Properties of Discretisation Method

In theory, when using computational methods, the numerical results should be indistinguishable from the 'exact' solution when the number of computational cells are indefinitely large. However, in CFD using FV approach, we always use a finite number of cells. Therefore, our numerical results are realistic when the discretisation method have certain properties. Here we discuss a few important properties:

- Conservativeness
- Stability
- Convergence
- Transportiveness
- Accuracy

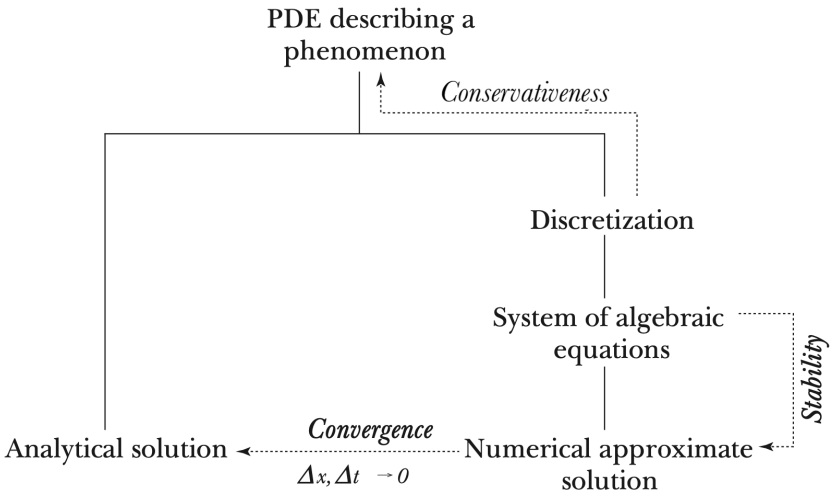

Figure 1: Role of Conservativeness, Stability, Transportiveness, Accuracy, and Convergence in CFD.

Conservativeness

Flow properties conserved over smooth flow as well as flow with steep interface. As you have seen the integration of advection-diffusion dominant flow involve the calculation of flux of properties, diffusive flux (appearing due to shearing rate) and advection fluxes. To ensure that the conservation of property is accounted for in the entire domain, we must ensure that the flux leaving the face of a certain cell, is **exactly equal** to the flux entering the adjacent cell. To achieve this, the flux through a common face should be calculated in a **consistent** manner, using the same expression, in the adjacent cells.
Consider the following system:

$$\frac{\partial u}{\partial t} + \frac{\partial uu}{\partial x} = S$$

Integrating this system over a mesh, and normalizing by Δx, we have:

$$\frac{1}{\Delta x}\int_w^e \frac{\partial u}{\partial t}dx + \frac{1}{\Delta x}\int_w^e \frac{\partial uu}{\partial x}dx = \frac{1}{\Delta x}\int_w^e Sdx$$

On the left, we can take the time derivative out of the integral, and we are left with the definition of a zone average, so this becomes simply$\partial < u > /\partial t$. On the right, we apply the divergence theorem, giving:

$$\frac{\partial < u >_i}{\partial t} + \frac{1}{\Delta x}[uu_{i+1/2} - uu_{i-1/2}] = \frac{1}{\Delta x}\int_w^e Sdx$$

Independent of how we discretize in time, notice that we have the cell-average on the left and that the RHS is simply a difference of fluxes through the interfaces of the zone. For the i + 1 zone, the update would be:

$$\frac{\partial < u >_{i+1}}{\partial t} + \frac{1}{\Delta x}[uu_{i+3/2} - uu_{i+1/2}] = \frac{1}{\Delta x}\int_w^e Sdx$$

Notice that this shares the flux at the i+1/2 interface, but with the opposite sign. When all of the updates are done, the flux through each boundary adds to one zone and subtracts from its neighbor, exactly conserving (to round-off error) the quantity u. This is assuming that $uu_{i+1/2}$ is calculated using same expression and in a **consistent** manner, in both i and $i + 1$ adjacent cells.

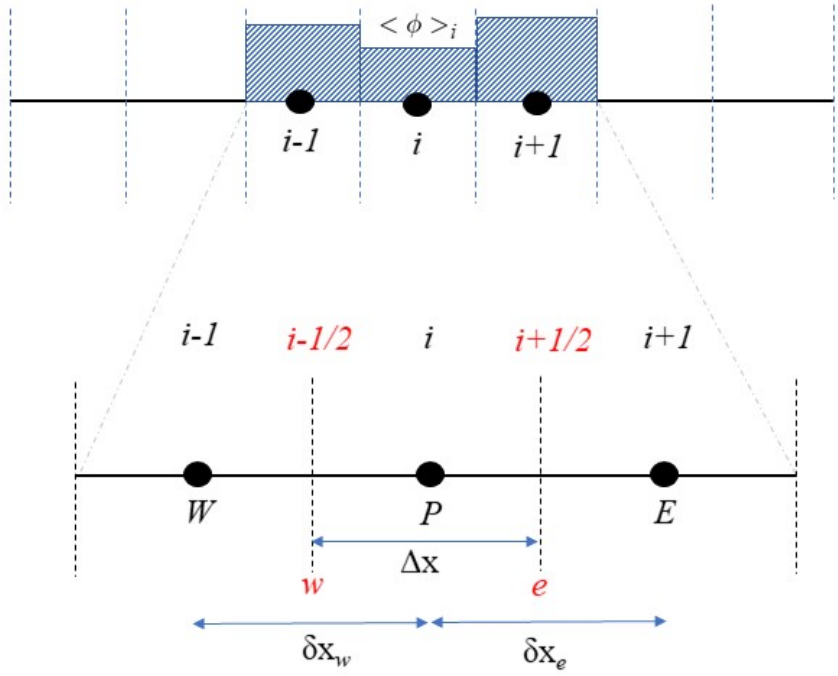

Figure 2: CVs for $i-1$, i, and $i+1$.

Note#1: Note that conservation is not the same as accuracy. We can construct the fluxes for our discretised equation by calling a random number generator and we'd still be conservative, but not at all accurate.
Note#2: This is one of the important short-comings of Finite Differencing methods. As seen, both FD and FV may lead to the same discretized equation, but conceptually the FD method does not ensure **conservativeness**.

Stability

It is a fact of life that numerical approximations to differential equations may exhibit unstable behavior. That is, computational results may include exponentially growing and sometimes oscillating features that bear no relation to the solution of the original differential equation. A scheme is stable if any initially finite perturbation remains bounded as time grows. A scheme is stable if initial errors or small errors at any time remain small while computation progresses. It is unstable if initial errors or small errors at any time get larger and larger, or

eventually get unbounded, as computation advances in time.
Though it may seem a very simple issue, it is interesting to mention that stability is an important property of the numerical methods which is not easy to notice and has not even been discovered by the one who defined the finite difference method for the first time. Will be discussed in the coming weeks!

Convergence

The CFD simulation has the objective of determining some quantity such as lift, drag, recovery, etc. One can track the values of such engineering quantities with respect to iteration and define iterative convergence when these quantities converge. A solution obtained by a numerical scheme is by definition convergent if it is closer and closer to the analytical (exact) solution of the differential equation when the grid size of the discretization tends to zero. The difference between the exact solution and the value of the solution obtained with numerical approximation is called solution error.
There are two different meanings of convergence in numerical analysis; if the discretized interval is getting finer and finer after discretizing the continuous problems, the solution is convergent to the true solution; and for an iterative scheme, convergence means the iteration gets closer and closer to the true solution as computation progresses.

Transportiveness

For a transport phenomenon may be affected by both advection and diffusion. We define a non-dimensional parameter, called Peclet number as the measure of strength of advection (or convection) and diffusion. Let's for instance, return to our 1D NS:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = S + \frac{\partial}{\partial x}(\frac{\mu}{\rho}\frac{\partial u}{\partial x})$$

The Peclet number can be defined as the ratio of advection to diffusion, where $[\mu] = Pa.s$:

$$Pe = \frac{\rho u L}{\mu} \tag{1}$$

For any other physical quantity, ϕ, that is subjected to advection and diffusion:

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = S + \frac{\partial}{\partial x}(K\frac{\partial \phi}{\partial x})$$

The Peclet number, in general, can be defined as:

$$Pe = \frac{uL}{K} \tag{2}$$

Note that in the case of NS equation, the coefficient of diffusivity is replaced with molecular viscosity. However, in the transport equation of mass and heat, this can be replaced with other diffusion coefficients. Figure 2 shows the flow direction and 2 sources of heat/mass/-momentum at w and e. If velocity is negligible or diffusivity is very strong, Figure 2(a) will happen, where the property spreads without being affected by advection:

- **In the case of no advection (convection) and pure diffusion:** $Pe \to 0$

In case of pure diffusion ($Pe \to 0$) the contours will be concentric circles. And the spread of the property will be in all directions. As Pe increases the countours change shapes from circles to elliptical and are shifted in the direction of the flow. Influencing becomes increasingly **biased towards upstream at large** Pe.

- **In the case of no diffusion and pure advection (convection):** $Pe \to \infty$

If velocity is strong or diffusivity is very weak, Figure 2(c) will happen, where the property moves with the flow without spreading. In such case of pure advection/convection ($Pe \to \infty$) the elliptical disappears and the property is simply moving with the flow and the property is transported from points w and e downstream. Therefore the condition at P **is only affected by** w **and not** e. It is important to understand the directionality of the influencing and the Peclet number.

Note#3: As you can see for NS equation, the definition of Pe is very similar to Reynolds number, $Re = uD/\nu$. In turbulent flow, where Reynolds number is high, the impact of molecular diffusion is small and $Pe \to \infty$. In flow with very low Reynolds number, on the other hand, $Pe \to 0$.

Accuracy

- **Truncation Error:** The smaller the discretization, the smaller is the truncation error. It also depends on the order of FD scheme used. To be discussed further later!!

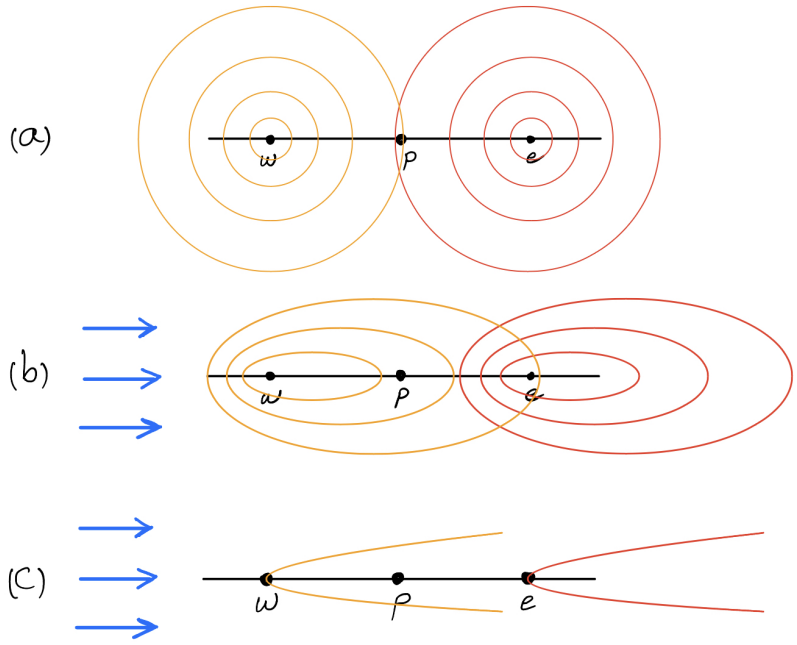

Figure 3: (a) $Pe \to 0$; (b) $Pe > 0$; $Pe \to \infty$.

- **Modeling Error:** human errors, selection of the wrong parameters, improper selection of the governing equations, for instance in selection of the momentum equation, viscosity or turbulent model.