
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 Section 4 it was shown how the flux and source terms could be discretised as

$$net\ \ flux - source = a_P\phi_P - \sum_F a_F\phi_F - b_P \tag{2}$$

In this section the time derivative will also be discretised.

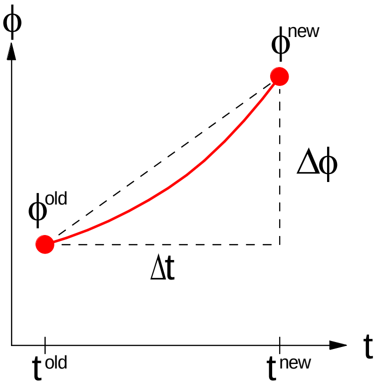
As a preliminary we first examine numerical methods for the first-order differential equation

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

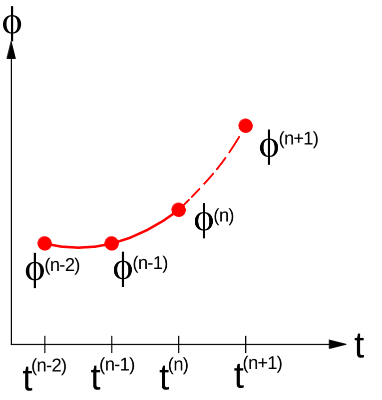
where F is an arbitrary **scalar** function of t and ϕ. Then we extend the methods to CFD (where ϕ and F refer to all nodes of the mesh).

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

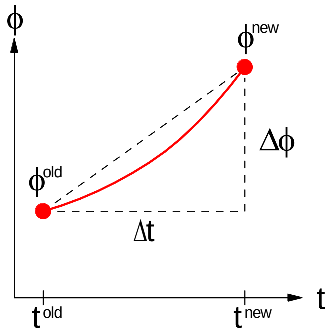
- *one-step* methods: use the value from the previous time level only;



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



6.2 One-Step Methods For Single Variables



For the first-order differential equation

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

By integration, or from the definition of average slope,

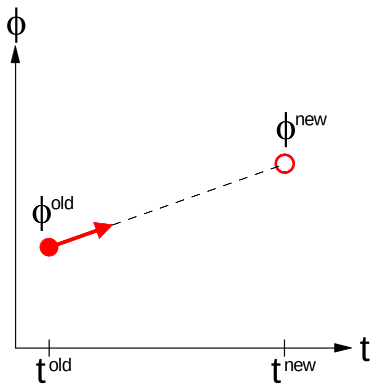
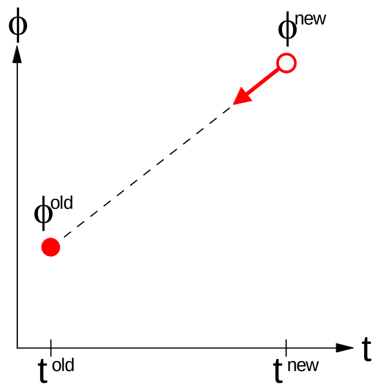
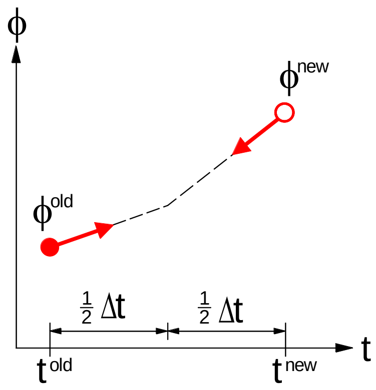
$$\frac{\Delta\phi}{\Delta t} = F^{av} \qquad \text{or} \qquad \Delta\phi = F^{av}\Delta t \tag{4}$$

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

Since derivative F depends on the unknown solution 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 Δt = 0.2 using:

(a) forward differencing;
(b) backward differencing;
(c) Crank-Nicolson.

Solve the equation analytically and compare with the numerical approximations.

Classroom Example 2

The equation

$$\frac{d\phi}{dt} = t - \phi^4\,, \qquad \phi = 2 \text{ when } t = 0,$$

is to be solved numerically, using a timestep Δt = 0.1. Solve this equation up to time t = 0.4 using the following approaches to time-marching:

(a) forward differencing (“fully-explicit”);
(b) backward differencing (“fully-implicit”);
(c) centred differencing (“semi-implicit”).

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

6.2.2 Other Methods

For equations of the form $\frac{\mathrm{d}\phi}{\mathrm{d}t} = F$, 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)

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

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

$$\Delta\phi_1 = \Delta t\, F(\phi^{old}, t^{old})$$
$$\Delta\phi_2 = \Delta t\, F(t^{old} + \tfrac{1}{2}\Delta t, \phi^{old} + \tfrac{1}{2}\Delta\phi_1)$$
$$\Delta\phi_3 = \Delta t\, F(t^{old} + \tfrac{1}{2}\Delta t, \phi^{old} + \tfrac{1}{2}\Delta\phi_2)$$
$$\Delta\phi_4 = \Delta t\, F(t^{old} + \Delta t, \phi^{old} + \Delta\phi_3)$$
$$\Delta\phi = \tfrac{1}{6}(\Delta\phi_1 + 2\Delta\phi_2 + 2\Delta\phi_3 + \Delta\phi_4)$$

For scalar ϕ, such methods are popular. Runge-Kutta 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 (evaluating flux and source terms) is very expensive. The majority of CFD calculations are performed with the simpler methods of 6.2.1.

Exercise. Using any computational tool 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:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V\phi_P) + net\ \ flux - source = 0 \tag{6}$$

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 could be discretised at any particular time level 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.

<u>Forward Differencing</u>

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

Rearranging, and dropping any "*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 simultaneous equations to be solved.
- Timestep restrictions; for boundedness, a positive coefficient of ϕ_p^{old} requires

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

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:

$$(\frac{\rho V}{\Delta t} + a_P)\phi_P - \sum a_F\phi_F = b_P + (\frac{\rho V\phi_P}{\Delta t})^{old} \qquad (10)$$

Assessment.

- Straightforward to implement; amounts to a simple change of coefficients:

$$a_P \to a_P + \frac{\rho V}{\Delta t} \qquad\qquad b_P \to b_P + (\frac{\rho V\phi_P}{\Delta t})^{old} \qquad (11)$$

- No timestep restrictions.

Crank-Nicolson

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

Rearranging, and dropping any "*new*" superscripts:

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

Multiplying by 2 for convenience:

$$(2\frac{\rho V}{\Delta t} + a_P)\phi_P - \sum a_F\phi_F = b_P + \left[(2\frac{\rho V}{\Delta t} - a_P)\phi_P + (b_P + \sum a_F\phi_F)\right]^{old} \qquad (12)$$

Assessment.

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

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

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

$$2\frac{\rho V}{\Delta t} - a_P \ge 0$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V \phi_P) \approx \theta F^{new} + (1-\theta) F^{old} \tag{14}$$

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

For $\theta \neq 0$ this so-called "θ 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

$$\Delta t < \frac{1}{1-\theta}\left(\frac{\rho V}{a_P}\right)^{old} \tag{15}$$

Example. Consider a 1-d time-dependent advection-diffusion problem

$$\frac{\partial}{\partial t}(\rho \phi) + \frac{\partial}{\partial x}\left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x}\right) = S$$

With the first-order upwind advection scheme on a uniform grid of spacing Δx, it is readily found that the coefficients in the flux-source discretisation are

$$a_W = D + C, \qquad a_E = D, \qquad a_P = a_W + a_E = 2D + C$$

where the mass flow rate C and diffusive transfer coefficient D are given by

$$C = \rho u A, \qquad D = \frac{\Gamma A}{\Delta x}$$

In the 1-d case the cross-sectional area $A = 1$ and the time-step restriction (15) becomes

$$\frac{2\Gamma \Delta t}{\rho (\Delta x)^2} + \frac{u \Delta t}{\Delta x} < \frac{1}{1-\theta}$$

Special cases are:–

- explicit (forward differencing; $\theta = 0$) and pure diffusion ($u = 0$): $\frac{(\Gamma/\rho)\Delta t}{(\Delta x)^2} < \frac{1}{2}$
- explicit (forward differencing; $\theta = 0$) and pure advection ($\Gamma = 0$): $\frac{u \Delta t}{\Delta x} < 1$
- implicit (backward differencing; $\theta = 1$): no restrictions.

<u>Courant Number</u>

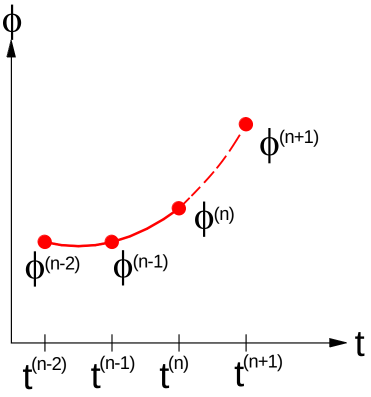
The *Courant number c* is defined by:

$$\boxed{c = \frac{u \Delta t}{\Delta x}} \tag{16}$$

It can be interpreted as the ratio of distance travelled at speed u in one timestep Δt to the mesh spacing Δx.

For the fully-explicit method the Courant-number restriction $c < 1$ 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 $t^{(n)}$ to calculate $(d\phi/dt)^{av}$.

Multi-step methods use the values of ϕ at earlier time levels as well: $\phi^{(n-1)}$, $\phi^{(n-2)}$, ...

One example is *Gear's method*:

$$\left(\frac{d\phi}{dt}\right)^{(n)} = \frac{3\phi^{(n)} - 4\phi^{(n-1)} + \phi^{(n-2)}}{2\Delta t} \tag{17}$$

This is second-order 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) *corrections*. A popular example of this type is the *Adams-Bashforth-Moulton* method:

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

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

Just as three-point advection schemes permit greater spatial accuracy than two-point schemes, so the use of multiple time levels allows greater temporal accuracy. However, there are a number of disadvantages which limit their application in CFD:

- **storage**: each computational variable has to be stored at all nodes at each time level;
- **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 stability 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.

In practice, 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* (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.

Examples

Q1.
Use: (a) forward-differencing; (b) backward-differencing to solve the equation

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

numerically over the interval $0 \le t \le 1$, using a timestep $\Delta t = 0.25$.

Q2.
Gear's scheme for the approximation of a time derivative is

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

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

Q3.
The semi-discretised version of the scalar transport equation

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

over a control volume, centred at node P and containing fluid mass ρV, can be written

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

(a) Show that time integration using backward differencing, with a timestep Δt, can be implemented by simple changes to the coefficients a_P, $\{a_F\}$ and b_P.

(b) Show that time integration using forward differencing is explicit, but imposes a maximum timestep for boundedness.

(c) Show that time integration using the Crank-Nicolson method, with a timestep Δt, can be implemented by changes to the coefficients a_P, $\{a_F\}$ and b_P and derive an expression for the maximum timestep for boundedness.

Q4. (Exam 2008 – part)

(a) Solve the first-order differential equation

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

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 one-dimensional 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 $\mathrm{d}\phi/\mathrm{d}t = f(t,\phi)$. Solve the equation

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

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)

time-stepping 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.

For the equation

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

use the following methods with a timestep $\Delta t = 0.25$ to find the value of ϕ at $t = 1$:

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

(b) backward differencing ("fully-implicit");

(c) centred differencing ("semi-implicit").

Q7. (Exam 2013 – part)

(a) For the equation

$$(t+\phi)\frac{\mathrm{d}\phi}{\mathrm{d}t} = -2\phi^3, \qquad \text{where } \phi = 1 \text{ at } t = 0,$$

use the following timestepping methods with timestep $\Delta t = 0.25$ to estimate the value of ϕ at $t = 1$:

(i) forward differencing (forward Euler);

(ii) centred differencing (Crank-Nicolson).

(b) For a fixed timestep, which of the integration methods in (a) might be expected to give the most accurate results, and why?