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CFD for Aerospace Applications Taylor Series and Finite Differencing

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Taylor Series and Finite Differencing

Introduction

- We have already reviewed in the previous lectures the Navier-Stokes equations that one typically solves in CFD.
- We have also studied basic potential flows and two panel methods that can be used to solve them in a fast and efficient way. However, these panel methods cannot be applied to non-potential flows.
- Generic viscous flow requires the use of more advanced methods to approximate the partial differential operators occurring in the Navier-Stokes equations.

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- Such methods include the finite element method, the finite volume method, and the earliest of them all the finite-difference method.
- Our main focus in this course is the finite volume method, which uses discrete differencing concepts from the finite-difference method.
- Therefore we need to study the finite-difference method first.
- And since the finite-difference method is based on Taylor series approximations, we will start by looking at Taylor series.
- This is all from chapter 7 in the course book by Vermeire, Pereira and Karbasian, with some minor modifications.

Taylor series

• The Taylor series, or expansion, is the direct result of Taylor's theorem, which allows approximating the value of a sufficiently smooth function at a point located at a distance Δx from another point at x, based on the value of the function and its derivatives at x.

Theorem

Let $n \ge 1$ and let f(x) be any smooth and sufficiently differentiable function, then

$$f(x + \Delta x) = f(x) + \frac{\partial f}{\partial x} \frac{\Delta x^{1}}{1!} + \frac{\partial^{2} f}{\partial x^{2}} \frac{\Delta x^{2}}{2!} + \dots + \frac{\partial^{n} f}{\partial x^{n}} \frac{\Delta x^{n}}{n!} + \dots$$
 (1)

 The Taylor series thus allows us to represent an entire smooth function based on its value and the value of its derivatives at one point. Examples

Taylor Series and Finite Differencing

- While there is no formal upper limit to the value of n it is usually sufficient to truncate the series at a finite value, leaving out terms of higher order and still retaining good accuracy.
- The order of the lowest order term left out is called the order of accuracy of the series. For example,

$$f(x + \Delta x) = f(x) + \frac{\partial f}{\partial x} \frac{\Delta x^{1}}{1!} + \frac{\partial^{2} f}{\partial x^{2}} \frac{\Delta x^{2}}{2!}$$

is a third order accurate series where the error is of order 3, proportional to $\frac{\partial^3 f}{\partial x^3} \frac{\Delta x^3}{3!}$, and formally denoted $O(\Delta x^3)$.

• For constant order we can further increase the accuracy of an expansion by reducing Δx .

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- We will demonstrate the accuracy dependence of the Taylor series on the order by expanding the function sin(x) around x = 0.
- Any high-order derivative of $f(x) = \sin(x)$ can be determined by,

$$\frac{\partial^n f}{\partial x^n} = \sin(x + n\frac{\pi}{2}). \tag{2}$$

- Therefore the function sin(x) is sufficiently smooth for $1 \le n < \infty$.
- The result of equation 2 is that even partial derivatives of sin(x) at x = 0 are equal to 0 and odd partial derivatives will alternate between 1 and -1 with a repeating pattern of period 4.

Example:

Taylor Series and Finite Differencing

• Let us denote $f_n(\Delta x)$ as the (n+1)th order Taylor expansion of $f(\Delta x)$. We have,

$$f_1(\Delta x) = \Delta x$$

$$f_3(\Delta x) = \Delta x - \frac{(\Delta x^3)}{3!}$$

$$f_5(\Delta x) = \Delta x - \frac{(\Delta x^3)}{3!} + \frac{(\Delta x^5)}{5!}$$

$$f_7(\Delta x) = \Delta x - \frac{(\Delta x^3)}{3!} + \frac{(\Delta x^5)}{5!} - \frac{(\Delta x^7)}{7!}$$

 Each of the equations above is a polynomial approximation of a sine function around x = 0 with increasing degree of accuracy.

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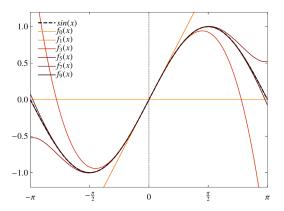


Figure 1: Taylor expansions of the sine function around x = 0 (obtained from Vermeire, Pereira and Karbasian).

• In figure 1 the polynomial approximations above are plotted together with the sine function in the interval $[-\pi,\pi]$.

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- We can make the following observations about the Taylor expansion.
- Close to x = 0 where Δx is very small all the expansions are very close to the sine function regardless of the order of accuracy.
- However, as we move away from x=0 where Δx is gradually increasing the accuracy is only retained with increasing order of the Taylor expansion.
- The highest order expansions shown, with 8th and 10th order accuracy, are practically indistinguishable from the sine function.
- These empirical observations confirm our earlier remarks about expansion accuracy depending on the size of Δx and the order of the error term.
- This concludes the Taylor expansion part of the lecture.

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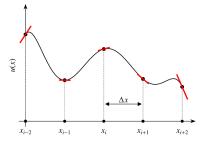


Figure 2: An arbitrary one-dimensional function (obtained from Vermeire, Pereira and Karbasian).

- Now we move to finite-difference approximations of differential operators.
- Consider an arbitrary one-dimensional function u(x) over the four consecutive intervals from x_{i-2} to x_{i+2}.

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Example:

- The index *i* increases with increasing *x* values and is used to identify points in this 1D subdivision of the *x*-axis.
- This indexed subdivision defines what is called a 1D mesh, or grid.
- It is a structured mesh because we can identify the points either by numbering them according to their location or by the index i.
- We are here looking at the approximation of u(x) over the discrete set of points x_{i-2} , x_{i-1} , x_i , x_{i+1} and x_{i+2} .
- We also have a constant grid spacing,

$$\Delta x = x_{i-1} - x_{i-2} = x_i - x_{i-1} = x_{i+1} - x_i = x_{i+2} - x_{i+1}.$$

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- Now consider the value of the function u(x) at x_i denoted $u_i = u(x_i)$.
- Using a Taylor expansion around x_i we can approximate u_{i-1} as,

$$u_{i-1} = u_i - \Delta x \frac{\partial u_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4).$$
 (3)

Similarly we can approximate u_{i+1} as,

$$u_{i+1} = u_i + \Delta x \frac{\partial u_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u_i}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4). \tag{4}$$

• We can also extract an expression for $\partial u_i/\partial x$ from equation 3 by simple manipulation,

$$\frac{\partial u_i}{\partial x} = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^3).$$
 (5)

- Note that even though we moved the error term to the other side of the equality operator we don't change its sign. This is by convention since we are only interested in the magnitude of the error, not its sign.
- Note also that as the grid spacing $\Delta x \to 0$ the terms with higher powers of Δx will tend to 0 even faster.
- In this case the Taylor approximation of the derivative at u_i truncated at order 1

$$\frac{\partial u_i}{\partial x} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x). \tag{6}$$

will converge to the actual value of the derivative as we refine.

• We can repeat the same exercise with equation 4 and get,

$$\frac{\partial u_i}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^3). \tag{7}$$

• This also leads to an approximation of $\partial u_i/\partial x$,

$$\frac{\partial u_i}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x). \tag{8}$$

- Therefore, knowing either u_{i-1} or u_{i+1} leads to an approximation of the derivative at u₁.
- We call the derivative in equation 6 a first order backward derivative since it uses u_{i-1} at the point x_{i-1} behind x_i and the error term is proportional to the first power of Δx.
- On the other hand the derivative in equation 8 is called a first order forward derivative since it uses u_{i+1} at the point x_{i+1} in front of x_i and the error term is proportional to the first power of Δx.

- The two forward and backward schemes derived here are called two-point stencils.
- The first order forward and backward derivatives are pretty robust, but they converge linearly, which is slow, to the exact value of the derivative at x_i as we decrease Δx since the error term is linear in Δx .
- Let's take an average of equations 5 and 7,

$$\frac{\partial u_i}{\partial x} = \frac{1}{2} \left(\frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} \right) +$$

$$\frac{1}{2} \left(\frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} \right) + O(\Delta x^3),$$

which leads to.

$$\frac{\partial u_i}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^3).$$

Examples

Taylor Series and Finite Differencing

The previous equation can be rewritten as,

$$\frac{\partial u_i}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2). \tag{9}$$

- Equation 9 is a second order approximation of the derivative at x_i since the error is proportional to the square of the grid spacing.
- It is called a central finite-difference derivative because the point x_i where the derivative is approximated is in the middle of the points used for the approximation, and is also a two-point stencil.
- The central derivative will converge quadratically to the exact value of the derivative as the spacing Δx is reduced since the error term is proportional to Δx^2 .
- This is much faster than linear error of the forward and backward two-point derivatives.

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Note that averaging the forward and backward derivatives gives you

$$\frac{\partial u_i}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x),$$

which is wrong since here the first order errors add up instead of canceling out.

- This is caused by our error magnitude convention which leaves out the error sign.
- Always derive schemes from the formal Taylor expansion and NOT from other schemes.

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Taylor Series and Finite Differencing

Generalization

- We have seen how to generate three finite differencing approximations for the first derivative using manipulations and truncations of the Taylor expansion, two being first order and one second order.
- Here we will generalize the previous approaches and show how to derive finite-difference approximations for derivatives and accuracy of arbitrary order.
- This will be illustrated by deriving a second-order accurate first derivative approximation using a three-point stencil at points x_i, x_{i-1} and x_{i-2}.
- The procedure will be broken down into four basic steps.

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Step 1, generating the Taylor expansion

• The Taylor expansion around x_i providing the value at x_{i-1} is given by equation 3 and we provide it here again,

$$u_{i-1} = u_i - \Delta x \frac{\partial u_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4).$$

• Similarly and keeping in mind that the distance between x_i and x_{i-2} is $2\Delta x$, the Taylor expansion around x_i providing the value at x_{i-2} is,

$$u_{i-1} = u_i - 2\Delta x \frac{\partial u_i}{\partial x} + \frac{(2\Delta x)^2}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{(2\Delta x)^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4). \quad (10)$$

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Step 2, isolating the required derivative

 We need equations for the first derivative so we move it to the LHS of equations 3 and 10, which gives us the following two equations,

$$\frac{\partial u_i}{\partial x} = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^3), \tag{11}$$

and,

$$\frac{\partial u_i}{\partial x} = \frac{u_i - u_{i-2}}{\Delta x} + \frac{2\Delta x}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{(2\Delta x)^2}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^3).$$
 (12)

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Step 3, eliminating the unnecessary error terms

- Equations 11 and 12 still have second derivatives on the RHS that are multiplied by Δx , which is first-order accurate.
- We need second-order accuracy so we need to manipulate the equations in a way that eliminates the first-order terms.
- Let's multiply equations 11 and 12 by two scalars coefficients a and b respectively.
- Judging from the multipliers of the first-order terms the only way to eliminate them would be to have,

$$a+2b=0. (13)$$

• Moreover, since we need to keep the first-order derivative $\partial u_i/\partial x$ on the LHS we also need to have,

$$a+b=1. (14)$$

• solving the system of two equations above yields a = 2 and b = -1

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Step 4, combining the equations for the final result

 Now that we have completed all the preparatory work we can just multiply equations 11 and 12 by a and b to get the final equation for the second-order accurate first derivative,

$$\frac{\partial u_i}{\partial x} = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + O(\Delta x^2). \tag{15}$$

- One thing we should point out here, and that can be verified by inspecting the three first derivative schemes with first-order accuracy as well, is that the sum of the coefficients of the point coordinates in the numerator is always zero.
- This is a check that one must always do after deriving a finite-difference scheme
- If you don't have it then your scheme is incorrect.

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- So we have just derived four finite-difference schemes for the first derivative, with varying number of points and orders of accuracy.
- We have also generalized the procedure.
- What about higher order derivatives like the Laplacian that represents the viscous diffusion in the Navier-Stokes equations?
- We will demonstrate here how to apply the generalized procedure to derive a second-order accurate scheme for the second derivative using the same three-point stencil as before.

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Taylor Series and Finite Differencing

We start again with step 1, the Taylor expansions around x_i providing the value at x_{i-1} and x_{i-2} as given by equations 3 and 10,

$$u_{i-1} = u_i - \Delta x \frac{\partial u_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4).$$

$$u_{i-1} = u_i - 2\Delta x \frac{\partial u_i}{\partial x} + \frac{(2\Delta x)^2}{2} \frac{\partial^2 u_i}{\partial x^2} - \frac{(2\Delta x)^3}{6} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^4).$$

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• Now in step 2, we rearrange the equations above to bring the second-derivative to the LHS giving us,

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{2(u_{i-1} - u_i)}{\Delta x^2} + \frac{2}{\Delta x} \frac{\partial u_i}{\partial x} + \frac{\Delta x}{3} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^2), \tag{16}$$

and

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{2(u_{i+1} - u_i)}{\Delta x^2} - \frac{2}{\Delta x} \frac{\partial u_i}{\partial x} - \frac{\Delta x}{3} \frac{\partial^3 u_i}{\partial x^3} + O(\Delta x^2). \tag{17}$$

• Note that the order of accuracy on the RHS of the equations above is now $O(\Delta x^2)$ since we divided both sides of the equations by Δx^2 .

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- Now in step 3 we need to determine the scalar coefficients a and b
 that will produce a second derivative on the LHS and eliminate the
 first and third derivatives on the RHS.
- The first condition requires that

$$a+b=1$$
,

and the second condition,

$$a-b=0$$
.

- solving the system of two equations above we readily get a = b = 1/2.
- Strictly speaking for two Taylor approximations you can use the second condition exlusively and then divide by whatever multiplier you end up with on the LHS.

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 Now in step 4 the final step, we combine equations 16 and 17 after multiplying them by a and b and get our finite-difference scheme for a second-order accurate second derivative,

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} + O(\Delta x^2).$$
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 Note that once again the sum of the coefficients of the terms in the numerator is zero. **AFRO 455**

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Summary of finite difference schemes

- Write down Taylor expansions at the points of the stencil, up to the order of accuracy desired.
- Isolate on the LHS the derivative you are interested in approximating.
- Figure out the scalar coefficients needed to eliminate the unneeded derivatives on the RHS and to retain the derivative on the LHS.
- Combine the equations after multiplying by the scalar coefficients.

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Examples

- Let us now apply what we learned in designing finite differencing schemes by discretizing three fundamental one-dimensional transport equations in partial differential form.
- These are:
 - The linear advection equation,
 - The Burgers equation,
 - The Linear diffusion equation.

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The linear advection equation

 The one-dimensional linear advection equation in partial differential form is,

$$\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} = 0. {19}$$

- Equation 19 consists of two terms:
 - The transient term $\partial u/\partial t$.
 - The advective term $\alpha \partial u/\partial x$.
- We are interested in the value of u_i as we advance in time and will get it by approximating each of these terms using the finite differencing schemes we derived earlier.
- Why is equation 19 linear?
- It is because the solution variable is not multiplied by other variables, only the constant advection velocity.

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The conservative inviscid Burgers equation

The linear diffusion

- But first we must point out that we are dealing with derivatives in t
 and x, so variations in time along the t-coordinate and in space
 along the x-coordinate.
- As far as finite differencing is concerned time is just another coordinate.
- The variation in space along the x-coordinate was shown in figure 2 and we derived our finite differencing schemes based on it.
- It implicitly assumed a constant time, where u_i and u_{i-1} are really u_i^t and u_{i-1}^t, and the ^t superscript indicates the time at which the variables are taken.
- For variation in time we do the opposite and apply the finite differencing over the t-coordinate with constant x (e.g. u_i^t , u_i^{t-1} , u_i^{t-1} , \cdots).

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The linear advection equation

The conservative inviscid Burgers equation

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- For the advective term the derivative is in x so the variation is along the x-coordinate and constant t.
- Let's apply the first-order backward difference scheme from equation 6 on the advective term.

$$\alpha \frac{\partial u_i}{\partial x} = \alpha \frac{u_i^t - u_{i-1}^t}{\Delta x} + O(\Delta x). \tag{20}$$

 For the transient term the derivative is in t so the variation is along the t-coordinate and constant x. We are moving forward in time and interested in u_i^{t+1} so let us apply the same first-order forward difference scheme from equation 8 on the transient term,

$$\frac{\partial u_i}{\partial t} = \frac{u_i^{t+1} - u_i^t}{\Delta t} + O(\Delta t). \tag{21}$$

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The linear advection

The conservative inviscid Burgers

The linear diffusion equation

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 Using equations 21 and 20 we can write the discretized form of the linear advection equation,

$$\frac{u_i^{t+1} - u_i^t}{\Delta t} + \alpha \frac{u_i^t - u_{i-1}^t}{\Delta x} + O(\Delta x, \Delta t) = 0.$$
 (22)

• Rearranging equation 22 we can write an equation approximating u_i^{t+1} ,

$$| u_i^{t+1} = u_i^t - \frac{\alpha \Delta t}{\Delta x} (u_i^t - u_{i-1}^t) + O(\Delta x, \Delta t).$$
 (23)

- Equation 23 provides an approximation of the solution at time t+1 as a function of the solution at time t, with an error term $O(\Delta x, \Delta t)$.
- Provided one knows the solution at the current time, it is then
 possible to approximate the solution at the next time step using
 equation 23 and so on...

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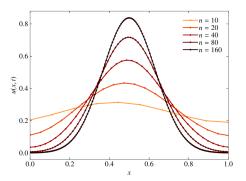


Figure 3: Finite-difference solution of the transport of a Gaussian bump using equation 23 (obtained from Vermeire, Pereira and Karbasian).

 Figure 3 shows the finite-difference solution of the transport of a Gaussian bell-shaped function, or bump, from left to right using equation 23.

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The linear advection equation

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The linear diffusion

- This example is taken from the Jupyter Python notebook in the course book and has the following initial and boundary conditions,
 - Domain length L = 1.
 - Advection speed a = 1.
 - Number of grid points n = 10, 20, 40, 80, 160.
 - Time step dt = 0.005.
 - Final time tf = 1.
- The solution is shown for several mesh sizes and increasing accuracy, clearly displaying the reduced error with reduced Δx .
- Accuracy is clearly linear when inspecting the change between successive refinements and it takes 4 levels of refinement to properly resolve the bell shape of the Gaussian function.
- It still does not look like we have reached grid independence though and we will need to refine more for that.

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The conservative inviscid Burgers equation

• We now move to a non-linear example, the conservative inviscid Burgers equation in one dimension,

$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = 0. {(24)}$$

- The conservative inviscid Burgers equation is a type of momentum transport equation used normally for flow with discontinuities.
- Let us use the same approach as we did for the linear advection equation but this time for u² as opposed to u.
- Why is equation 24 non-linear?
- It's because its advective velocity is the actual velocity variable and not a constant like α in the linear advection example.

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Taylor Series and Finite Differencing

Backward differencing for the advective term yields,

$$\frac{\partial u_i^2}{\partial x} = \frac{(u_i^t)^2 - (u_{i-1}^t)^2}{\Delta x} + O(\Delta x). \tag{25}$$

 Forward differencing for the transient term is the same as the linear advection example,

$$\frac{\partial u_i}{\partial t} = \frac{u_i^{t+1} - u_i^t}{\Delta t} + O(\Delta t). \tag{26}$$

Inserting the differencing equations obtained in the Burgers equation,

$$\frac{u_i^{t+1} - u_i^t}{\Delta t} + \frac{(u_i^t)^2 - (u_{i-1}^t)^2}{\Delta x} + O(\Delta x, \Delta t) = 0.$$
 (27)

 Yet again, we derive an approximation of the solution at the next time step as a function of the known solution at the current time step,

$$u_i^{t+1} = u_i^t - \frac{1}{2} \frac{\Delta t}{\Delta x} \left((u_i^t)^2 - (u_{i-1}^t)^2 \right) + O(\Delta x, \Delta t).$$
 (28)

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- Equation 28 is very similar in structure to equation 23, its counterpart for the linear advection equation.
- This makes sense since we used the same finite differencing.
- The difference is in the advection terms,

$$\frac{\Delta t}{\Delta x} (\alpha u_i^t - \alpha u_{i-1}^t) \quad \text{vs.} \quad \frac{1}{2} \frac{\Delta t}{\Delta x} \left((u_i^t)^2 - (u_{i-1}^t)^2 \right).$$

- In the linear advection example the advection speed is the constant α .
- In the Burgers equation the advection speed is the variable flow velocity itself.
- However, we linearized it by using $(u_i^t)^2$ and $(u_{i-1}^t)^2$ which are known constants in the next time step t+1.

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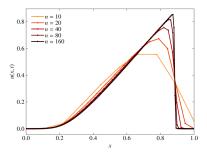


Figure 4: Finite-difference solution of the transport of a Gaussian bump using the conservative inviscid Burgers equation 28 (obtained from Vermeire, Pereira and Karbasian).

- Figure 4 shows the finite-difference solution of the transport of a Gaussian bump using equation 28.
- The solution is shown for several mesh sizes and increasing accuracy, clearly displaying the reduced error with reduced Δx .

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- Note the discontinuous shock wave-like profile introduced by the conservative inviscid Burgers equation. Why is that?
- It is because unlike the linear advection equation where the advection velocity is the constant α , the advection velocity in the Burgers equation is the variable velocity itself and gets updated at every time step.
- We end up having more advection in the flow compared to the linear advection example.
- Since there is no diffusion (Laplacian of velocity) the flow "piles up" in a shock that stays sharp.
- This is possible thanks to the conservative properties of the inviscid conservative Burgers equation.
- Note that unlike the linear advection example we have practically reached grid independence here in four refinements.

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The linear diffusion equation

- The linear diffusion equation is the final fundamental transport equation we will solve with the finite-difference method.
- It is defined as,

$$\frac{\partial u}{\partial t} - \beta \frac{\partial^2 u}{\partial x^2} = 0. {(29)}$$

- It is a transient Laplace equation.
- The diffusion coefficient β is equivalent to dissipation (of momentum, heat, mass, etc.).
- Why should it always be positive?
- We will answer this question in a couple of slides.

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- Let's follow the same steps as before to discretize equation 29 using finite differencing.
- We are dealing with a second derivative so we will use the second-order accurate finite-difference approximation of the second derivative from equation 15,

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{u_{i-1}^t - 2u_i^t + u_{i+1}^t}{\Delta x^2} + O(\Delta x^2).$$
 (30)

 The transient term is handled as before with the first-order accurate forward difference,

$$\frac{\partial u_i}{\partial t} = \frac{u_i^{t+1} - u_i^t}{\Delta t} + O(\Delta t). \tag{31}$$

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 Taking the previous two equations together we get the discretized finite-difference form of the linear diffusion equation,

$$\frac{u_i^{t+1} - u_i^t}{\Delta t} - \beta \frac{u_{i-1}^t - 2u_i^t + u_{i+1}^t}{\Delta x^2} + O(\Delta x^2, \Delta t) = 0.$$
 (32)

- Equation 32 is a finite-difference equation that is second-order accurate in space and first-order accurate in time.
- This means that the spatial error will drop faster than the transient error as we refine the mesh.
- We continue as before and derive an approximation for the solution at the next time step as a function of the solution at the current time step.

$$u_i^{t+1} = u_i^t + \frac{\beta \Delta t}{\Delta x^2} (u_{i-1}^t - 2u_i^t + u_{i+1}^t) + O(\Delta x^2, \Delta t).$$
 (33)

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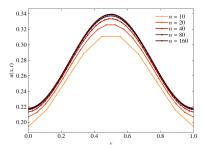


Figure 5: Finite-difference solution of the transport of a Gaussian bump using the linear diffusion equation equation 33 (obtained from Vermeire, Pereira and Karbasian).

- Note that the solution reaches grid independence in just three refinements thanks to the second-order accurate scheme in space.
- It would be even faster with second-order accuracy in time, but you
 would need the solution at time level t 2 as well.

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The linear diffusion equation

- Remember the question about why β needs to be positive? Let's answer it now.
- Diffusive transport always happens from high concentration zones to low ones, with the implication that high concentration zones will drop in concentration over time, or $u_i^{t+1} < u_i^t$.
- Take the point of maximum concentration at the middle of the curves in figure5. The concentrations at either side of the maximum are lower so the term between parentheses in equation 33 will always be negative.
- Since $\beta > 0$ we get $\frac{\beta \Delta t}{\Delta x^2} > 0$, which leads to $u_i^{t+1} < u_i^t$ and is the expected physical result.
- On the other hand, if β < 0 we end up with the a non-physical $u_i^{t+1} > u_i^t$.

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- This concludes our finite differencing lecture.
- In the next lecture we start looking at the finite volume method.