The University of British Columbia
MECH 479

# Module 3
# Taylor Series & Finite Difference Approximation

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# Taylor Series & Finite Difference Method

This module introduces finite difference methods to discretize partial differential equations. The finite difference methods work by approximating the solution of PDEs defined on a continuous domain on a grid (i.e. mesh) composed of a finite number of points. The partial derivatives in PDEs at each point are approximated from the neighborhood information via Taylor's theorem. *This module should be treated as means to transform a PDE problem into the finite difference equation (FDE) and ordinary differential equation (ODE).*

## 1 Taylor Series Expansion

Taylor series expansion is a powerful method that will allow us to construct a Finite Difference (FD) scheme to any order of accuracy that we desire. It can also be used to check the consistency of a given FD scheme. The general single variable Taylor series expansion of function $u(x)$ (expanded around $x_0$) is given as

$$u\left(x_0+\Delta x\right)=u\left(x_0\right)+(\Delta x)\left.\frac{\partial u}{\partial x}\right|_{x=x_0}+\frac{1}{2!}(\Delta x)^2\left.\frac{\partial^2 u}{\partial x^2}\right|_{x=x_0}+\frac{1}{3!}(\Delta x)^3\left.\frac{\partial^3 u}{\partial x^3}\right|_{x=x_0}+\cdots$$

Using the formulation above, we can generate FD schemes to any desired order of accuracy for derivatives of any order.

## 2 Differential and Difference Operators

1. Differential operators are *unique* designations,

$$\frac{\partial u}{\partial x},\frac{\partial^2 u}{\partial x^2},\frac{\partial u}{\partial t},\ldots$$

2. Difference operators are discretization-dependent approximations of differential operators, thus being *non-unique* and giving different (n) orders of accuracy. e.g.: in Central differencing (to n = 2 which is second order

of accuracy),

$$
\begin{aligned}
(\bar{\delta}_x U)_j &= \frac{U_{j+1} - U_{j-1}}{2\Delta x} \\
&= \left(\frac{\partial u}{\partial x}\right)_j + \frac{1}{6}\Delta x^2 \left(\frac{\partial^3 u}{\partial x^3}\right)_j + \cdots \\
&= \left(\frac{\partial u}{\partial x}\right)_j + O(\Delta x^2) + \cdots
\end{aligned}
$$

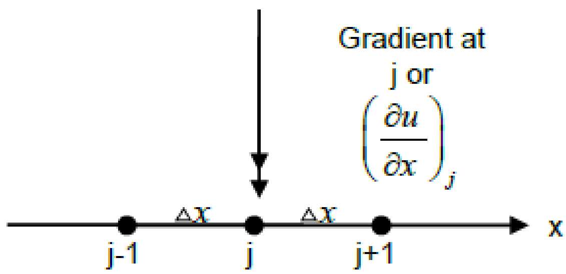
in Forward differencing (to n = 1 which is first order of accuracy),

$$
\begin{aligned}
(\vec{\delta}_x U)_j &= \frac{U_{j+1} - U_j}{\Delta x} \\
&= \left(\frac{\partial u}{\partial x}\right)_j + \frac{1}{2}\Delta x \left(\frac{\partial^2 u}{\partial x^2}\right)_j + \cdots \\
&= \left(\frac{\partial u}{\partial x}\right)_j + O(\Delta x) + \cdots
\end{aligned}
$$

in Backward differencing (to n = 1 which is first order of accuracy),

$$
\begin{aligned}
(\overleftarrow{\delta}_x U)_j &= \frac{U_j - U_{j-1}}{\Delta x} \\
&= \left(\frac{\partial u}{\partial x}\right)_j + O(\Delta x) + \cdots
\end{aligned}
$$

As shown, difference operators are *non-unique* with different (n) orders



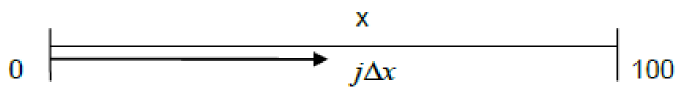

of approximation depending on the nodal points employed. In general, in order to get higher order of approximation (i.e. more accurately), one would require more nodal points for representation of the differential operator.

# 3 Generation of differencing scheme using Taylor series expansion

Let $u = u(x)$, then for small $h = \Delta x$ and $x = j\Delta x$,

$$\begin{aligned}
u(x+h) &= u(x) + \left.\frac{\partial u}{\partial x}\right|_x h + \left.\frac{\partial^2 u}{\partial x^2}\right|_x \frac{h^2}{2!} + \frac{\partial^3 u}{\partial x^3}\,|\,\frac{h^3}{3!} + \cdots \\
&= u(x) + u'(x)h + u''(x)\frac{h^2}{2!} + u'''(x)\frac{h^3}{3!} + \cdots \\
&= u_j + u_j'h + u_j''\frac{h^2}{2!} + u_j'''\frac{h^3}{3!} + \cdots
\end{aligned} \tag{1}$$

Similarly,




$$\begin{aligned}
u(x-h) =&u(x) - u'(x)h + u''(x)\frac{h^2}{2!} - u'''(x)\frac{h^3}{3!} + \cdots \\
&= u_j - u_j'h + u_j''\frac{h^2}{2!} - u_j'''\frac{h^3}{3!} + \cdots
\end{aligned} \tag{2}$$

**Adding** equations (1) and (2), we have upto second order $O(\Delta x^2)$

$$\begin{aligned}
u(x+h) + u(x-h) &= 2u(x) + h^2u''(x) + o\left(h^4\right) + \cdots \\
\therefore u''(x) &= \tfrac{1}{h^2}\{u(x+h) - 2u(x) + u(x-h)\} + o\left(h^2\right) + \ldots \\
&\equiv \tfrac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2}
\end{aligned}$$

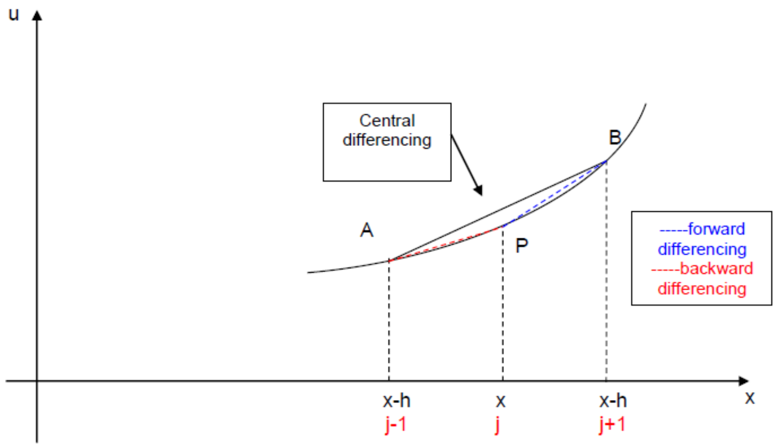
**Subtracting** equation (2) from (1), we have upto second order $O(\Delta x^2)$

$$\begin{aligned}
u'(x) &= \frac{1}{2h}\{u(x+h) - u(x-h)\} + o\left(h^2\right) + \ldots \\
&\equiv \frac{U_{j+1} - U_{j-1}}{2\Delta x}
\end{aligned}$$

The above two expressions are sometimes called the "Central Difference Approximation" to $\frac{\partial^2 u}{\partial x^2} \& \frac{\partial u}{\partial x}$. (One can perform more complex addition and subtraction with coefficients). Graphically, the central difference approximation for $\left[\frac{\partial u}{\partial x}\right]$ can be viewed as thus:

The exact gradient $\left(\frac{\partial u}{\partial x}\right)_x$ at $P$ is given by the slope $AB$, i.e.

$$\begin{aligned}
&\tfrac{u(x+h) - u(x-h)}{2h}(h \equiv \Delta x) \\
&\equiv \tfrac{U_{j+1} - U_{j-1}}{2\Delta x}
\end{aligned}$$




For forward difference approximation, the gradient $\left(\frac{\partial u}{\partial x}\right)_p$ at $P$ is given by the slope $BP$, i.e.

$$\frac{u(x+h)-u(x)}{h} \equiv \frac{U_{j+1}-U_j}{\Delta x}$$

For backward difference approximation, the gradient $\left(\frac{\partial u}{\partial x}\right)_p$ at $P$ is given by the slope $AP$, i.e.

$$\frac{u(x)-u(x-h)}{h} \equiv \frac{U_j-U_{j-1}}{\Delta x}$$

## 4 Systematic way of generating difference scheme to different orders

Taylor series expansion of functions about a fixed point provides a mean for constructing finite-difference point-operators of any order. The constructing process can be formulated as Taylor tables, which brings simplicity and ease to the calculation.

Suppose we are interested in obtaining the difference operator for $\frac{\partial u}{\partial x}$ up to order $\mathrm{O}(\Delta x)^p$ with function values $U_{j-n}\cdots, U_{j-1}, U_j, U_{j+1}, \cdots, U_{j+n}$. The idea is to determine values of $\alpha_{-n}, \cdots, \alpha_{-1}, \alpha_0, \alpha_1, \cdots \alpha_n$ such that

$$U_j' + \alpha_{-n}U_{j-n}\cdots + \alpha_{-1}U_{j-1} + \alpha_0 U_j + \alpha_1 U_{j+1} + \cdots + \alpha_n U_{j+n} = O(\Delta x^p)$$

$U_j'-$ Difference operator for the approximation of differential operator $\frac{\partial u}{\partial x}$ to have minimum truncation error $O(\Delta x^p)^*$
That is, to express $U_j'$ in terms of function value at nodal points. To do so, we need to expand $U_{j-1}, U_j, U_{j+1}, \ldots$ about $U_j$ with Taylor expansion and present them in a table; see below.
Adding up in each column, we have

$$\text{LHS} = \text{RHS1} + \text{RHS2} + \text{RHS3} + \text{RHS4} + \ldots$$

| | | $U_j$ | $U_j'$ | $U_j''$ | $U_j'''$ | ...... |
|---|---|---|---|---|---|---|
| $U_j'$ | = | 0 | 1 | 0 | 0 | |
| $\alpha_{-1}U_{j-1}$ | = | $\alpha_{-1}$ | $-\Delta x\alpha_{-1}$ | $\frac{\Delta x^2}{2}\alpha_{-1}$ | $-\frac{\Delta x^3}{6}\alpha_{-1}$ | |
| $\alpha_0 U_j$ | = | $\alpha_0$ | 0 | 0 | 0 | |
| $\alpha_1 U_{j+1}$ | = | $\alpha_1$ | $\Delta x\alpha_1$ | $\frac{\Delta x^2}{2}\alpha_1$ | $\frac{\Delta x^3}{6}\alpha_1$ | |
| LHS | = | RHS1 + | RHS2 + | RHS3 + | RHS4 + … | |

where

$$
\begin{aligned}
LHS &= U_j' + \textstyle\sum_{k=-1}^{k=1} \alpha_k U_{j+k} \\
RHS1 &= \left[\alpha_{-1} + \alpha_0 + \alpha_1\right] U_j \\
RHS2 &= \left[1 + \Delta x \alpha_{-1} + \Delta x \alpha_1\right] U_j' \\
RHS3 &= \left[\tfrac{1}{2}\Delta x^2 \left(\alpha_{-1} + \alpha_1\right)\right] U_j'' \\
RHS4 &= \tfrac{\Delta x^3}{6}\left(\alpha_1 - \alpha_{-1}\right) U_j'''
\end{aligned}
$$

Now we seek to make as many as possible RHS (starting from the lowest order of $\Delta x$ to higher order , i.e., from the left or $1^{\text{st}}$ column and progressing towards the right) to vanish by appropriate choices of $\alpha_k$. Let's say that we have only 3 unknowns $\alpha_{-1}, \alpha_0, \alpha_1$ hence we can set three equations of $RHS$ equal to zero (starting from $1^{\text{st}}$ column ), i.e.

$$
\begin{aligned}
RHS1 &= 0 \\
RHS2 &= 0 \\
RHS3 &= 0
\end{aligned}
$$

and hence 3 independent equations with 3 unknowns $(\alpha_k)$. Expanding or re-arranging, we therefore have

$$
\begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_{-1} \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{1}{\Delta x} \\ 0 \end{pmatrix}
$$

Solving, we obtain

$$
\begin{aligned}
\alpha_{-1} &= \tfrac{1}{2\Delta x} \\
\alpha_0 &= 0 \\
\alpha_1 &= -\tfrac{1}{2\Delta x}
\end{aligned}
$$

and the first non-zero term on the right hand side, $RHS4 = -\frac{\Delta x^2}{6} U_j'''$. Substituting back, we get

$$
U_j' - \frac{1}{2\Delta x}\left(U_{j+1} - U_{j-1}\right) = -\frac{1}{6}\Delta x^2 U_j''' + \ldots
$$

The error terms on the RHS $\frac{1}{6}\Delta x^2 U_j''' + \ldots$. are referred to as truncation error. The lowest order error term, i.e. the leading error term $\frac{1}{6}\Delta x^2 U_j'''$ (which gives the maximum error given $\Delta x$ is a small value) indicate the order of accuracy for the difference approximation $U_j'$ (or the order $p$ of approximation ). Hence

$$U_j' = \frac{U_{j+1} - U_{j-1}}{2\Delta x} + O(\Delta x)^2$$

i.e. $p = 2$ as worked out*. In general, more nodal points which also means more $\alpha'$s can be used eliminated the RHS, thus giving higher order approximation of the differential operator.
The term $O(\Delta x^2)$ with $p = 2$ is therefore $2^{nd}$ order accurate central finite difference representation for $\left(\frac{\partial u}{\partial x}\right)_j$. Of course, using the same method, we can construct a $2^{nd}$ order *one-sided* (i.e. setting $k$ either to the right or left of $j$) finite difference approximation for $\left(\frac{\partial u}{\partial x}\right)_j$ and others.
In this one-sided approximation case (with nodal points on the right of $U_j$ ), we set

$$U_j' + \beta U_j + \beta_1 U_{j+1} + \beta_2 U_{j+2} + \ldots = O(\Delta x)^p$$

That is we set all the nodal points to be on one side of $U_j$ and proceed as before. Note that in the above example, on the LHS the index for u is greater or equal to j.
Similarly, we set the nodal points to be on the opposite one side of $U_j$. such that:

$$U_j' + \beta U_j + \beta_1 U_{j-1} + \beta_2 U_{j-2} + \ldots = O(\Delta x)^p$$

Or we can even set the nodal points to be non-symmetrical about the $U_j$ with nodal points to the left and right, and we would obtain different type and orders of representation for $U_j'$.

# 5 Another approach to (general) discretization

Assume that we have $u$ values at each mesh point. We want to approximate the $n$ -th order derivative $\left(u^{(n)} \equiv \frac{d^n u}{dt^n}\right)$ of the function with $p$ -th order accuracy $\left(O\left(\Delta x^p\right)\right)$ using a Taylor expansion.

Suppose we have function values $u(x), u(x + \Delta x_1), u(x + \Delta x_2), \cdots$ For generality, we assume that the mesh spacing is non-uniform, i.e.

$$\Delta x_2 \neq 2\Delta x_1, \Delta x_n \neq n\Delta x_1$$

To begin with, we expand $u\left(x + \Delta x_1\right)$ at $u\left(x\right)$:

$$u(x + \Delta x_1) = u(x) + u^{(1)}\Delta x_1 + \cdots + \frac{1}{n!}u^{(n)}(\Delta x_1)^n + \cdots + \frac{1}{(n+p-1)!}u^{(n+p-1)}(\Delta x_1)^{n+p-1} + O(\Delta x_1)^{n+p}$$

Rearranging all the terms on one side of the equation and multiplying the equation with $\frac{n!}{(\Delta x_1)^n}$, we have:

$$n!\frac{u(x)-u(x+\Delta x_1)}{(\Delta x_1)^n}+\cdots+u^{(n)}+\frac{n!}{(n+p-1)!}u^{n+p-1}(\Delta x_1)^{p-1}+O((\Delta x_1)^p)=0$$

It can be shown from the above equations that, in order to have $p$ -th order of accuracy for the approximation of $u^{(n)}$, $u\left(x+\Delta x_1\right)$ should be expanded to the term $\frac{1}{(n+p-1)!}u^{(n+p-1)}(\Delta x_1)^{(n+p-1)}$ with the truncation error of $O\left(\Delta x_1^{n+p}\right)$

The equation can be viewed as an algebraic equation:

$$c_1+c_2u^{(1)}+\cdots+c_{n+p}u^{(n+p-1)}=O((\Delta x_1)^p). \tag{3}$$

It has $(n+p-1)$ unknowns namely $u^{(1)},u^{(2)},u^{(3)},\cdots,u^{(n+p-1)}$. As a result, we need $(n+p-1)$ equations to close the system. In other words, we need $(n+p-1)$ **neighbouring points** to be expanded by Taylor series. After the system has been closed, eliminate all the unknowns except for $u^(n)$ with the Gaussian elimination to form the finite difference scheme. We proceed to study a few examples.

**Case 1:**

$n=1\Rightarrow\frac{\partial u}{\partial x}$ and $p=1\Rightarrow O(\Delta x)$. Hence $(n+p-1)=1$. The Taylor series expansion is then

$$\begin{aligned}
&u(x+\Delta x)=u(x)+u^{(1)}\cdot\Delta x+O\left(\Delta x^2\right)\\
&u^{(1)}=\tfrac{u(x+\Delta x)-u(x)}{\Delta x}+\tfrac{O\left(\Delta x^2\right)}{\Delta x}\\
&\tfrac{\partial u}{\partial x}\Big|_i=\tfrac{u(x+\Delta x)-u(x)}{\Delta x}+O(\Delta x)
\end{aligned}$$

This FD scheme is known as explicit forward Euler scheme.

**Case 2:**

$n=1\Rightarrow\frac{\partial u}{\partial x}$ but $p=2\Rightarrow O\left(\Delta x^2\right)$ so $(n+p-1)=2$.

We need 2 Taylor series expansion this time

$$\begin{aligned}
&u(x+\Delta x)=u(x)+u^{(1)}\cdot\Delta x+1/2!u^{(2)}\cdot(\Delta x)^2+O\left(\Delta x^3\right)\\
&u(x-\Delta x)=u(x)-u^{(1)}\cdot\Delta x+1/2!u^{(2)}\cdot(\Delta x)^2+O\left(\Delta x^3\right)\\
&\Rightarrow\tfrac{\partial u}{\partial x}\Big|_i=\tfrac{u(x+\Delta x)-u(x-\Delta x)}{2\Delta x}+O\left(\Delta x^2\right)
\end{aligned}$$

This FD scheme is known as central difference scheme or leapfrog scheme. If the mesh spacing is uniform, using $(n+p-1)$ neighbouring points may generate a scheme with $(p+1)^{th}$ order of accuracy.

For example, $n=2\Rightarrow\frac{\partial^2 u}{\partial x^2}$ and $p=1\Rightarrow O(\Delta x)$. Hence $(n+p-1)=2$. As above, we need 2 Taylor expansions.

$$\begin{aligned}
u(x+\Delta x)&=u(x)+u^{(1)}\cdot\Delta x+1/2!u^{(2)}\cdot(\Delta x)^2+1/3!u^{(3)}\cdot(\Delta x)^3+O\left(\Delta x^4\right)\\
u(x-\Delta x)&=u(x)-u^{(1)}\cdot\Delta x+1/2!u^{(2)}\cdot(\Delta x)^2-1/3!u^{(3)}\cdot(\Delta x)^3+O\left(\Delta x^4\right)
\end{aligned}$$

We add the 2 equations to obtain

$$\frac{\partial^2 u}{\partial x^2}\Big|_i=\frac{u(x+\Delta x)-2u(x)+u(x-\Delta x)}{(\Delta x)^2}+O\left(\Delta x^2\right)$$

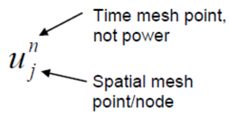
If $i$ happens to be the boundary point, the neighbouring point is no longer symmetric about the local point. Instead we have,

$$u(x+\Delta x) = u(x) + u^{(1)} \cdot \Delta x + 1/2! u^{(2)} \cdot (\Delta x)^2 + O\left(\Delta x^3\right)$$
$$u(x+2\Delta x) = u(x) + u^{(1)} \cdot (2\Delta x) + \frac{1}{2!} u^{(2)} \cdot (2\Delta x)^2 + O\left(\Delta x^3\right)$$
$$\Rightarrow \left.\frac{\partial^2 u}{\partial x^2}\right|_i = \frac{u(x) - 2u(x+\Delta x) + u(x+2\Delta x)}{(\Delta x)^2} + O(\Delta x)$$

The Taylor series expansion can also be used to determine the order of accuracy of a given FD scheme, or whether an FDE is consistent to the PDE or not. For example, say the PDE of interest is $\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$ which can describe diffusion. The FD scheme we are going to use is called Dufort-Frankel scheme and is given as

$$u_j^{n+1} = u_j^{n-1} + \frac{2\nu\Delta t}{\Delta x^2}\left[u_{j-1}^n - \left(u_j^{n+1} + u_j^{n-1}\right) + u_{j+1}^n\right]$$

The usual convention we will be using is




That is, the superscript of $u$ denotes the time mesh point while the subscript denotes spatial mesh point. Using Taylor series to expand the terms $u_j^{n+1}, u_j^{n-1}, u_{j-1}^n$ and $u_{j+1}^n$ about point $\left(x = x_j, t = t_n\right)$ and substituting them into the FD scheme gives an equivalent PDE as follows

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2} - v\left(\frac{\Delta t}{\Delta x}\right)^2 \frac{\partial^2 u}{\partial t^2} + O\left(\Delta t^2\right) + O\left(\Delta x^2\right)$$

We find that in general, this is not consistent with our original diffusion PDE since

$$\lim_{\Delta t, \Delta x \to 0} \frac{\Delta t}{\Delta x} \neq 0$$

However, if we choose $\Delta t = c\Delta x^2$ where $c$ is some constant, then

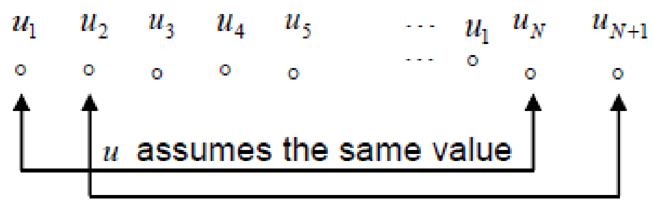
$$\lim_{\Delta t, \Delta x \to 0} \frac{\Delta t}{\Delta x} = \lim_{\Delta t, \Delta x \to 0} c\Delta x = 0$$

For a general case, even though the FDE has shown to be not consistent with the equivalent PDE, the FDE can be stable as long as the truncation error is small.

# 6 Boundary Conditions for Spatial Discretization

There are 3 common types of Boundary Conditions which are

1. *Dirichlet* - function $u$ is given at boundary points which may or may not depend on time.
2. *Neumann* - the spatial derivative of function $\frac{\partial u}{\partial x}$, is given at boundary points.
3. *Periodic* - function $u$ is to repeat itself again and again after certain fixed spatial dimension.




A less common type is the mixed boundary condition (also known as Robin boundary condition). For example

$$u(x = 2\pi) = u_0 + \left.\frac{\partial u}{\partial x}\right|_{x=2\pi} = 0$$

# 7 FDE for 1-D diffusion equation

Consider the generation of FDE of the 1 -D diffusion equation

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2}, \quad x \in [0, \pi]$$

First, we divide the interval $x \in [0, \pi]$ into equal segments of $\Delta x$ with $N = M + 2$ total number of grid points. Therefore, $\Delta x = \frac{\pi}{M+1} = \frac{\pi}{N-1}$ and the coordinates of the grid points are $x_j = (j)\Delta x$ where $j = 0, 1, \ldots, M + 1$ Next, we generate the FDE using truncated Taylor series

$$\begin{aligned}
u_j &= u(x_j) \\
u_{j+1} &= u(x_j + \Delta x) = u_j + \Delta x u_j^{(1)} + \frac{\Delta x^2}{2!}u_j^{(2)} + \frac{\Delta x^3}{3!}u_j^{(3)} + \cdots \\
u_{j-1} &= u(x_j - \Delta x) = u_j - \Delta x u_j^{(1)} + \frac{\Delta x^2}{2!}u_j^{(2)} - \frac{\Delta x^3}{3!}u_j^{(3)} + \cdots
\end{aligned}$$

We can then approximate $u_j^{(2)} \equiv \frac{\partial^2 u}{\partial x^2}$ by appropriate linear combination of $u_j$ $u_{j+1}$ and $u_{j-1}$ with an error term, $\varepsilon$.

$$u_j^{(2)} + \varepsilon = au_{j-1} + bu_j + cu_{j+1}$$

Or course, if we wish to have $\varepsilon \to 0$ then we will need an infinite order of terms. We choose the coefficients $a, b$ and $c$ to eliminate $u_j$ and $u_j^{(1)}$. Finally, we obtain

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j + \varepsilon = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} = u_j^{(2)} + \underbrace{\frac{\Delta x^2}{12} u_j^{(4)} + O\left(\Delta x^4\right)}_{=\varepsilon}$$

So, $\varepsilon \in O\left(\Delta x^2\right)$ and $\varepsilon \to 0$ as $\Delta x \to 0$

(Convince yourself this is the case; hint $a = c = 1/\Delta x^2, b = -2/\Delta x^2\Big)$

The above FD scheme for the $2^{\text{nd}}$ derivative $u_j^{(2)} = \frac{\partial^2 u}{\partial x^2}$ is sometimes called the 3-point central difference scheme, yielding
$\left(\frac{\partial u}{\partial t}\right)_j = \frac{v}{\Delta x^2}\left(u_{j-1} - 2u_j + u_{j+1}\right) + O\left(\Delta x^2\right)$ for $j = 1, 2, \ldots, M$ (interior points)

The boundary condition is either $u$ or $\frac{\partial^2 u}{\partial x^2}$ at $j = 0, M+1$ It should be noted that the use of FDE necessarily implied that we are actually solving

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2} - \frac{\Delta x^2}{12} u_j^{(4)} + \cdots$$

which suggests a discretization error of $O\left(\Delta x^2\right)$

**Truncation Error**

To discretize the temporal and spatial derivatives, the finite difference approach is discussed earlier. As a result, a PDE is approximated by a finite difference equation (FDE). We can then define truncation error (TE) as

$$TE = PDE - FDE$$

The truncation error is an intrinsic error in any numerical method whereas the round-off error comes from finite precision arithmetic.

**Consistency**

A finite difference representation of a PDE is said to be consistent if

$$\lim_{\text{mesh}\to 0} \text{TE} = \lim_{\text{mesh}\to 0} \text{PDE} - \text{FDE} = 0$$

**Order of accuracy (OOA)**

This term refers to the order of the truncation error. For example, if we consider the FD corresponding to the first derivative of the function $u(x)$ i.e. $\frac{\partial u}{\partial x}$, using **backward** difference, where

$$\frac{\partial u}{\partial x} \approx \frac{u_i - u_{i-1}}{\Delta x}$$

then

$$\text{TE} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2}(\Delta x)$$

Hence, the OOA of the backward difference method is 1, i.e. O($\Delta x$).
If we use **central** difference instead, where

$$\frac{\partial u}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

then

$$\text{TE} = \frac{1}{6}\frac{\partial^3 u}{\partial x^3}(\Delta x)^2$$

The OOA of the central difference method is 2, i.e. O($\Delta x^2$).Furthermore, the OOA of a PDE takes the lowest OOA of each derivative approximation. For example if we have

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2}$$

Say we use backward difference method for the $\frac{\partial u}{\partial t}$ term where OOA is 1 and we use the central difference for the $\frac{\partial^2 u}{\partial x^2}$ term (with OOA = 2), then the OOA of the whole PDE is equal to 1.

**Stability**

A stable FD scheme means that any error that arises from sources such as round-off, truncation or mistakes are not permitted to grow in the sequence of numerical computation. Basically, stability involves the actual solution and exact solution of an FDE.

**Convergence**

The solution to the FDE should approach the true solution of the PDE (provided they have the same initial and boundary conditions) as the mesh is refined. The determination of convergence involves exact solutions of PDE and FDE. Usually, it is very difficult to show that an FD scheme would or would not converge at all since the exact solution to the PDE is not known. This difficulty can be removed by using Lax's equivalence theorem: *For a linear, well-posed initial value problem, a consistent FD approximation is convergent if and only if it is stable.* With this theorem, we only need to prove that an FD method is stable to guarantee convergence. Although Lax's equivalence theorem is only proven for linear initial value problems, it has been widely applied to nonlinear and boundary value/initial-boundary value problems in engineering.

# 8 Formulation of FDE in terms of Matrices

We can write out the above FDE at each interior point where $j$ =1,2,$\cdots$,M.

$$\frac{du_1}{dt} = \frac{v}{\Delta x^2}\left(u_0 - 2u_1 + u_2\right)$$
$$\frac{du_2}{dt} = \frac{v}{\Delta x^2}\left(u_1 - 2u_2 + u_3\right)$$
$$\frac{du_M}{dt} = \frac{v}{\Delta x^2}\left(u_{M-1} - 2u_M + u_{M+1}\right)$$

In matrix form, we have

$$\frac{d}{dt}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{M-1} \\ u_M \end{bmatrix} = \frac{v}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & \\ 0 & 1 & -2 & \ddots \\ 0 & & \ddots & 1 \\ 0 & 1 & -2 & \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{M-1} \\ u_M \end{bmatrix} + \begin{bmatrix} \frac{v}{\Delta x^2}u_0 \\ 0 \\ \vdots \\ 0 \\ \frac{v}{\Delta x^2}u_{M+1} \end{bmatrix}$$

Let $\vec{u} = \begin{bmatrix} u_1 & u_2 & \cdots & u_{M-1} & u_M \end{bmatrix}^T$ and $\overrightarrow{BC} = \begin{bmatrix} \frac{v}{\Delta x^2}u_0 & 0 & \cdots & 0 & \frac{v}{\Delta x^2}u_{M+1} \end{bmatrix}^T$.
The size of matrix $\mathbf{A}$ is $M$ by $M$. The difference form of the equation becomes

$$\frac{d\vec{u}}{dt} = \mathbf{A}\vec{u} + \overrightarrow{BC}$$

We have managed to convert a continuous PDE, $\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2}$ into a semidiscrete equation, $\frac{d\vec{u}}{dt} = \mathbf{A}\vec{u} + \overrightarrow{BC}$
We shall see that expressing finite difference schemes in vector-matrix forms is essential to subsequent analysis be it a finite difference, finite element, finite volume or spectral method schemes. All of them can be expressed in matrix form and the analysis /evaluation follows similar procedure.

# 9 Summary

We have seen that finite difference discretization converts PDE into a coupled set of ODE. For example, the model equation for linear convection is $\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$ and can be approximated by a coupled set of ODE given as

$$\frac{d\vec{u}}{dt} = -\frac{c}{2\Delta x}[B(-1,0,1)\vec{u} + \overrightarrow{BC}] + O\left(\Delta x^2\right)$$

where Dirichlet boundary condition have been imposed. For periodic boundary condition, the coupled ODE becomes

$$\frac{d\vec{u}}{dt} = -\frac{c}{2\Delta x}\left[B_p(-1,0,1)\vec{u}\right] + O\left(\Delta x^2\right)$$

Note that there is no boundary condition vector. We show another example which is the diffusion equation, $\frac{\partial u}{\partial t} = \nu\frac{\partial^2 u}{\partial x^2}$. We have for Dirichlet and periodic boundary conditions respectively

$$\begin{aligned} \frac{d\bar{u}}{dt} &= \frac{\nu}{\Delta x^2}[B(1,-2,1)\vec{u} + \overrightarrow{BC}] + O\left(\Delta x^2\right) \\ \frac{d\vec{u}}{dt} &= \frac{\nu}{\Delta x^2}\left[B_p(1,-2,1)\bar{u}\right] + O\left(\Delta x^2\right) \end{aligned}$$

Thus far, we have only used 3 points FD scheme for spatial discretization of $\frac{\partial u}{\partial x}$ and $\frac{\partial^2 u}{\partial x^2}$ where we have obtained banded matrices that are tridiagonal. If we use more mesh points to generate higher order FD scheme, we will increase the band width of the matrices. In all cases, if spatial discretization is only applied to PDE, keeping the time derivative continuous, the PDE is converted to

$$\frac{d\vec{u}}{dt} = \mathbf{A}\vec{u} + \overrightarrow{BC} + O\left(\Delta x^p\right) \longleftrightarrow \text{ Error term of order } p$$

which is a coupled set of ODEs. The discrete FD form of the Euler equations and Navier-Stokes equations are composed of aforementioned basic discrete FD forms.