

Take-home Midterm

AERO 455 - CFD for Aerospace Applications

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Given: 11th March 2022
Due: 5pm EST on 25th March 2022
Total points: 160/130
No extensions!

1 Fluid Dynamics (45 points)

This part tests you on the content of lectures 01 to 04.

1.1 The substantial derivative (9 points)

Answer the following questions.

1. What is the formula of the substantial derivative? *(2 points)*
2. Explain what each part means and give real-life examples. *(5 points)*
3. When is it appropriate to use the substantial derivative? *(2 points)*

1.2 Conservation Forms (6 points)

Answer the following questions.

1. When is it appropriate to use a transport equation in conservation form? *(2 points)*
2. Give an example. *(2 points)*
3. Which fluid model leads directly to a conservation form and why? *(2 points)*

1.3 The Total Energy Equation (20 points)

1.3.1 The total energy moving infinitesimal element (10 points)

Answer the following questions.

1. Draw the total energy moving infinitesimal element with fluxes in the y-direction and explain the meaning of each term. Assume a Newtonian stress model and thermal conduction for surface heat transfer. *(5 points)*
2. Repeat the same exercise for fluxes in the z-direction. *(5 points)*

1.3.2 The integral conservative total energy equation (10 points)

Derive the integral conservative total energy equation and use the divergence theorem where appropriate to transform volume integrals into surface integrals. Do not assume a particular form for the viscous stresses and surface heat transfer.

1.4 Potential Flow (10 points)

Answer the following questions.

1. Which panel method studied in class is used for non-lifting flow and which flow property can you get from it? *(2.5 points)*
2. Which panel method studied in class is used for lifting flow and which flow property can you get from it? *(2.5 points)*
3. Which panel method studied in class leads to an ill-defined algebraic system and how do you fix that in practice? *(2.5 points)*
4. What is the Kutta-Joukowski theorem and which panel method uses it? *(2.5 points)*

2 Finite Differencing, Stability and the Finite Volume Method (85 points)

All questions below relate to lectures 05, 06 and 07.

2.1 Finite Differencing and Stability (30 points)

Consider the second order accurate central difference scheme of the first derivative using a two-point stencil,

$$\frac{\partial q_i}{\partial x} = \frac{q_{i+1} - q_{i-1}}{2\Delta x} + O(\Delta x^2). \quad (2.1)$$

Consider also the second order accurate backward difference scheme of the first derivative using a three-point stencil,

$$\frac{\partial q_i}{\partial x} = \frac{3q_i - 4q_{i-1} + q_{i-2}}{2\Delta x} + O(\Delta x^2). \quad (2.2)$$

The 1D linear advection equation of a scalar q is given by,

$$\frac{\partial q}{\partial t} + a \frac{\partial q}{\partial x} = 0, \quad (2.3)$$

where a is a constant advection velocity.

1. Using a linear Neumann stability analysis, determine whether 2.3 is stable when using the scheme of equation 2.1 to approximate the first spatial derivative and under which conditions. Use a first order

forward difference in time for the transient term and an explicit formulation. You may assume an exponential time variation or a generic one, as was shown in lecture 07, slides 36 to 50. *(10 points)*

2. What is the applicable form of the Courant number here and what is its physical meaning compared to the grid velocity as shown in slides 54 to 56 of lecture 07? *(5 points)*
3. Repeat the previous exercises in 1 and 2 using the second order scheme from equation 2.2 for the first derivative. Compare your results to what you got with the central scheme. *(15 points)*

2.2 The Finite Volume Method (10 points)

Answer the following questions.

1. What is the Riemann problem? *(2.5 points)*
2. What is the advantage of the finite volume method over the finite difference method? *(2.5 points)*
3. What is flux upwinding? *(2.5 points)*
4. What is the MUSCL scheme and what is its order of accuracy? How does it maintain stability? *(2.5 points)*

2.3 Coding (45 points)

The Python script provided with the midterm is a finite difference discretization of the 1D linear advection equation using a first order forward difference two-point scheme in time for the transient term, and a first order backward difference two-point scheme in space for the advection term. The advection velocity is $a = 1$ and the domain length is $L = 1$. At the end of the script the solution of the advection of a step function is plotted against the x-axis.

2.3.1 2nd order accurate central differencing (20 points)

1. Add the second order accurate central two-point scheme of equation 2.1 to the script and plot its results on the same plot as the first-order backward difference two-point scheme at time $t = 0.75$. (10 points)
2. Keeping the Courant number limitations of both schemes in mind, can you refine the time step and mesh spacing until you your results stop varying at time $t = 0.75$? This is called time step and mesh independence. (10 points)

2.3.2 2nd order accurate backward differencing (20 points)

1. Add the second order accurate backward three-point scheme of equation 2.2 to the script and plot its results on the same plot as the first order scheme of the first derivative at time $t = 0.75$. (10 points)
2. Keeping the Courant number limitations of both schemes in mind, can you refine the time step and mesh spacing until you your results stop varying at time $t = 0.75$? Which time step and mesh spacing achieve time step and mesh independence? (10 points)

2.3.3 Comparing all three schemes (5 points)

Plot the solutions of all three schemes on the same plot at time $t = 0.75$ and answer the following questions.

3. Which of the three schemes exhibits the most oscillations and why? (2.5 points)
4. Which well-known stability theorem about the order of accuracy of a stable linear scheme applies to your results? (2.5 points)

3 Bonus Problem (30 points)

The 1D linear advection-diffusion equation is given by,

$$\frac{\partial q}{\partial t} + a \frac{\partial q}{\partial x} = \beta \frac{\partial^2 q}{\partial x^2}, \quad (3.1)$$

where $a = 1$ is a constant advection velocity and $\beta = 10^{-3}$ is a constant diffusion coefficient.

1. Modify the linear advection script from problem 2.3 by adding the following 2nd order accurate three-point central difference approximation of the second derivative,

$$\frac{\partial^2 q}{\partial x^2} = \frac{q_{i-1} - 2q_i + q_{i+1}}{\Delta x^2} + O(\Delta x^2). \quad (3.2)$$

Since the diffusion operator is a second derivative you will need to add another boundary condition at the outlet of the domain. Use a zero-gradient boundary condition, which can be implemented by setting the solution value of the last point of the domain equal to that of the preceding point. Obviously, you will not need to solve for the solution at the last point anymore. (*15 points*)

2. Using the 2nd order accurate scheme of equation 2.2 for the advection term, simulate the transport of the same step function as in problem 2.3. Keep refining the time step and mesh spacing until you reach time step and mesh independence at time $t = 0.75$. Show it by plotting the results of successive time and space refinements on the same plot and mention which time-step and mesh spacing achieved time step and mesh independence. (*5 points*)

3. Once you have reached time step and mesh independence, run the script again for $\beta = 10^{-5}$, 10^{-4} , 10^{-2} , 10^{-1} and plot your results on the same plot for $t = 0.75$ with the baseline solution at $\beta = 10^{-3}$. (5 points)
4. How do your results for each β value compare to the baseline solution at $\beta = 10^{-3}$? Which solution has the most oscillations and what do you attribute that to? (5 points)

1.1.1) For a generic function $f(t, x_1, x_2, x_3)$ we have the substantial derivative given as follows

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \vec{V} \cdot \nabla f = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_1} v_1 + \frac{\partial f}{\partial x_2} v_2 + \frac{\partial f}{\partial x_3} v_3$$

1.1.2) The substantial derivative simply represents the time rate of change on a moving fluid element. It is the physical equivalent of the total derivative w.r.t time, & consists of 2 parts.

$\frac{\partial f}{\partial t}$ is the local derivative. A physical example of this would be the change in temperature you would feel if you stood still & the local temperature of the room changed.

$\vec{V} \cdot \nabla f = \frac{\partial f}{\partial x_1} v_1 + \frac{\partial f}{\partial x_2} v_2 + \frac{\partial f}{\partial x_3} v_3$ is the convective derivative. A physical example of this would be the change in temperature you felt as you walk through a spatial temperature gradient. For example, as you walk from a heated room through the hall way into the cold outdoors.

1.1.3) It is appropriate to use the substantial derivative when the analysis at hand deals with the time rate of change as the control volume moves with the flow.

1.2.1) When you want to solve the transport equation in divergence form you should use the conservation form. This involves the local time rate of change & flux derivatives. In this case the fluid element will be fixed.

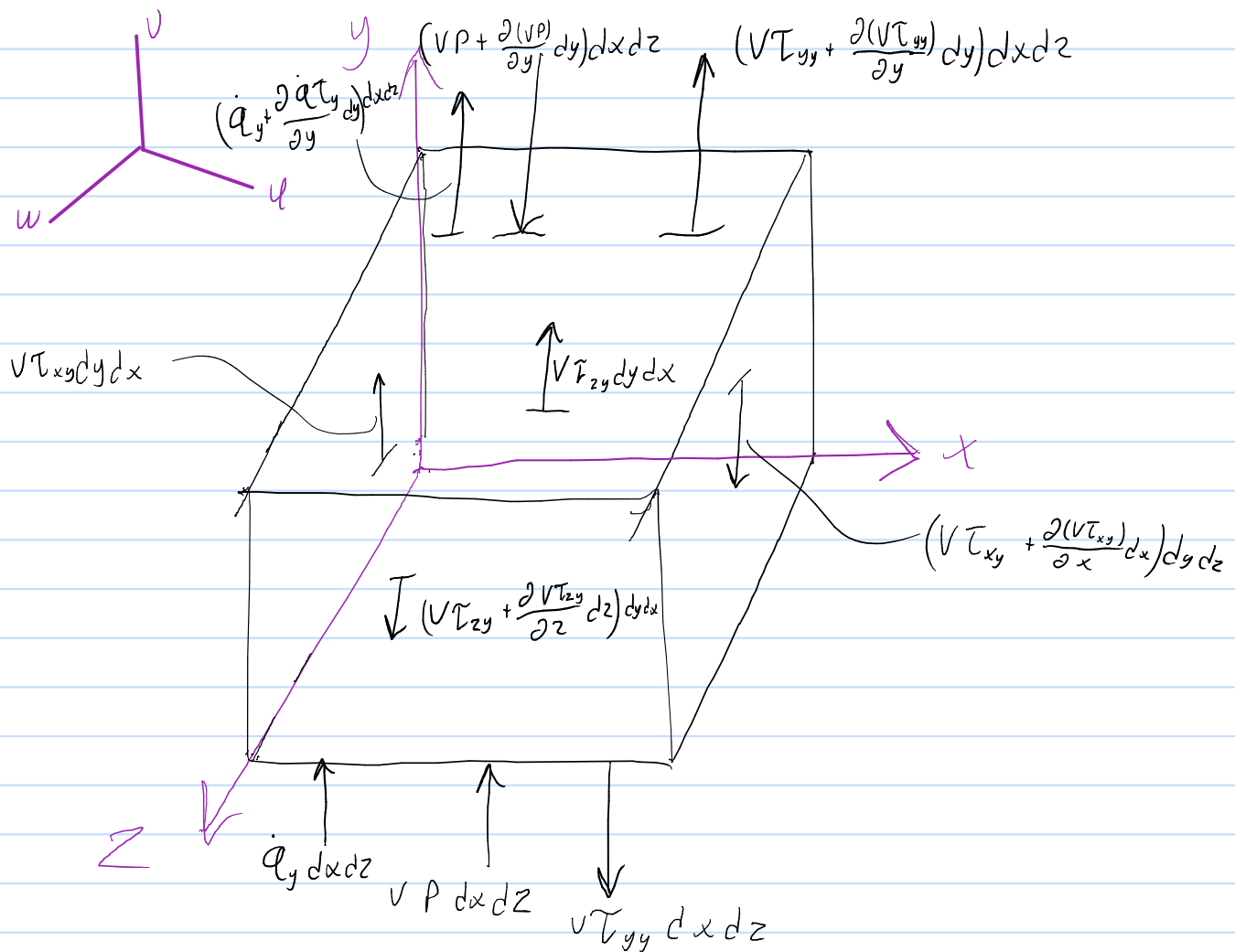
1.2.2) As an example we can look at the integral form of the conservation of mass equation, applied to a fixed finite control volume

$$\frac{\partial}{\partial t} \iiint_V \rho dV + \iint_S \rho \vec{V} \cdot d\vec{S} = 0$$

Since we wanted to analyze this for a fixed finite volume, we must use the conservation form of the equation.

1.2.3) When the equations are directly obtained from a fixed control volume, they will be in conservation form. This is because the fluid flow equations derived from a fixed control volume directly lead to the conservation form. Upon converting to the differential equations from the integral equations, the conservation form will be kept.

1.3.1.1)

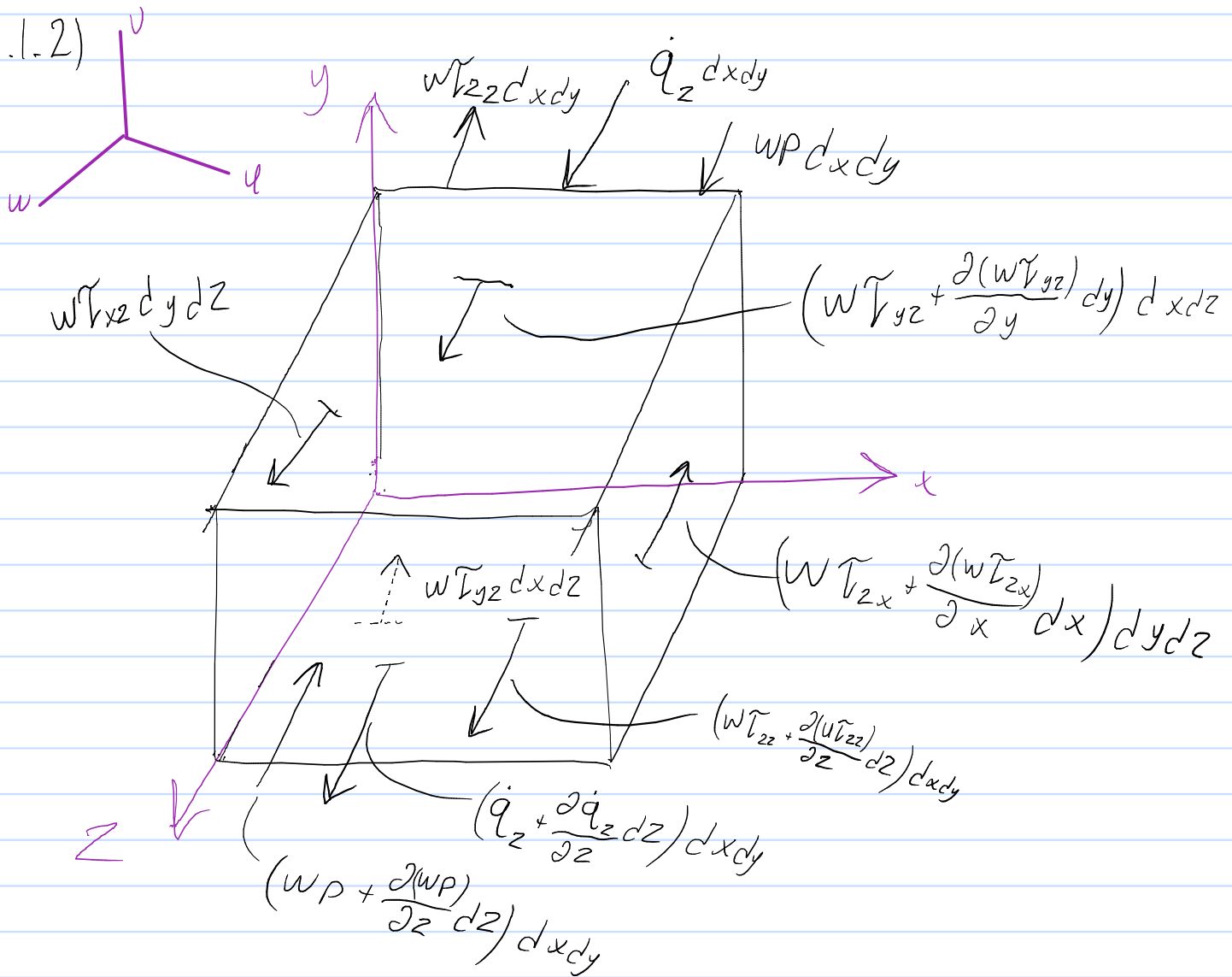


$-VT_{xy} dy dx$, $(VT_{xy} + \frac{\partial(VT_{xy})}{\partial x} dx) dy dz$, $VT_{yy} dx dz$, $(VT_{yy} + \frac{\partial(VT_{yy})}{\partial y} dy) dx dz$, $VT_{zy} dy dx$ & $(VT_{zy} + \frac{\partial(VT_{zy})}{\partial z} dz) dy dx$ all represent the rate of work done on the fluid element by the Shear forces.

$-VP dx dz$ & $(VP + \frac{\partial(VP)}{\partial z} dz) dx dy$ represent the rate of work by the pressure forces on the fluid element

$q_y dx dz$ & $(q_y + \frac{\partial q_y}{\partial y} dy) dx dz$ represent the heat transferred into the fluid by thermal conduction.

1.3.1.2)



- $wT_{yz} dy dz$, $(wT_{zx} \frac{\partial(wT_{zx})}{\partial x} dx) dy dz$, $wT_{yz} dx dz$, $(wT_{yz} + \frac{\partial(wT_{yz})}{\partial y} dy) dx dz$, $wT_{zz} dxdy$, & $(wT_{zz} + \frac{\partial(wT_{zz})}{\partial z} dz) dxdy$
all represent the rate of work done on the fluid element by the shear forces.

- $w p dxdy$ & $(w p + \frac{\partial(w p)}{\partial z} dz) dxdy$ represent the rate of work by the pressure forces on the fluid element

- $\dot{q}_z dxdy$ & $(\dot{q}_z + \frac{\partial \dot{q}_z}{\partial z} dz) dxdy$ represent the heat transferred into the fluid by thermal conduction.

1.3.2)

Useful equations:

First Law of thermodynamics

$$Q = \Delta E + W = \Delta E + W_{\text{shaft}} + W_{\text{viscous}} + W_{\text{pressure}} + W_{\text{body}}$$

$$W_{\text{shaft}} = 0, \quad W_{\text{pressure}} = - \oint_S (p dS) \vec{V}, \quad W_{\text{body}} = \iiint_V (\rho f dV) \vec{V}, \quad W_{\text{viscous}} = 0$$

$$\text{Net energy into control volume} = \oint_S (\rho \vec{V} dS) (e + \frac{V^2}{2})$$

$$\text{Change in energy inside the control volume} = \frac{d}{dt} \iiint_V \rho (e + \frac{V^2}{2}) dV$$

$$\text{Heat addition: } Q = 0, \quad \text{Internal Energy} = U = C_v T$$

Assume viscous stresses & heat transfer are 0.

$$\text{First Law: } 0 = \Delta E + W_{\text{shaft}} + W_{\text{viscous}} + W_{\text{pressure}} + W_{\text{body}}$$

$$0 = \underbrace{\oint_S (\rho \vec{V} dS) (e + \frac{V^2}{2})}_{\Delta E \text{ net in control volume}} + \underbrace{\frac{d}{dt} \iiint_V \rho (e + \frac{V^2}{2}) dV}_{\Delta E \text{ Change in control volume}} - \underbrace{\oint_S (p \vec{V}) dS}_{W_{\text{pressure}}} + \underbrace{\iiint_V (\rho f dV)}_{W_{\text{body}}} \quad [1.3.2]$$

$$\text{from divergence theorem we have } \iiint_V (\nabla \cdot \vec{V}) dxdydz = \oint_S \vec{V} \cdot \hat{n} dS$$

Above we have the energy equation in integral form. We can also apply the divergence theorem to the differential form to land at the same result

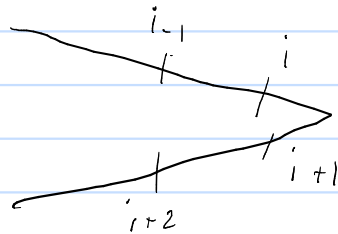
$$\frac{d}{dt} [\rho (e + \frac{V^2}{2})] + \nabla \cdot [\rho (e + \frac{V^2}{2}) \vec{V}] = - \frac{\partial (uP)}{\partial x} - \frac{\partial (vP)}{\partial y} - \frac{\partial (wP)}{\partial z} + \rho \vec{f} \cdot \vec{V}$$

We can integrate the above equation & apply divergence theorem. Doing this we will give us the same result as equation 1.3.2.

1.4.1) The source panel method is the panel method we studied for non-lifting flow. This method uses the source flow to describe the flow, & it provides the velocity distribution around the body. From this the pressure can also be found.

1.4.2) The vortex panel method is the method we studied for lifting bodies. This method uses the vortex flow to describe the flow & provides a variety of things. It can provide the circulation around the body & from this you can use the Kutta-Joukowski theorem to find the lift. We can also find the velocity & pressure.

1.4.3) The vortex panel method describes an algebraically incomplete system as we have 1 more unknown than we do equations. To get around this we apply the Kutta-Condition, in which the circulation at the trailing edge is 0. In practice we simply place two control points close to the trailing edge labelled i & $i+1$.



Then we calculate the circulation of i & set the circulation of $i+1$ to be the negative of this value.

$$\gamma_i = -\gamma_{i+1}$$

1.4.4) The Kutta-Joukowski theorem is a theorem which allows us to determine the lift from the total circulation around a lifting body. It is used in the vortex panel method to calculate lift from the following properties,

$$\Gamma = \sum_{j=1}^N \gamma_j S_j \text{ where } \gamma \text{ is the circulation of a panel \& } S \text{ is the length of it.}$$

$$L = \rho_{\infty} V_{\infty} \Gamma \quad (\text{Kutta-Joukowski theorem})$$

2.1.1) We have $\frac{\partial a}{\partial t} + a \frac{\partial a}{\partial x}$ for linear advection [2.1]

Using a second order accurate central difference scheme with a two point stencil we have

$$\frac{\partial a}{\partial x} = \frac{a_{i+1} - a_{i-1}}{2\Delta x} + O(\Delta x^2) \quad [2.2]$$

We can choose the discrete scheme as follows

$$\frac{a_i^{t+1} - a_i^t}{\Delta t} + \alpha \frac{a_{i+1}^t - a_{i-1}^t}{2\Delta x} = 0 \quad [2.3]$$

We know the wavelike solution for this as follows

$$a_i^t = e^{a^t} e^{ik_m x}$$

$$a_i^{t+1} = e^{a^{t+1}} e^{ik_m x}$$

$$a_{i+1}^t = e^{a^t} e^{ik_m (x+\Delta x)}$$

$$a_{i-1}^t = e^{a^t} e^{ik_m (x-\Delta x)}$$

We can plug these into [2.3] to get the following

$$\frac{e^{a^{t+1}} e^{ik_m x} - e^{a^t} e^{ik_m x}}{\Delta t} + \alpha \frac{e^{a^t} e^{ik_m (x+\Delta x)} - e^{a^t} e^{ik_m (x-\Delta x)}}{2\Delta x} = 0$$

We can simplify this as follows

$$\frac{e^{a\Delta t} - 1}{\Delta t} + \alpha \frac{1 - e^{-ik_m 2\Delta x}}{2\Delta x} = 0$$

Rearranging yields

$$e^{a\Delta t} = 1 - \sigma + \sigma e^{-ik_m 2\Delta x} \quad \text{where } \sigma = \frac{\alpha \Delta t}{2\Delta x} \quad \text{which is our Courant number}$$

from this we see our amplification factor is

$$|e^{a\Delta t}| = |1 - \sigma + \sigma e^{-ikm2\Delta x}|$$

Based on this we know our function is stable if our Courant number is in the range

$$0 \leq \sigma \leq 1$$

2.1.2) Our Courant number is $\sigma = \frac{\alpha \Delta t}{2\Delta x}$

Physically this means that if a particle is travelling fast enough that it is able to travel further than half of a gridcell the solution will be unstable.

2.1.3) Here we can see the 2nd order accurate backward difference scheme of the 1st derivative using a 3 point stencil.

$$\frac{\partial a_i}{\partial x} = \frac{3a_i - 4a_{i-1} + a_{i-2}}{2\Delta x} + O(\Delta x^2)$$

We can write our discrete scheme as

$$\frac{a_i^{++1} - a_i^+}{\Delta t} + \alpha \frac{3a_i^+ - 4a_{i-1}^+ + a_{i-2}^+}{2\Delta x} = 0$$

We can apply the wavelike solution as follows.

$$a_i^+ = e^{at} e^{ikmx}$$

$$a_i^{++1} = e^{a(t+\Delta t)} e^{ikmx}$$

$$a_{i-1}^+ = e^{at} e^{ikm(x-\Delta x)}$$

$$a_{i-2}^+ = e^{at} e^{ikm(x-2\Delta x)}$$

from this we get

$$\frac{e^{a(t+\Delta t)} e^{ik_m x} - e^{at} e^{ik_m x}}{\Delta t} + \alpha \frac{3e^{at} e^{ik_m x} - 4e^{at} e^{ik_m(x-\Delta x)} + e^{at} e^{ik_m(x-2\Delta x)}}{2\Delta x}$$

Rearranging

$$\frac{e^{a\Delta t} e^{ik_m x} - e^{at} e^{ik_m x}}{\Delta t} + \alpha \frac{3e^{at} e^{ik_m x} - 4e^{at} e^{ik_m x} e^{-ik_m \Delta x} + e^{at} e^{ik_m x} e^{-2ik_m \Delta x}}{2\Delta x} = 0$$

Dividing by $e^{at} e^{ik_m x}$ we get

$$\frac{e^{a\Delta t} - 1}{\Delta t} + \alpha \frac{3 - 4e^{-ik_m \Delta x} + e^{-2ik_m \Delta x}}{2\Delta x} = 0$$

Multiplying by Δt

$$e^{a\Delta t} - 1 + \frac{\alpha \Delta t}{2\Delta x} (3 - 4e^{-ik_m \Delta x} + e^{-2ik_m \Delta x}) = 0$$

rearranging

$$e^{a\Delta t} = 1 - 3\sigma + 4\sigma e^{-ik_m \Delta x} - \sigma e^{-2ik_m \Delta x} \quad \text{where } \sigma = \frac{\alpha \Delta t}{2\Delta x}$$

Here we have an amplification factor $|e^{a\Delta t}| = |1 - 3\sigma + 4\sigma e^{-ik_m \Delta x} - \sigma e^{-2ik_m \Delta x}|$

Our Courant number is $\sigma = \frac{\alpha \Delta t}{2\Delta x}$

Our second order accurate linear advection will be stable as long as

$$0 \leq \sigma \leq 1$$

Physically this means if a particle travels fast enough that it passes half the grid cell or more in 1 time step the solution will be unstable

2.2.1) The Riemann problem occurs when using finite volume discretization. Normally with finite difference the value of the flux will be $\vec{F} = \vec{F}(\vec{u})$ but with finite volume we will have two solutions for the flux at the face. However these two solutions are expected to yield a single value for flux.

2.2.2) The advantage to the finite volume is that it is integral & as such can be used on unstructured meshes.

2.2.3) Flux upwinding is when the solution is computed from the left-hand side to the right-hand side at each interface in the domain.

2.2.4) The MUSCL scheme is a finite volume method that can provide stable & highly accurate results, even for flows with discontinuities. It is 2nd order accurate. It is able to maintain stability by extending Godunov's method with piecewise linear reconstruction of the face values resulting in an average of neighbouring cells.

2.3.1 – 2nd Order Accurate Central Differencing (20 points)

1. Add the second order accurate central two-point scheme of equation 2.1 to the script and plot its results on the same plot as the first order backward difference two-point scheme at time $t = 0.75$. (10 points).

The python code provided for the midterm was modified to add second order central differencing. This was then plotted alongside first order backward differencing, as can be seen in Figure 1.

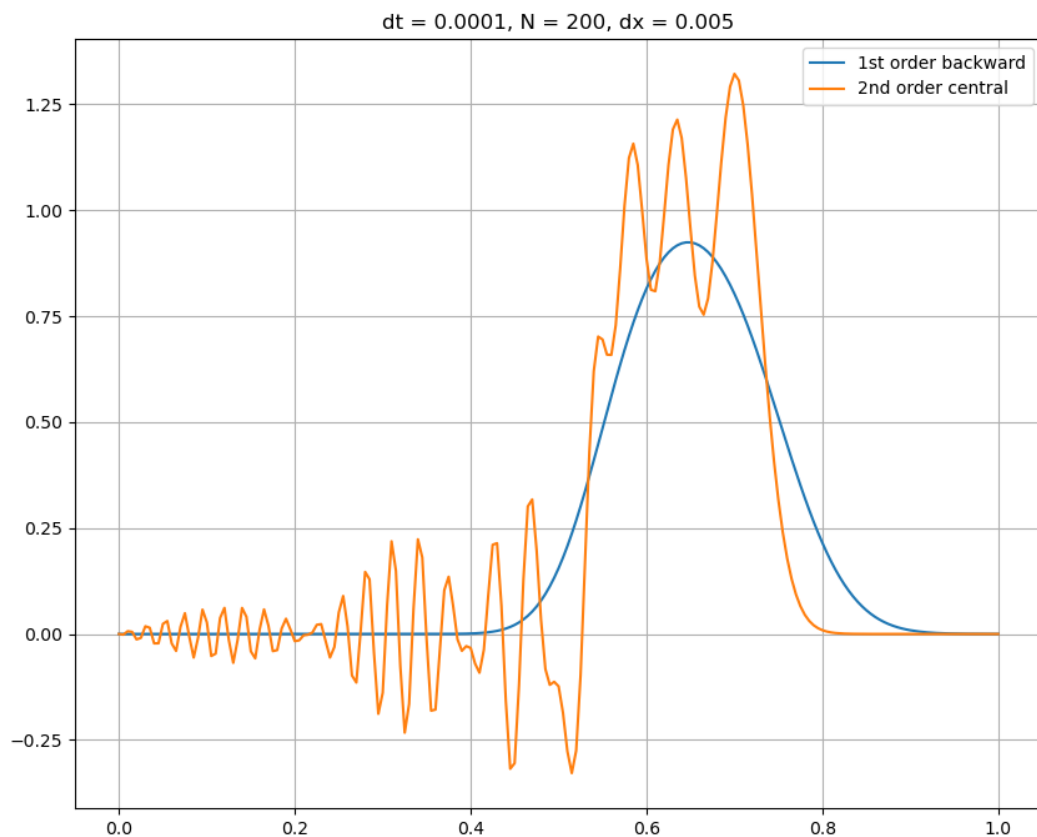


Figure 1: 2nd Order Central Vs. 1st Order Backward

2. Keeping the Courant number limitations of both schemes in mind, can you refine the time step and mesh spacing until your results stop varying at time $t = 0.75$? This is called time step and mesh independence. (10 points)

A new function was added to the code provided in the midterm which would only calculate the values for the second order central scheme. This allowed looping to be used to iteratively compare multiple time and mesh spacings. This was done by first running for a range of different mesh spacings, and then reducing the timestep until suitable results were achieved. The results can be seen in Figure 2.

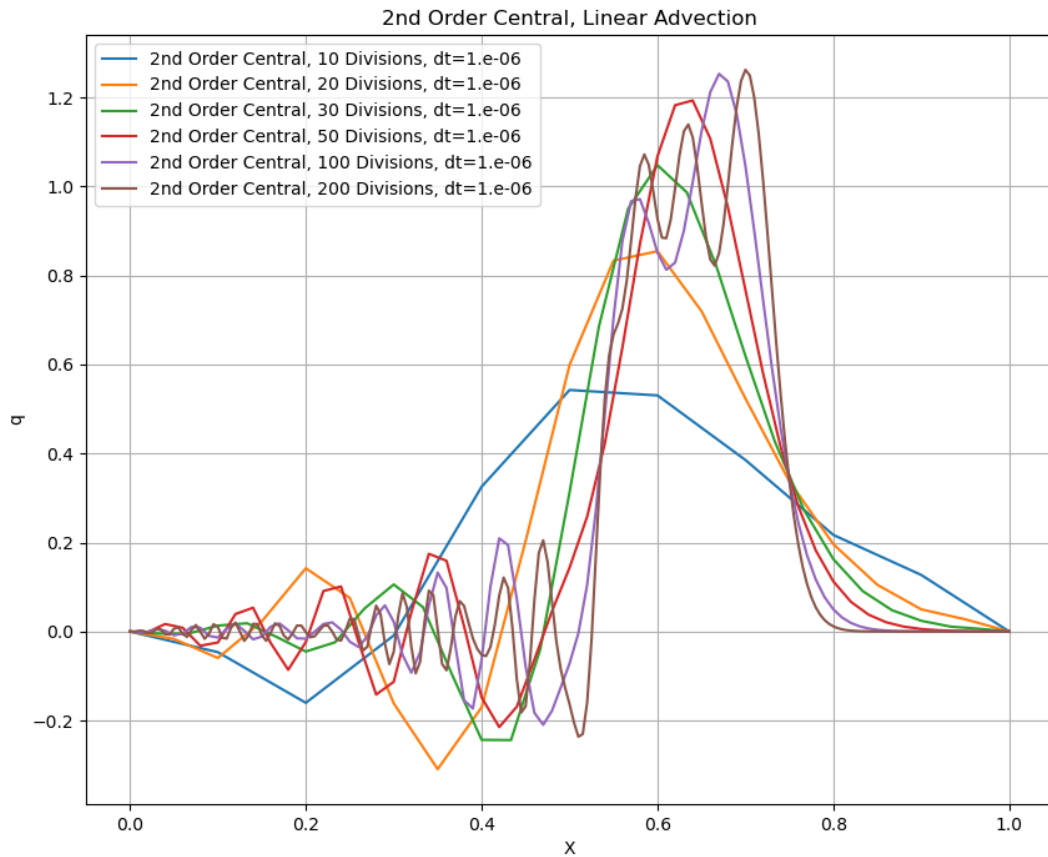


Figure 2: 2nd Order Central Mesh and Time Independence

In this case the best results were obtained with a timestep of 1e-6, and a mesh step as low as 20 divisions. With these values, the courant number is 2.5e-8. This lies within the range of values for which the central scheme is expected to be stable.

2.3.2 – 2nd Order Accurate Backward Differencing (25 Points)

1. Add the second order accurate backward three-point scheme of equation 2.2 to the script and plot its results on the same plot as the first order scheme of the first derivative at time $t = 0.75$. (10 points)

Similar to question 2.3.1.1, the provided midterm code was modified to add the second order backward differencing. These results were then plotted alongside first order backward differencing, which can be seen in Figure 3.

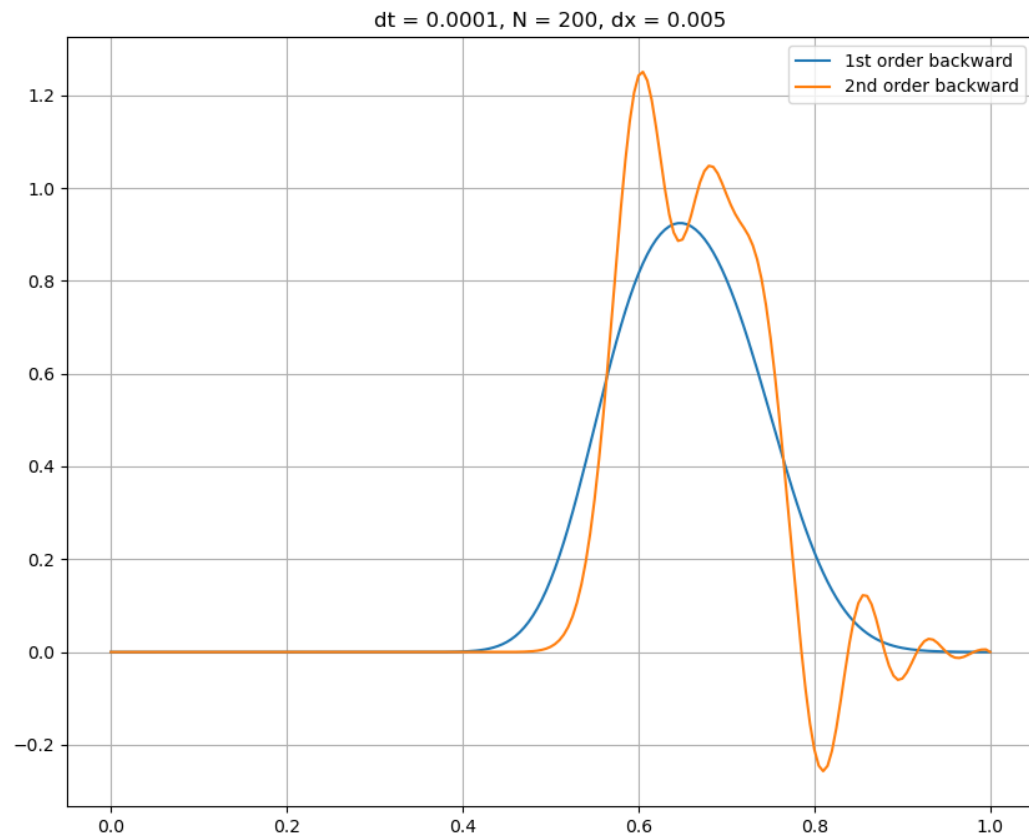


Figure 3: 2nd Order Backward Vs. 1st Order Central

2. Keeping the Courant number limitations of both schemes in mind, can you refine the time step and mesh spacing until your results stop varying at time $t = 0.75$? This is called time step and mesh independence. (10 points)

Similar to question 2.3.1.2, a separate function was created which would only calculate values for the second order central backwards. This makes it easy to loop through ranges of values and test for mesh independence and time independence. Instead of testing a variety of different timesteps in this case however, the courant number was set to be a constant value of 0.05, and the timestep was calculated based on the number of divisions and the courant number. The results were then plotted, and can be seen in Figure 4.

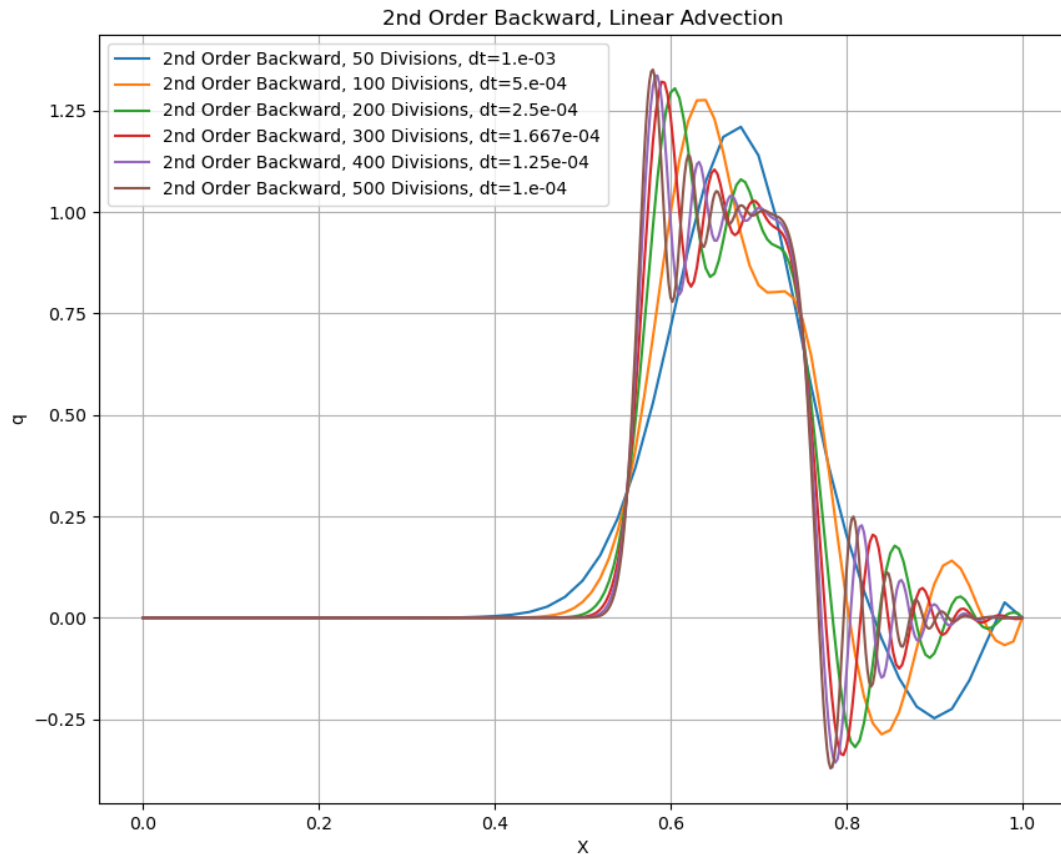


Figure 4: 2nd Order Backward Mesh and Time Independence

In this case the best results were determined to be 200 divisions. This led to a timestep of $2.5e-4$.

2.3.3 – Comparing All 3 Schemes (5 Points)

Plot the solutions of all three schemes on the same plot at time $t = 0.75$ and answer the following questions.

In order to directly compare the 3 methods, the code was run 3 times. The first time involved running the code with a timestep of $1e-4$, and 200 divisions. The code was then run again using the respective maximum timestep and number of divisions found in 2.3.1 and 2.3.2. The first order backward scheme was kept constant at 200 divisions with a timestep of $1e-4$. Finally, the code was run using the timesteps found in 2.3.1 and 2.3.2, but with 200 divisions for each scheme. The results for these can be found in Figure 5, Figure 6, and Figure 7.

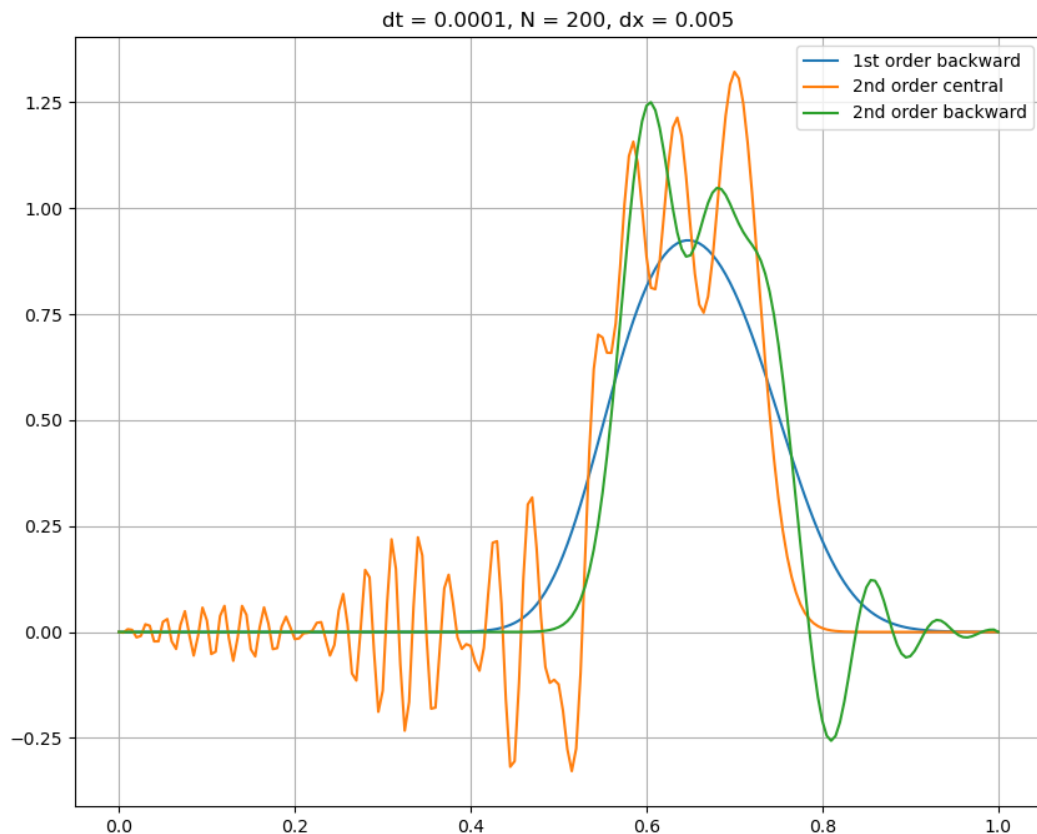


Figure 5: Comparison of all 3 schemes with $dt = 1e-4$, and 200 divisions

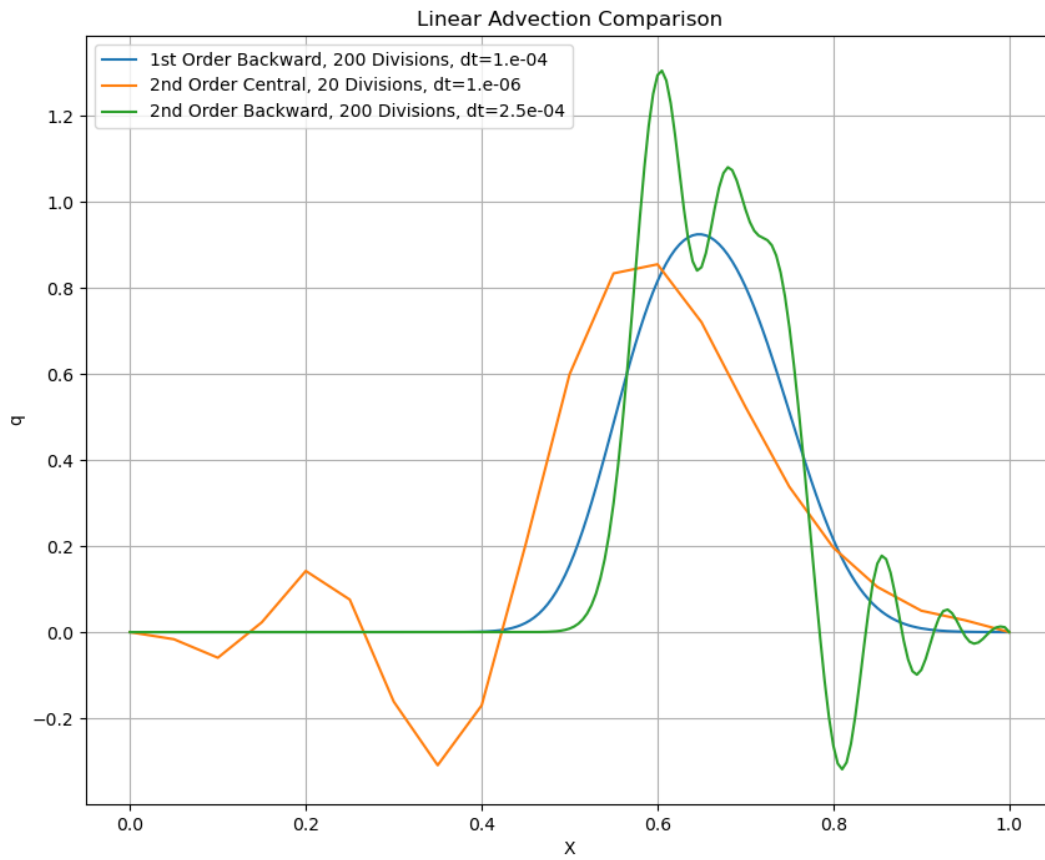


Figure 6: Comparison of all 3 schemes with ideal timestep and mesh spacing

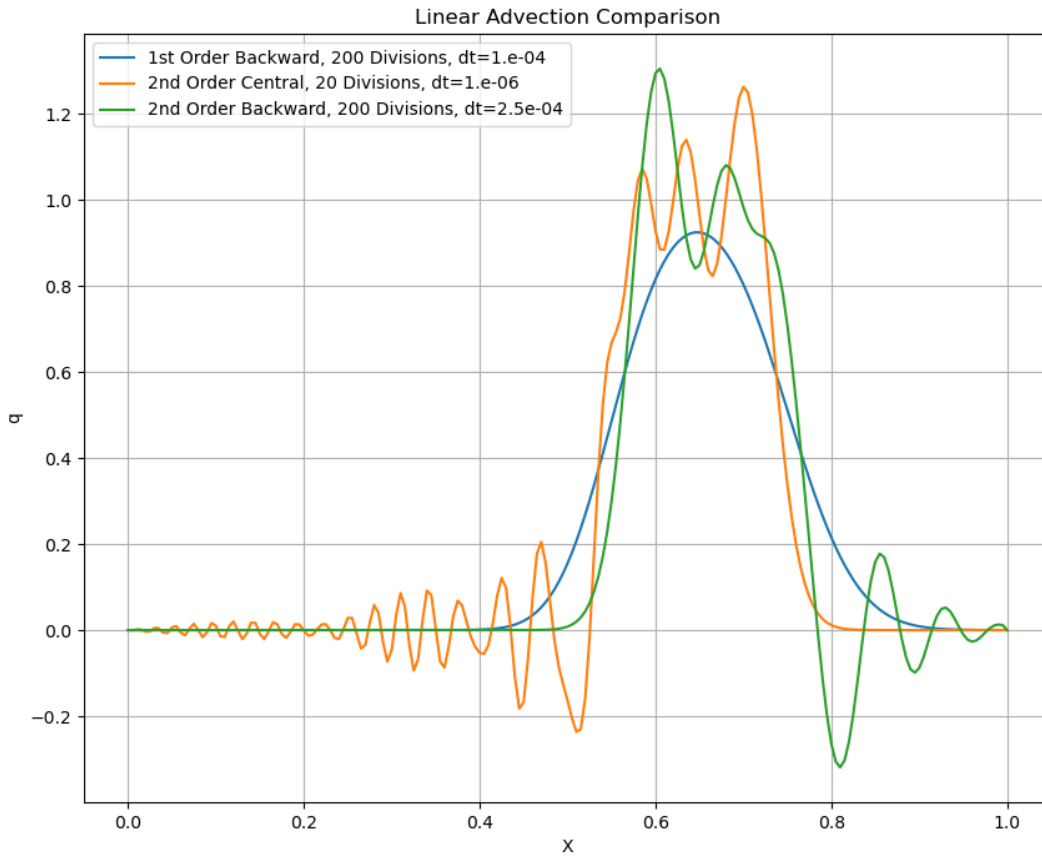


Figure 7: Comparison of all 3 schemes with ideal timestep and 200 divisions

1. Which of the 3 schemes exhibits the most oscillations and why? (2.5 points)

Referring to Figure 5, Figure 6, and Figure 7 it becomes clear that the second order central scheme exhibits the most oscillations. This is expected, as the central scheme has the highest accuracy. Both the forward and backward schemes converge linearly, while central scheme converges quadratically to the value. This can be seen when looking at the equations.

$$\frac{\partial u_i}{\partial x} = \frac{(u_i - u_{i-1})}{\Delta x} + O(\Delta x) - \text{Backward difference scheme}$$

$$\frac{\partial u_i}{\partial x} = \frac{(u_{i+1} - u_i)}{\Delta x} + O(\Delta x) - \text{Forward difference scheme}$$

$$\frac{\partial u_i}{\partial x} = \frac{(u_{i+1} - u_{i-1})}{2\Delta x} + O(\Delta x^2) - \text{Central difference scheme}$$

The central difference scheme has an order of accuracy proportional to Δx^2 , while the other two schemes only have an order of accuracy proportional to Δx . Schemes with higher of orders of accuracy are subject to higher oscillatory behaviour, and as such it is expected that the central scheme will have more oscillations. It is for this reason that a common tactic used in CFD is to run simulations initially using a lower order of accuracy scheme, and then switching to a higher order of accuracy scheme once the solution begins to converge. This allows the solution to stabilize quickly initially, while obtaining the desired accuracy afterwards.

2. Which well-known stability theorem about the order of accuracy of a stable linear scheme applies to your results? (2.5 points)

The Neumann stability analysis theory applies to the results obtained. This can be seen in the derivations obtained in questions 2.1.1 and 2.1.3.

3.1 – Bonus Problem

Modify the linear advection script from problem 2.3 by adding the following 2nd order accurate three-point central difference approximation of the second derivative,

$$\frac{\partial^2 q}{\partial x^2} = \frac{q_{i-1} - 2q_i + q_{i+1}}{\Delta x^2} + O(\Delta x^2) \quad (3.2)$$

Since the diffusion operator is a second derivative you will need to add another boundary condition at the outlet of the domain. Use a zero-gradient boundary condition, which can be implemented by setting the solution value of the last point of the domain equal to that of the preceding point. Obviously, you will not need to solve for the solution at the last point anymore. (15 points)

For the bonus problem, a new code was created which included the diffusion part described in equation 3.1 on the midterm. A 3-point 2nd order accurate central difference approximation of the second derivative was added to the linear advection equation found in question 2. This allowed for the solving of the linear advection-diffusion equation. This code will also be included in the final package handed in, and can be verified. It will be named `linear_advection_diffusion.py`.

3.2 - Using the 2nd order accurate scheme of equation 2.2 for the advection term, simulate the transport of the same step function as in problem

2.3. Keep refining the time step and mesh spacing until you reach time step and mesh independence at time $t = 0.75$. Show it by plotting the results of successive time and space refinements on the same plot and mention which time-step and mesh spacing achieved time step and mesh independence. (5 points)

The time step and mesh independence analysis were performed similarly to that which was done in question 2.3.2. That is, a function was created which would output the linear advection-diffusion results, and the courant number was set to be a constant value. In this case the courant number was set to be 0.05. The timestep was then calculated based on the courant number and the mesh spacing. Finally multiple mesh spacings were iterated through. The results can be seen in Figure 8. It can be seen that after 400 divisions with a timestep of $1.25e-4$ the results begin to converge.

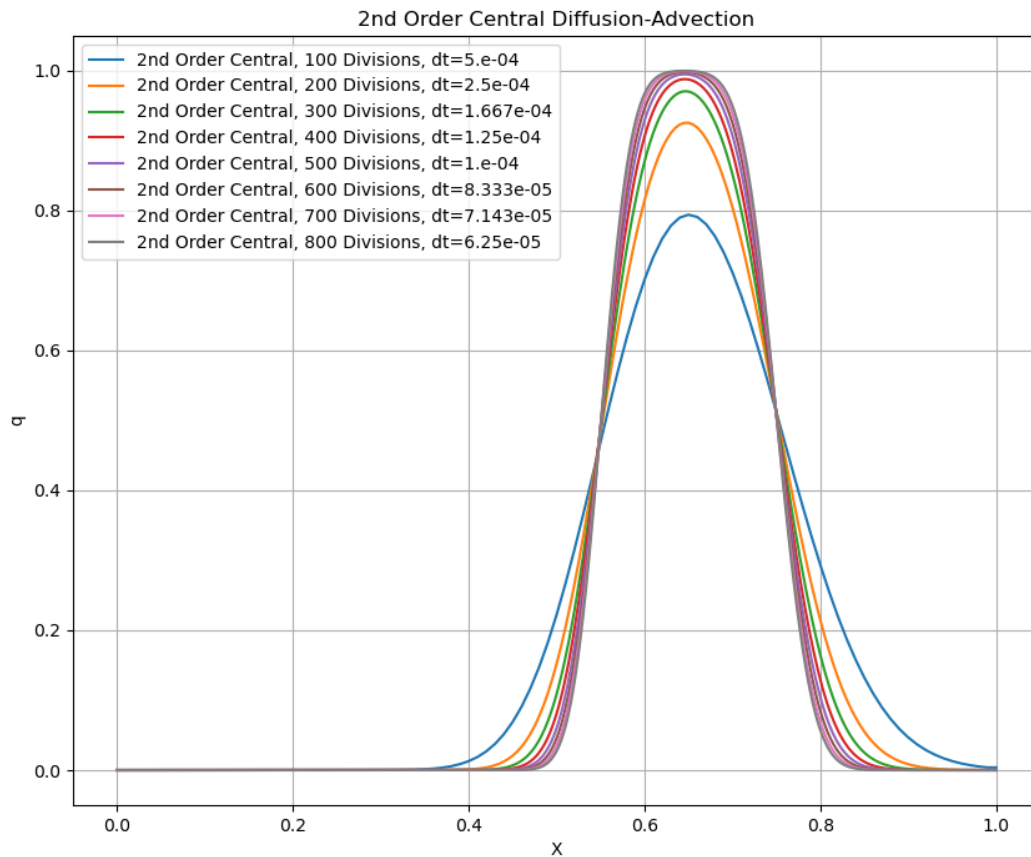


Figure 8: 2nd Order Central Diffusion-Advection

The results found in Figure 8 demonstrate the linear advection diffusion equation using a first order backward scheme for the first derivative. The same thing was coded for both the second order central scheme as well as the second order backward scheme for the second derivative. The results for this can be seen in Figure 9.

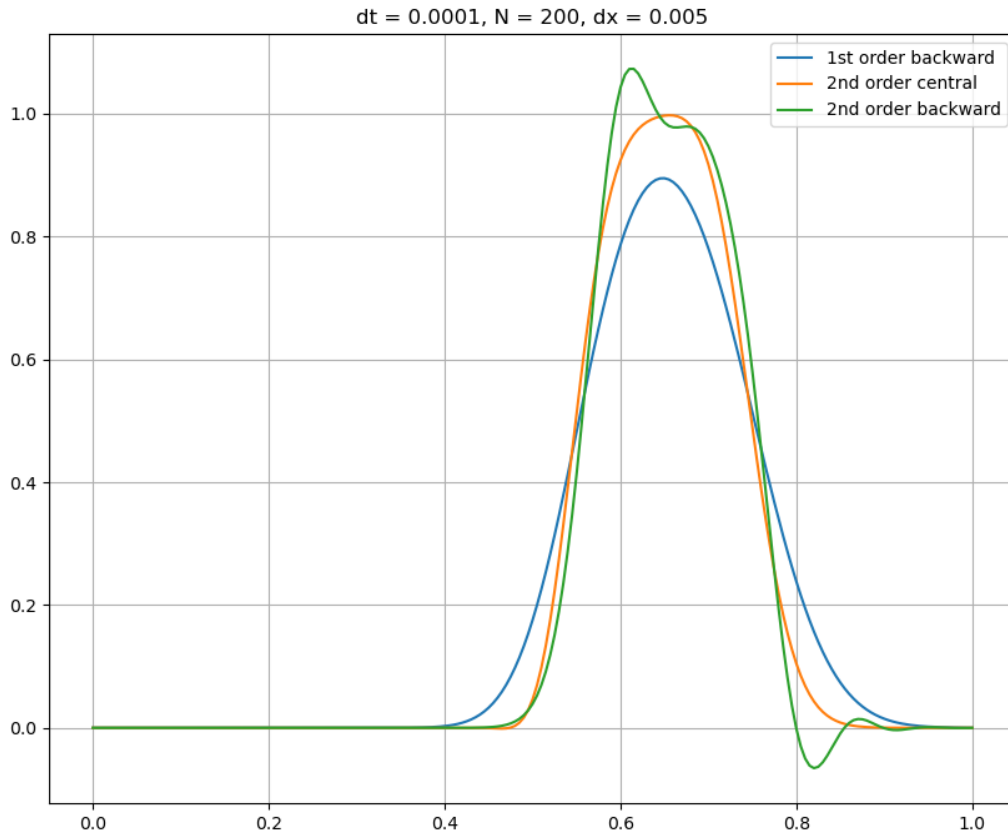


Figure 9: Linear Advection-Diffusion Comparison

3.3 - Once you have reached time step and mesh independence, run the script again for $\beta = 10^{-5}$, 10^{-4} , 10^{-2} , 10^{-1} and plot your results on the same plot for $t = 0.75$ with the baseline solution at $\beta = 10^{-3}$. (5 points)

The following plots were created for the varying beta values.

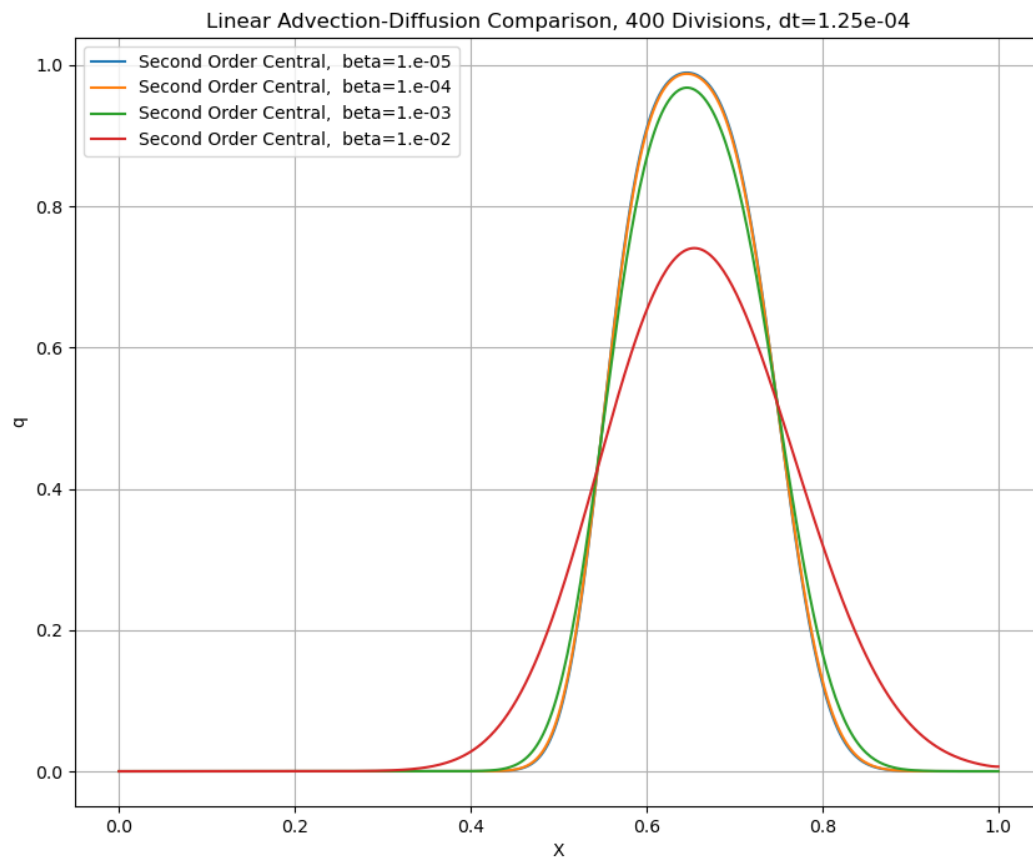


Figure 10: Beta value comparison with first order backward method for the first derivative

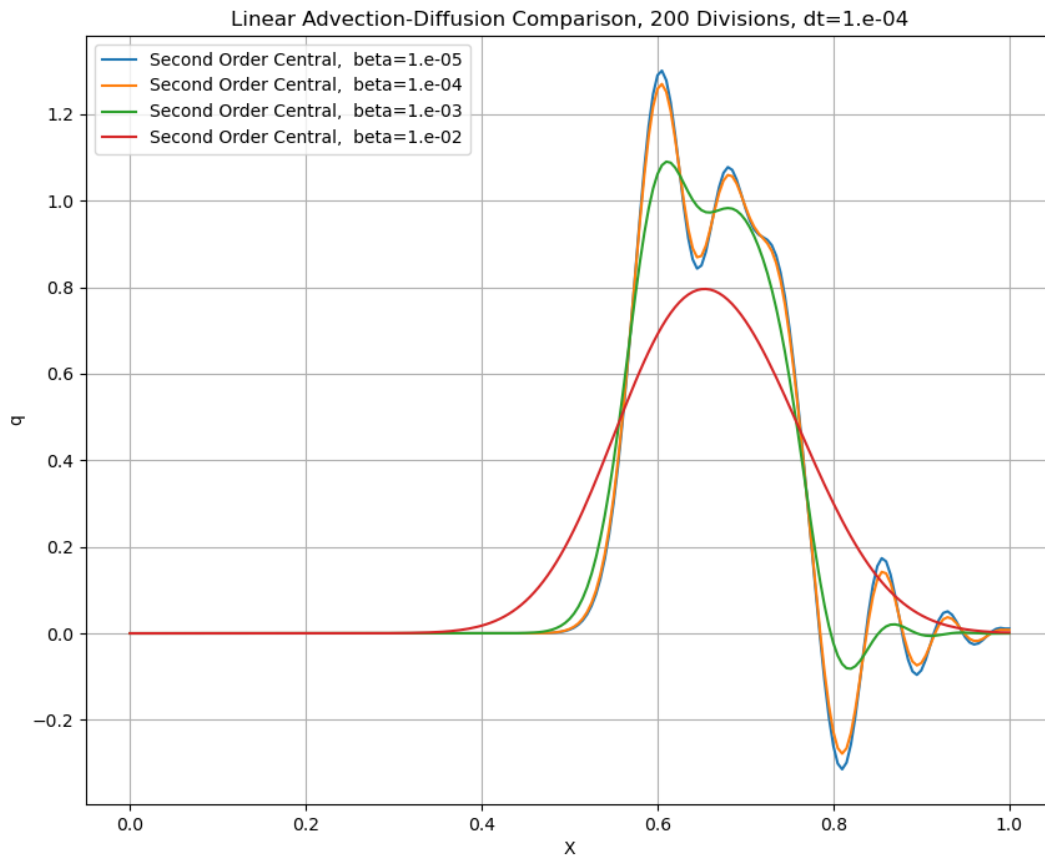


Figure 11: Beta value comparison with second order backward method for the first derivative

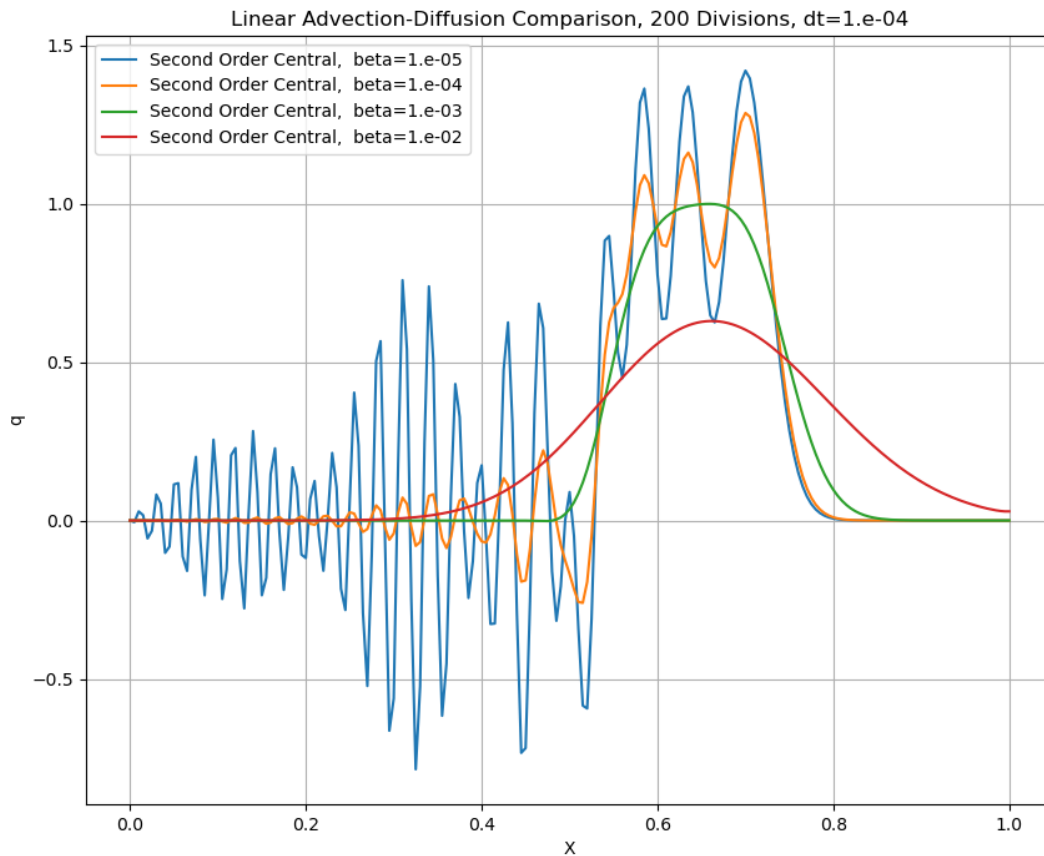


Figure 12: Beta value comparison with second order central method for the first derivative

3.4 - How do your results for each β value compare to the baseline solution at $\beta = 10^{-3}$? Which solution has the most oscillations and what do you attribute that to? (5 points)

Figure 10, Figure 11, and Figure 12 show how the results obtained with varying beta for each different method used. Each method used the second order central difference scheme for the second derivative, but varied the method used for the first derivative. Unfortunately, when beta was set to $1e-1$, the code consistently crashed. It was due to overflow, indicating the values obtained blew up with this value for beta. Overflow simply means that the values were too large to be captured by numpy. In this case, numpy double precision was used, and as such the value was outside of the range $[-1.79769313486e+308, 1.79769313486e+308]$. It is unclear as to why this occurred. However, for the results obtained the most oscillations were found with the central second order method for the first derivative, when beta was $1e-5$. It was explained in question 2.3.1 why using the

central second order method will cause the most oscillations. However, what is interesting is the fact that the diffusion coefficient changing also caused oscillations to occur. This may have occurred, as in the equation beta is the coefficient which the second derivative is multiplied by. Changing beta will change the value of what gets added for the second derivative term, and induce oscillations.