditions require special treatment to maintain consistency at the domain edges. Ghost zones are introduced to handle these boundary values effectively. We define the boundary conditions for $W(x_{\text{min}}) = W_{\text{min}}$ and $W(x_{\text{max}}) = W_{\text{max}}$.

To determine the values of the ghost zones, W_{-1} and W_J, the slopes at the boundaries must agree:

$$\frac{W_0 - W_{\text{min}}}{\Delta x/2} = \frac{W_0 - W_{-1}}{\Delta x},$$

$$\frac{W_{\text{max}} - W_{J-1}}{\Delta x/2} = \frac{W_J - W_{J-1}}{\Delta x}.$$

Solving for W_{-1} and W_J, we find:

$$W_{-1} = 2W_{\text{min}} - W_0,$$

$$W_J = 2W_{\text{max}} - W_{J-1}.$$

The Explicit Equation (Central Differencing)

First step
Formula:

$$\frac{W_j^{n+1} - W_j^n}{\Delta t} = b\left(\frac{\partial^2 U}{\partial x^2} W_j^n + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^n - W_{j-1}^n}{2\Delta x}\right)\right) + D\left(\frac{W_{j+1}^n - 2W_j^n + W_{j-1}^n}{\Delta x^2}\right)$$

$$W_j^{n+1} = -b\Delta t\left(\frac{\partial^2 U}{\partial x^2} W_j^n + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^n - W_{j-1}^n}{2\Delta x}\right)\right) - D\Delta t\left(\frac{W_{j+1}^n - 2W_j^n + W_{j-1}^n}{\Delta x^2}\right) + W_j^n$$

Further step
Formula:

$$\frac{W_j^{n+1} - W_j^{n-1}}{2\Delta t} = b\left(\frac{\partial^2 U}{\partial x^2} W_j^n + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^n - W_{j-1}^n}{2\Delta x}\right)\right) + D\left(\frac{W_{j+1}^n - 2W_j^n + W_{j-1}^n}{\Delta x^2}\right)$$

$$W_j^{n+1} = -2b\Delta t\left(\frac{\partial^2 U}{\partial x^2} W_j^n + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^n - W_{j-1}^n}{2\Delta x}\right)\right) - 2D\Delta t\left(\frac{W_{j+1}^n - 2W_j^n + W_{j-1}^n}{\Delta x^2}\right) + W_j^{n-1}$$

Explicit Equation continued

First step coefficients:

$$\alpha = D\frac{\Delta t}{\Delta x^2},$$

$$\beta(x) = -\frac{b\Delta t}{2\Delta x}\frac{\partial U}{\partial x} + \alpha,$$

$$\gamma(x) = b\Delta t\frac{\partial^2 U}{\partial x^2} - 2\alpha,$$

$$\delta(x) = \frac{b\Delta t}{2\Delta x}\frac{\partial U}{\partial x} + \alpha.$$

First Time Step Using the coefficients $\beta(x)$, $\gamma(x)$, and $\delta(x)$, the update for the first time step is:

$$W_j^{(1)} = \beta(j\Delta x)W_{j-1}^{(0)} + \gamma(j\Delta x)W_j^{(0)} + \delta(j\Delta x)W_{j+1}^{(0)} + W_j^{(0)},$$

where $W^{(0)}$ represents the initial condition.

Second step and beyond:

$$\epsilon(x) = 2\beta(x),$$

$$\zeta(x) = 2b\Delta t\frac{\partial^2 U}{\partial x^2} - 4\alpha,$$

$$\eta(x) = 2\delta(x).$$

Subsequent Time Steps For $n \geq 2$, the update rule uses the coefficients $\epsilon(x)$, $\zeta(x)$, and $\eta(x)$:

$$W_j^{(n)} = W_j^{(n-2)} + \epsilon(j\Delta x)W_{j-1}^{(n-1)} + \zeta(j\Delta x)W_j^{(n-1)} + \eta(j\Delta x)W_{j+1}^{(n-1)}.$$

Stability Considerations

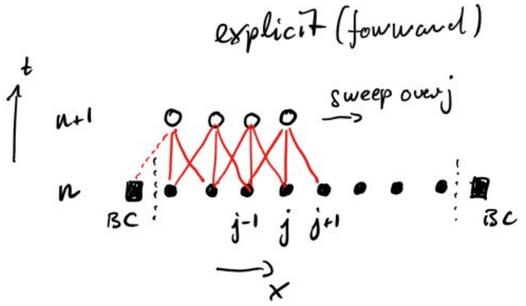
Von Neumann Stability Analysis

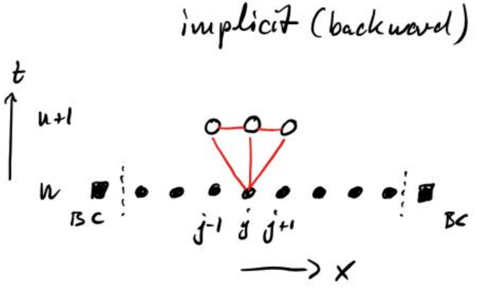
Assume the solution is a Fourier mode, $W_i^n = G^n e^{iki\Delta x}$ where $|G| \leq 1$

Central Difference Scheme in Space is Unstable for Advection

Forward and backward differences is chosen for stability due to directionality and strong advection effects

$$\frac{F\Delta t}{\Delta x} < 1 \qquad \Delta t < \frac{\Delta x^2}{2D}$$



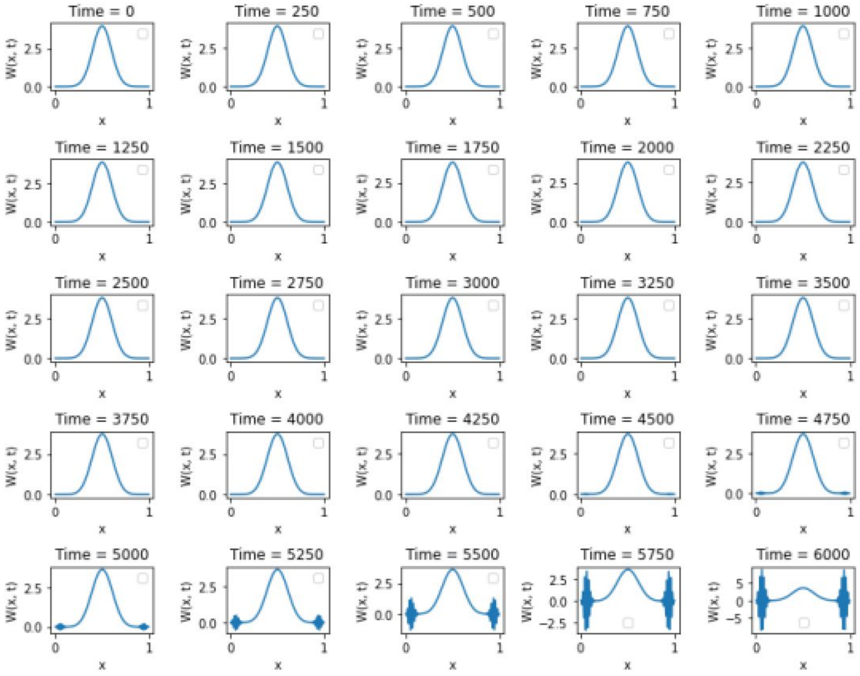


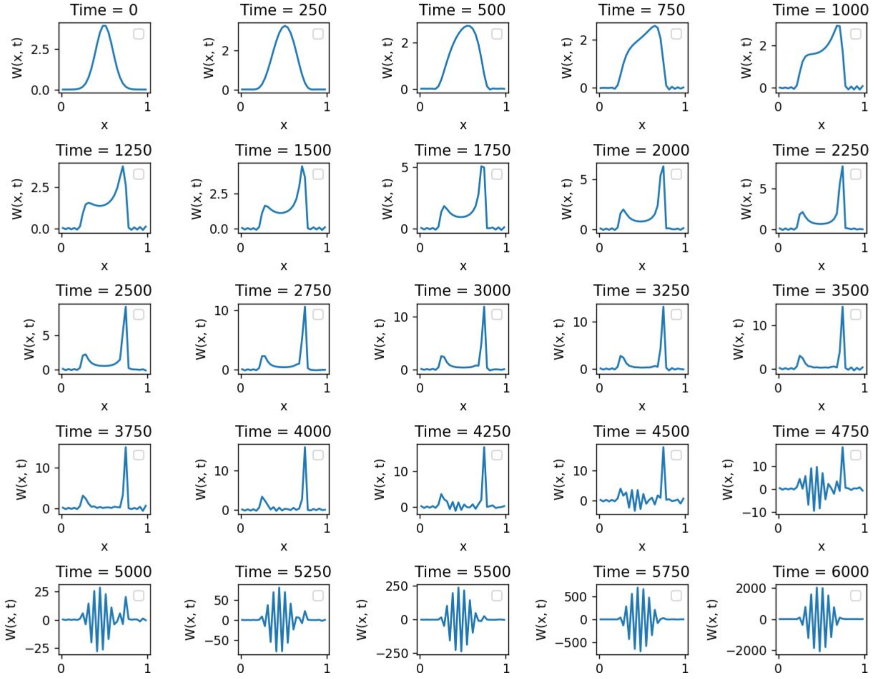
Explicit Results - Central Difference Scheme

D = 1 J = 100 $\mu = 0.5$
$t = 0.1\mu s$ $\sigma = 0.1$

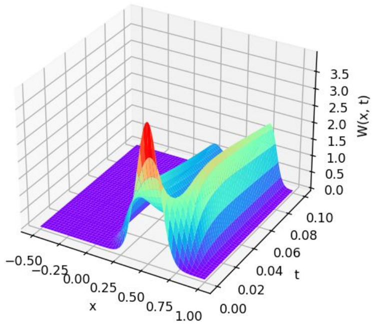
Takeaway: Central Differencing scheme works to a point, but always seems to encounter some instability

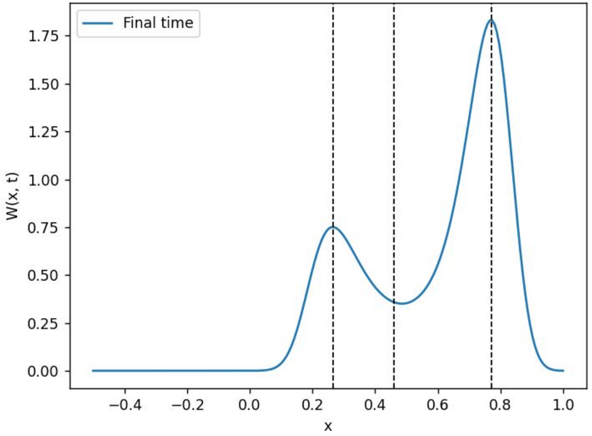
D = 0.1 J = 100 $\mu = 0.5$
t = 0.1ms $\sigma = 0.1$

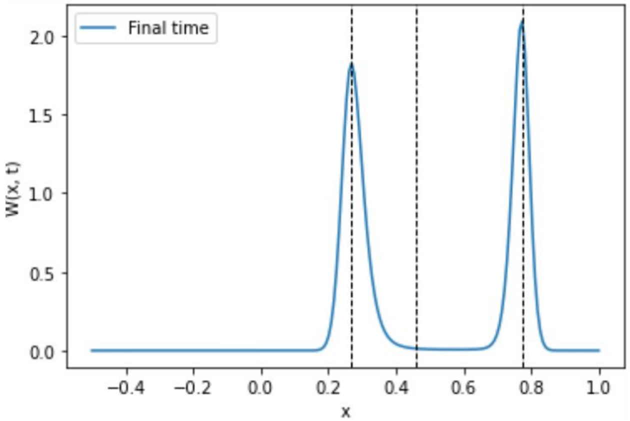




Explicit Results (Upwind Scheme)







$D = 1$ $J = 100$ $\mu = 0.5$ $t = 0.1\mu s$ $\sigma = 0.1$

$D = 0.1$ $J = 100$ $\mu = 0.5$ $t = 0.1ms$ $\sigma = 0.1$

The Implicit Equation

$$\frac{W_j^{n+1} - W_j^n}{\Delta t} = b\left(\frac{\partial^2 U}{\partial x^2} W_j^{n+1} + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^{n+1} - W_{j-1}^{n+1}}{2\Delta x}\right)\right) + D\left(\frac{W_{j+1}^{n+1} - 2W_j^{n+1} + W_{j-1}^{n+1}}{\Delta x^2}\right)$$

$$W_j^n = \; -b\Delta t\left(\frac{\partial^2 U}{\partial x^2} W_j^{n+1} + \frac{\partial U}{\partial x}\left(\frac{W_{j+1}^{n+1} - W_{j-1}^{n+1}}{2\Delta x}\right)\right) - D\Delta t\left(\frac{W_{j+1}^{n+1} - 2W_j^{n+1} + W_{j-1}^{n+1}}{\Delta x^2}\right) + W_j^{n+1}$$

$$W_j^n = \underbrace{\left(\frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2}\right)}_{\beta} W_{j-1}^{n+1} + \underbrace{\left(-b\Delta t\frac{\partial^2 U}{\partial x^2} + \frac{2D\Delta t}{\Delta x^2} + 1\right)}_{\gamma} W_j^{n+1} + \underbrace{\left(-\frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2}\right)}_{\delta} W_{j+1}^{n+1}$$

$$\boxed{\alpha \equiv \frac{D\Delta t}{\Delta x^2}}$$

$$\beta \equiv \frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2} = \frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \alpha$$

$$\gamma \equiv -b\Delta t\frac{\partial^2 U}{\partial x^2} + \frac{2D\Delta t}{\Delta x^2} + 1 = -b\Delta t\frac{\partial^2 U}{\partial x^2} + 2\alpha + 1$$

$$\delta \equiv -\frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2} = -\frac{\partial U}{\partial x}\frac{b\Delta t}{2\Delta x} - \alpha$$

$$\boxed{W_j^n = \beta W_{j-1}^{n+1} + \gamma W_j^{n+1} + \delta W_{j+1}^{n+1}}$$

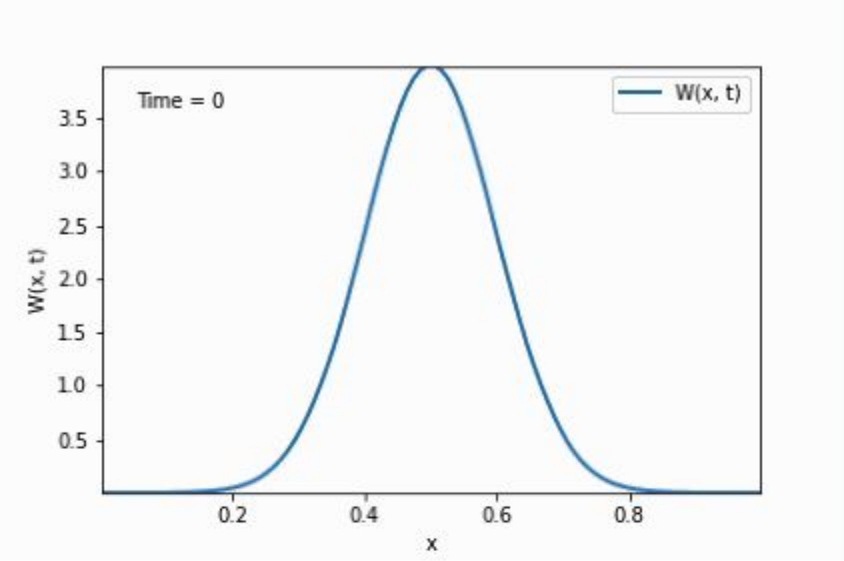
$$
\begin{pmatrix} W_0^n \\ \boxed{W_1^n} \\ W_2^n \\ \vdots \\ W_{J+1}^n \end{pmatrix} = \begin{pmatrix} \gamma & \delta & 0 & 0 & 0 & 0 \\ \beta & \gamma & \delta & 0 & 0 & 0 \\ 0 & \beta & \gamma & \delta & 0 & 0 \\ 0 & 0 & \beta & \ddots & \ddots & \vdots \\ & & & \ddots & \ddots & \delta \\ 0 & 0 & 0 & \cdots & \beta & \gamma \end{pmatrix} \begin{pmatrix} W_0^{n+1} \\ W_1^{n+1} \\ W_2^{n+1} \\ \vdots \\ W_{J+1}^{n+1} \end{pmatrix}
$$

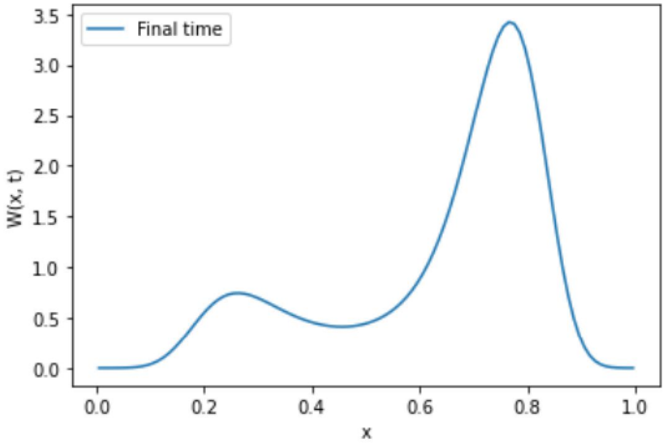
$$
W^n = \mathbf{A} W^{n+1}
$$

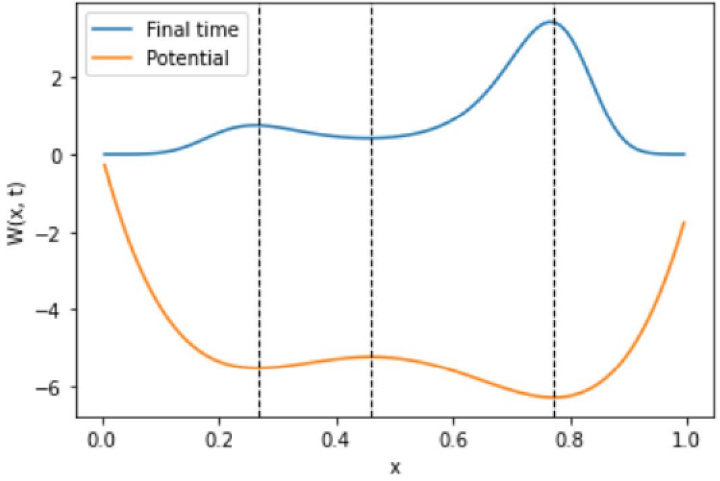
$$
\mathbf{A}^{-1} W^n = \mathbf{A}^{-1} \mathbf{A} W^{n+1}
$$

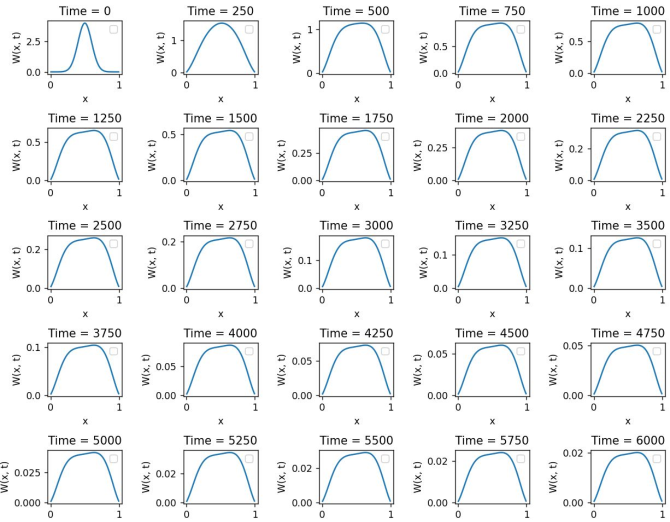
$$
\boxed{W^{n+1} = \mathbf{A}^{-1} W^n}
$$

Results - Implicit



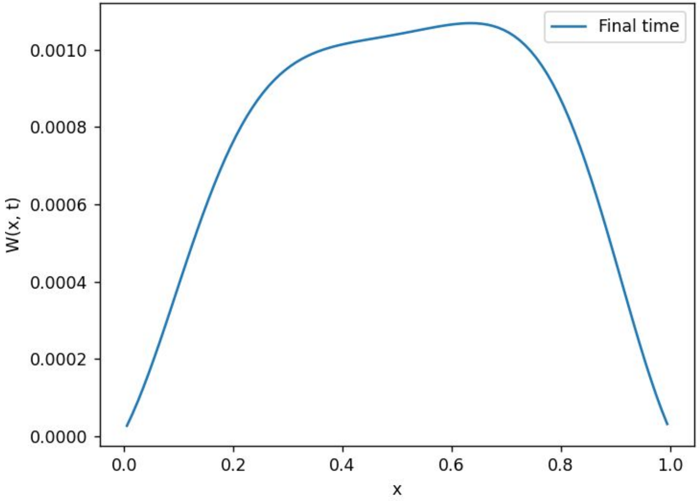


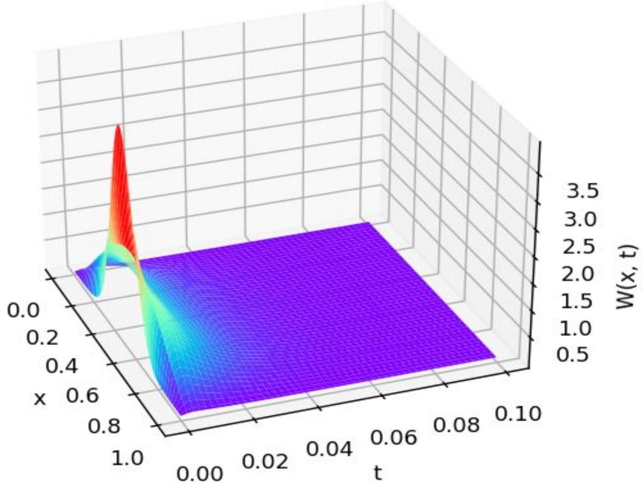




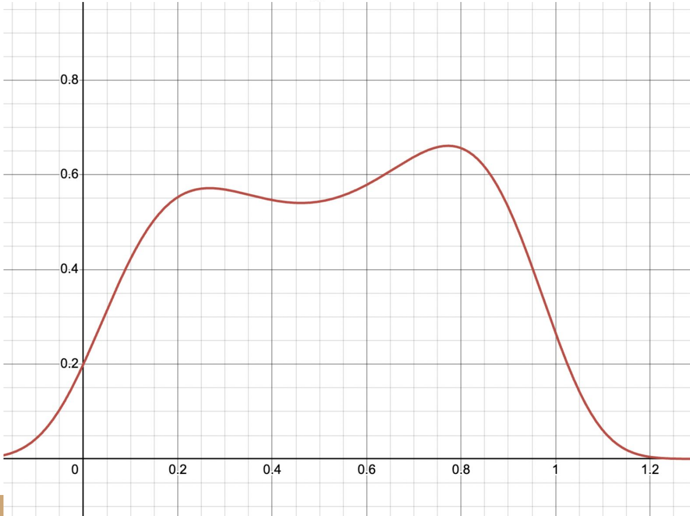
- J = 100
- dt = 0.01ms
- D = 10

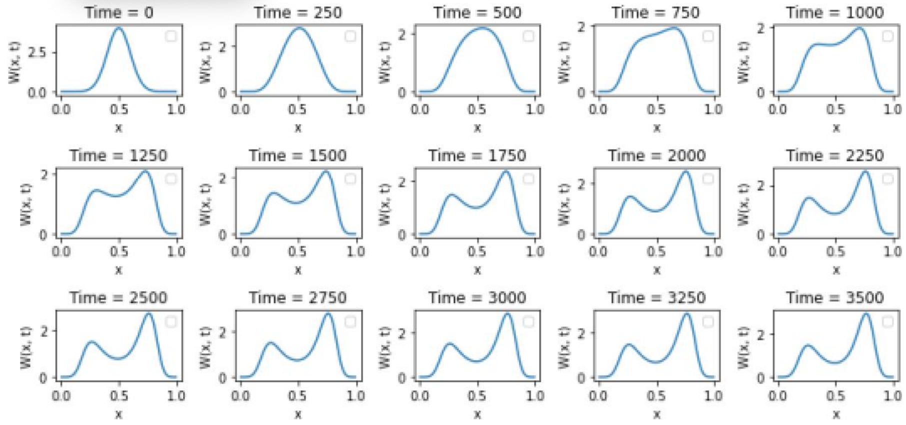
- μ = 0.5
- σ = 0.1





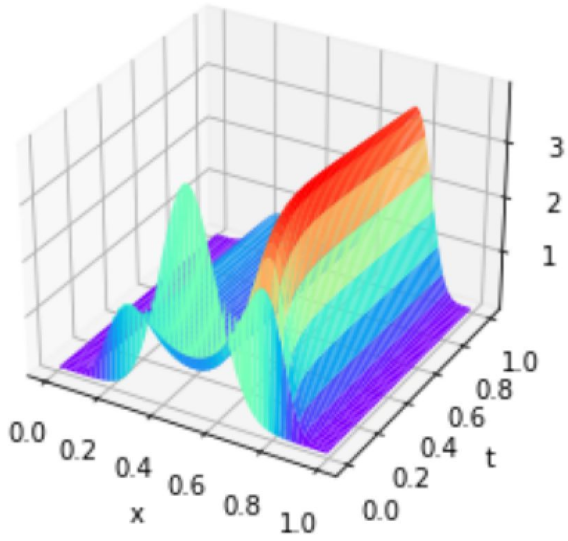
Look Familiar?

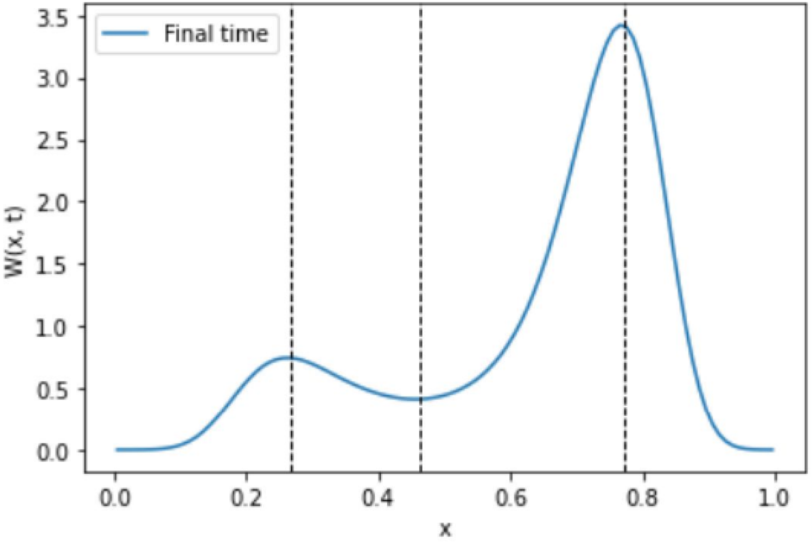


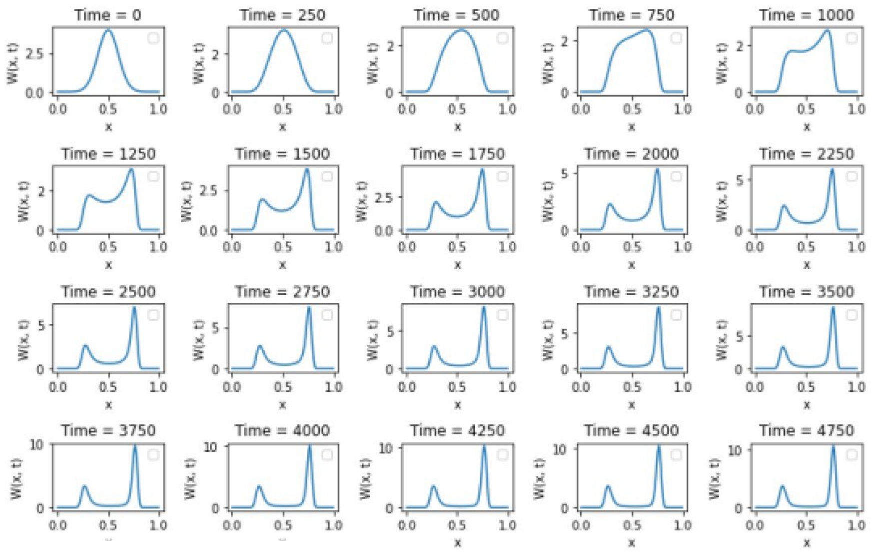


- J = 100
- dt = 0.01ms
- D = 1

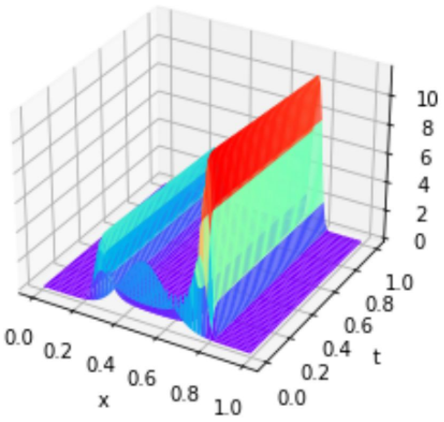
- $\mu = 0.5$
- $\sigma = 0.1$

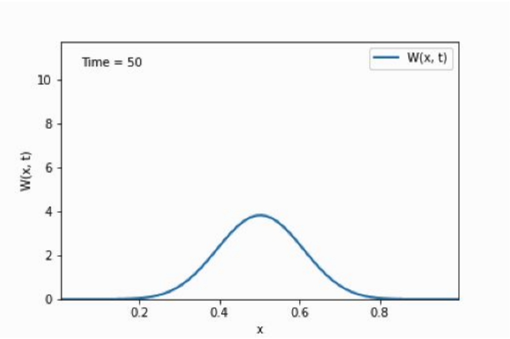


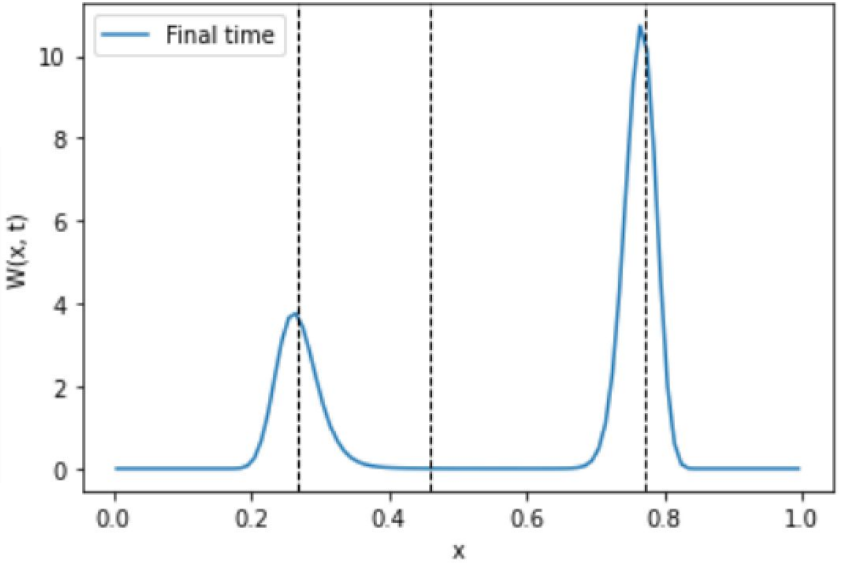


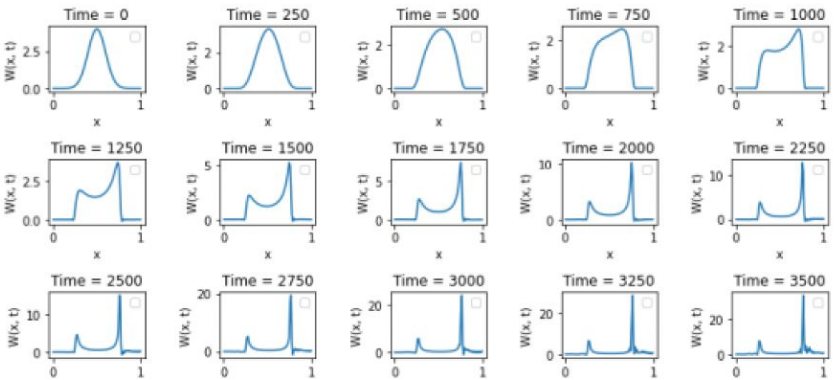


- J = 100
- dt = 0.01ms
- D = 0.1
- $\mu = 0.5$
- $\sigma = 0.1$



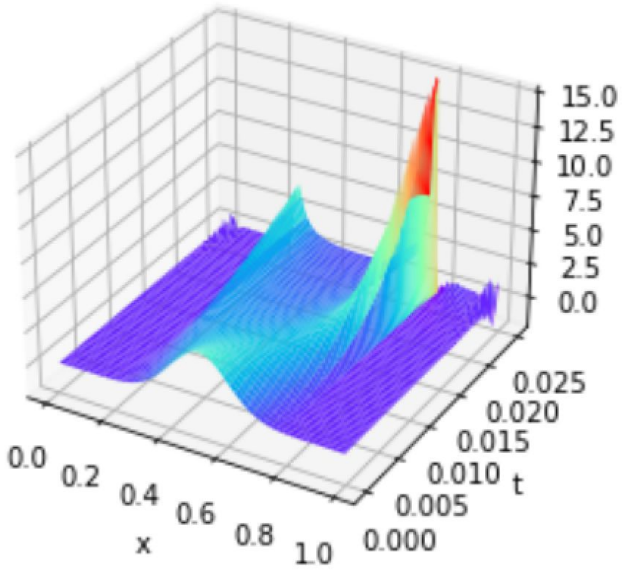


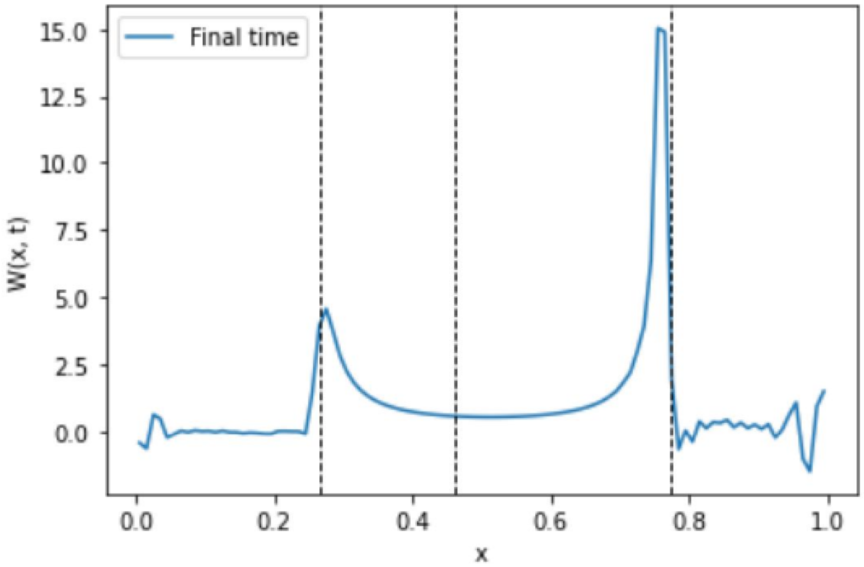


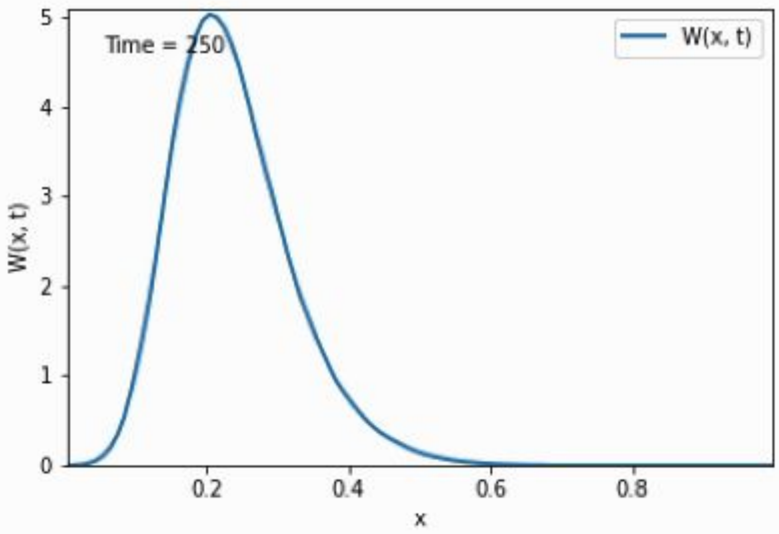


- J = 100
- dt = 0.01ms
- D = 0.01

- $\mu = 0.5$
- $\sigma = 0.1$

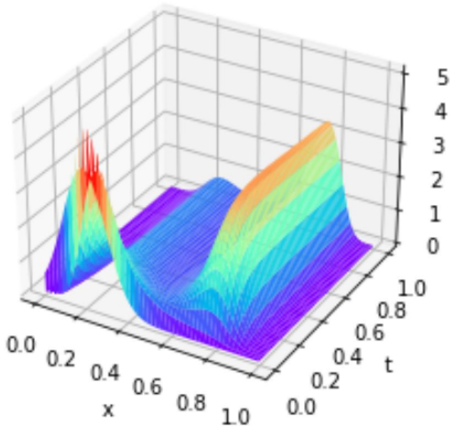


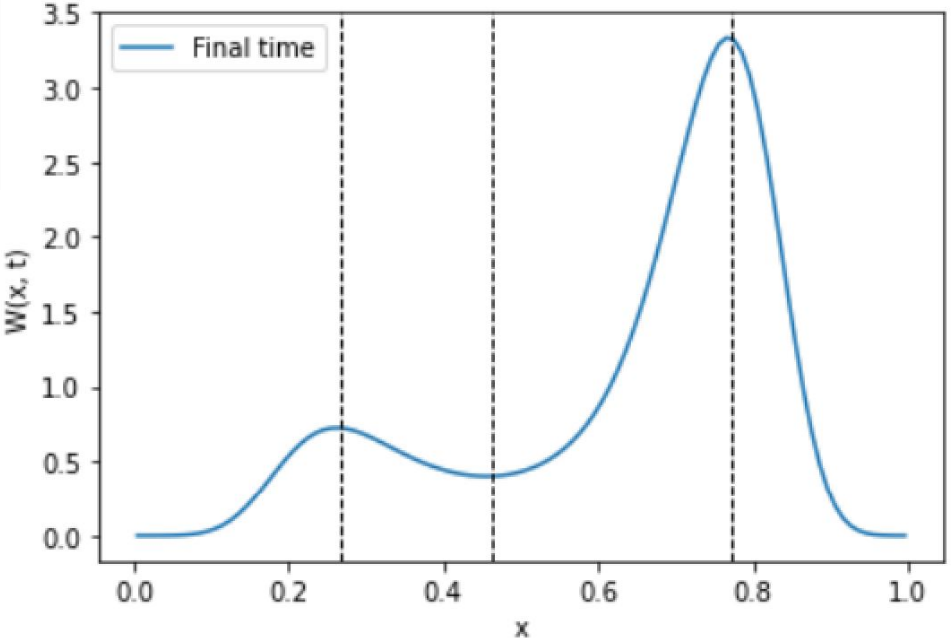


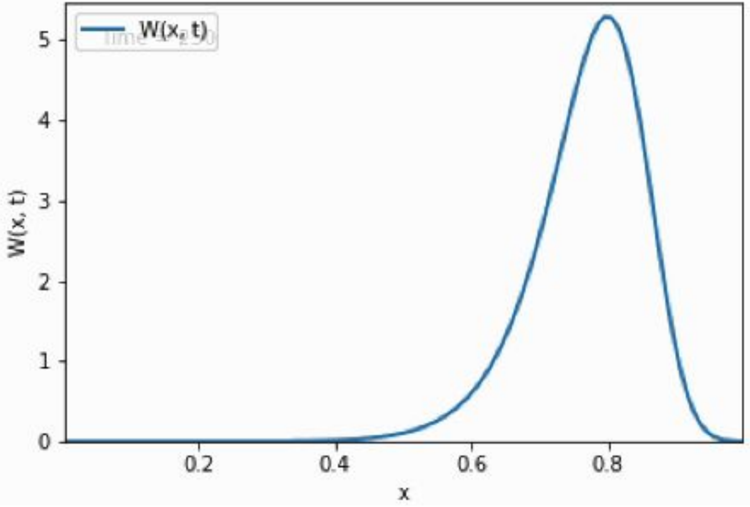


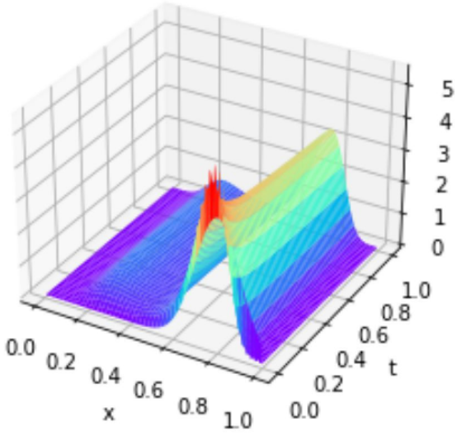
- $J = 100$
- $dt = 0.01\text{ms}$
- $D = 1$

- $\mu = 0.2$
- $\sigma = 0.1$

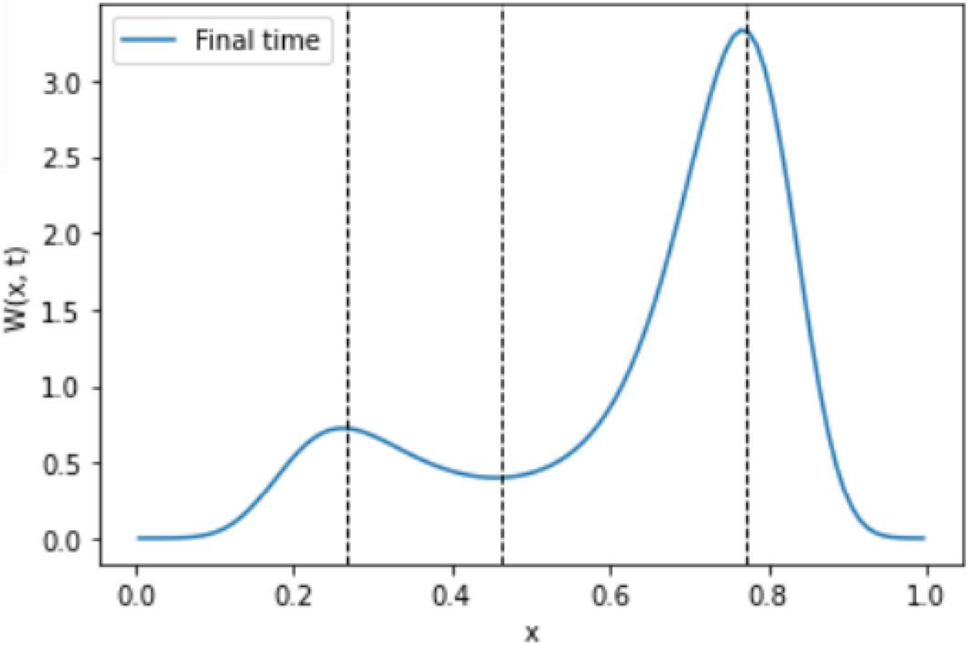


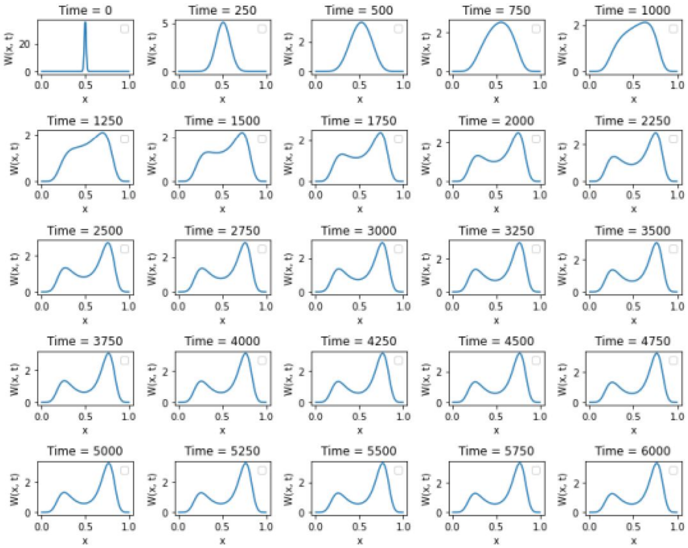






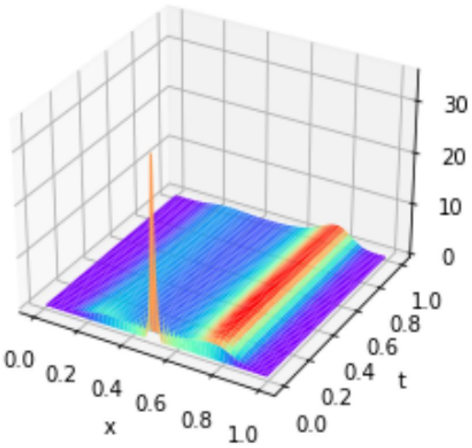
- $J = 100$
- $dt = 0.01ms$
- $D = 1$
- $\mu = 0.8$
- $\sigma = 0.1$

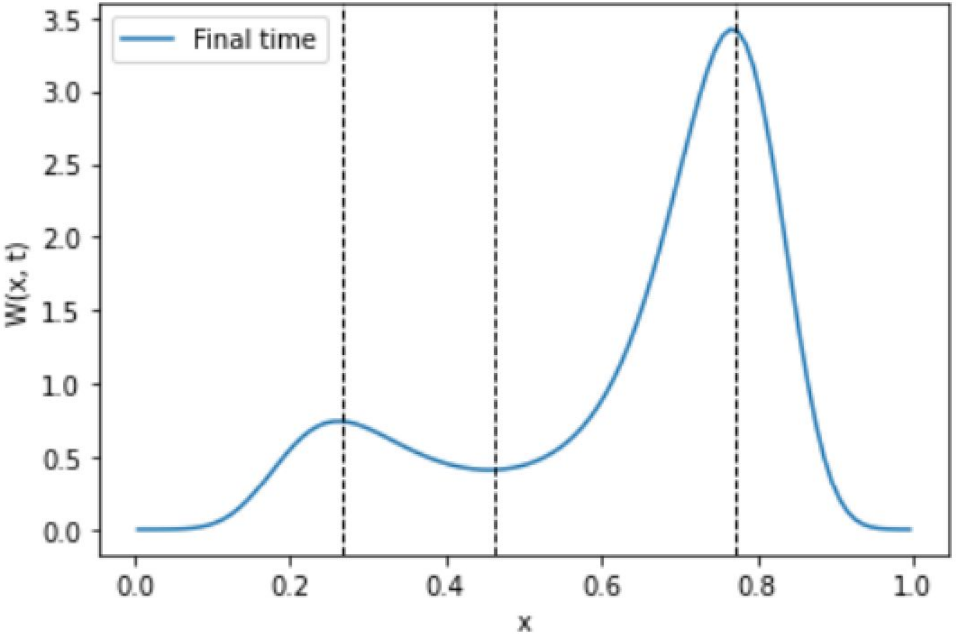




- $J = 100$
- $dt = 0.01\text{ms}$
- $D = 1$

- $\mu = 0.5$
- $\sigma = 0.01$





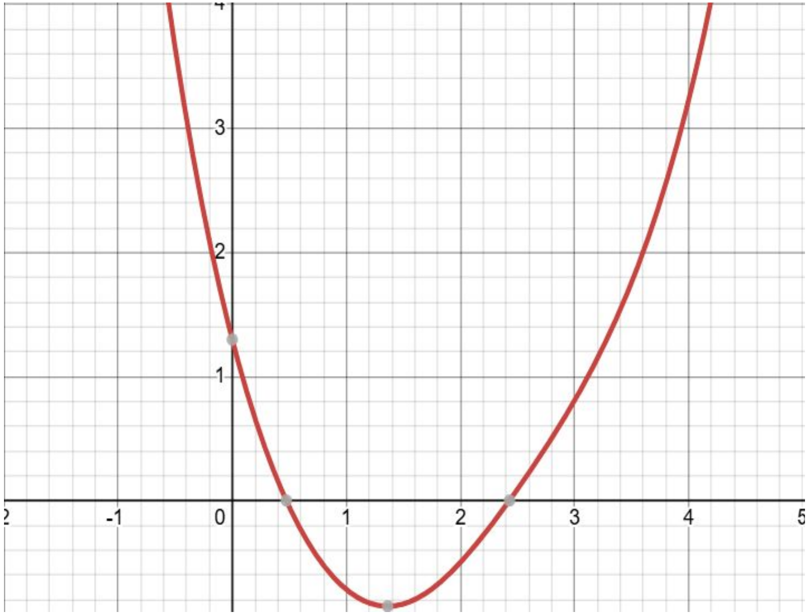
Effects of Another Potential

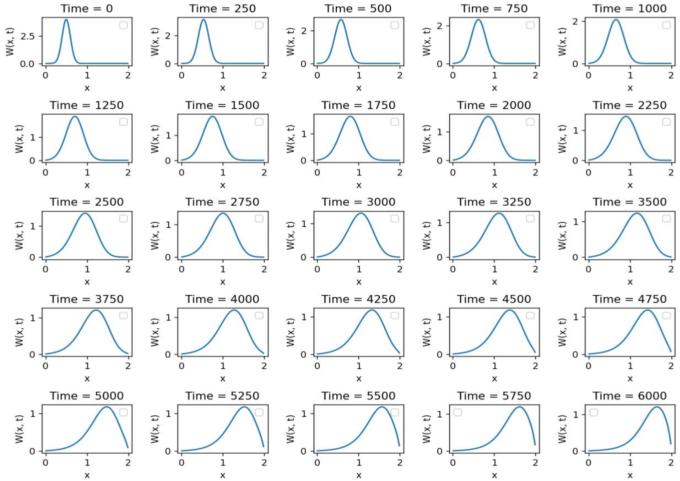
We generate a new arbitrary force/potential regime:

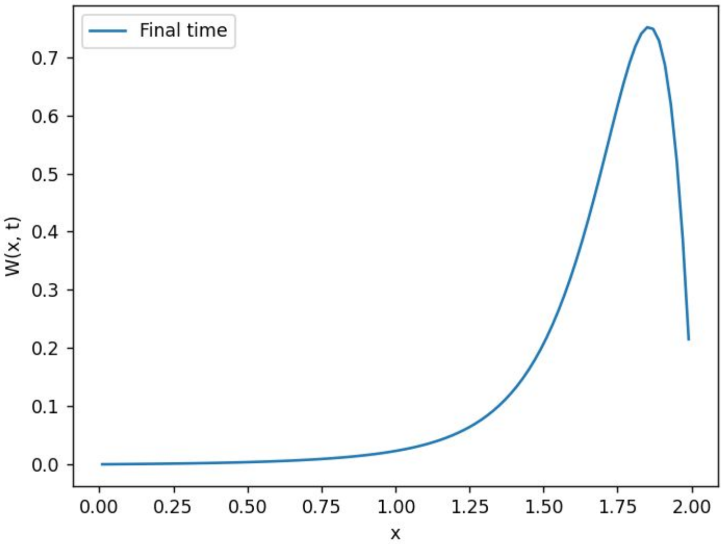
$$F(x) = -[sinh(x-2) + ln(cosh(x-2)) + 1.5x]$$

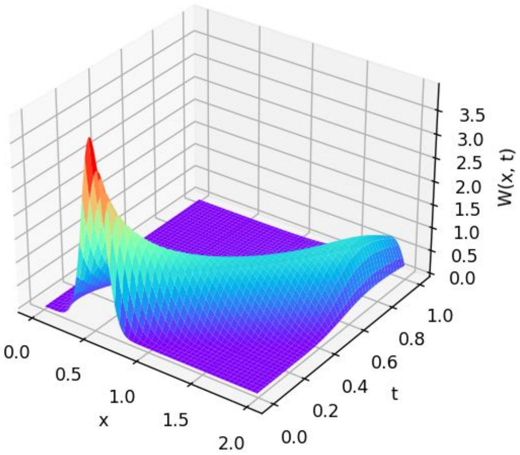
$$U = cosh(x-2) + tanh(x-2) + 1.5$$

$$\frac{\partial U}{\partial x} = sinh(x-2) + sech(x-2)$$



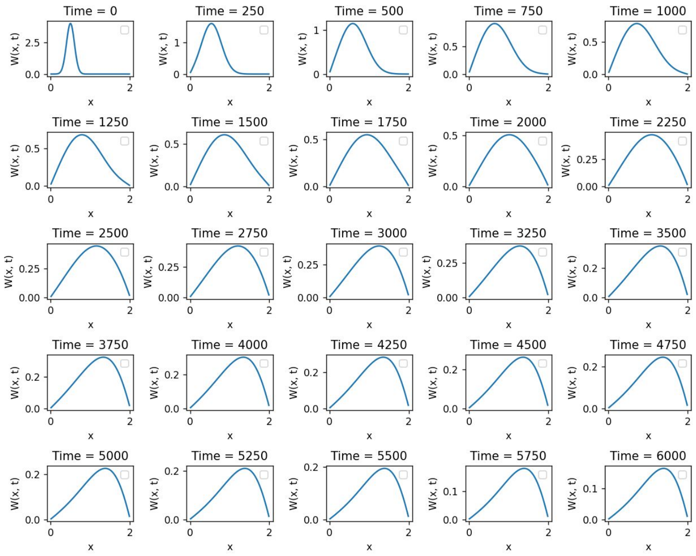


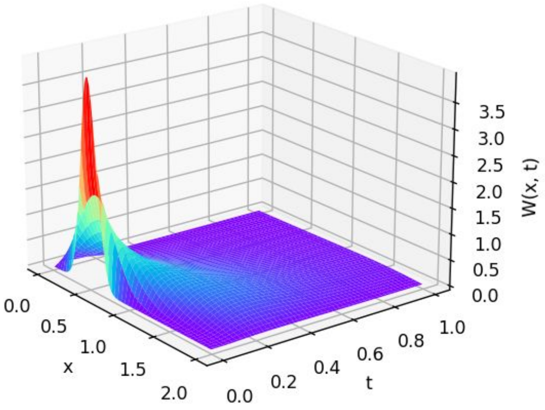


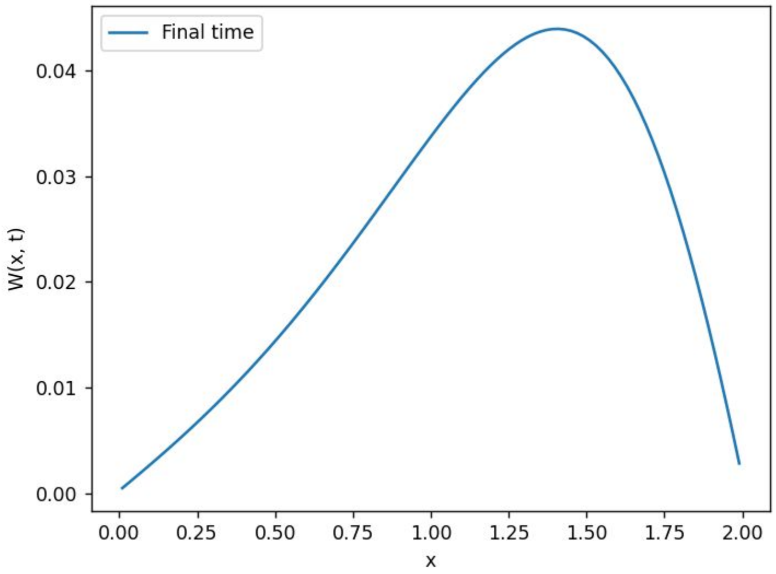


- J = 100
- dt = 0.1ms
- D = 0.1

- $\mu = 0.5$
- $\sigma = 0.1$







- J = 100
- dt = 0.1ms
- D = 1.0
- μ = 0.5
- σ = 0.1

Applications

- Physics
  - Brownian Motion
  - Diffusion Processes
  - Statistical Mechanics
  - Quantum Computing
- Chemistry
  - Chemical Reaction dynamics
- Finance
  - Option pricing
  - Risk management
- Engineering
  - Control systems
  - Signal Processing
  - Aerospace Applications

Future Directions/General Conclusions

- With more powerful computers, such as access to a supercomputer, it may be possible to take timesteps small enough for the explicit equation to be more generally stable
  - No real point to this other than curiosity when the implicit method works so much better
  - For very expensive problems may be viable
- Other solvers besides explicit and implicit exist, examples include Crank Nicholson

- **Observations**
  - Explicit - Computationally cheap, however more stability constraints
  - Implicit - More computationally expensive, fewer stability constraints
  - More resolution (support points), more accurate solutions but more computationally expensive

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