FUNDAMENTALS OF THE FINITE DIFFERENCE METHOD

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OUTLINE

Generalities

Basic concepts and techniques in the formulation of Finite-Difference (FD herafter):

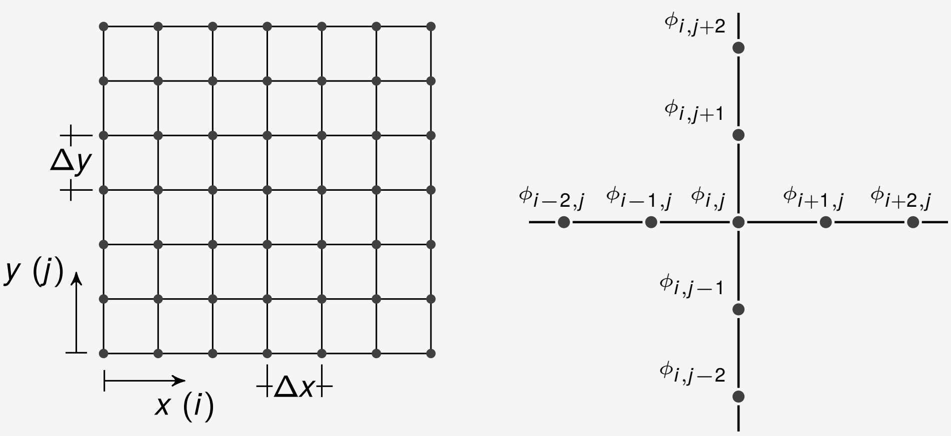
- The most fundamental statement of conservation principles, like e.g. mass, energy, momentum, et., applies to a fixed quantity of matter;
- From that, it is possible to develop conservation statements applicable to both a fixed region in space and at a point, in the limit of a vanishing volume;
- The conservation statement applicable to a point appears as a *Partial Differential Equation* (PDE) and the statement for a fixed region in space as an equation involving *integrals*;
- In the *finite difference* - FD - formulation, the continuous problem domain is discretized, so that the dependent variables are considered to exist only at discrete points:
  - The FD method is based on the properties of Taylor (Maclaurin) expansions and on the definition of derivatives.
  - The PDE form of the conservation principle is converted to an algebraic equation by approximating derivatives as *differences*.
- In the *finite volume* - FV - methodology, the continuous problem domain is divided up into regions called control volumes (CV):
  - The dependent variables are considered to exists at a specified location within the volumes or on the boundaries of the volumes;
  - The integrals in the conservation statement are approximated algebraically.
- For both methods - FD and FV - a problem involving calculus has been transformed into an algebraic problem.

The Finite Difference Method, E. Nobile | Introduction | Generalities and notation

Definition and notation

In order to establish a finite difference procedure for solving a PDE, we need to replace the continuous problem domain with a finite difference *grid* or *mesh*:

- As an example, suppose we wish to solve a PDE for which $\phi(x, y)$ is the dependent variable in the 2D (two-dimensional) square domain $0 \leq x \leq 1$, $0 \leq y \leq 1$.
- We establish a grid on the domain by replacing $\phi(x, y)$ by $\phi(i\Delta x, j\Delta y)$, as illustrated in the figure.



- Points on the grid can be easily located according to the values of i and j, so difference equations are usually written in terms of the general point (i, j) and its neighbors.

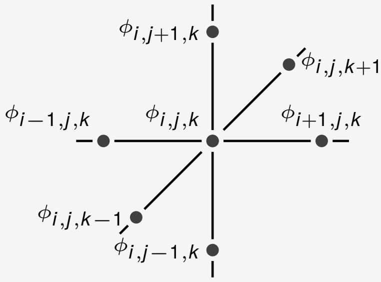
Definition and notation - cont.

Thus, if we think of $\phi_{i,j}$ as $\phi(x_0, y_0)$, then:

$$\begin{aligned}
\phi_{i+1,j} &= \phi(x_0 + \Delta x, y_0) \\
\phi_{i-1,j} &= \phi(x_0 - \Delta x, y_0) \\
\phi_{i,j+1} &= \phi(x_0, y_0 + \Delta y) \\
\phi_{i,j-1} &= \phi(x_0, y_0 - \Delta y) \\
\phi_{i+2,j} &= \phi((x_0 + 2\Delta x, y_0) \\
&\ldots\ldots
\end{aligned}$$

For 3D problems we would have:

$$\begin{aligned}
\phi_{i+1,j,k} &= \phi(x_0 + \Delta x, y_0, z_0) \\
\phi_{i,j+1,k} &= \phi(x_0, y_0 + \Delta y, z_0) \\
\phi_{i,j,k+1} &= \phi(x_0, y_0, z_0 + \Delta z) \\
&\ldots\ldots
\end{aligned}$$



For *marching problems*, e.g. time-dependent problems, the variation of the marching coordinate is usually indicated by a superscript, such as $\phi_{i,j}^{n+1}$, rather than a subscript.

Many different finite-difference formulations are possible for any given PDE (Partial Differential Equation), according to:

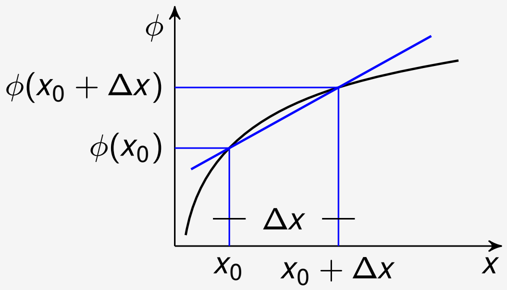
- Accuracy
- Economy (computational costs)
- Simplicity (implementation/programming).

Definition of derivative

Definition of derivative

$$\frac{\partial \phi}{\partial x} = \lim_{\Delta x \to 0} \frac{\phi(x_0 + \Delta x, y_0) - \phi(x_0, y_0)}{\Delta x} \tag{1}$$

Here, if ϕ is continuous, it is expected that $[\phi(x_0 + \Delta x, y_0) - \phi(x_0, y_0)]/\Delta x$ will be a reasonable approximation to $\partial \phi / \partial x$ for a sufficiently small, but finite, Δx.



Mean-value theorem: the difference representation is *exact* for some point within the Δx interval.

Developing a Taylor series expansion:

$$\begin{aligned}
\phi(x_0 + \Delta x, y_0) = \phi(x_0, y_0) + \left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!} \\
+ \ldots + \left(\frac{\partial^{n-1} \phi}{\partial x^{n-1}}\right)_0 \frac{(\Delta x)^{n-1}}{(n-1)!} + \left(\frac{\partial^n \phi}{\partial x^n}\right)_\xi \frac{(\Delta x)^n}{(n)!} \qquad x_0 \le \xi \le (x_0 + \Delta x)
\end{aligned} \tag{2}$$

where the last term can be identified as the *remainder*, and the subscript 0 indicates (x_0, y_0).

Forward difference

We can now form the *forward difference* by rearranging the previous equation (2):

$$\left(\frac{\partial \phi}{\partial x}\right)_{(x_0,y_0)} = \frac{\phi(x_0+\Delta x, y_0) - \phi(x_0,y_0)}{\Delta x} - \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)}{2!} - \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^2}{3!} - \dots \quad (3)$$

Switching to the index notation:

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} + \text{T.E} \quad (4)$$

Truncation Error

The difference between the partial derivative and its finite difference representation is the *truncation error*, or TE for short.

We can characterize the limiting behavior of the T.E. by using the order of (O) notation:

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} + O(\Delta x)$$

When the T.E. is written as $O(\Delta x)$, it means that

$$\|T.E.\| \leq K\|\Delta x\|$$

for $\Delta x \to 0$ (sufficiently small Δx), and K is a positive real constant.

Truncation error

- In practical terms, the order of the T.E. is found to be Δx raised to the largest power that is common to all terms of the T.E.
- More general definition of the O notation:
  - When we say $f(x) = O[\phi(x)]$, we mean that there exists a positive constant K, independent of x, such that:

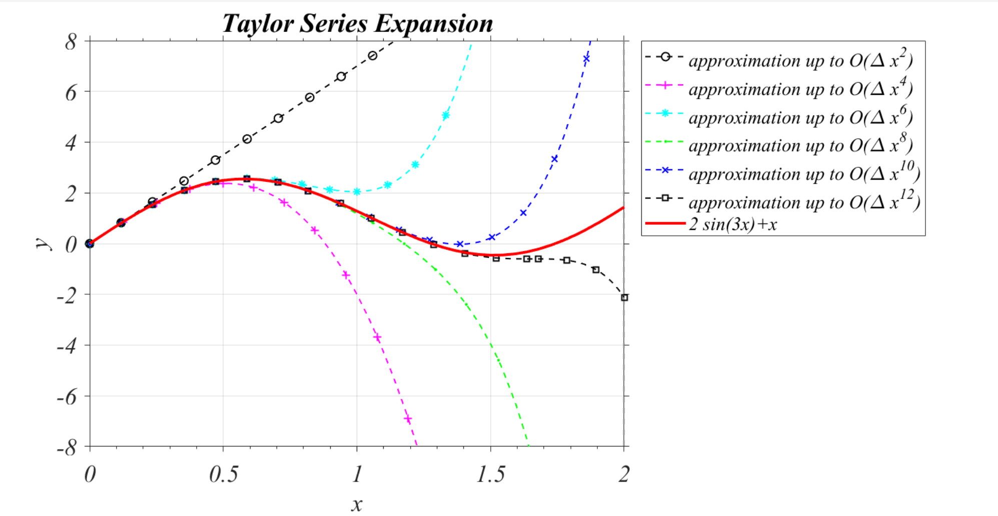
    $$|f(x)| \leq K\,|\phi(x)| \quad \forall\, x \in S$$

    where f and ϕ are real or complex functions defined in S. For finite difference applications, we restrict S by $x \to 0$, i.e. sufficiently small x.
- Note that $O(\Delta x)$ does not say anything about the *size* of the T.E., but rather *how* it behaves as Δx tends towards zero.
- If another finite difference expression had a $T.E. = O((\Delta x)^2)$, we might expect, or hope, that the T.E. of this second representation would be smaller than the previous one for a convenient Δx, but we could only be *sure* that this would be true if we refined the mesh *sufficiently*:
  - *Sufficiently* is a quantity that is extremely difficult to estimate, since it is very case-dependent.

A remark on Taylor expansions

The Taylor expansion, eq. (2), has several important implications:

- The *left-hand side* (lhs) is the value of the function ϕ at an arbitrary distance Δx from point x_0, with *no restriction* on Δx.
- In the *right-hand side* (rhs), all quantities are evaluated at point x_0: it means that we can know the value of the function at *arbitrary distance* from point x_0, if we know all the derivatives at this *single point* x_0.
- In practical terms, it is possible to evaluate the function at a point $x_0 + \Delta x$, with a given accuracy, from the knowledge of a *finite* number of derivatives at point x_0.



The Finite Difference Method, E. Nobile | Finite Differences

Backward and central difference

- An infinite number of difference representations can be found for $(\partial\phi/\partial x)_{i,j}$.
- For example we can expand *backward*:

$$
\begin{aligned}
\phi(x_0 - \Delta x, y_0) = \phi(x_0, y_0) - \left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!} \\
- \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!} + O((\Delta x)^4)
\end{aligned}
\tag{5}
$$

and obtain the *backward difference* representation:

$$
\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} + O(\Delta x) \tag{6}
$$

Backward and central difference - cont.

- We can subtract eq. (5) from eq. (2):

$$\phi(x_0+\Delta x, y_0) - \phi(x_0-\Delta x, y_0) = \cancel{\phi(x_0,y_0)} - \cancel{\phi(x_0,y_0)} + \left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x + \left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x$$
$$+ \cancel{\left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!}} - \cancel{\left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!}} + \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!} + \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!} + \dots \quad (7)$$

- Rearranging we obtain the *central difference* representation:

$$\left(\frac{\partial \phi}{\partial x}\right)_{(x_0,y_0)} = \frac{\phi(x_0+\Delta x, y_0) - \phi(x_0-\Delta x, y_0)}{2\Delta x} + O((\Delta x)^2)$$

and in index notation:

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta x} + O((\Delta x)^2) \quad (8)$$

- Since the T.E. of a first order FD formula is proportional to the second derivative, as seen from eq. (3), it results that a first order FD approximation is *exact* for a linear function.
- Similarly, a second order formula has its T.E. proportional to the third derivative - see eq. (7) - and therefore it is exact for a quadratic function.

Second derivative

- We can also add equations (5) and (2) and rearrange to obtain an approximation to the second derivative:

$$\phi(x_0+\Delta x, y_0) + \phi(x_0-\Delta x, y_0) = \phi(x_0,y_0) + \phi(x_0,y_0) + \cancel{\left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x} - \cancel{\left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x}$$
$$+ \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!} + \cancel{\left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!}} - \cancel{\left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!}} + O((\Delta x)^4)$$

- Rearranging and in index notation:

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{(\Delta x)^2} + O((\Delta x)^2) \quad (9)$$

- It should be emphasized that these are only a few examples of the possible ways in which first and second derivatives can be approximated.

Forward and Backward difference operators

- First forward-difference of $\phi_{i,j}$ with respect to x at point i, j, Δ_x:

$$\boxed{\Delta_x \phi_{i,j} = \phi_{i+1,j} - \phi_{i,j}} \qquad (10)$$

and thus

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\Delta_x \phi_{i,j}}{\Delta x} + O(\Delta x)$$

Similarly:

$$\Delta_y \phi_{i,j} = \phi_{i,j+1} - \phi_{i,j}$$
$$\left(\frac{\partial \phi}{\partial y}\right)_{i,j} = \frac{\Delta_y \phi_{i,j}}{\Delta y} + O(\Delta y)$$

- First backward-difference of $\phi_{i,j}$ with respect to x at point i, j, ∇_x:

$$\boxed{\nabla_x \phi_{i,j} = \phi_{i,j} - \phi_{i-1,j}} \qquad (11)$$

It follows

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\nabla_x \phi_{i,j}}{\Delta x} + O(\Delta x)$$

Central difference, averaging and identity operators

- Central difference operators $\overline{\delta}$, δ and δ^2:

$$\overline{\delta_x} \phi_{i,j} = \phi_{i+1,j} - \phi_{i-1,j} \qquad (12)$$
$$\delta_x \phi_{i,j} = \phi_{i+1/2,j} - \phi_{i-1/2,j} \qquad (13)$$
$$\begin{aligned} \delta_x^2 \phi_{i,j} &= \delta_x(\delta_x \phi_{i,j}) = \delta_x(\phi_{i+1/2,j} - \phi_{i-1/2,j}) \\ &= (\phi_{i+1,j} - \phi_{i,j}) - (\phi_{i,j} - \phi_{i-1,j}) \\ &= \phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j} \end{aligned} \qquad (14)$$

- Averaging operator μ:

$$\boxed{\mu_x \phi_{i,j} = \frac{\phi_{i+1/2,j} + \phi_{i-1/2,j}}{2}} \qquad (15)$$

- Identity operator I:

$$\boxed{I \phi_{i,j} = \phi_{i,j}} \qquad (16)$$

Shift and derivative operators

- Shift operator E:

$$E_x^{+1}\phi_{i,j} = E_x\phi_{i,j} = \phi_{i+1,j} \quad (17)$$
$$E_x^{-1}\phi_{i,j} = \phi_{i-1,j} \quad (18)$$
$$E_y\phi_{i,j} = \phi_{i,j+1} \quad (19)$$

where the superscript, if it is equal to $+1$, is usually omitted.
It also follows that:

$$E_x^{+2}\phi_{i,j} = \phi_{i+2,j}$$
$$E_x^{+1/2}\phi_{i,j} = \phi_{i+1/2,j}$$
$$E_x^{+n}\phi_{i,j} = \phi_{i+n,j}$$

- Derivative operator D:

$$D_x\phi_{i,j} = \left(\frac{\partial \phi}{\partial x}\right)_{i,j} \quad (20)$$

All these operators satisfy the commutative, associative and distributive laws satisfied by real or complex numbers.

Finite Difference operators relations

- We say that two operators are *equal* when both produce the same result when applied to any function for which both operations are defined.
- With this understanding, it follows immediately that:

$$\Delta_x = (E_x - I) \quad (21a)$$
$$\nabla_x = (I - E_x^{-1}) \quad (21b)$$
$$\delta_x = E_x^{1/2} - E_x^{-1/2} \quad (21c)$$

- Other useful relations are of the form:

$$\Delta_x = E_x^{1/2}\delta_x = E_x\nabla_x \quad (22a)$$
$$\delta_x = E_x^{1/2}\nabla_x = E_x^{-1/2}\Delta_x \quad (22b)$$
$$\nabla_x = E_x^{-1/2}\delta_x = E_x^{-1}\Delta_x \quad (22c)$$
$$\nabla_x\Delta_x = \Delta_x\nabla_x = \Delta_x - \nabla_x = \delta_x^2 \quad (22d)$$
$$\mu_x = \frac{1}{2}(E_x^{1/2} + E_x^{-1/2}) \quad (22e)$$

- Any of the difference operators taken to a given power n, is interpreted as n repeated actions of this operator, e.g.:

$$\Delta_x^2 = \Delta_x\Delta_x = E_x^2 - 2E_x + 1 \quad (23a)$$
$$\Delta_x^3 = (E_x - I)^3 = E_x^3 - 3E_x^2 + 3E_x - 1 \quad (23b)$$

Finite Difference operators relations - cont.

Let's prove eq. (22a)

$$\begin{aligned}
E_x \nabla_x \phi_{i,j} &= E_x(\phi_{i,j} - \phi_{i-1,j}) \\
&= \phi_{i+1,j} - \phi_{i,j} \\
&= \Delta_x \phi_{i,j}
\end{aligned}$$

$$\begin{aligned}
E_x^{1/2} \delta_x \phi_{i,j} &= E_x^{1/2}(\phi_{i+1/2,j} - \phi_{i-1/2,j}) \\
&= \phi_{i+1,j} - \phi_{i,j} \\
&= \Delta_x \phi_{i,j}
\end{aligned}$$

Finite Difference operators relations - cont.

Let's prove eq. (22d)

$$\begin{aligned}
\nabla_x \Delta_x \phi_{i,j} &= \nabla_x(\phi_{i+1,j} - \phi_{i,j}) \\
&= \phi_{i+1,j} - \phi_{i,j} - \phi_{i,j} + \phi_{i-1,j} \\
&= \phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j} \\
&= \delta_x^2 \phi_{i,j}
\end{aligned}$$

$$\begin{aligned}
\Delta_x \nabla_x \phi_{i,j} &= \Delta_x(\phi_{i,j} - \phi_{i-1,j}) \\
&= \phi_{i+1,j} - \phi_{i,j} - \phi_{i,j} + \phi_{i-1,j} \\
&= \delta_x^2 \phi_{i,j}
\end{aligned}$$

$$\begin{aligned}
(\Delta_x - \nabla_x)\phi_{i,j} &= \phi_{i+1,j} - \phi_{i,j} - \phi_{i,j} + \phi_{i-1,j} \\
&= \delta_x^2 \phi_{i,j}
\end{aligned}$$

Finite Difference operators relations - cont.

- Difference representations can be indicated by using combinations of E and I as, for example:

$$\Delta_x \phi_{i,j} = (E_x - I)\phi_{i,j} = \phi_{i+1,j} - \phi_{i,j}$$

- The specific operators defined for certain common central differences are convenient, although two of them can be expressed in terms of first difference operators:

$$\begin{aligned} \overline{\delta_x}\phi_{i,j} &= \Delta_x \phi_{i,j} + \nabla_x \phi_{i,j} \\ &= \phi_{i+1,j} - \phi_{i,j} + \phi_{i,j} - \phi_{i-1,j} \\ &= \phi_{i+1,j} - \phi_{i-1,j} \end{aligned} \tag{24}$$

$$\begin{aligned} \delta_x^2\phi_{i,j} &= \Delta_x \phi_{i,j} - \nabla_x \phi_{i,j} \\ &= \phi_{i+1,j} - \phi_{i,j} - \phi_{i,j} + \phi_{i-1,j} \\ &= \phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j} \end{aligned} \tag{25}$$

$$\begin{aligned} \delta_x^2\phi_{i,j} &= \Delta_x \nabla_x \phi_{i,j} \\ &= \nabla_x \phi_{i+1,j} - \nabla_x \phi_{i,j} \\ &= \phi_{i+1,j} - \phi_{i,j} - \phi_{i,j} + \phi_{i-1,j} \\ &= \phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j} \end{aligned} \tag{26}$$

Finite Difference operators relations - cont.

- Using the newly defined operators, the central difference representation for the first partial derivative can be written as:

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta x} + O[(\Delta x)^2] = \frac{\overline{\delta_x}\phi_{i,j}}{2\Delta x} + O[(\Delta x)^2] \tag{27}$$

- The central difference representation for the second partial derivative can be written as:

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{(\Delta x)^2} + O[(\Delta x)^2] = \frac{\delta_x^2\phi_{i,j}}{(\Delta x)^2} + O[(\Delta x)^2] \tag{28}$$

- Higher order forward and backward difference operators are defined recursively as:

$$\Delta_x^n \phi_{i,j} = \Delta_x(\Delta_x^{n-1}\phi_{i,j}) \tag{29}$$

$$\nabla_x^n \phi_{i,j} = \nabla_x(\nabla_x^{n-1}\phi_{i,j}) \tag{30}$$

Finite Difference operators relations - cont.

Forward second-order derivative approximation:

$$\frac{\Delta_x^2 \phi_{i,j}}{(\Delta x)^2} = \frac{\Delta_x(\phi_{i+1,j} - \phi_{i,j})}{(\Delta x)^2} = \frac{\phi_{i+2,j} - 2\phi_{i+1,j} + \phi_{i,j}}{(\Delta x)^2} = \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} + O(\Delta x)$$

Finite Difference operators relations - cont.

Backward third-order derivative approximation:

$$\frac{\nabla_x^3 \phi_{i,j}}{(\Delta x)^3} = \frac{\nabla_x(\nabla_x^2 \phi_{i,j})}{(\Delta x)^3} = \frac{\nabla_x \nabla_x(\phi_{i,j} - \phi_{i-1,j})}{(\Delta x)^3} = \frac{\nabla_x(\phi_{i,j} - 2\phi_{i-1,j} + \phi_{i-2,j})}{(\Delta x)^3} = \frac{\phi_{i,j} - 3\phi_{i-1,j} + 3\phi_{i-2,j} - \phi_{i-3,j}}{(\Delta x)^3} = \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i,j} + O(\Delta x)$$

Finite Difference operators relations - cont.

- In general, it can be shown that forward- and backward-difference approximations to derivative of any order can be obtained from:

$$\left(\frac{\partial^n \phi}{\partial x^n}\right)_{i,j} = \frac{\Delta_x^n \phi_{i,j}}{(\Delta x)^n} + O(\Delta x) \quad (31)$$

$$\left(\frac{\partial^n \phi}{\partial x^n}\right)_{i,j} = \frac{\nabla_x^n \phi_{i,j}}{(\Delta x)^n} + O(\Delta x) \quad (32)$$

- Central difference representations of derivatives greater than second-order can be expressed in terms of Δ_x, ∇_x and δ, and will be illustrated in some detail in sect. 8.

Simple 1st order derivative

- Most of the PDEs arising in fluid mechanics and heat transfer involve only 1st and 2nd order partial derivatives and, generally, it is convenient, for practical purposes, to represent these derivatives using function values at only two or three grid points.
- With these limitations, the most frequently used first-derivative approximations on a grid for which $\Delta x = \text{const.}$, are

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} + O(\Delta x) \quad (33)$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} + O(\Delta x) \quad (34)$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta x} + O((\Delta x)^2) \quad (35)$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{-3\phi_{i,j} + 4\phi_{i+1,j} - \phi_{i+2,j}}{2\Delta x} + O((\Delta x)^2) \quad (36)$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{3\phi_{i,j} - 4\phi_{i-1,j} + \phi_{i-2,j}}{2\Delta x} + O((\Delta x)^2) \quad (37)$$

Simple 2nd order derivative

- The most common three-point second-derivative approximations on a grid for which $\Delta x =$ const., are

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} = \frac{\phi_{i,j} - 2\phi_{i+1,j} + \phi_{i+2,j}}{(\Delta x)^2} + O(\Delta x) \tag{38}$$

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} = \frac{\phi_{i,j} - 2\phi_{i-1,j} + \phi_{i-2,j}}{(\Delta x)^2} + O(\Delta x) \tag{39}$$

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{(\Delta x)^2} + O((\Delta x)^2) \tag{40}$$

Derivatives with more than three grid points - First order derivative

- Some difference approximations for first order derivatives that involve more than three grid points, on a grid for which $\Delta x =$ const., are given here

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{-\phi_{i+2,j} + 8\phi_{i+1,j} - 8\phi_{i-1,j} + \phi_{i-2,j}}{12\Delta x} + O((\Delta x)^4) \tag{41}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{3\phi_{i+1,j} + 10\phi_{i,j} - 18\phi_{i-1,j} + 6\phi_{i-2,j} - \phi_{i-3,j}}{12\Delta x} + O((\Delta x)^3) \tag{42}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{25\phi_{i,j} - 48\phi_{i-1,j} + 36\phi_{i-2,j} - 16\phi_{i-3,j} + 3\phi_{i-4,j}}{12\Delta x} + O((\Delta x)^3) \tag{43}$$

Derivatives with more than three grid points - Second order derivative

- Some difference approximations for second order derivatives that involve more than three grid points, on a grid for which Δx = const., are given here

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{-\phi_{i+2,j} + 16\phi_{i+1,j} - 30\phi_{i,j} + 16\phi_{i-1,j} - \phi_{i-2,j}}{12(\Delta x)^2} + O((\Delta x)^4) \quad (44)$$

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{2\phi_{i,j} - 5\phi_{i+1,j} + 4\phi_{i+2,j} - \phi_{i+3,j}}{(\Delta x)^2} + O((\Delta x)^2) \quad (45)$$

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{2\phi_{i,j} - 5\phi_{i-1,j} + 4\phi_{i-2,j} - \phi_{i-3,j}}{(\Delta x)^2} + O((\Delta x)^2) \quad (46)$$

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{35\phi_{i,j} - 104\phi_{i-1,j} + 114\phi_{i-2,j} - 56\phi_{i-3,j} + 11\phi_{i-4,j}}{12(\Delta x)^2} + O((\Delta x)^3) \quad (47)$$

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{11\phi_{i+1,j} - 20\phi_{i,j} + 6\phi_{i-1,j} + 4\phi_{i-2,j} - \phi_{i-3,j}}{12(\Delta x)^2} + O((\Delta x)^3) \quad (48)$$

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j} = \frac{45\phi_{i,j} - 154\phi_{i-1,j} + 214\phi_{i-2,j} - 156\phi_{i-3,j} + 61\phi_{i-4,j} - 10\phi_{i-5,j}}{12(\Delta x)^2} + O((\Delta x)^4) \quad (49)$$

Compact FD - Introduction

- In the standard FD approach considered so far, the e.g. first derivative $(\partial\phi/\partial x)_{i,j}$ depends *explicitly* on the function values at *nodes near i*.
- In the spectral methods the values of $(\partial\phi/\partial x)_{i,j}$ depends on *all the nodal values*.
- The *Padé* or *compact* finite difference schemes mimic this global dependence and are derived by writing approximations such as

$$\beta\left(\frac{\partial\phi}{\partial x}\right)_{i-2,j} + \alpha\left(\frac{\partial\phi}{\partial x}\right)_{i-1,j} + \left(\frac{\partial\phi}{\partial x}\right)_{i,j} + \alpha\left(\frac{\partial\phi}{\partial x}\right)_{i+1,j} + \beta\left(\frac{\partial\phi}{\partial x}\right)_{i+2,j} = c\frac{\phi_{i+3,j} - \phi_{i-3,j}}{6\,\Delta x} + b\frac{\phi_{i+2,j} - \phi_{i-2,j}}{4\,\Delta x} + a\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\,\Delta x} \quad (50)$$

- In this case it is not possible to compute explicitly $(\partial\phi/\partial x)_{i,j}$like in the standard schemes, since it depends also on the values of $(\partial\phi/\partial x)$ in the near nodes.
- The relation between the coefficients a, b, c and α, β are derived by matching the Taylor series coefficients of various orders. The first unmatched coefficient determines the formal truncation error of the approximation (50).
- It can be proved that, according to the terms used in the series, it is possible to obtain an accuracy up to $O((\Delta x)^{10})$ and a *resolution* (see later) closed to that of spectral schemes.
- An expression analogous to (50) can be written for the second derivative.

Compact 4th order FD schemes

- Considering, for example, 4th order schemes, it can be proved that the computational molecule can be reduced by setting, in eq.(50), the following values of the coefficients

$$\beta = 0, \quad c = 0, \quad a = \frac{2}{3}(\alpha + 2), \quad b = \frac{1}{3}(4\alpha - 1) \tag{51}$$

- As $\alpha \to 0$ this family merges into the already seen 4th order central difference scheme (41).
- For $\alpha = \frac{1}{4}$ the classical Padé scheme is recovered, while for $\alpha = \frac{1}{3}$ the leading truncation error coefficient vanishes and the scheme is thus formally 6th order accurate. Its coefficients are

$$\beta = 0, \quad c = 0, \quad \alpha = \frac{1}{3}, \quad a = \frac{14}{9}, \quad b = \frac{1}{9} \tag{52}$$

  and therefore eq. (50) becomes

$$\frac{1}{3}\left(\frac{\partial \phi}{\partial x}\right)_{i-1,j} + \left(\frac{\partial \phi}{\partial x}\right)_{i,j} + \frac{1}{3}\left(\frac{\partial \phi}{\partial x}\right)_{i+1,j} = \frac{1}{9}\,\frac{\phi_{i+2,j} - \phi_{i-2,j}}{4\,\Delta x} + \frac{14}{9}\,\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\,\Delta x} \tag{53}$$

- The application of (53) for each node, can be solved together as a linear tridiagonal system of equations for the unknown derivative values.

Pros and cons of Compact FD schemes

The use of compact FD provides a number of advantages compared to traditional (i.e. explicit) FD schemes:

- They require a computational molecule smaller than the corresponding traditional FD scheme with the same order of accuracy.
- Compared to the traditional FD approximations, compact FD schemes provide a better representation of the shorter length scales. This feature brings them closer to the spectral methods, while the freedom in choosing the mesh geometry and the boundary conditions is maintained.
- Their *resolution* characteristic - rather than their formal order of accuracy - make them an ideal candidate for the DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation) of turbulent flows, where the interest is to capture the smallest possible turbulent structures for a given grid.

There are, however, some disadvantages:

- They increase the computational cost, since they require the solution of banded - tridiagonal or pentadiagonal - linear system of equations in order to evaluate the first (or second) derivative.
- The derivation of similar high-order Compact FD expressions for the boundary nodes is not straightforward.

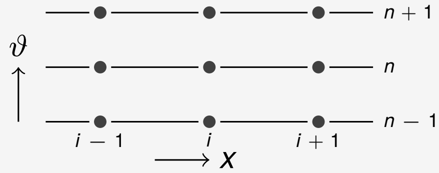
1D heat conduction equation

Let's consider first the unsteady one-dimensional (1D) heat conduction equation, where $\alpha = k/\rho c$

$$\frac{\partial T}{\partial \vartheta} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{54}$$

Using a *forward-difference* representation for the time derivative ($\vartheta = n\,\Delta\vartheta$) and the simplest *central-difference* for the second derivative, we can approximate the heat conduction equation by:

$$\frac{T_i^{n+1} - T_i^n}{\Delta\vartheta} = \frac{\alpha}{(\Delta x)^2}\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right) \tag{55}$$



However, we already found that TE (Truncation Errors) were associated with the forward and central-difference representations used in eq. (55)

$$\underbrace{\frac{\partial T}{\partial \vartheta} - \alpha \frac{\partial^2 T}{\partial x^2}}_{\text{PDE}} = \underbrace{\frac{T_i^{n+1} - T_i^n}{\Delta\vartheta} - \frac{\alpha}{(\Delta x)^2}\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)}_{\text{FDE}}$$
$$+ \underbrace{\left[-\left(\frac{\partial^2 T}{\partial \vartheta^2}\right)_{n,i}\frac{\Delta\vartheta}{2} + \alpha\left(\frac{\partial^4 T}{\partial x^4}\right)_{n,i}\frac{(\Delta x)^2}{12} + \dots\right]}_{\text{TE}} \tag{56}$$

where PDE is the *partial differential equation* and FDE is the *finite-difference equation*.

1D heat conduction equation - cont.

- The TEs associated with all derivatives in any one PDE should be obtained by Taylor expansion about the same point (n, i in the previous example of the unsteady 1D heat conduction).
- The difference representation given by eq. (55) will be referred to as the *simple explicit scheme* for the heat conduction equation[1]:
  - For an explicit scheme, only one unknown appears in the difference equation, in a manner that permits an economical evaluation in terms of known quantities.
  - An implicit scheme, which would lead to three unknowns in each equation, would results if the 2nd derivative was approximated by T at the $(n+1)$ time level. This, in turn, requires the solution of a sparse (tridiagonal in this case) system of linear equations at each time-step.
- The TE is defined as

$$\text{TE} = \text{PDE} - \text{FDE}$$

  which, in this case, if of $O[\Delta\vartheta, (\Delta x)^2]$.

[1] A detailed examination of several temporal integration schemes will be given during the presentation of the Finite Volume method.

Round-Off Error

- *Round-Off error*: difference between the calculated approximation of a number and its exact mathematical value. It is due to the use of a finite number of digits in the arithmetic operations.
  - In FD (and Finite Volume and Finite Element methods as well) they may became very important because of the large number of dependent repetitive operations that are usually involved. Sometimes the magnitude of the Round-Off error is proportional to the number of grid points: in this case, refining the grid may decrease the TE but increase the Round-Off error (use of double-precision representation).
- *Discretization error*: caused by replacing the continuous problem with a discrete one, and is defined as the difference between the exact solution of the PDE (Round-Off error free) and the exact solution of the FDE (Round-Off error free). It is caused by the TE plus any error introduced by the treatment of boundary conditions.
- The difference between the exact solution of the PDE and the computer solution of the FDE is equal to the sum of the discretization error and and Round-Off error (associated with the finite difference calculation).
- It will be seen that, in general, we have also to consider other type of errors:
  - *Modelling error*: associated with the use of simplified mathematical models of complex phenomena like, i.e., turbulence, combustion, multiphase et.
  - *Convergence error*: associated to the use of *iterative* methods for the solution of the non-linear set of PDEs which usually arise in CFD.

Steady 2D heat conduction

Another example: let's consider the 2D steady heat conduction equation without sources

$$\nabla^2 T = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{57}$$

We already found - eq. (9) - that

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + O((\Delta x)^2) \tag{58a}$$

$$\frac{\partial^2 T}{\partial y^2} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} + O((\Delta y)^2) \tag{58b}$$

Replacing eqs.(58) in (57)

$$\underbrace{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}}_{PDE} = \underbrace{\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2}}_{FDE} + \underbrace{O\left[(\Delta x)^2, (\Delta y)^2\right]}_{TE} \tag{59}$$

Steady 2D heat conduction - cont.

The previous FDE (59) can be re-arranged as

$$\left[2(\Delta x)^2 + 2(\Delta y)^2\right] T_{i,j} - (\Delta y)^2 T_{i+1,j} - (\Delta y)^2 T_{i-1,j} - (\Delta x)^2 T_{i,j+1} - (\Delta x)^2 T_{i,j-1} = 0 \qquad (60)$$

and, in the particular case $\Delta x \equiv \Delta y$, eq. (60) can be simplified in the following one

$$4T_{i,j} - T_{i+1,j} - T_{i-1,j} - T_{i,j+1} - T_{i,j-1} = 0 \qquad (61)$$

or

$$T_{i,j} = \frac{1}{4}\left[T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}\right] \qquad (62)$$

and finally in *compact form*

$$T_{i,j} = \frac{1}{4}\sum_{nb} T_{nb} \qquad (63)$$

where *nb* means *neighbors*.

- It is interesting to observe, from eq. (62), that, for uniform and constant grid spacing, the temperature value of a node *must* be equal to the average value of its 4 neighboring nodes in 2D (2 and 6 in 1D and 3D, respectively).
- Tridiagonal (1D), pentadiagonal (2D) and eptadiagonal (3D) systems of equations.

Steady 2D heat conduction - cont.

Another possibility would be to use a 4^{th} order approximation of the second-order derivative, i.e. eq. (44), resulting in

$$\underbrace{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}}_{PDE} = \underbrace{\frac{-T_{i+2,j} + 16T_{i+1,j} - 30T_{i,j} + 16T_{i-1,j} - T_{i-2,j}}{12\,(\Delta x)^2} + \frac{-T_{i,j+2} + 16T_{i,j+1} - 30T_{i,j} + 16T_{i,j-1} - T_{i,j-2}}{12\,(\Delta y)^2}}_{FDE} + \underbrace{O\left[(\Delta x)^4, (\Delta y)^4\right]}_{TE} \qquad (64)$$

Steady 2D heat conduction - cont.

Clearly, in order to maintain the same order of accuracy throughout all the domain, expressions of 2^{nd} derivative of the same order have to be used at the boundary, using i.e. eqs. (46) and (49) for $O((\Delta x)^2, (\Delta y)^2)$ and $O((\Delta x)^4, (\Delta y)^4)$, respectively.
Again, in the particular case $\Delta x \equiv \Delta y$, eq (64) can be written as

$$60T_{i,j} - 16T_{i+1,j} - 16T_{i-1,j} - 16T_{i,j+1} - 16T_{i,j-1} + T_{i+2,j} + T_{i-2,j} + T_{i,j+2} + T_{i,j-2} = 0 \qquad (65)$$

Equations (64) and (65) leads to a symmetrical, bounded (ennea-diagonal) system of linear equations.

Overview of boundary conditions

In order to attain closure to the system of discrete equations, additional equations are required, and these came from the boundary conditions.
Although boundary conditions encountered in engineering can take a myriad of forms, the vast majority of them can be classified under three canonical types:

1. Dirichlet, *e.g.* fixed value of the variable.
2. Neumann, *e.g.* fixed value of the first derivative (flux).
3. Robin or convective, *e.g.* a linear combination of the values of the variable and the values of its derivative on the boundary of the domain.

We reserve the term *boundary condition* for conditions applied to to spatial operators, and *initial condition* for conditions applied to temporal operators.

Dirichlet boundary condition

TBD.

Neumann Boundary condition

TBD

Robin (convective) boundary condition

Let's consider, for simplicity, the unsteady one-dimensional (1D) heat conduction equation, where $\alpha = k/\rho c$ [m^2/s] is the thermal diffusivity, k [W/kg K] is the thermal conductivity, ρ [kg/m^3] is the density and c [J/kg K] is the specific heat.

$$\frac{\partial T}{\partial \vartheta} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{66}$$

Using a *backward-difference* representation for the time derivative ($\vartheta = n\,\Delta\vartheta$), and the simplest 2^{nd} order *central-difference* for the second derivative, we can approximate the heat conduction equation by

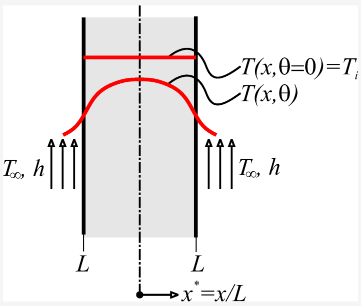
$$\frac{T_i^{n+1} - T_i^n}{\Delta\vartheta} = \frac{\alpha}{(\Delta x)^2}\left(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}\right) \tag{67}$$

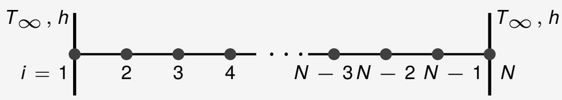
which can be written as

$$-\frac{\alpha}{\Delta x^2} T_{i-1}^{n+1} + \left(\frac{1}{\Delta\vartheta} + \frac{2\alpha}{\Delta x^2}\right) T_i^{n+1} - \frac{\alpha}{\Delta x^2} T_{i+1}^{n+1} = \frac{T_i^n}{\Delta\vartheta} \tag{68}$$

The equation (68) should be written for all nodes $i = 1 \ldots N$ and will result in a *tridiagonal* system of equations.

Robin (convective) boundary condition - cont.





As common, we may assume that, for the slab sketched, convective heat transfer - in this case cooling - occurs at both ends

$$h\,(T_1 - T_\infty) - k\left.\frac{\partial T}{\partial x}\right|_{i=1} = 0 \tag{69}$$

$$h\,(T_N - T_\infty) + k\left.\frac{\partial T}{\partial x}\right|_{i=N} = 0 \tag{70}$$

The previous equations can be expressed using different formulations for $\partial T/\partial x$.

1. First order expression for $\partial T/\partial x$.

$$h\left(T_1^{n+1} - T_\infty\right) - k\,\frac{T_2^{n+1} - T_1^{n+1}}{\Delta x} = 0 \tag{71}$$

$$h\left(T_N^{n+1} - T_\infty\right) + k\,\frac{T_N^{n+1} - T_{N-1}^{n+1}}{\Delta x} = 0 \tag{72}$$

which can be expressed as

$$\left(h + \frac{k}{\Delta x}\right) T_1^{n+1} - \frac{k}{\Delta x} T_2^{n+1} = hT_\infty \tag{73}$$

$$\left(h + \frac{k}{\Delta x}\right) T_N^{n+1} - \frac{k}{\Delta x} T_{N-1}^{n+1} = hT_\infty \tag{74}$$

Robin (convective) boundary condition - cont.

2. Second order expression for $\partial T / \partial x$.

$$h\left(T_1^{n+1} - T_\infty\right) - k\frac{-3T_1^{n+1} + 4T_2^{n+1} - T_3^{n+1}}{2\,\Delta x} = 0 \tag{75}$$

$$h\left(T_N^{n+1} - T_\infty\right) + k\frac{T_N^{n+1} - 4T_{N-1}^{n+1} + T_{N-2}^{n+1}}{2\,\Delta x} = 0 \tag{76}$$

which, again, can be expressed in a form convenient for the numerical solution

$$\left(h + \frac{3k}{2\,\Delta x}\right)T_1^{n+1} - \frac{2k}{\Delta x}T_2^{n+1} + \frac{k}{2\,\Delta x}T_3^{n+1} = hT_\infty \tag{77}$$

$$\left(h + \frac{3k}{2\,\Delta x}\right)T_N^{n+1} - \frac{2k}{\Delta x}T_{N-1}^{n+1} + \frac{k}{2\,\Delta x}T_{N-2}^{n+1} = hT_\infty \tag{78}$$

As a final note it should be observed that a better, more accurate, approach, would ensure that *both* the boundary condition *and* the governing equation are satisfied at the boundary.

Available procedures

- As we start with a given PDE and a Finite-Difference mesh, several procedures are available to developing FDEs:
  1. Taylor-series expansions
  2. Polynomial fitting
  3. Difference operators
  4. Integral method (or micro-integral method).
- It is sometimes possible to obtain exactly the same FD representation by using all four methods.
- In general we will lean most heavily on method 1., using method 2. in treating boundary conditions.
- Method 3 is very general and it will be described in a separate section.

Taylor-series expansions

Formal approach with Taylor-series expansions, satisfying specified constraints, to develop difference expressions.

- Suppose we want to develop a difference approximation for $(\partial\phi/\partial x)_{i,j}$ having a TE of $O[(\Delta x)^2]$ using at most values $\phi_{i-2,j}$, $\phi_{i-1,j}$ and $\phi_{i,j}$.
- With these constraints and objectives:
  1. Write Taylor-series expansions for $\phi_{i-2,j}$ and $\phi_{i-1,j}$, expanding about point (i,j).
  2. Attempt to solve for $(\partial\phi/\partial x)_{i,j}$ from the resulting equations in such a way to obtain a TE of $O[(\Delta x)^2]$.

$$\phi_{i-2,j} = \phi_{i,j} + \left(\frac{\partial\phi}{\partial x}\right)_{i,j}(-2\Delta x) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j}\frac{(2\Delta x)^2}{2!} + \left(\frac{\partial^3\phi}{\partial x^3}\right)_{i,j}\frac{(-2\Delta x)^3}{3!} + \cdots \quad (79)$$

$$\phi_{i-1,j} = \phi_{i,j} + \left(\frac{\partial\phi}{\partial x}\right)_{i,j}(-\Delta x) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j}\frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3\phi}{\partial x^3}\right)_{i,j}\frac{(-\Delta x)^3}{3!} + \cdots \quad (80)$$

It is often possible to determine the required form of the difference representation by inspection or simple substitution. Proceeding by substitution, we rearrange eq. (79) to put $(\partial\phi/\partial x)_{i,j}$ on the left-hand side:

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j} = \frac{\phi_{i,j}}{2\Delta x} - \frac{\phi_{i-2,j}}{2\Delta x} + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j}\Delta x + O[(\Delta x)^2]$$

Taylor-series expansions - cont.

- As is, the representation is $O(\Delta x)$ because of the term $(\partial^2\phi/\partial x^2)_{i,j}\Delta x$.
- We can then substitute for $(\partial^2\phi/\partial x^2)_{i,j}$ in the previous equation, using eq. (80), to obtain the desired result. From eq. (80):

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_{i,j}\Delta x = \frac{2(\phi_{i-1,j} - \phi_{i,j})}{\Delta x} + 2\left(\frac{\partial\phi}{\partial x}\right)_{i,j} - \left(\frac{\partial^3\phi}{\partial x^3}\right)_{i,j}\frac{(-\Delta x)^2}{3!} + \cdots$$

which, substituted in the previous expression of $(\partial\phi/\partial x)_{i,j}$:

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j} = \frac{\phi_{i,j}}{2\Delta x} - \frac{\phi_{i-2,j}}{2\Delta x} + \frac{2\phi_{i-1,j}}{\Delta x} - \frac{2\phi_{i,j}}{\Delta x} + 2\left(\frac{\partial\phi}{\partial x}\right)_{i,j} + O[(\Delta x)^2]$$

and rearranging we finally obtain:

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j} = \frac{\phi_{i-2,j} - 4\phi_{i-1,j} + 3\phi_{i,j}}{2\Delta x} + O[(\Delta x)^2] \quad (81)$$

Taylor-series expansions - cont.

In a more formal way:

1. Multiply eq. (79) by "*a*" and eq. (80) by "*b*".
2. Add the two resulting equations:

$$a\phi_{i-2,j} + b\phi_{i-1,j} - (a+b)\,\phi_{i,j}$$
$$= \left(\frac{\partial \phi}{\partial x}\right)_{i,j} [-2a - b]\,\Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,j} \frac{[4a+b]}{2!}(\Delta x)^2 + O[(\Delta x)^3]$$

3. Impose that the coefficient of $(\partial\phi/\partial x)_{i,j}$ is equal to 1

$$-2a - b = 1$$

4. Impose that the coefficient of $(\partial^2\phi/\partial x^2)_{i,j}$ is equal to zero, in order to have a TE of $O[(\Delta x)^2]$

$$2a + b/2 = 0$$

5. Solve for *a* and *b*

$$a = 1/2; \quad b = -2$$

   and therefore, from the previous expressions, we obtain again

$$\left(\frac{\partial \phi}{\partial x}\right)_{i,j} = \frac{\phi_{i-2,j} - 4\phi_{i-1,j} + 3\phi_{i,j}}{2\Delta x} + O[(\Delta x)^2]$$

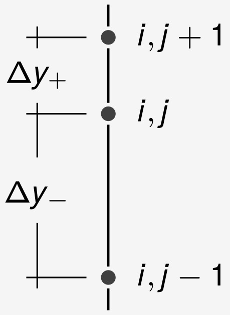
Taylor-series expansions - cont.

Some considerations

- We observe that it was in fact necessary, in this example, to include the terms involving $(\partial^3\phi/\partial x^3)_{i,j}$ in the Taylor-series expansions - see eqns. (79) and (80) - in order to determine whether or not these terms would cancel in the algebraic operations and reduce the TE even further to $O[(\Delta x)^2]$. Fortuitous cancellation of terms occurs frequently enough to warrant close attention to this point.
- It is sometimes necessary to carry out the inverse of the previous process. That is, suppose that we had obtained, by some other means, the approximation represented by eq. (37), and we wanted to investigate the *consistency* and TE of such an expression. For this, the use Taylor-series expansions would be invaluable, and the recommended procedure would be to substitute the Taylor-series expressions from eqns. (79) and (80) for $\phi_{i-2,j}$ and $\phi_{i-1,j}$ into the difference representation to obtain an expression of the form $(\partial\phi/\partial x)_{i,j}$ + TE on the right-hand side. In this way the TE has been identified, and if $\lim_{\Delta x \to 0}(TE) = 0$, the difference representation is consistent.
- Our main interest is in correctly approximating an entire PDE at an arbitrary point in the problem domain. For this reason, we must be careful to use the same expansion point in approximating all derivatives in the PDE by the Taylor-series method. If this is done, than the TE for the entire equation can be obtained by adding the TE for each derivative.

Case of non-uniform grid

In this case we use the following notation



where

$\Delta y_+ = y_{i,j+1} - y_{i,j}$ and $\Delta y_- = y_{i,j} - y_{i,j-1}$

We recall that, for equal spacing, the CD (Central Difference) representation for the first derivative was equivalent to the arithmetic average of a forward and backward representation, that is, for $\Delta y_+ = \Delta y_- = \Delta y$ (eqs. (24) and (27)):

$$\left(\frac{\partial \phi}{\partial y}\right)_{i,j} = \frac{\overline{\delta_y}\phi_{i,j}}{2\Delta y} = \frac{\Delta_y \phi_{i,j} + \nabla_y \phi_{i,j}}{2\Delta y} + O[(\Delta y)^2]$$

Is the 2^{nd} order accuracy preserved also for unequal spacing using a geometrical weighted average ?

$$\left(\frac{\partial \phi}{\partial y}\right)_{i,j} \stackrel{?}{=} \frac{\Delta_y \phi_{i,j}}{\Delta y_+}\left(\frac{\Delta y_-}{\Delta y_+ + \Delta y_-}\right) + \frac{\nabla_y \phi_{i,j}}{\Delta y_-}\left(\frac{\Delta y_+}{\Delta y_+ + \Delta y_-}\right) \tag{82}$$

We can verify it by use of Taylor-series expansion about point (i,j).

Case of non-uniform grid - cont.

Letting $\Delta y_+ / \Delta y_- = \alpha$, one obtains

$$\begin{aligned}\phi_{i,j+1} = \phi_{i,j} &+ \left(\frac{\partial \phi}{\partial y}\right)_{i,j} \alpha \Delta y_- + \left(\frac{\partial^2 \phi}{\partial y^2}\right)_{i,j} \frac{(\alpha \Delta y_-)^2}{2!} \\ &+ \left(\frac{\partial^3 \phi}{\partial y^3}\right)_{i,j} \frac{(\alpha \Delta y_-)^3}{3!} + \left(\frac{\partial^4 \phi}{\partial y^4}\right)_{i,j} \frac{(\alpha \Delta y_-)^4}{4!} + \ldots\end{aligned} \tag{83}$$

$$\begin{aligned}\phi_{i,j-1} = \phi_{i,j} &+ \left(\frac{\partial \phi}{\partial y}\right)_{i,j} (-\Delta y_-) + \left(\frac{\partial^2 \phi}{\partial y^2}\right)_{i,j} \frac{(-\Delta y_-)^2}{2!} \\ &+ \left(\frac{\partial^3 \phi}{\partial y^3}\right)_{i,j} \frac{(-\Delta y_-)^3}{3!} + \left(\frac{\partial^4 \phi}{\partial y^4}\right)_{i,j} \frac{(-\Delta y_-)^4}{4!} + \ldots\end{aligned} \tag{84}$$

As already done before, we will multiply eq.(83) by a, and eq.(84) by b, add the results and solve for $(\partial \phi / \partial y)_{i,j}$.

Case of non-uniform grid - cont.

Requiring that the coefficient of $(\partial\phi/\partial y)_{i,j}\Delta y_-$ be equal to 1 after the addition gives

$$a\alpha - b = 1$$

In order to have a TE of $O[(\Delta y)^2]$ or better, the coefficient of $(\partial^2\phi/\partial y^2)_{i,j}$ must be zero after the addition, which requires that

$$\alpha^2 a + b = 0$$

A solution to these two algebraic equations can be obtained readily as

$$\begin{cases} a = \dfrac{1}{\alpha(\alpha+1)} \\ b = -\dfrac{\alpha}{\alpha+1} \end{cases}$$

The final result can be written as

$$\boxed{\left(\frac{\partial\phi}{\partial y}\right)_{i,j} = \frac{\phi_{i,j+1} + (\alpha^2-1)\phi_{i,j} - \alpha^2\phi_{i,j-1}}{\alpha(\alpha+1)\Delta y_-}} \qquad (85)$$

Equation (85) can be rearranged further in the form given by eq. (82).

Polynomial fitting - Laplace equation

- This technique can be used to develop the entire finite-difference representation for a PDE. However, the technique is perhaps most commonly employed in the treatment of boundary conditions or in gathering information from the solution in the neighborhood of the boundary. In the following we consider some specific examples.
- Consider again the 2D steady heat conduction (Laplace equation)

$$\nabla^2 T = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

- We suppose that both the x and y dependency of temperature can be expressed by a 2nd degree polynomial. In particular, holding $y = y_0$ fixed, we assume that temperatures at various x locations in the neighborhood of point (i,j) can be determined from

$$T(x, y_0) = a + bx + cx^2$$

where $(x,y)_{i,j} = (x_0, y_0)$ and, for convenience, we let $x = 0$ at point (i,j), and $\Delta x = const$. Clearly

$$\left(\frac{\partial T}{\partial x}\right)_{i,j} = b$$

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} = 2c$$

Polynomial fitting - Laplace equation - cont.

- The coefficients a, b and c can be evaluated in terms of temperatures at specific grid points and Δx. The choice of neighboring grid points used in the evaluation determines the geometric arrangement of the difference molecule, that is, whether the resulting derivative approximations are *central*, *forward* or *backward* differences.
- Here we will choose points $(i-1,j)$, (i,j) and $(i+1,j)$ and obtain:

$$T_{i,j} = a \quad (86a)$$

$$T_{i+1,j} = a + b\Delta x + c(\Delta x)^2 \quad (86b)$$

$$T_{i-1,j} = a - b\Delta x + c(\Delta x)^2 \quad (86c)$$

from which, subtracting (86c) from (86b):

$$b = \left(\frac{\partial T}{\partial x}\right)_{i,j} = \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x}$$

while summing (86b) and (86c):

$$c = \frac{1}{2}\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{2\,(\Delta x)^2}$$

Polynomial fitting - Laplace equation - cont.

- Thus

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{2\,(\Delta x)^2} \quad (87)$$

  The TE of expression (87) can be determined by substituting Taylor-series expansions about point (i,j) for $T_{i+1,j}$ and $T_{i-1,j}$ into eq. (87).
  The TE is found to be of $O((\Delta x)^2)$.
- A finite-difference approximation for $(\partial^2 T/\partial y^2)_{i,j}$ can be found in a similar manner.
- We notice that arbitrary decisions need to be made in the process of polynomial fitting, which will influence the form and TE of the result: in particular, these decisions influence which of the neighboring points will appear in the difference expression.
- We also observe that there is nothing unique about the polynomial fitting procedure that guarantees that the difference approximation for the PDE is the best in any sense or that the numerical scheme is stable when used for marching problems.

Estimation of the heat flux at the wall

- Suppose that we have solved the finite-difference form of the energy equation for the temperature distribution near a solid boundary and we need to estimate the *heat flux* at that location.
- From Fourier's law

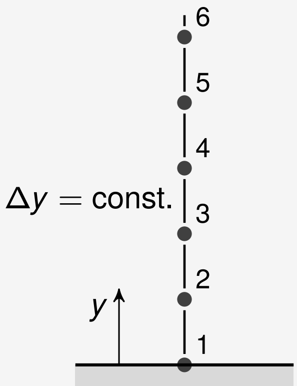
$$q_w = -k \left(\frac{\partial T}{\partial y} \right)_{y=0}$$

  thus we need to approximate $(\partial T/\partial y)_{y=0}$ by a difference representation that uses the temperature obtained from the FD solution of the energy equation.
- One way to proceed is to assume that the temperature distribution near the boundary is a polynomial, and to *fit* such a polynomial, that is, straight line, parabola, 3^{rd} degree polynomial *et.* to the FD solution that has been determined at discrete points.
- By requiring that the polynomial matches the FD solution for T at certain discrete points, the unknown coefficients in the polynomial can be determined.

Estimation of the heat flux at the wall - cont.

Example 1

Assume that the temperature distribution near the boundary is again a 2nd degree polynomial of the form $T = a + by + cy^2$, then, referring to the following figure, we note that $(\partial T/\partial y)_{y=0} = b$.



Furthermore, for $\Delta y = const$, we can write:

$$T_1 = a$$
$$T_2 = a + b\Delta y + c(\Delta y)^2$$
$$T_3 = a + b(2\Delta y) + c(2\Delta y)^2$$

The resulting solutions for a, b, and c are:

$$a = T_1$$
$$b = \frac{-3T_1 + 4T_2 - T_3}{2\Delta y}$$
$$c = \frac{T_1 - 2T_2 + T_3}{2(\Delta y)^2}$$

This and other algebraic problems have been solved by the MATLAB® Symbolic toolbox.

Estimation of the heat flux at the wall - cont.

Thus, we can evaluate the wall heat flux by the approximation

$$q_w = -k\left(\frac{\partial T}{\partial y}\right)_{y=0} \cong -kb = \frac{k}{2\Delta y}\left(3T_1 - 4T_2 + T_3\right)$$

What is the TE of this approximation for $(\partial T/\partial y)_{y=0}$?

- This may be found by expressing T_2 and T_3 in terms of Taylor-series expansions about the boundary point and substituting these evaluations into the difference expression of $(\partial T/\partial y)_{y=0}$.
- Alternatively, we can identify the 2nd degree polynomial as a truncated Taylor-series expansion about $y = 0$.
- Second degree polynomial:

$$T = a + by + cy^2$$

- Taylor series:

$$T = \underbrace{T(0)}_{a} + \underbrace{\left(\frac{\partial T}{\partial y}\right)_{y=0}}_{b} y + \underbrace{\left(\frac{\partial^2 T}{\partial y^2}\right)_{y=0}}_{2c} \frac{y^2}{2!} + \underbrace{\left(\frac{\partial^3 T}{\partial y^3}\right)_{y=0} \frac{y^3}{3!}}_{TE} + \ldots$$

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Estimation of the heat flux at the wall - cont.

- Thus the approximation

$$T \cong a + by + cy^2$$

  is equivalent to utilizing the first three terms of a Taylor-series expansion with the resulting TE in the expression for T being $O[(\Delta y)^3]$.
- Solving the Taylor series for an expression for $(\partial T/\partial y)_{y=0}$ involves division by Δy, which reduces the TE in the expression for $(\partial T/\partial y)_{y=0}$ to $O[(\Delta y)^2]$

Estimation of the heat flux at the wall - cont.

Example 2

Assume now that that the temperature distribution near the boundary is a 4th degree polynomial:

$$T = a + by + cy^2 + dy^3 + ey^4$$

Then we have again

$$\left(\frac{\partial T}{\partial y}\right)_{y=0} = b$$

and, for $\Delta y = const$, we can write

$$\begin{aligned}
T_1 &= a \\
T_2 &= a + b\,\Delta y + c(\Delta y)^2 + d(\Delta y)^3 + e(\Delta y)^4 \\
T_3 &= a + b\,2\Delta y + c(2\Delta y)^2 + d(2\Delta y)^3 + e(2\Delta y)^4 \\
T_4 &= a + b\,3\Delta y + c(3\Delta y)^2 + d(3\Delta y)^3 + e(3\Delta y)^4 \\
T_5 &= a + b\,4\Delta y + c(4\Delta y)^2 + d(4\Delta y)^3 + e(4\Delta y)^4
\end{aligned}$$

Estimation of the heat flux at the wall - cont.

Solving for a, b, c, d and e by means of MATLAB® Symbolic toolbox, one obtains:

$$\begin{aligned}
a &= T_1 \\
b &= \frac{-25T_1 + 48T_2 - 36T_3 + 16T_4 - 3T_5}{12\,\Delta y} \\
c &= \frac{35T_1 - 104T_2 + 114T_3 - 56T_4 + 11T_5}{24(\Delta y)^2} \\
d &= \frac{-5T_1 + 18T_2 - 24T_3 + 14T_4 - 3T_5}{12(\Delta y)^3} \\
e &= \frac{T_1 - 4T_2 + 6T_3 - 4T_4 + T_5}{24(\Delta y)^4}
\end{aligned}$$

Then, as before:

$$q_w = -k\left(\frac{\partial T}{\partial y}\right)_{y=0} \cong -kb = \frac{k}{12\,\Delta y}\left(25T_1 - 48T_2 + 36T_3 - 16T_4 + 3T_5\right)$$

Estimation of boundary value

- Suppose that now, for the energy equation, the wall heat flux is specified as a boundary condition.
- We may then want to use *polynomial fitting* to obtain an expression for the boundary temperature that is called for in the FD equation for internal points.
- In other words, if $q_w = -k(\partial T/\partial y)_{y=0}$ is given, how can we evaluate T at $y = 0$, that is, T_1 in terms of q_w/k and T_2, T_3, etc. ?
- Assume that

$$T = a + by + cy^2 + dy^3$$

near the wall, and that $(\partial T/\partial y)_{y=0} = b = -q_w/k$ (given).

- Our objective is to evaluate T_1, which in this case equals a. Referring to the previous figure, we can write:

$$T_2 = a - \frac{q_w}{k}\Delta y + c(\Delta y)^2 + d(\Delta y)^3$$
$$T_3 = a - \frac{q_w}{k}2\Delta y + c(2\Delta y)^2 + d(2\Delta y)^3$$
$$T_4 = a - \frac{q_w}{k}3\Delta y + c(3\Delta y)^2 + d(3\Delta y)^3$$

Estimation of boundary value - cont.

- Solving for a, c and d in terms of T_2, T_3, T_4, q_w/k and Δy (by means, in this case, of MATLAB® Symbolic toolbox):

$$a = \frac{1}{11\,k}(18T_2\,k - 9T_3\,k + 2T_4\,k + 6q_w\,\Delta y)$$
$$c = -\frac{1}{22\,k\,(\Delta y)^2}(19T_2\,k - 26T_3\,k + 7T_4\,k - 12q_w\,\Delta y)$$
$$d = \frac{1}{22\,k\,(\Delta y)^3}(5T_2\,k - 8T_3\,k + 3T_4\,k - 2q_w\,\Delta y)$$

- The derived result T_1 follows directly from $T_1 = a$ and is given by:

$$T_1 = \frac{1}{11\,k}(18T_2\,k - 9T_3\,k + 2T_4\,k + 6q_w\,\Delta y) + O[(\Delta y)^4] \quad (88)$$

- The TE in eq.(88) can be found by substituting Taylor-series expansions about the boundary point for the temperatures on the right-hand side, or by identifying the polynomial as a truncated series by inspection.

Expressions for wall value of derivative

Expressions for wall values of the first derivative of a function in terms of values of the function, with the assumption that $\Delta y = const$.

$$\left(\frac{\partial T}{\partial y}\right)_{i,j} = \frac{T_{i,j+1} - T_{i,j}}{\Delta y} + O[\Delta y] \tag{89}$$

$$\left(\frac{\partial T}{\partial y}\right)_{i,j} = \frac{1}{2\,\Delta y}\left(-3T_{i,j} + 4T_{i,j+1} - T_{i,j+2}\right) + O[(\Delta y)^2] \tag{90}$$

$$\left(\frac{\partial T}{\partial y}\right)_{i,j} = \frac{1}{6\,\Delta y}\left(-11T_{i,j} + 18T_{i,j+1} - 9T_{i,j+2} + 2T_{i,j+3}\right) + O[(\Delta y)^3] \tag{91}$$

$$\left(\frac{\partial T}{\partial y}\right)_{i,j} = \frac{1}{12\,\Delta y}\left(-25T_{i,j} + 48T_{i,j+1} - 36T_{i,j+2} + 16T_{i,j+3} - 3T_{i,j+4}\right) + O[(\Delta y)^4] \tag{92}$$

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Expressions for wall value of a function

Expressions for wall values of a function in terms of the values of the function and its first derivative at the wall, with the assumption that $\Delta y = const$.

$$T_{i,j} = T_{i,j+1} - \Delta y \left(\frac{\partial T}{\partial y}\right)_{i,j} + O[(\Delta y)^2] \tag{93}$$

$$T_{i,j} = \frac{1}{3}\left[4T_{i,j+1} - T_{i,j+2} - 2\Delta y \left(\frac{\partial T}{\partial y}\right)_{i,j}\right] + O[(\Delta y)^3] \tag{94}$$

$$T_{i,j} = \frac{1}{11}\left[18T_{i,j+1} - 9T_{i,j+2} + 2T_{i,j+3} - 6\Delta y \left(\frac{\partial T}{\partial y}\right)_{i,j}\right] + O[(\Delta y)^4] \tag{95}$$

$$T_{i,j} = \frac{1}{25}\left[48T_{i,j+1} - 36T_{i,j+2} + 16T_{i,j+3} - 3T_{i,j+4} - 12\Delta y \left(\frac{\partial T}{\partial y}\right)_{i,j}\right] + O[(\Delta y)^5] \tag{96}$$

Generalities

- In section 3, where we defined the *Finite Difference operators*, we have introduced some simple recursive formulas for first-order accurate forward- and backward-difference approximations to derivative of any order.
- In the following we will see a general methodology for the generation of arbitrary FD formulas with prescribed order.
- They are also based on the *Finite Difference operators* defined in sect. (3).
- For the derivation of these and other FD formulas, it is convenient to use a *symbolic manipulator*, like the MATLAB *Symbolic Math Toolbox*^{TM} and its associated function/tools: `taylor`, `taylortool` et.

Relation between D and E operators

The important point, for generating Finite difference formulas, lies in the relation between the *Shift operator*, eq. (17), and the *Derivative operator*, eq. (20).
This relation is obtained from the Taylor expansion[2]

$$\phi(x+\Delta x) = \phi(x) + \left(\frac{\partial \phi}{\partial x}\right)_0 \Delta x + \left(\frac{\partial^2 \phi}{\partial x^2}\right)_0 \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 \phi}{\partial x^3}\right)_0 \frac{(\Delta x)^3}{3!} + \dots \tag{97}$$

and in operator form

$$E\phi(x) = \phi(x)\left(1 + \Delta x D + \frac{(\Delta x D)^2}{2!} + \frac{(\Delta x D)^3}{3!} + \dots\right) \tag{98}$$

Remembering that

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots + \frac{x^n}{n!} + \dots$$

the relation (98) can be written as

$$E\phi(x) = \phi(x)\, e^{\Delta x D} \tag{99}$$

[2] In the following and subsequent equations, unless necessary, we will either omit the indices, or use just a single index for brevity.

Relation between D and E operators - cont.

The relation (99) can be expressed symbolically as

$$\boxed{E = e^{\Delta x D}} \tag{100}$$

- This relation should be interpreted as giving identical results when acting on the exponential function e^{ax} and on any polynomial of degree n.
- For a polynomial of degree n, the expansion on the r.h.s. has only n terms and therefore all the expressions presented in the following *are exact up to n terms*.
- Equation (100) can be used in the inverse way, leading to

$$\boxed{\Delta x\, D = \ln E} \tag{101}$$

Forward differences

- The formulas for forward differences are obtained by taking into account the relation (21a), e.g.

$$\Delta_x = (E_x - I)$$

  This leads to

$$\begin{aligned} \Delta x\, D = \ln E &= \ln(1 + \Delta_x) && (102)\\ &= \Delta_x - \frac{\Delta_x^2}{2} + \frac{\Delta_x^3}{3} - \frac{\Delta_x^4}{4} + \dots && (103)\\ &= \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\Delta_x^n}{n} \end{aligned}$$

- The order of accuracy increases with the number of terms kept in the r.h.s. of eq. (103), and the first neglected term gives the *T.E.*.
- Keeping the first term only, leads to the first order formula (4) and a T.E. equal to $(\partial^2\phi/\partial x^2)\Delta x/2$:

$$D\phi_i = \frac{1}{\Delta x}(\phi_{i+1} - \phi_i)$$

Forward differences - cont.

- If the first two terms of (103) are considered, we obtain

$$D\phi_i = \frac{1}{\Delta x}\left(\Delta_x - \frac{\Delta_x^2}{2}\right)\phi_i = \frac{1}{\Delta x}\left(\phi_{i+1} - \phi_i\right) - \frac{\Delta_x}{2\Delta x}\left(\phi_{i+1} - \phi_i\right)$$
$$= \frac{1}{2\Delta x}\left(-3\phi_i + 4\phi_{i+1} - \phi_{i+2}\right)$$

  i.e. the second order formula (36) with the truncation error $\Delta x^2/3\ (\partial^3\phi/\partial x^3)$.
- Therefore, the relation (103) leads to various FD formulas for the first derivative with increasing order of accuracy.
- Since the forward difference operator can be written as $\Delta_x = \Delta x\,(\partial/\partial x) + O(\Delta x^2)$, it follows that the first neglected operator Δ_x^n is of order n, showing that the associated T.E. is $O(\Delta x^{n-1})$.

Backward differences

- Backward difference formulas can be obtained, with increasing order of accuracy, by application of eq. (21b), e.g.

$$\nabla_x = (I - E_x^{-1})$$

  which leads to

$$\Delta x\, D = \ln E = -\ln(1 - \nabla_x) \tag{104}$$
$$= \nabla_x + \frac{\nabla_x^2}{2} + \frac{\nabla_x^3}{3} + \frac{\nabla_x^4}{4} + \frac{\nabla_x^5}{5} + \dots \tag{105}$$
$$= \sum_{n=1}^{\infty} \frac{\nabla_x^n}{n}$$

- Again, keeping the first term only, leads to the first order formula (6) and a T.E. equal to $(\partial^2\phi/\partial x^2)\Delta x/2$

$$D\phi_i = \frac{1}{\Delta x}\left(\phi_i - \phi_{i-1}\right)$$

- Keeping the first two terms we obtain

$$D\phi_i = \frac{1}{2\Delta x}\left(3\phi_i - 4\phi_{i-1} + \phi_{i-2}\right)$$

  i.e. the second order formula (37) with the truncation error $\Delta x^2/3\ (\partial^3\phi/\partial x^3)$.

Central differences

- Central differences are obtained from eq. (21c), i.e.

$$\delta_x \phi_i = \phi_{i+1/2} - \phi_{i-1/2} = \left(E_x^{1/2} - E_x^{-1/2}\right) \phi_i$$

- Remembering that

$$\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \ldots = \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!} \tag{106}$$

it follows that

$$\delta_x = e^{\Delta x D/2} - e^{-\Delta x D/2} = 2 \sinh\left(\frac{\Delta x D}{2}\right) \tag{107}$$

- The Taylor expansion of $\text{arsinh}\,\phi$ (e.g. $\sinh^{-1})\phi$ is

$$\text{arsinh}\, x = \sum_{n=0}^{\infty} \frac{(-1)^n\,(2n)!}{4^n (n!)^2 (2n+1)} x^{2n+1} \tag{108}$$

therefore, inversion of equation (107) leads to

$$\begin{aligned} \Delta x\, D &= 2\ \text{arsinh}\, \delta_x/2 \\ &= 2\left[\frac{\delta_x}{2} - \frac{1}{2\cdot 3}\left(\frac{\delta_x}{2}\right)^3 + \frac{1\cdot 3}{2\cdot 4\cdot 5}\left(\frac{\delta_x}{2}\right)^5 - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6\cdot 7}\left(\frac{\delta_x}{2}\right)^7 + \ldots\right] \\ &= \delta_x - \frac{\delta_x^3}{24} + \frac{3\,\delta_x^5}{640} - \frac{5\,\delta_x^7}{7168} + \ldots \end{aligned} \tag{109}$$

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Central differences - cont.

- Equation (109) generates a family of central difference schemes of first order derivatives $(\partial\phi/\partial x)_i$ based on values of ϕ at half-integer grid point locations, and are not reported here.
- To derive expressions involving only integer grid points, we could apply the same procedure to the operator $\overline{\delta_x}$

$$\overline{\delta_x} = \left(E_x^{+1} - E_x^{-1}\right) = \left(e^{\Delta x D} - e^{\Delta x D}\right) = 2\sinh(\Delta x D) \tag{110}$$

and therefore

$$\begin{aligned} \Delta x\, D &= \text{arsinh}\, \overline{\delta_x}/2 \\ &= \frac{\overline{\delta_x}}{2} - \frac{1}{2\cdot 3}\left(\frac{\overline{\delta_x}}{2}\right)^3 + \frac{1\cdot 3}{2\cdot 4\cdot 5}\left(\frac{\overline{\delta_x}}{2}\right)^5 + \ldots \\ &= \frac{\overline{\delta_x}}{2} - \frac{\overline{\delta_x}^3}{48} + \frac{3\,\overline{\delta_x}^5}{1280} + \ldots \end{aligned} \tag{111}$$

- This formula, however, is of little help, since the second term leads to a fourth order scheme for $(\partial\phi/\partial x)_i$ involving the four points $i-3$, $i-1$, $i+1$ and $i+3$, rather than $i-2$, $i-1$, $i+1$ and $i+2$.

Central differences - cont.

- A better approach, in order to obtain a general formula for central difference representation of $(\partial \phi / \partial x)_i$, is to start from the identity (22e)

$$\mu_x = \frac{1}{2}(E_x^{1/2} + E_x^{-1/2})$$

It follows

$$\mu_x^2 = \frac{1}{4}\left(E_x^{+1} + E_x^{-1} + 2\,E_x^{1/2}\,E_x^{-1/2}\right) = 1 + \frac{\delta_x^2}{4} \tag{112}$$

and then, using e.g. function `taylor` of the MATLAB *Symbolic Math Toolbox*^{TM}

$$\boxed{\begin{aligned} 1 &= \mu_x \left(1 + \frac{\delta_x^2}{4}\right)^{-1/2} \\ &= \mu_x \left(1 - \frac{\delta_x^2}{8} + \frac{3\delta_x^4}{128} - \frac{5\delta_x^6}{1024} + \frac{35\delta_x^8}{32768} + \dots\right) \end{aligned}} \tag{113}$$

- Observing that

$$\mu_x \delta_x \phi_i = \frac{\overline{\delta_x}}{2}\phi_i$$

we can now multiply equation (113) by equation (109)

Central differences - cont.

- The result is

$$\boxed{\Delta x\, D = \frac{\overline{\delta_x}}{2}\left(1 - \frac{\delta_x^2}{6} + \frac{\delta_x^4}{30} - \frac{\delta_x^6}{140} + \frac{689\,\delta_x^8}{1720320} + \dots\right)} \tag{114}$$

- We can now recover the second order accurate central difference scheme of the first derivative, eq. (8) with a T.E. equal to $(\partial^3\phi/\partial x^3)\Delta x^2/6$, by keeping only the first term of eq.(114)

$$\begin{aligned} D\phi_i &= \frac{\overline{\delta_x}}{2\Delta x}\phi_i \\ &= \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} \end{aligned} \tag{115}$$

- Keeping the first two terms of (114), will result in the 4th order accurate central difference scheme, eq. (41)

$$\begin{aligned} D\phi_i &= \frac{1}{2\Delta x}\overline{\delta_x}\left(1 - \frac{\delta_x^2}{6}\right)\phi_i \\ &= \frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\,\Delta x} \end{aligned} \tag{116}$$

with a T.E equal to $(\partial^5\phi/\partial x^5)\Delta x^4/30$.

Higher order derivatives

- Higher order derivatives can be obtained, with the same approach seen for the first derivative, using the FD operators.
- In CFD the major interest is in second order derivatives.
- For completeness, however, we show some general formulas for *n-th* order derivatives.

Forward differences

- From equation (102)

$$
\begin{aligned}
\left(\frac{\partial^n \phi}{\partial x^n}\right)_i &= D^n \phi_i = \frac{1}{\Delta x^n}\left[\ln\left(1+\Delta_x\right)\right]^n \phi_i \\
&= \frac{\Delta_x^n}{\Delta x^n}\left[1 - \frac{n}{2}\Delta_x + \frac{n(3n+5)}{24}\Delta_x^2 - \frac{n(n+2)(n+3)}{48}\Delta_x^3 + \dots\right]\phi_i
\end{aligned}
\qquad (117)
$$

- It is easy to see that:
  - For $n = 1$ (first order derivative) and keeping only the first term of (117), we recover equation (4), while keeping the first two terms, we obtain the formula (36).
  - For $n = 2$ (second order derivative), we obtain eq.(38) if we keep only the first term, and equation (45) if the first two terms are considered.
  - For arbitrary n (nth order derivative), by keeping just the first term of eq.(117) we recover eq.(31).

Backward differences

- From equation (104)

$$\left(\frac{\partial^n \phi}{\partial x^n}\right)_i = D^n \phi_i = -\frac{1}{\Delta x^n}\left[\ln\left(1-\nabla_x\right)\right]^n \phi_i$$
$$= -\frac{\nabla_x^n}{\Delta x^n}\left[1+\frac{n}{2}\nabla_x+\frac{n(3n+5)}{24}\nabla_x^2+\frac{n(n+2)(n+3)}{48}\nabla_x^3+\dots\right]\phi_i \qquad (118)$$

- Also in this case, one can see that:
  - For $n = 1$ (first order derivative) and keeping just the first term of (118), we obtain equation(6), while keeping also the second term we recover equation (37).
  - For $n = 2$ (second order derivative) and keeping only the first term, it is easy to see that we obtain eq. (39), and we recover eq. (46) by adding also the second term of the formula (118).
  - For arbitrary n (nth order derivative), by keeping only the first term of eq.(118) we recover eq.(32).

Central differences

- Central differences for n *even* can be obtained from equation (109)

$$\left(\frac{\partial^n \phi}{\partial x^n}\right)_i = D^n \phi_i = \left(\frac{2}{\Delta x}\operatorname{arsinh}\delta_x/2\right)^n \phi_i$$
$$= \frac{1}{\Delta x^n}\left[\delta_x - \frac{\delta_x^3}{24}+\frac{3}{640}\delta_x^5-\frac{5}{7168}\delta_x^7+\dots\right]^n \phi_i$$
$$= \frac{1}{\Delta x^n}\delta_x^n\left[1-\frac{n}{24}\delta_x^2+\frac{n}{5760}(22+5n)\,\delta_x^4 - \frac{n}{4^5}\left(\frac{5}{7}+\frac{n-1}{5}+\frac{(n-1)(n-2)}{81}\right)\delta_x^6+\dots\right]\phi_i \qquad (119)$$

- In this case
  - For $n = 2$ (second derivative) and keeping only the first term of formula (119), lead to the well-known three-point expression (9).
  - For $n = 2$ but keeping also the second term, it is easy to verify that we recover equation (44).

Central differences - cont.

- In case of *n odd* (uneven), a general formula can be obtained from eq. (113)

$$\left(\frac{\partial^n \phi}{\partial x^n}\right)_i = D^n \phi_i = \frac{\mu_x}{\left[1 + \delta_x^2/4\right]^{1/2}} \left(\frac{2}{\Delta x} \operatorname{arsinh} \delta_x/2\right)^n \phi_i$$
$$= \frac{\mu_x}{\Delta x^n} \delta_x^n \left[1 - \frac{n+3}{24}\delta_x^2 + \frac{(5n+27)(n+5)}{5760}\delta_x^4 + \dots\right] \phi_i \qquad (120)$$

- For this case
  - For $n = 1$ (first derivative), eq. (8) is obtained from the previous formula keeping only the first term.
  - For $n = 1$ but keeping also the second term of formula (**??**), we recover eq. (41).