
6.1 The Time-Dependent Scalar-Transport Equation

The time-dependent scalar-transport equation for an arbitrary control volume is

$$\frac{\mathrm{d}}{\mathrm{d}t}(amount) + net\ \ flux = source \tag{1}$$

In discrete form, for every control volume:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V\phi_P) + a_P\phi_P - \sum_F a_F\phi_F = b_P \tag{2}$$

This is a coupled set of equations for solution vector (ϕ_P).

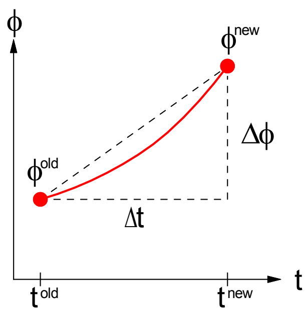
As a preliminary we examine numerical methods for the first-order differential equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = F(t,\phi), \qquad\qquad \phi(0) = \phi_0 \tag{3}$$

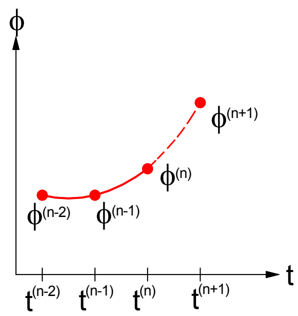
where F is an arbitrary *scalar* function of t and ϕ. Then we extend the methods to CFD, where ϕ and F are vectors corresponding to all nodes of the mesh.

Initial-value problems of the form (3) are solved by *time-marching*. There are two main types of method:

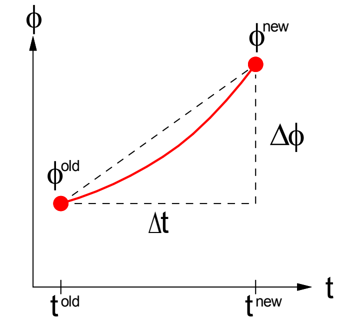
- *one-step* methods: use the value from the previous time level only;



- *multi-step* methods: use values from several previous times.



6.2 One-Step Methods For Single Variables



Consider the first-order differential equation

$$\frac{d\phi}{dt} = F$$

By integration, or from the definition of average slope,

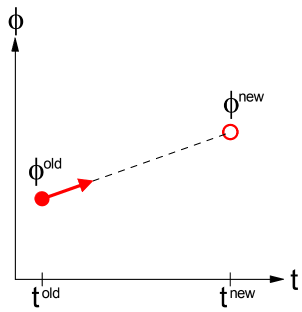
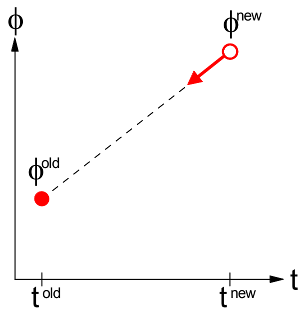
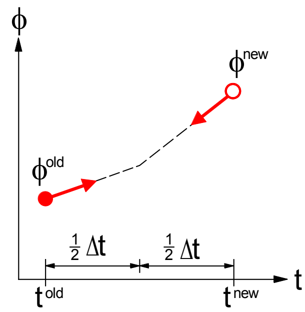
$$\frac{\Delta\phi}{\Delta t} = F^{av} \qquad \text{or} \qquad \Delta\phi = F^{av}\Delta t \tag{4}$$

$$\Rightarrow \qquad \phi^{new} = \phi^{old} + F^{av}\Delta t \tag{5}$$

Since the derivative F depends on the unknown ϕ, the average slope must be estimated.

6.2.1 Simple Estimate of Derivative

There are three obvious methods of estimating the average derivative.

Forward Differencing (Euler Method)	**Backward Differencing (Backward Euler)**	**Centred Differencing (Crank-Nicolson)**
Take F^{av} as the derivative at the *start* of the time-step: $\phi^{new} = \phi^{old} + F^{old}\Delta t$  	Take F^{av} as the derivative at the *end* of the time-step: $\phi^{new} = \phi^{old} + F^{new}\Delta t$  	Take F^{av} as the *average* of derivatives at the beginning and end. $\phi^{new} = \phi^{old} + \frac{1}{2}(F^{old} + F^{new})\Delta t$ 
For: • Easy to implement because *explicit* (the RHS is known).	**For:** • In CFD, no time-step restrictions.	**For:** • Second-order accurate in Δt.
Against: • Only *first-order* in Δt. • In CFD there are time-step restrictions.	**Against:** • Only *first-order* in Δt. • *Implicit*, so needs iteration (but in CFD, no worse than the steady case).	**Against:** • *Implicit*, so needs iteration (but in CFD, no worse than the steady case). • In CFD there are time-step restrictions.

Classroom Example 1

The following differential equation is to be solved on the interval [0,1]:

$$\frac{d\phi}{dt} = t - \phi \ , \qquad \phi(0) = 1$$

Solve this numerically, with a step size $\Delta t = 0.2$ using:
(a) forward differencing;
(b) backward differencing;
(c) centred differencing.

Solve the equation analytically and compare with the numerical approximations.

Classroom Example 2 (Exam 2015 – part)

Solve the equation

$$\frac{d\phi}{dt} = t^2 - 2\phi^2, \qquad \phi(0) = 1$$

numerically on the interval $0 \le t \le 2$, using a timestep $\Delta t = 0.5$, by:
(i) the forward-Euler (explicit) method;
(ii) the backward-Euler (implicit) method.
(iii) the Crank-Nicolson (semi-implicit) method.

Note. Be very careful how you rearrange the implicit schemes for iteration.

6.2.2 Other Methods

For equations of the form $\frac{d\phi}{dt} = F$, improved solutions may be obtained by making successive estimates of the average gradient. Examples include:

Modified Euler method (2 function evaluations; similar to Crank-Nicolson, but explicit)

$$\Delta\phi_1 = \Delta t\, F(t^{old}, \phi^{old})$$

$$\Delta\phi_2 = \Delta t\, F(t^{old} + \Delta t, \phi^{old} + \Delta\phi_1)$$

$$\Delta\phi = \frac{1}{2}(\Delta\phi_1 + \Delta\phi_2)$$

Runge-Kutta (4 function evaluations; strictly this is "4th-order explicit Runge-Kutta")

$$\Delta\phi_1 = \Delta t\, F(\phi^{old}, \qquad t^{old})$$

$$\Delta\phi_2 = \Delta t\, F(t^{old} + \frac{1}{2}\Delta t, \phi^{old} + \frac{1}{2}\Delta\phi_1)$$

$$\Delta\phi_3 = \Delta t\, F(t^{old} + \frac{1}{2}\Delta t, \phi^{old} + \frac{1}{2}\Delta\phi_2)$$

$$\Delta\phi_4 = \Delta t\, F(t^{old} + \Delta t, \phi^{old} + \Delta\phi_3)$$

$$\Delta\phi = \frac{1}{6}(\Delta\phi_1 + 2\Delta\phi_2 + 2\Delta\phi_3 + \Delta\phi_4)$$

For scalar ϕ, such methods are popular. The Runge-Kutta version above is probably the single most widely-used method in engineering. However, in CFD, ϕ and F represent vectors of nodal values, and calculating the derivative F (i.e. evaluating flux and source terms) is very expensive. The majority of CFD calculations are performed with the simpler methods of the previous subsection.

Exercise. Using any computational tool or programming language, solve the Classroom Examples from the previous subsection using Modified-Euler and Runge-Kutta methods.

6.3 One-Step Methods in CFD

General scalar-transport equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V \phi_P) + net\ \ flux = source \tag{6}$$

For one-step methods the time derivative is always discretised as

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V \phi_P) \quad \rightarrow \quad \frac{(\rho V \phi_P)^{new} - (\rho V \phi_P)^{old}}{\Delta t} \tag{7}$$

Flux and source terms are discretised as

$$net\ flux\ -\ source = a_P \phi_P - \sum a_F \phi_F - b_P \tag{8}$$

Different time-marching schemes depend on the time level at which (8) is evaluated.

Forward Differencing

$$\frac{(\rho V \phi_P)^{new} - (\rho V \phi_P)^{old}}{\Delta t} + \left[a_P \phi_P - \sum a_F \phi_F - b_P \right]^{old} = 0$$

Rearranging, and dropping "*new*" superscripts as tacitly understood:

$$\frac{\rho V}{\Delta t} \phi_P = \left[(\frac{\rho V}{\Delta t} - a_P) \phi_P + b_P + \sum a_F \phi_F \right]^{old} \tag{9}$$

Assessment.

- Explicit; no iteration.
- Timestep restrictions: for boundedness, a positive coefficient of ϕ_P^{old} requires

  $$\frac{\rho V}{\Delta t} - a_P \geq 0$$

  i.e.

  $$\Delta t \leq \frac{\rho V}{a_P} \tag{10}$$

- Only first-order accurate in time.

Backward Differencing

$$\frac{(\rho V\phi_P)^{new}-(\rho V\phi_P)^{old}}{\Delta t}+\left[a_P\phi_P-\sum a_F\phi_F-b_P\right]^{new}=0$$

Rearranging, and dropping any "*new*" superscripts as tacitly understood:

$$(\frac{\rho V}{\Delta t}+a_P)\phi_P-\sum a_F\phi_F=b_P+(\frac{\rho V\phi_P}{\Delta t})^{old} \qquad (11)$$

Assessment.

- Implicit (but better than steady-state: more diagonally dominant).
- Straightforward to implement; amounts to a simple change of coefficients:

$$a_P\to a_P+\frac{\rho V}{\Delta t}, \qquad b_P\to b_P+(\frac{\rho V\phi_P}{\Delta t})^{old} \qquad (12)$$

- No timestep restrictions for boundedness.
- Only first-order accurate in time.

Crank-Nicolson

$$\frac{(\rho V\phi_P)^{new}-(\rho V\phi_P)^{old}}{\Delta t}+\frac{1}{2}\left[a_P\phi_P-\sum a_F\phi_F-b_P\right]^{old}+\frac{1}{2}\left[a_P\phi_P-\sum a_F\phi_F-b_P\right]^{new}=0$$

Rearranging, and dropping any "*new*" superscripts as tacitly understood:

$$(\frac{\rho V}{\Delta t}+\frac{1}{2}a_P)\phi_P-\frac{1}{2}\sum a_F\phi_F=\frac{1}{2}b_P+\left[(\frac{\rho V}{\Delta t}-\frac{1}{2}a_P)\phi_P+\frac{1}{2}(b_P+\sum a_F\phi_F)\right]^{old}$$

Multiplying by 2 for convenience:

$$(2\frac{\rho V}{\Delta t}+a_P)\phi_P-\sum a_F\phi_F=b_P+\left[(2\frac{\rho V}{\Delta t}-a_P)\phi_P+(b_P+\sum a_F\phi_F)\right]^{old} \qquad (13)$$

Assessment.

- Implicit.
- Fairly straightforward to implement; amounts to a change of coefficients:

$$a_P\to a_P+2\frac{\rho V}{\Delta t}\ , \qquad b_P\to b_P+\left[(2\frac{\rho V}{\Delta t}-a_P)\phi_P+(b_P+\sum a_F\phi_F)\right]^{old} \qquad (14)$$

- Timestep restrictions: for boundedness, a positive coefficient of ϕ_p^{old} requires

$$2\frac{\rho V}{\Delta t}-a_P\geq 0 \qquad (15)$$

- Second-order accurate in time.

In general, weightings $1-\theta$ and θ can be applied to derivatives at each end of the timestep:

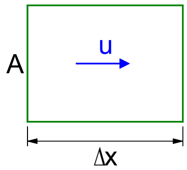
$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V \phi_P) \approx \theta F^{new} + (1-\theta)F^{old} \tag{16}$$

This "θ method" includes the special cases of forward differencing ($\theta = 0$), backward differencing ($\theta = 1$) and Crank-Nicolson ($\theta = ½$).

For $\theta \neq 0$ the method can be implemented by a simple change in matrix coefficients. For $\theta \neq 1$ (i.e. anything other than fully-implicit backward-differencing), boundedness imposes a timestep restriction:

$$\Delta t \leq \frac{1}{1-\theta}\left(\frac{\rho V}{a_P}\right)^{old} \tag{17}$$

Example. Consider a 1-d time-dependent advection problem with no sources:



$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x}(\rho u \phi) = 0$$

Integrating over a cell of length Δx and cross-sectional area A:

$$A\Delta x \frac{(\rho\phi_P)^{new} - (\rho\phi_P)^{old}}{\Delta t} + \rho u A \phi_e^{av} - \rho u A \phi_w^{av} = 0$$

Using the simplest advection scheme – first-order upwind ($\phi_e = \phi_P$, $\phi_w = \phi_W$) – and forward differencing ("*av*" → "old") gives, on multiplying by Δt and dividing by $\rho A \Delta x$:

$$\phi_P^{new} - \phi_P^{old} + \frac{u\Delta t}{\Delta x}(\phi_P^{old} - \phi_W^{old}) = 0$$

or

$$\phi_P^{new} = (1 - \frac{u\Delta t}{\Delta x})\phi_P^{old} + \frac{u\Delta t}{\Delta x}\phi_W^{old} = 0 \tag{18}$$

From the sign of the bracketed term multiplying ϕ_P^{old}, this is *bounded* (i.e. produces no wiggles in time) provided

$$\frac{u\Delta t}{\Delta x} \leq 1$$

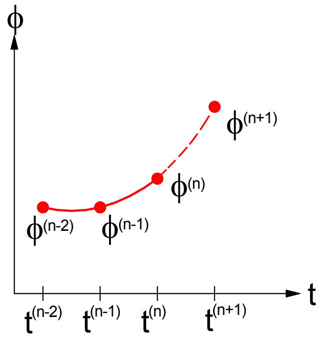
The quantity

$$\boxed{c = \frac{u\Delta t}{\Delta x}} \tag{19}$$

is called the *Courant number*. It can be interpreted physically as the ratio of the distance travelled in one timestep, $u\Delta t$, to the mesh spacing Δx.

For the fully-explicit method the Courant-number restriction $c \leq 1$ means that the distance which information can be advected in one timestep should not exceed the mesh spacing.

6.4 Multi-Step Methods



One-step methods use only information from time level n to calculate $(\mathrm{d}\phi/\mathrm{d}t)^{av}$.

Multi-step methods use the values of ϕ at earlier time levels $n-1$, $n-2$, … as well.

One example is *Gear's method*:

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)^{(n)} = \frac{3\phi^{(n)} - 4\phi^{(n-1)} + \phi^{(n-2)}}{2\Delta t} \qquad (20)$$

This is second-order-accurate in Δt. (*Exercise*: prove it).

A wider class of schemes is furnished by so-called *predictor-corrector* methods which refine their initial *prediction* with one or more explicit *corrections*. A popular example of this type is the *Adams-Bashforth-Moulton* method:

predictor: $$\phi^{n+1}_{pred} = \phi^n + \frac{1}{24}\Delta t\,[-9F^{n-3} + 37F^{n-2} - 59F^{n-1} + 55F^n] \qquad (21)(a)$$

corrector: $$\phi^{n+1} = \phi^n + \frac{1}{24}\Delta t\,[F^{n-2} - 5F^{n-1} + 19F^n + 9F^{n+1}_{pred}] \qquad (21)(b)$$

Advantages:
- high-order time accuracy, stemming from use of multiple time levels;
- good efficiency: fourth-order method stemming from only two new evaluations of F per timestep (Runge-Kutta needs four).

This is a very good scheme for a *scalar* equation; however two particular disadvantages limit its application in CFD:
- *storage*: computational variables have to be stored at all nodes for several time levels;
- *start-up*: initially, only data at time $t = 0$ is available; the first step requires a single-step method (or other information).

6.5 Uses of Time-Marching in CFD

Time-dependent schemes are used in two ways:
(1) for a genuinely time-dependent problem;
(2) for time marching to steady state.

In case (1), accuracy and boundedness often impose restrictions on the timestep and hence how fast one can advance the solution in time. Because all nodal values must be updated at the same rate the timestep Δt is *global*; i.e. the same at all grid nodes.

In case (2), one is not seeking high accuracy so one simply adopts a bounded algorithm: usually backward differencing. Alternatively, if using an explicit or semi-implicit scheme, the timestep can be *local*, i.e. vary from cell to cell, in order to satisfy Courant-number restrictions in each cell individually.

For incompressible flow with fixed domain boundaries, steady flow should be computable without time-marching. This is not the case in compressible flow, where time-marching is necessary in transonic calculations (flows with both subsonic and supersonic regions).

Summary

- The time-dependent fluid-flow equations are first-order in time and are solved by time-marching.

- Time-marching schemes may be *explicit* (average time derivative known at the start of the timestep) or *implicit* (require iteration at each timestep).

- Common one-step methods are forward differencing (explicit), backward differencing (implicit) and Crank-Nicolson (semi-implicit).

- One-step methods are easily implemented via changes to the matrix coefficients. For the backward-differencing scheme this amounts to:

$$a_P \quad \to \quad a_P + \frac{\rho V}{\Delta t} \; , \qquad\qquad b_P \quad \to \quad b_P + \frac{(\rho V \phi_P)^{old}}{\Delta t}$$

- The only unconditionally-bounded two-time-level scheme is backward differencing. Other schemes have time-step restrictions: typically, an upper limit on the *Courant number*

$$c = \frac{u\Delta t}{\Delta x}$$

- The Crank-Nicolson scheme is second-order accurate in Δt. The backward-differencing and forward-differencing schemes are both first order in Δt, which means they need smaller timesteps to achieve the same time accuracy.

- *Multi-step* methods may be used to achieve higher accuracy. However, these are less favoured in CFD because of large storage overheads.

- Time-accurate solutions require a *global* timestep. A *local* timestep may be used for time-marching to steady state. In the latter case, high time accuracy is not required and backward differencing is favoured because it is unconditionally bounded and does not affect the final state.

Examples

Q1. (Exam 2010 – part; minor rewording)

(a) The equation

$$\frac{d\phi}{dt} = t + \phi^2, \qquad \phi(0) = 1.0,$$

is to be solved numerically, using a time step $\Delta t = 0.1$. Solve this equation up to time $t = 0.5$ using

(i) forward differencing ("fully-explicit");

(ii) backward differencing ("fully-implicit").

(b) Define what is meant in general by *explicit* and *implicit* schemes for timestepping, and state an advantage and disadvantage for each.

(c) Both of the methods in part (a) are first-order accurate in time. Define a second-order accurate method for equations of the type

$$\frac{d\phi}{dt} = f(t, \phi)$$

for arbitrary function $f(t, \phi)$, using only two time levels.

Q2.

Gear's scheme for the approximation of a time derivative is

$$\left(\frac{d\phi}{dt}\right)^{(n)} = \frac{3\phi^{(n)} - 4\phi^{(n-1)} + \phi^{(n-2)}}{2\Delta t}$$

where superscripts $(n-2)$, $(n-1)$, (n) denote successive time levels. Show that this scheme is second-order accurate in time.

Q3. (Exam 2014 – part)

Use time-centred differencing to solve the differential equation

$$\frac{d\phi}{dt} = t - 2\phi^2, \qquad \phi(1) = 2$$

on the interval $1 \le t \le 2$, using a timestep $\Delta t = 0.5$.

Q4. (Exam 2008 – part)

(a) Solve the first-order differential equation

$$\frac{1}{\phi^2}\frac{d\phi}{dt} = 1 - \phi t \ , \qquad \phi(0) = 1$$

with a timestep $\Delta t = 0.25$ on the interval $0 \le t \le 1$, using:

(i) forward differencing;

(ii) backward differencing.

(b) State (without mathematical detail) the advantages and disadvantages of using:

(i) forward-differencing

(ii) backward-differencing

methods in computational fluid dynamics.

Q5. (Exam 2012)

The 1-d time-dependent advection-diffusion equation for a scalar ϕ can be written

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x}(\rho u\phi - \Gamma\frac{\partial\phi}{\partial x}) = s \qquad (*)$$

where ρ is density, u is velocity, Γ is diffusivity and s is source density.

(a) By integrating over an interval $[x_w, x_e]$ (a 1-d volume) show that equation (*) can be written in a corresponding conservative integral form. State what is meant by *fluxes* in this context, identify the advective and diffusive fluxes and explain in what sense their treatment is *conservative*.

(b) Time-stepping schemes similar to those used for solving the unsteady advection-diffusion equation may be used to solve simpler ordinary differential equations of the form $d\phi/dt = f(t, \phi)$. Solve the equation

$$\frac{d\phi}{dt} = 1 - t - \phi^2, \qquad \phi(0) = 1,$$

for $\phi(t)$ in the domain $0 \le t \le 2$ with a time step $\Delta t = 0.5$ using:

(i) forward-differencing

(ii) backward-differencing

(iii) centred-differencing (Crank-Nicolson)

timestepping schemes.

(c) State the advantages and disadvantages of each of the timestepping schemes in part (b) when used to solve the time-dependent advection-diffusion equation.

Q6. (Exam 2017 – part)
The equation

$$(\phi + t)\frac{\mathrm{d}\phi}{\mathrm{d}t} = -\phi^2, \qquad \phi(0) = 2$$

is to be solved numerically with timestep $\Delta t = 0.25$.

(a) Find the value of ϕ at $t = 1$ using the:
 (i) forward-Euler (fully-explicit) method;
 (ii) Crank-Nicolson (semi-implicit) method.

(b) State which of the schemes in part (a) you expect to give a more accurate answer and explain your reasoning.