Assignment 4: Adjoint of unsteady 1D Euler Equations

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Abstract

1 Summary

For this assignment, the following functionalities have been implemented:

- derived the continuous adjoint equation of unsteady 1D Euler equation given the specific functional;
- derived the discrete adjoint equation of unsteady 1D Euler with Crank-Nicolson discretization;
- solved the unsteady adjoint equation;
- computed the total derivative of the functional with respect to the source using adjoint variable.

1.1 How to run the code

```
julia assign4_example.jl
```

Note to turn on the finite difference verification of DJ/Ds, just change value of `FD_verification` to `true`.

2 Continuous adjoint equation

We first derive the Frechet derivative for the nonlinear differential operator $N(q) = \frac{\partial F}{\partial x}$:

$$N'[q]w = [\frac{\partial}{\partial \epsilon}\frac{\partial F(q+\epsilon w)}{\partial x}]_{\epsilon=0} = \frac{\partial (Aw)}{\partial x} \tag{1}$$

where $A = \frac{\partial F}{\partial q}$ is the flux Jacobian matrix. This is followed by the corresponding adjoint differential operator:

$$\begin{aligned}
(\psi, N'[q]w)_\Omega &= \int_\Omega \psi^T (\frac{\partial Aw}{\partial x}) \mathrm{d}\Omega \\
&= -\int_\Omega w^T A^T \frac{\partial \psi}{\partial x}\mathrm{d}\Omega + \int_{\partial\Omega} w^T A^T \psi \mathrm{d}\Gamma \\
&= -\int_\Omega w^T A^T \frac{\partial \psi}{\partial x}\mathrm{d}\Omega + \int_{\partial\Omega} w^T A^T \psi \mathrm{d}\Gamma \\
&= -\int_0^1 w^T A^T \frac{\partial \psi}{\partial x}\mathrm{d}x + [w^T A^T \psi]|_{x=1} - [w^T A^T \psi]|_{x=0}
\end{aligned} \tag{2}$$

Then we derive the Frechet derivative of the functional:

$$J'[q]w = \int_0^2 \int_0^1 w^T \kappa (p - p_{targ}) p'[q] \mathrm{d}x\mathrm{d}t \tag{3}$$

By definition, the Lagrangian is

$$L = J(q) - \int_0^2 (\psi, R(q))_\Omega dt - \int_0^2 [\psi^T A(q - q(0,t))]|_{x=0} \mathrm{d}t - \int_0^1 [\psi^T (q - q(x,0))]_{t=0} \mathrm{d}x \tag{4}$$

As can be seen, in addition to the primal PDE, we have also involved the boundary conditions and the initial conditions. Taking the derivative of the Lagrangian with a variant w, we get

$$\begin{aligned}
L'[q]w &= J'[q]w - \int_0^2 (\psi, R'[q]w)_\Omega dt - \int_0^2 [w^T A^T \psi]_{x=0} \mathrm{d}t - \int_0^1 [w^T \psi]_{t=0} \mathrm{d}x \\
&= J'[q]w - \int_0^2 (\psi, \frac{\partial w}{\partial t} + N'[q])w)_\Omega dt - \int_0^2 [w^T A^T \psi]_{x=0} \mathrm{d}t - \int_0^1 [w^T \psi]_{t=0} \mathrm{d}x \\
&= \int_0^2 \int_0^1 w^T \kappa (p - p_{targ}) p'[q] \mathrm{d}x\mathrm{d}t + \int_0^2 \int_0^1 w^T \frac{\partial \psi}{\partial t} \mathrm{d}x\mathrm{d}t - \int_0^1 [w^T \psi]|_{t=2} \mathrm{d}x \\
&+ \int_0^2 \int_0^1 w^T A^T \frac{\partial \psi}{\partial x} \mathrm{d}x\mathrm{d}t - \int_0^2 [w^T A^T \psi]_{x=1} \mathrm{d}t \\
&= \int_0^2 \int_0^1 w^T (\frac{\partial \psi}{\partial t} + A^T \frac{\partial \psi}{\partial x} + \kappa (p - p_{targ} p'[q])) \mathrm{d}x\mathrm{d}t \\
&- \int_0^1 [w^T \psi]_{t=1} \mathrm{d}x - \int_0^2 [w^T A^T \psi]_{x=1} \mathrm{d}t
\end{aligned} \tag{5}$$

By the definition of duality, all three terms should vanish since the variant w is involved in these three terms. This leads to the continuous adjoint problem:

$$\begin{aligned}
\frac{\partial \psi}{\partial t} + A^T \frac{\partial \psi}{\partial x} + \kappa (p - p_{targ}) p'[q] = 0, &\qquad x, t \in [0,1] \times [0,2] \\
\psi(x, 2) = 0, &\qquad x \in [0,1] \\
\psi(1, t) = 0, &\qquad t \in [0,2]
\end{aligned} \tag{6}$$

3 Discrete adjoint

3.1 Derivation of discrete adjoint equation

The residual of implicit Crank-Nicholson is

$$\hat{R}_h^{(n+1)} = \mathsf{M}(q_h^{(n+1)} - q_h^{(n)}) + \frac{\Delta t}{2} [R_h(q_h^{(n+1)}, s_h^{(n+1)}) + R_h(q_h^{(n)}, s_h^{(n)})], \quad n = 0, \ldots, N-1 \tag{7}$$

The functional is discretized as

$$J_h = \sum_{n=0}^{N} w_n \Delta t \int_0^1 \frac{1}{2} \kappa (p^{(n)} - p_{targ})^2 \mathrm{d}x = \sum_{n=0}^{N} w_n \Delta t g_n \tag{8}$$

where $g_n = \int_0^1 \frac{1}{2} \kappa (p^{(n)} - p_{targ})^2 \mathrm{d}x$, and w_n is the weight coefficient:

$$w_n = \begin{cases} 1 & 0 < n < N \\ 0.5 & n = 0 \text{ or } n = N \end{cases} \tag{9}$$

The discrete Lagrangian is defined by subtracting the adjoint-weighted residual from the functional:

$$\begin{aligned} L_{h,\Delta t} &= \sum_{n=0}^{N} \Delta t w_n g_n - \sum_{n=0}^{N-1} (\psi_h^{(n+1)})^T \hat{R_h}^{(n+1)} \\ &= \sum_{n=0}^{N} \Delta t w_n g_n - \sum_{n=0}^{N-1} (\psi_h^{(n+1)})^T (\mathsf{M}(q_h^{(n+1)} - q_h^{(n)}) + \frac{\Delta t}{2}[R_h(q_h^{(n+1)}, s_h^{(n+1)}) + R_h(q_h^{(n)}, s_h^{(n)})]) \end{aligned} \tag{10}$$

The discrete adjoint can be found by setting the derivative of the Lagrangian with respect to the primal solution $q_h^{(n)}$ to zero. For $n = 1, \dots, N-1$, we have

$$\frac{\partial L_{h,\Delta t}}{\partial q_h^{(n)}} = \Delta t w_n \frac{\partial g_n}{\partial q_h^{(n)}} - \mathsf{M}^T (\psi_h^{(n)} - \psi_h^{(n+1)}) - \frac{\Delta t}{2} (\frac{\partial R_h}{\partial q_h^{(n)}})^T (\psi_h^{(n)} + \psi_h^{(n+1)}) \tag{11}$$

For $n = N$, we have

$$\frac{\partial L_{h,\Delta t}}{\partial q_h^{(N)}} = \Delta t w_N \frac{\partial g_N}{\partial q_h^{(N)}} - \mathsf{M}^T \psi_h^{(N)} - \frac{\Delta t}{2} (\frac{\partial R_h}{\partial q_h^{(N)}})^T \psi_h^{(N)} \tag{12}$$

Hence, the discrete adjoint equations are as follows

$$\begin{aligned} \mathsf{M}^T (\psi_h^{(n)} - \psi_h^{(n+1)}) + \frac{\Delta t}{2} (\frac{\partial R_h}{\partial q_h^{(n)}})^T (\psi_h^{(n)} + \psi_h^{(n+1)}) - \Delta t w_n \frac{\partial g_n}{\partial q_h^{(n)}} &= 0, \qquad n = 1 \dots, N-1 \\ \mathsf{M}^T \psi_h^{(N)} + \frac{\Delta t}{2} (\frac{\partial R_h}{\partial q_h^{(N)}})^T \psi_h^{(N)} - \Delta t w_N \frac{\partial g_N}{\partial q_h^{(N)}} &= 0 \end{aligned} \tag{13}$$

As we can see, when $\Delta t \to 0$, the second equation in (13) gives $\psi_h^{(N)} \to 0$ which is consistent with the the terminal condition in (6). For $n = 1, \dots, N-1$, the temporal discretization in the adjoint equation is also Crank-Nicolson, which is second-order accurate; that is to say, the discretization is adjoint consistent.

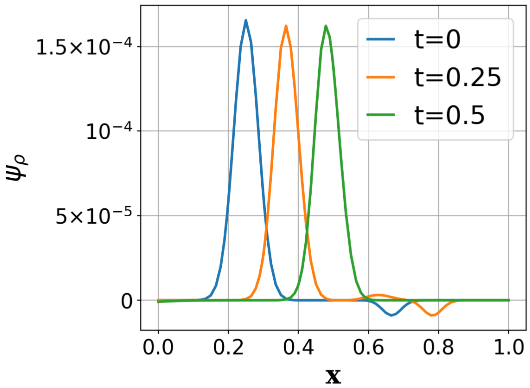
3.2 Results

To solve (13), we do a backwards sweep: first the second equation in (13) is solved for $\psi^{(N)}$; then the first equation in (13) is solved backwards in time, i.e., $n = N-1, N-2, \dots, 0$.

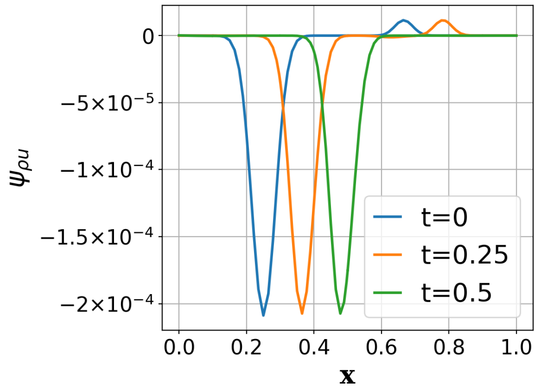
The following results verifies the correct derivation and implementation of the adjoint:

- in Figure 1 we can see the adjoint wave propagating upstream, as expected;
- as shown in Figure 2, the adjoint solution at $t = 2$, $\psi_h(x, 2)$, is nearly zero, which agrees with the terminal condition in (6);
- we will see later in Section 4, the total derivative of the functional with respect to the source obtained using adjoint-based approach matches that computed using finite difference.

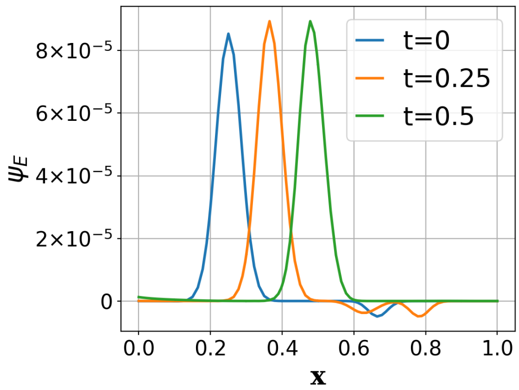
A further verification to do would be the convergence study.



(a) adjoint solution for ρ



(b) adjoint solution for ρu



(c) adjoint solution for E

Figure 1: Adjoint solution at 3 time stations

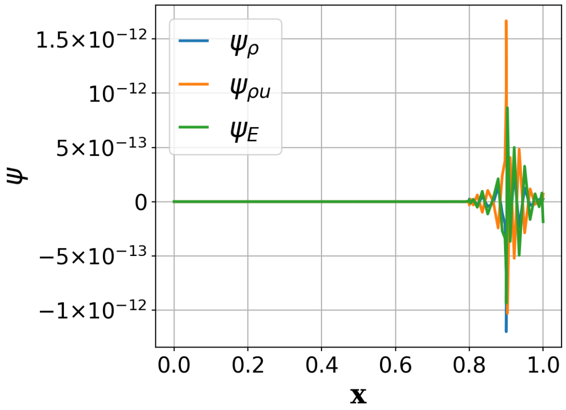


Figure 2: Adjoint solution at $t = 2$

4 Total derivative of functional

According to (10),

$$\begin{aligned}
\frac{DJ_h}{Ds^{(i)}} &= \frac{\partial L_{h,\Delta t}}{\partial s^{(i)}} \\
&= \frac{\partial J_h}{\partial s^{(i)}} - \sum_{n=0}^{N-1} (\psi_h^{(n+1)})^T \frac{\partial \hat{R}_h^{(n+1)}}{\partial s^{(i)}} \\
&= \begin{cases} -(\psi_h^{(i)})^T \frac{\partial \hat{R}_h^{(i)}}{\partial s^{(i)}} - (\psi_h^{(i+1)})^T \frac{\partial \hat{R}_h^{(i+1)}}{\partial s^{(i)}}, & 0 < i < N \\ -(\psi_h^{(i+1)})^T \frac{\partial \hat{R}_h^{(i+1)}}{\partial s^{(i)}}, & i = 0 \\ -(\psi_h^{(i)})^T \frac{\partial \hat{R}_h^{(i)}}{\partial s^{(i)}}, & i = N \end{cases} \\
&= \begin{cases} -\frac{\Delta t}{2} (\psi_h^{(i)} + \psi_h^{(i+1)})^T \frac{\partial R_h^{(i)}}{\partial s^{(i)}}, & 0 < i < N \\ -\frac{\Delta t}{2} (\psi_h^{(i+1)})^T \frac{\partial R_h^{(i)}}{\partial s^{(i)}}, & i = 0 \\ -\frac{\Delta t}{2} (\psi_h^{(i)})^T \frac{\partial R_h^{(i)}}{\partial s^{(i)}}, & i = N \end{cases}
\end{aligned} \tag{14}$$

In the above equation, we have utilized the fact that $\frac{\partial J_h}{\partial s^{(i)}} = 0$, and that $\hat{R}_h^{(n)} = \hat{R}_h(s^{(n)}, s^{(n+1)})$ and $\frac{\partial \hat{R}^{(n+1)}}{\partial s^{(n)}} = \frac{\partial \hat{R}^{(n)}}{\partial s^{(n)}} = \frac{\Delta t}{2} \frac{\partial R^{(n)}}{\partial s^{(n)}}$. We can see that in addition to the discrete adjoint variable $\psi_h^{(n)}$, $n = 1, \dots, N$, the partial derivative of the residual with respect s, $\frac{\partial \hat{R}}{\partial s^{(n)}}$, is also required to compute the total derivative of the functional.

The result is shown in Figure 3. For verification, we compare the derivatives for several time steps using adjoint-based approach to that using the finite difference method. For all time steps, the relative difference between two approaches is less than 0.02%, and the absolute difference is on the order of 10^{-11}.

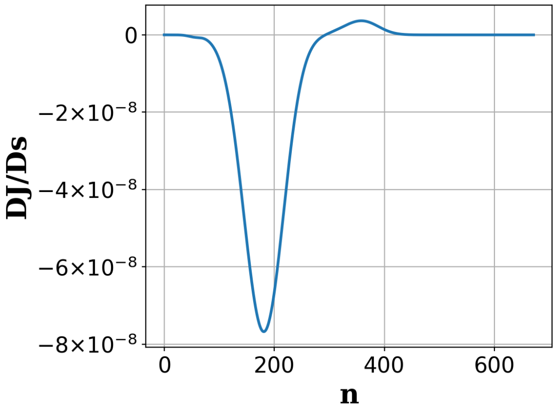


Figure 3: Adjoint solution at $t = 2$

Table 1: Comparison of $DJDs$ between adjoint-based approach and finite difference

n	adjoint	FD	diff(%)
200	-6.649642178447126e-8	-6.650801120737715e-8	0.0174286414139
201	-6.547562653134201e-8	-6.548721076713906e-8	0.0176924397837
202	-6.441868649339054e-8	-6.443026535579894e-8	0.01797438451276
203	-6.332777721431136e-8	-6.333935056083499e-8	0.01827530829712
204	-6.220512517227239e-8	-6.221669284582214e-8	0.0185960136206
205	-6.105300004457184e-8	-6.106456191230011e-8	0.01893742767731