

Mihai Research

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The equation that we have is

$$u_t = \delta u_{xx} - \delta^{-1} V'(u), V(u) = \frac{1}{4}(1 - u^2)^2$$

So, by using the finite difference scheme, the second-order centred differences for partial derivative and the Euler method in time,

$$u_{xx} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}, u_t = \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

So, the equation becomes that, for $\forall j \in 1, 2, 3, \dots, N-1$ and $\forall n \in 0, 1, \dots, T-2$, we have

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \delta \left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} \right) - \frac{1}{\delta} ((u_j^n)^3 - u_j^n)$$

which is equivalent to

$$\begin{aligned} u_j^{n+1} &= u_j^n + \frac{\delta \Delta t}{h^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) - \frac{\Delta t}{\delta} ((u_j^n)^3 - u_j^n) \\ &= \left(1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}\right) u_j^n + \frac{\delta \Delta t}{h^2} u_{j+1}^n + \frac{\delta \Delta t}{h^2} u_{j-1}^n - \frac{\Delta t}{\delta} (u_j^n)^3 \end{aligned}$$

Since we have the Dirichlet boundary condition that

$$u(0, t) = u(1, t) = 0, u(x, 0) = u_+(x), u(x, T) = u_-(x)$$

so in our numerical simulation, we have 100×100 points in discretization, so $N = 99, T = 99$.

Note that u_j^n denotes the point at the j -th position at time n .

We only need to consider the case when $j = 1, 2, \dots, 98$ and $n = 0, 1, \dots, 97$.

Thus, the system of equations that we have is:

For $n = 0$,

$$\begin{cases} u_1^1 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_1^0 + \frac{\delta \Delta t}{h^2} u_2^0 + \frac{\delta \Delta t}{h^2} u_0^0 - \frac{\Delta t}{\delta} (u_1^0)^3 = (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_1^0 + \frac{\delta \Delta t}{h^2} u_2^0 - \frac{\Delta t}{\delta} (u_1^0)^3 \\ u_2^1 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_2^0 + \frac{\delta \Delta t}{h^2} u_3^0 + \frac{\delta \Delta t}{h^2} u_1^0 - \frac{\Delta t}{\delta} (u_2^0)^3 \\ &\vdots \\ u_{98}^1 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_{98}^0 + \frac{\delta \Delta t}{h^2} u_{99}^0 + \frac{\delta \Delta t}{h^2} u_{97}^0 - \frac{\Delta t}{\delta} (u_{98}^0)^3 = (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_{98}^0 + \frac{\delta \Delta t}{h^2} u_{97}^0 - \frac{\Delta t}{\delta} (u_{98}^0)^3 \end{cases}$$

For $n = 1$,

$$\begin{cases} u_1^2 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_1^1 + \frac{\delta \Delta t}{h^2} u_2^1 + \frac{\delta \Delta t}{h^2} u_0^1 - \frac{\Delta t}{\delta} (u_1^1)^3 = (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_1^1 + \frac{\delta \Delta t}{h^2} u_2^1 - \frac{\Delta t}{\delta} (u_1^1)^3 \\ u_2^2 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_2^1 + \frac{\delta \Delta t}{h^2} u_3^1 + \frac{\delta \Delta t}{h^2} u_1^1 - \frac{\Delta t}{\delta} (u_2^1)^3 \\ &\vdots \\ u_{98}^2 &= (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_{98}^1 + \frac{\delta \Delta t}{h^2} u_{99}^1 + \frac{\delta \Delta t}{h^2} u_{97}^1 - \frac{\Delta t}{\delta} (u_{98}^1)^3 = (1 + \frac{\Delta t}{\delta} - 2 \frac{\delta \Delta t}{h^2}) u_{98}^1 + \frac{\delta \Delta t}{h^2} u_{97}^1 - \frac{\Delta t}{\delta} (u_{98}^1)^3 \end{cases}$$

For $n = 97$,

$$\begin{cases} u_1^{98} &= (1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2})u_1^{97} + \frac{\delta\Delta t}{h^2}u_2^{97} + \frac{\delta\Delta t}{h^2}u_0^{97} - \frac{\Delta t}{\delta}(u_1^{97})^3 = (1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2})u_1^{97} + \frac{\delta\Delta t}{h^2}u_2^{97} - \frac{\Delta t}{\delta}(u_1^{97})^3 \\ u_2^{98} &= (1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2})u_2^{97} + \frac{\delta\Delta t}{h^2}u_3^{97} + \frac{\delta\Delta t}{h^2}u_1^{97} - \frac{\Delta t}{\delta}(u_2^{97})^3 \\ &\vdots \\ u_{98}^{98} &= (1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2})u_{98}^{97} + \frac{\delta\Delta t}{h^2}u_{99}^{97} + \frac{\delta\Delta t}{h^2}u_{97}^{97} - \frac{\Delta t}{\delta}(u_{98}^{97})^3 = (1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2})u_{98}^{97} + \frac{\delta\Delta t}{h^2}u_{97}^{97} - \frac{\Delta t}{\delta}(u_{98}^{97})^3 \end{cases}$$

If we write the iteration in the form of a linear system, we would have,

$$\begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{98}^{n+1} \end{bmatrix} = \begin{bmatrix} 1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2} & \frac{\delta\Delta t}{h^2} & 0 & 0 & \dots & 0 \\ \frac{\delta\Delta t}{h^2} & 1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2} & \frac{\delta\Delta t}{h^2} & 0 & \dots & 0 \\ 0 & \frac{\delta\Delta t}{h^2} & 1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2} & \frac{\delta\Delta t}{h^2} & \dots & 0 \\ \vdots & 0 & \frac{\delta\Delta t}{h^2} & \ddots & \ddots & \vdots \\ \vdots & 0 & 0 & \ddots & \ddots & 0 \\ \vdots & 0 & 0 & 0 & \frac{\delta\Delta t}{h^2} & 1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2} \\ \vdots & 0 & 0 & 0 & \frac{\delta\Delta t}{h^2} & 1 + \frac{\Delta t}{\delta} - 2\frac{\delta\Delta t}{h^2} \end{bmatrix} \begin{bmatrix} u_1^n \\ u_2^n \\ u_3^n \\ \vdots \\ \vdots \\ \vdots \\ u_{98}^n \end{bmatrix} + \begin{bmatrix} (u_1^n)^3 \\ (u_2^n)^3 \\ (u_3^n)^3 \\ \vdots \\ \vdots \\ \vdots \\ (u_{98}^n)^3 \end{bmatrix}$$

After discuss with Prof Mihai, we decided to set

$$u_+(x) = u(x, 0) = \sin(\pi x), u_-(x) = -\sin(\pi x)$$

, and we discretize the space-time domain $[0, 1] \times [0, 1]$ with sizes $\Delta x = \frac{1}{99}$, $\Delta t = \frac{1}{99}$.

To make our life easier, we just try to construct the function $u(x, t)$ on the domain as simple as possible with the boundary condition above. So, we set

$$\begin{aligned} u(x, t) &= -t\sin(\pi x) + (1 - t)\sin(\pi x) \\ &= -2t\sin(\pi x) + \sin(\pi x) \\ &= (1 - 2t)\sin(\pi x) \end{aligned}$$

Firstly I use Matlab to plot the 3D plot of this function on the domain. And then I get the matrix U , where the last row of U is $u(x, 0)$ while the top row is $u(x, 1)$.

```

1 x = linspace(0, 1, 100);
2 t = linspace(0, 1, 100);
3
4 U = zeros(100, 100);
5
6 for idx_t = 1:length(t)
7     current_t = t(idx_t);
8     U(101 - idx_t, :) = (1 - 2 * current_t) * sin(pi * x);
9 end
10
11 [X, T] = meshgrid(x, t);
12
13 figure;
14 surf(X, T, flipud(U));
15 xlabel('x');
16 ylabel('t');
17 zlabel('u(x,t)');
18 title('u(x,t) = (1 - 2t)sin(\pi x)');
19 shading interp;
20 colorbar;
```

And then I get the matrix U , where the row on the top is $u(x, 0)$ while the row in the bottom is $u(x, 1)$. Next we try to find matrix P where P is the numerical approximation to

$$p(x, t) = u_t - \delta u_{xx} + \delta^{-1} V'(u)$$

The formula is given by

$$P_{i,j+\frac{1}{2}} = \frac{U_{i,j+1} - U_{i,j}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{i,j+1} + U_{i,j}}{2} \right) - \frac{\delta}{2} \left(\frac{U_{i+1,j+1} - 2U_{i,j+1} + U_{i-1,j+1}}{\Delta x^2} + \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{\Delta x^2} \right)$$

where $i = 1, \dots, 98$, $j = 0, \dots, 98$, $\delta = 0.05$, $\Delta x = \frac{1}{99}$, $\Delta t = \frac{1}{99}$ and recall that

$$V(u) = \frac{1}{4}(1 - u^2)^2, V'(u) = u^3 - u$$

After we get P , we calculate $S_T(U)$ which is defined as

$$S_T(U) = \frac{1}{2} \Delta x \Delta t \sum_{i=1}^{98} \sum_{j=0}^{98} P_{i,j+\frac{1}{2}}^2$$

And since the boundary condition, S_T is actually a function of variables $U_{i,j}$ where $i = 1, \dots, 98$, $j = 1, \dots, 98$, and the gradient of S_T with respect to each variable is given by

$$\begin{aligned} \frac{\partial S_T}{\partial U_{i,j}} &= \left(2\Delta x + \frac{\Delta x \Delta t}{\delta} V'' \left(\frac{U_{i,j-1} + U_{i,j}}{2} \right) + \frac{2\delta \Delta t}{\Delta x} \right) P_{i,j-\frac{1}{2}} \\ &\quad - \left(2\Delta x - \frac{\Delta x \Delta t}{\delta} V'' \left(\frac{U_{i,j} + U_{i,j+1}}{2} \right) - \frac{2\delta \Delta t}{\Delta x} \right) P_{i,j+\frac{1}{2}} \\ &\quad - \frac{\delta \Delta t}{\Delta x} \left(P_{i-1,j-\frac{1}{2}} + P_{i-1,j+\frac{1}{2}} + P_{i+1,j-\frac{1}{2}} + P_{i+1,j+\frac{1}{2}} \right) \end{aligned}$$

Well, actually the function S_T is a function of the whole matrix U , so there should be 100×100 random variables, but since the boundary condition, the boundaries are constant so their derivatives are 0. So the gradient is

$$\nabla S_T(U) = \begin{bmatrix} \mathbf{0} \\ 0 \\ \frac{\partial S_T}{\partial U_{1,1}} \\ \vdots \\ \frac{\partial S_T}{\partial U_{98,1}} \\ 0 \\ 0 \\ \frac{\partial S_T}{\partial U_{1,2}} \\ \vdots \\ \frac{\partial S_T}{\partial U_{98,2}} \\ 0 \\ \vdots \\ 0 \\ \frac{\partial S_T}{\partial U_{1,98}} \\ \vdots \\ \frac{\partial S_T}{\partial U_{98,98}} \\ 0 \\ \mathbf{0} \end{bmatrix}$$

and the **BFGS** method is presented as follows,

$$U_0 = U$$

For $k = 0, 1, 2, \dots$,

$$U_{k+1} = U_k + \alpha_k p_k$$

where the step length α_k is chosen by the wolfe condition

$$S_T(U_{k+1}) \leq S_T(U_k) + c_1 \alpha_k \nabla S_T(U_k)^T p_k$$

and

$$\nabla S_T(U_{k+1})^T p_k \geq c_2 \nabla S_T(U_k)^T p_k$$

with $0 < c_1 < c_2 < 1$

The descent direction p_k is given by

$$p_k = -H_k \nabla f_k$$

where H_k is defined recursively by

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T$$

where $s_k = U_{k+1} - U_k$, $y_k = \nabla S_T(U_{k+1}) - \nabla S_T(U_k)$, and $\rho_k = \frac{1}{y_k^T s_k}$.

For H_0 , we firstly consider

$$H_0 = \gamma_1 I$$

where $\gamma_1 = \frac{y_0^T s_0}{y_0^T y_0}$

The algorithm is follows

Algorithm 1 BFGS Method

- 1: **Input:** Initial matrix $U_0 = U$, tolerance $\epsilon = 10^{-4}$, $\delta = 0.05$, $\Delta x = \frac{1}{99}$, $\Delta t = \frac{1}{99}$.
- 2: **Initialize:** $H_0 = \gamma_1 I$, where $\gamma_1 = \frac{y_0^T s_0}{y_0^T y_0}$.
- 3: **for** $k = 0, 1, 2, \dots$ **do**
- 4: Compute descent direction: $p_k = -H_k \nabla S_T(U_k)$.
- 5: Choose step length α_k satisfying the Wolfe conditions:

$$\begin{aligned} S_T(U_{k+1}) &\leq S_T(U_k) + c_1 \alpha_k \nabla S_T(U_k)^T p_k, \\ \nabla S_T(U_{k+1})^T p_k &\geq c_2 \nabla S_T(U_k)^T p_k, \end{aligned}$$

where $0 < c_1 < c_2 < 1$.

- 6: Update U : $U_{k+1} = U_k + \alpha_k p_k$.
 - 7: Compute $s_k = U_{k+1} - U_k$ and $y_k = \nabla S_T(U_{k+1}) - \nabla S_T(U_k)$.
 - 8: Compute $\rho_k = \frac{1}{y_k^T s_k}$.
 - 9: Update H_k by:
$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T.$$
 - 10: **if** $\|\nabla S_T(U_{k+1})\| \leq \epsilon$ **then**
 - 11: **Stop** and return U_{k+1} .
 - 12: **end if**
 - 13: **end for**
-

Then, we move to finding the initial boundary condition for $u_+(x, 0)$ and $u_-(x, 0)$. These two functions come from the stable equilibrium states of the function

$$\mathbb{E}[u] = \frac{1}{2} \int_0^1 (\delta u_x^2 + 2\delta^{-1} \mathbb{V}(u)) dx$$

Similarly, we set $q(x) = \delta u_x^2 + 2\delta^{-1} \mathbb{V}(u)$, so the energy function can be written as

$$\mathbb{E}[u] = \frac{1}{2} \int_0^1 q(x) dx$$

We use the midpoint rule to compute the temporal integral, and obtaining

$$E(U) = \frac{1}{2} \Delta x \sum_{i=1}^{I-1} P_i$$

and since here we have 100 points so $I = 100$, and P_i is the numerical approximation of $q(x_i)$ by central finite difference

$$P_i = 2\delta^{-1}\mathbb{V}(U_i) + \delta\left(\frac{U_{i+1} - U_{i-1}}{2\Delta x}\right)^2$$

For the boundary condition of U , we have $U_0 = U_{100} = 0$ and the BFGS method requires the gradient, which is given by

$$\begin{aligned}\frac{\partial E}{\partial U_1} &= \frac{1}{2}\Delta x \left[\delta^{-1}(1 - U_1^2)(-2U_1) + 2\delta\left(\frac{U_3 - U_1}{2\Delta x}\right)\left(-\frac{1}{2\Delta x}\right) \right] \\ \frac{\partial E}{\partial U_2} &= \frac{1}{2}\Delta x \left[2\delta\frac{U_2}{2\Delta x}\left(\frac{1}{2\Delta x}\right) + \delta^{-1}(1 - U_2^2)(-2U_2) + 2\delta\left(\frac{U_4 - U_2}{2\Delta x}\right)\left(-\frac{1}{2\Delta x}\right) \right] \\ \frac{\partial E}{\partial U_i} &= \frac{1}{2}\Delta x \left[2\delta\left(\frac{U_i - U_{i-2}}{2\Delta x}\right)\left(\frac{1}{2\Delta x}\right) + \delta^{-1}(1 - U_i^2)(-2U_i) + 2\delta\left(\frac{U_{i+2} - U_i}{2\Delta x}\right)\left(-\frac{1}{2\Delta x}\right) \right], \quad \text{for } i = 3, \dots, 97 \\ \frac{\partial E}{\partial U_{98}} &= \frac{1}{2}\Delta x \left[2\delta\left(\frac{U_{98} - U_{96}}{2\Delta x}\right)\left(\frac{1}{2\Delta x}\right) + \delta^{-1}(1 - U_{98}^2)(-2U_{98}) + 2\delta\frac{-U_{98}}{2\Delta x}\left(-\frac{1}{2\Delta x}\right) \right] \\ \frac{\partial E}{\partial U_{99}} &= \frac{1}{2}\Delta x \left[2\delta\left(\frac{U_{99} - U_{97}}{2\Delta x}\right)\left(\frac{1}{2\Delta x}\right) + \delta^{-1}(1 - U_{99}^2)(-2U_{99}) \right]\end{aligned}$$

And the BFGS method present as follow. $\mathbf{U}_0 = \sin(\pi x)$, $H_0 = I$

The BFGS method defines the next one as

$$\mathbf{U}_{k+1} = \mathbf{U}_k + \alpha_k p_k$$

, where α_k is chosen to satisfy the wolfe conditions

$$E(U_{k+1}) \leq E(\mathbf{U}_k) + c_1 \alpha_k \nabla E(\mathbf{U}_k)^T p_k$$

and

$$\nabla E(\mathbf{U}_{k+1})^T p_k \geq c_2 \nabla E(\mathbf{U}_k)^T p_k$$

with $0 < c_1 < c_2 < 1$

The search direction p_k is given by

$$p_k = -H_k \nabla E_k$$

where H_k is defined recursively by

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T$$

, where

$$s_k = E(\mathbf{U}_{k+1}) - E(\mathbf{U}_k), \quad y_k = \nabla E_{k+1} - \nabla E_k, \quad \rho_k = \frac{1}{y_k^T s_k}$$

and finally the iteration would stop if the norm of the gradient is smaller than $\epsilon = 10^{-4}$.

Unfortunately, we saw strong oscillation in the figure output and so we try to fix the formula of P_i into

$$2\delta^{-1}\mathbb{V}(U_i) + \frac{1}{2}\delta \left[\left(\frac{U_{i+1} - U_i}{\Delta x} \right)^2 + \left(\frac{U_i - U_{i-1}}{\Delta x} \right)^2 \right]$$

And the gradient becomes

$$\begin{aligned}\frac{\partial E}{\partial U_1} &= \frac{1}{2}\Delta x \left[\delta^{-1}(1 - U_1^2)(-2U_1) - 2\delta\frac{U_2 - U_1}{(\Delta x)^2} + \delta\frac{U_1}{(\Delta x)^2} \right] \\ \frac{\partial E}{\partial U_i} &= \frac{1}{2}\Delta x \left[2\delta\frac{U_i - U_{i-1}}{(\Delta x)^2} - 2\delta^{-1}(1 - U_i^2)U_i - 2\delta\frac{U_{i+1} - U_i}{(\Delta x)^2} \right], \quad \forall i = 2, \dots, 98 \\ \frac{\partial E}{\partial U_{99}} &= \frac{1}{2}\Delta x \left[2\delta\frac{U_{99} - U_{98}}{(\Delta x)^2} - 2\delta^{-1}(1 - U_{99}^2)U_{99} + \delta\frac{U_{99}}{(\Delta x)^2} \right]\end{aligned}$$

Then I re-calculate the gradient of $ST(U)$ with respect to $U_{i,j}$. The formula is given below.

When $j = 1, \dots, 99$, $i = 1$,

$$\begin{aligned}
\frac{\partial ST(U)}{\partial U_{j,i}} = & \frac{1}{2} \Delta x \Delta t \left[2 \left(\frac{U_{j,i} - U_{j-1,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) \right. \right. \\
& - \frac{\delta}{2} \left(\frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} + \frac{U_{j-1,i+1} - 2U_{j-1,i} + U_{j-1,i-1}}{(\Delta x)^2} \right) \Bigg) \\
& \cdot \left(\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j,i+1} - U_{j-1,i+1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i+1} + U_{j-1,i+1}}{2} \right) \right. \\
& - \frac{\delta}{2} \left(\frac{U_{j,i+2} - 2U_{j,i+1} + U_{j,i}}{(\Delta x)^2} + \frac{U_{j-1,i+2} - 2U_{j-1,i+1} + U_{j-1,i}}{(\Delta x)^2} \right) \Bigg) \cdot \frac{\delta}{(\Delta x)^2} \\
& + 2 \left(\frac{U_{j+1,i} - U_{j,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) \right. \\
& - \frac{\delta}{2} \left(\frac{U_{j+1,i+1} - 2U_{j+1,i} + U_{j+1,i-1}}{(\Delta x)^2} + \frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} \right) \Bigg) \\
& \cdot \left(-\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j+1,i+1} - U_{j,i+1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i+1} + U_{j,i+1}}{2} \right) \right. \\
& - \frac{\delta}{2} \left(\frac{U_{j+1,i+2} - 2U_{j+1,i+1} + U_{j+1,i}}{(\Delta x)^2} + \frac{U_{j,i+2} - 2U_{j,i+1} + U_{j,i}}{(\Delta x)^2} \right) \Bigg) \cdot \frac{\delta}{(\Delta x)^2} \Bigg]
\end{aligned}$$

When $j = 1, \dots, 99, i = 2, \dots, 98$,

$$\begin{aligned}
\frac{\partial ST(U)}{\partial U_{j,i}} = & \frac{1}{2} \Delta x \Delta t \left[\right. \\
& \left(\frac{U_{j,i-1} - U_{j-1,i-1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i-1} + U_{j-1,i-1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j,i} - 2U_{j,i-1} + U_{j,i-2}}{(\Delta x)^2} + \frac{U_{j-1,i} - 2U_{j-1,i-1} + U_{j-1,i-2}}{(\Delta x)^2} \right) \right) \cdot \left(\frac{-\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j+1,i-1} - U_{j,i-1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i-1} + U_{j,i-1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j+1,i} - 2U_{j+1,i-1} + U_{j+1,i-2}}{(\Delta x)^2} + \frac{U_{j,i} - 2U_{j,i-1} + U_{j,i-2}}{(\Delta x)^2} \right) \right) \cdot \left(\frac{\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j,i+1} - U_{j-1,i+1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i+1} + U_{j-1,i+1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j,i+2} - 2U_{j,i+1} + U_{j,i}}{(\Delta x)^2} + \frac{U_{j-1,i+2} - 2U_{j-1,i+1} + U_{j-1,i}}{(\Delta x)^2} \right) \right) \cdot \left(\frac{\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j+1,i+1} - U_{j,i+1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i+1} + U_{j,i+1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j+1,i+2} - 2U_{j+1,i+1} + U_{j+1,i}}{(\Delta x)^2} + \frac{U_{j,i+2} - 2U_{j,i+1} + U_{j,i}}{(\Delta x)^2} \right) \right) \cdot \left(\frac{\delta}{(\Delta x)^2} \right) \\
& + 2 \left(\frac{U_{j,i} - U_{j-1,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} + \frac{U_{j-1,i+1} - 2U_{j-1,i} + U_{j-1,i-1}}{(\Delta x)^2} \right) \right) \\
& \quad \cdot \left(\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \\
& + 2 \left(\frac{U_{j+1,i} - U_{j,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j+1,i+1} - 2U_{j+1,i} + U_{j+1,i-1}}{(\Delta x)^2} + \frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} \right) \right) \\
& \quad \cdot \left(-\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \left. \right]
\end{aligned}$$

When $j = 1, \dots, 99, i = 99$

$$\begin{aligned}
\frac{\partial ST(U)}{\partial U_{j,i}} = & \frac{1}{2} \Delta x \Delta t \left[\right. \\
& 2 \left(\frac{U_{j,i} - U_{j-1,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} + \frac{U_{j-1,i+1} - 2U_{j-1,i} + U_{j-1,i-1}}{(\Delta x)^2} \right) \right) \\
& \quad \cdot \left(\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j,i} + U_{j-1,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \\
& + 2 \left(\frac{U_{j+1,i} - U_{j,i}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j+1,i+1} - 2U_{j+1,i} + U_{j+1,i-1}}{(\Delta x)^2} + \frac{U_{j,i+1} - 2U_{j,i} + U_{j,i-1}}{(\Delta x)^2} \right) \right) \\
& \quad \cdot \left(-\frac{1}{\Delta t} + \frac{\delta^{-1}}{2} V'' \left(\frac{U_{j+1,i} + U_{j,i}}{2} \right) + \frac{\delta}{(\Delta x)^2} \right) \\
& - \left(\frac{U_{j,i-1} - U_{j-1,i-1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j,i-1} + U_{j-1,i-1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j,i} - 2U_{j,i-1} + U_{j,i-2}}{(\Delta x)^2} + \frac{U_{j-1,i} - 2U_{j-1,i-1} + U_{j-1,i-2}}{(\Delta x)^2} \right) \right) \cdot \frac{\delta}{(\Delta x)^2} \\
& - \left(\frac{U_{j+1,i-1} - U_{j,i-1}}{\Delta t} + \delta^{-1} V' \left(\frac{U_{j+1,i-1} + U_{j,i-1}}{2} \right) \right. \\
& \quad \left. - \frac{\delta}{2} \left(\frac{U_{j+1,i} - 2U_{j+1,i-1} + U_{j+1,i-2}}{(\Delta x)^2} + \frac{U_{j,i} - 2U_{j,i-1} + U_{j,i-2}}{(\Delta x)^2} \right) \right) \cdot \frac{\delta}{(\Delta x)^2} \left. \right]
\end{aligned}$$