Advection and Diffusion

$$\frac{\partial c}{\partial t} + u\,\frac{\partial c}{\partial x} + v\,\frac{\partial c}{\partial y} + w\,\frac{\partial c}{\partial z} =$$
$$\frac{\partial}{\partial x}\left(\mathcal{A}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mathcal{A}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\kappa\frac{\partial c}{\partial z}\right) + S - Kc,$$

First and Second Moments of Advection-Diffusion of Tracer

1 Mean over a volume

When we integrate Equation (6.2) over the domain volume $\mathcal{V}$, we can readily integrate the diffusion terms and, if the flux is zero at all boundaries, these vanish, and we obtain:

$$\frac{d}{dt}\int_{\mathcal{V}} c\, d\mathcal{V} \;=\; -\int_{\mathcal{V}}\left(u\,\frac{\partial c}{\partial x}+v\,\frac{\partial c}{\partial y}+w\,\frac{\partial c}{\partial z}\right) d\mathcal{V} \;+\; \int_{\mathcal{V}} S\, d\mathcal{V} \;-\; \int_{\mathcal{V}} K c\, d\mathcal{V}.$$

After an integration by parts, the first set of terms on the right can be rewritten as

$$\frac{d}{dt}\int_{\mathcal{V}} c\, d\mathcal{V} \;=\; +\int_{\mathcal{V}} c\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right) d\mathcal{V} \;+\; \int_{\mathcal{V}} S\, d\mathcal{V} \;-\; \int_{\mathcal{V}} K c\, d\mathcal{V},$$

as long as there is no flux or no advection at all boundaries. Invoking the continuity equation (4.21d) reduces the first term on the right to zero, and we obtain simply:

$$\frac{d}{dt}\int_{\mathcal{V}} c\, d\mathcal{V} \;=\; \int_{\mathcal{V}} S\, d\mathcal{V} \;-\; \int_{\mathcal{V}} K c\, d\mathcal{V}. \tag{6.4}$$

2 Variance over a volume

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{\mathcal{V}} c^2\, d\mathcal{V} \;&=\; -\int_{\mathcal{V}}\left[\mathcal{A}\left(\frac{\partial c}{\partial x}\right)^2+\mathcal{A}\left(\frac{\partial c}{\partial y}\right)^2+\kappa\left(\frac{\partial c}{\partial z}\right)^2\right] d\mathcal{V}\\ &\quad+\; \int_{\mathcal{V}} S c\, d\mathcal{V} \;-\; \int_{\mathcal{V}} K c^2\, d\mathcal{V}.\end{aligned} \tag{6.5}$$

This conservation property can be extended, still in the absence of diffusion, source and sink, to any power c^p of c, by multiplying the equation by c^{p-1} before integration. The

Hard to find numerical schemes that conserve all the higher moments.

3

Advection only redistributes existing values, thus not changing either minimum and maximum, max/min property
numerical scheme that have this properties are called *monotonic schemes* or *monotonicity preserving.* Also, c should always remain positive --> *positiveness*

3 properties: conservation of tracer, variance and min/max

Advection vs Diffusion

$$\frac{\text{advection}}{\text{diffusion}} = \frac{U\Delta c/L}{D\Delta c/L^2} = \frac{UL}{D}.$$

Peclet Number

If $Pe \gg 1$ (in practice, if $Pe > 10$)

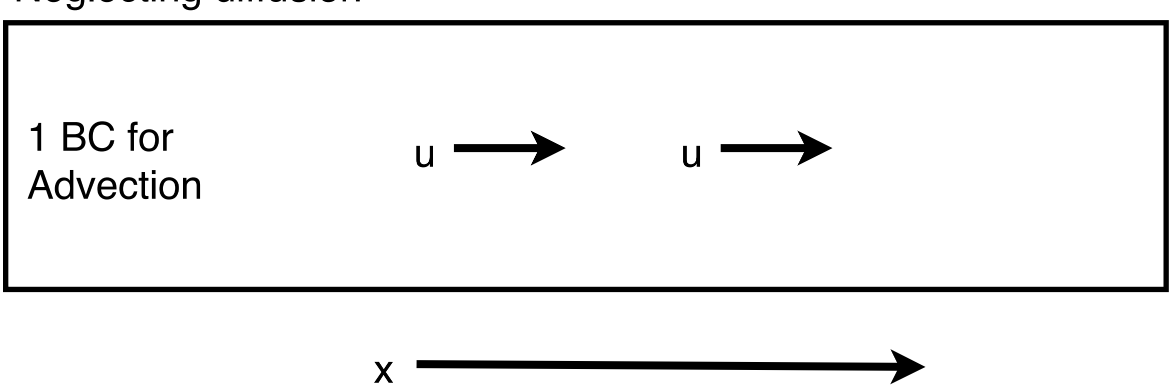
Advection dominated regime

Advection may dominate the horizontal while diffusion may dominate the vertical

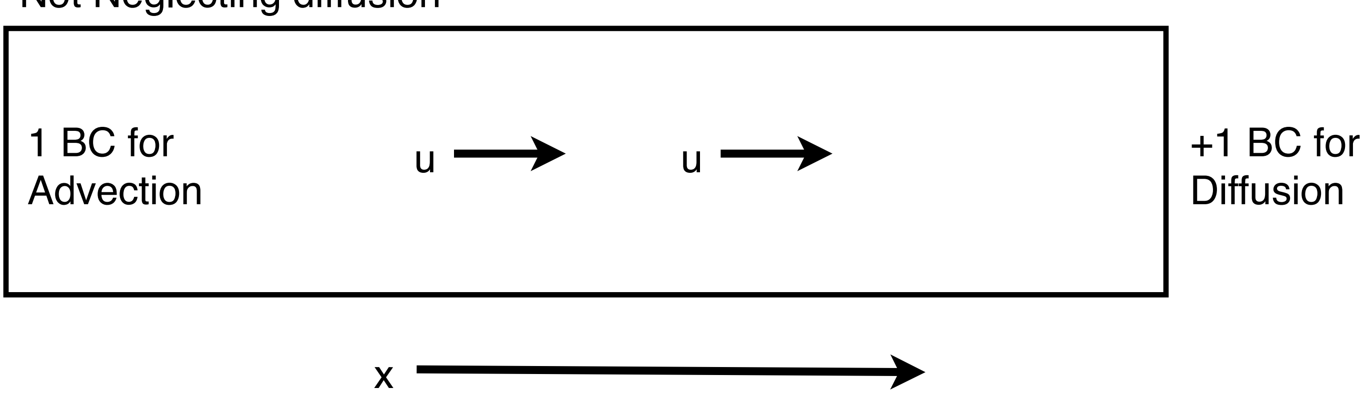
$$\frac{\partial c}{\partial t} + u\,\frac{\partial c}{\partial x} + v\,\frac{\partial c}{\partial y} = \frac{\partial}{\partial z}\left(\kappa\frac{\partial c}{\partial z}\right) + S - Kc.$$

(e.g. in ocean models, horizontal advection may be resolved while vertical advection needs parameterization)

Neglecting diffusion



Not Neglecting diffusion

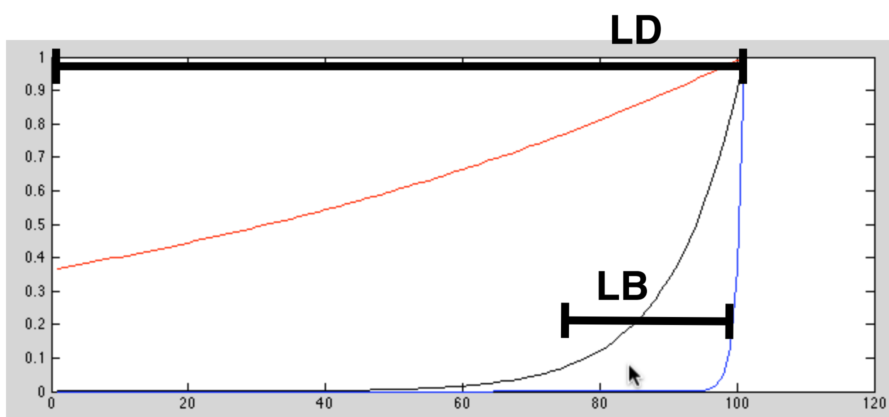


$$u \frac{dc}{dx} = \mathcal{A} \frac{d^2 c}{dx^2},$$

$$c(x) = C_0 + C_1 \, e^{ux/\mathcal{A}}.$$

u/A = L/T / L2/T =1/LB e-folding length scale

Peclet Number = **LD / LB**



Peclet Number = **LD / LB**

If **LX / LD > LB / LD**
that is the grid size of the model is larger than the boundary later, than diffusion must be neglected

grid size LX

6.4 Centered and upwind advection schemes

In GFD, advection is generally dominant compared to diffusion, and we therefore begin with the case of pure advection of a tracer concentration $c(x,t)$ along the x–direction. The aim is to solve numerically the following equation:

$$\frac{\partial c}{\partial t} + u\,\frac{\partial c}{\partial x} = 0. \tag{6.10}$$

If u>0 and constant

$$c(x,t) = c_0(x - ut)$$

$$\frac{d\bar{c}_i}{dt} + \frac{q_{i+1/2} - q_{i-1/2}}{\Delta x} = 0, \qquad q_{i-1/2} = uc\big|_{i-1/2},$$

finite volume approach

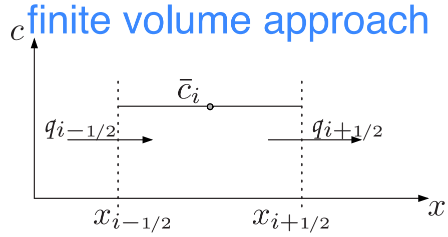


Figure 6-3 One-dimensional finite-volume approach with fluxes at the interfaces between grid cells for a straightforward budget calculation.

approximation of the flux in between cells

$$\tilde{q}_{i-1/2} = u\left(\frac{\bar{c}_i + \bar{c}_{i-1}}{2}\right)$$

resulting equation

$$\frac{d\bar{c}_i}{dt} = -\,u\,\frac{\bar{c}_{i+1} - \bar{c}_{i-1}}{2\Delta x}.$$

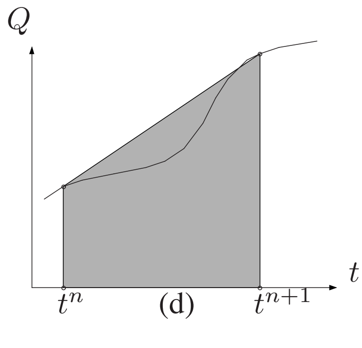
this form of the equation conserves the total amount of substance and its variance (only for semi-discrete form, properties are lost when adding time discretization)

$$\textstyle\sum_i \bar{c}_i \text{ and } \sum_i (\bar{c}_i)^2$$

An example of time-discretization that conserves variance.

Trapezoidal

Recall Trapezoidal scheme or Euler semi-implicit



$$u(t^{n+1}) = u(t^n) + \int_{t^n}^{t^{n+1}} Q\, dt,$$

$$\boxed{\tilde{u}^{n+1} = \tilde{u}^n + \frac{\Delta t}{2}\left(Q^n + Q^{n+1}\right)}$$

$$\frac{d\tilde{c}_i}{dt} + \mathcal{L}(\tilde{c}_i) = 0, \tag{6.15}$$

where $\mathcal{L}$ stands for a linear discretization operator applied to the discrete field $\tilde{c}_i$. For our centered advection, the operator is $\mathcal{L}(\tilde{c}_i) = u(\tilde{c}_{i+1} - \tilde{c}_{i-1})/(2\Delta x)$. Suppose that the operator is designed to satisfy conservation of variance, which demands that at any moment t and for any discrete field $\tilde{c}_i$ the following relation holds:

$$\sum_i \tilde{c}_i \mathcal{L}(\tilde{c}_i) = 0, \tag{6.16}$$

because only then does $\sum_i \tilde{c}_i \, d\tilde{c}_i/dt$ vanish according to (6.15) and (6.16). The trapezoidal time discretization applied to (6.15) leads to

$$\boxed{\frac{\tilde{c}_i^{n+1} - \tilde{c}_i^n}{\Delta t} = -\frac{\mathcal{L}(\tilde{c}_i^{n+1}) + \mathcal{L}(\tilde{c}_i^n)}{2}} = -\frac{1}{2}\mathcal{L}(\tilde{c}_i^{n+1} + \tilde{c}_i^n), \tag{6.17}$$

where the last equality follows from the linearity of operator $\mathcal{L}$. Multiplying this equation by $(\tilde{c}_i^{n+1} + \tilde{c}_i^n)$ and summing over the domain then yields

$$\sum_i \frac{(\tilde{c}_i^{n+1})^2 - (\tilde{c}_i^n)^2}{\Delta t} = -\frac{1}{2}\sum_i (\tilde{c}_i^{n+1} + \tilde{c}_i^n)\mathcal{L}(\tilde{c}_i^{n+1} + \tilde{c}_i^n). \tag{6.18}$$

The term on the right is zero by virtue of (6.16). Therefore, any spatial discretization scheme that conserves variance continues to conserve variance if the trapezoidal scheme is used for the time discretization. As an additional benefit, the resulting scheme is also unconditionally stable. This does not mean, however, that the scheme is satisfactory, as Numerical Exercise 6-9 shows for the advection of the top-hat signal. Furthermore, there is a price to pay for stability because a system of simultaneous linear equations needs to be solved at each time step if the operator $\mathcal{L}$ uses several neighbors of the local grid point i.

An example of time-discretization

Leapfrog from t-1 to t+1 (2 timesteps)

$$\bar{c}_i^{n+1} = \bar{c}_i^{n-1} - 2\,\frac{\Delta t}{\Delta x}\left(\hat{q}_{i+1/2} - \hat{q}_{i-1/2}\right)$$

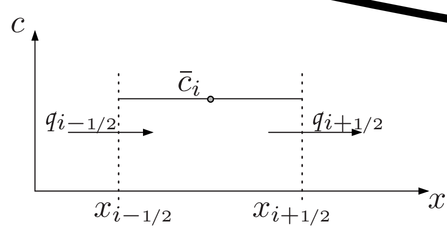


Figure 6-3 One-dimensional finite-volume approach with fluxes at the interfaces between grid cells for a straightforward budget calculation.

average flux between time interval

$$\hat{q}_{i-1/2} = \frac{1}{2\Delta t}\int_{t^{n-1}}^{t^{n+1}} uc\big|_{i-1/2}\, dt \quad \rightarrow \quad \tilde{q}_{i-1/2} = u\left(\frac{\tilde{c}_i^n + \tilde{c}_{i-1}^n}{2}\right),$$

solve equation to obtain

$$\tilde{c}_i^{n+1} = \tilde{c}_i^{n-1} - \mathsf{C}\left(\tilde{c}_{i+1}^n - \tilde{c}_{i-1}^n\right),$$

where the coefficient C is defined as

Courant number or CFL parameter $\quad \mathsf{C} = \dfrac{u\Delta t}{\Delta x}.$

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0.$$

If u>0 and constant

$$c(x,t) = c_0(x-ut)$$

$$c(x-ut) = \text{constant}.$$

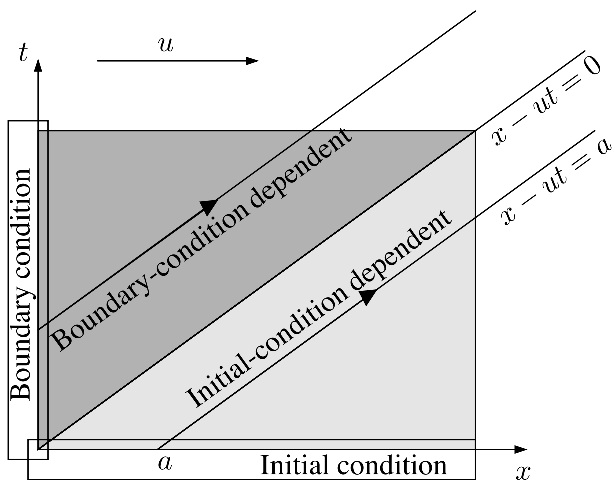
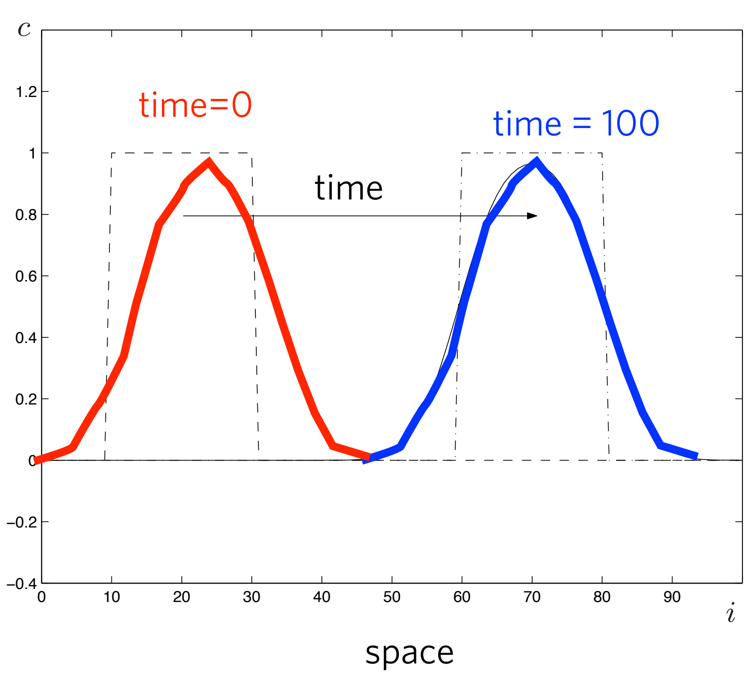


Figure 6-4 The characteristic line $x - ut = a$ propagates information from the initial condition or boundary condition into the domain. If the boundary is located at $x = 0$ and the initial condition given at $t = 0$, the line $x = ut$ divides the space-time frame into two distinct regions: For $x \leq ut$ the boundary condition defines the solution whereas for $x \geq ut$ the initial condition defines the solution.



no need of BC at this boundary, however numerical scheme needs one (artificial boundary condition)

Figure 6-8 Upwind scheme with $\mathsf{C} = 0.5$ applied to the advection of a "top-hat" signal after 100 times steps. Ideally the signal should be translated without change in shape by 50 grid points, but the solution is characterized by a certain diffusion and a reduction in gradient.

m=right boundary

$$\tilde{c}_i^{n+1} = \tilde{c}_i^{n-1} - \mathsf{C}\left(\tilde{c}_{i+1}^n - \tilde{c}_{i-1}^n\right),$$

$$\tilde{c}_m^{n+1} = \tilde{c}_m^{n-1} - 2\mathsf{C}\left(\tilde{c}_m^n - \tilde{c}_{m-1}^n\right)$$

Stability analysis (see book for details on the Newman method)

$$\tilde{c}_i^n = A\, e^{\mathrm{i}\,(k_x\; i\Delta x \,-\, \tilde{\omega}\; n\Delta t)}$$

$$\tilde{c}_i^{n+1} = \tilde{c}_i^{n-1} - \mathsf{C}\left(\tilde{c}_{i+1}^n - \tilde{c}_{i-1}^n\right),$$

Conditionally stable

$$\mathsf{C} = \frac{u\Delta t}{\Delta x}.$$

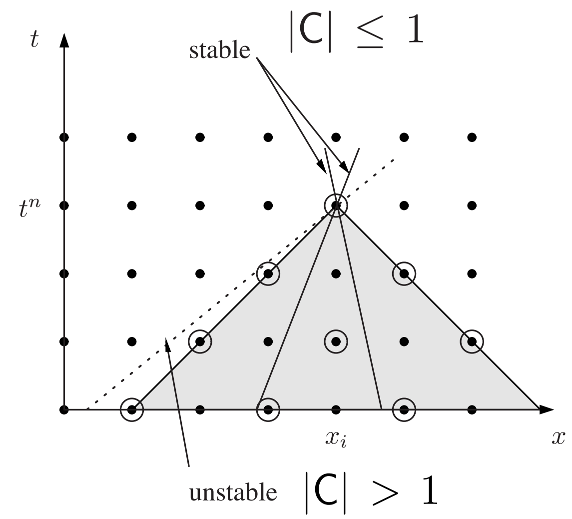
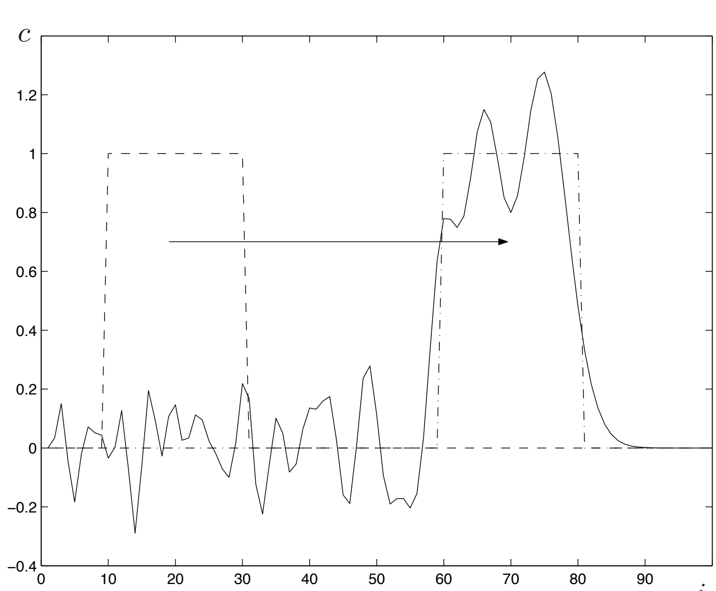


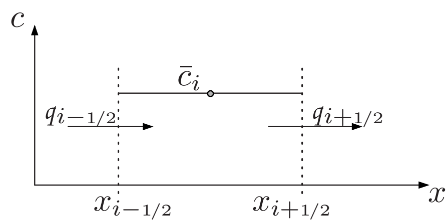
Figure 6-5 Numerical domain of dependence of the leapfrog scheme (in gray) covered by the points (circled dots) that influence the calculation at point i, n. This network of points is constructed recursively by identifying the grid points involved in prior calculations. The physical solution is only influenced by values along the characteristic. If the characteristic falls into the numerical domain of dependence (one of the solid lines for example), this value can be captured by the numerical grid. On the contrary, when the physical characteristic is not included in the numerical domain of dependence (dashed line for example), the numerical scheme uses only information that is physically unrelated to the advection process, and the scheme is unstable. Also note that for the leapfrog scheme the domain of dependence defines a checkerboard pattern and that the grid in (x, t) space includes two numerically independent sets of values (circled and non-circled dots).



the scheme ignores the physical bias of advection (e.g. only upstream information should be used)

Figure 6-6 Leapfrog scheme applied to the advection of a "top-hat" signal with $\mathsf{C} = 0.5$ for 100 times steps. The exact solution is a mere translation from the initial position (dashed curve on the left) by 50 grid points downstream (dash-dotted curve on the right). The numerical method generates a solution that is roughly similar to the exact solution, with the solution varying around the correct value.

upwind or *donor cell* scheme



First-order upwind scheme [edit]

The simplest upwind scheme possible is the first-order upwind scheme. It is given by[2]

$$(1) \qquad \frac{u_i^{n+1}-u_i^n}{\Delta t}+a\frac{u_i^n-u_{i-1}^n}{\Delta x}=0 \quad \text{for} \quad a>0$$

$$(2) \qquad \frac{u_i^{n+1}-u_i^n}{\Delta t}+a\frac{u_{i+1}^n-u_i^n}{\Delta x}=0 \quad \text{for} \quad a<0$$

Compact form [edit]

Defining

$$a^+=\max(a,0)\,, \qquad a^-=\min(a,0)$$

and

$$u_x^-=\frac{u_i^n-u_{i-1}^n}{\Delta x}\,, \qquad u_x^+=\frac{u_{i+1}^n-u_i^n}{\Delta x}$$

the two conditional equations (1) and (2) can be combined and written in a compact form as

$$(3) \qquad u_i^{n+1}=u_i^n-\Delta t\left[a^+u_x^-+a^-u_x^+\right]$$

Equation (3) is a general way of writing any upwind-type schemes.

Stability [edit]

The upwind scheme is stable if the following Courant–Friedrichs–Lewy condition (CFL) condition is satisfied.[3]

$$c=\left|\frac{a\Delta t}{\Delta x}\right|\leq 1.$$

A Taylor series analysis of the upwind scheme discussed above will show that it is first-order accurate in space and time

For a positive velocity (e.g. downstream)

$$\tilde{c}_i^{n+1} = \tilde{c}_i^n - \mathrm{C}\left(\tilde{c}_i^n-\tilde{c}_{i-1}^n\right).$$

upwind or *donor cell* scheme

upwind scheme

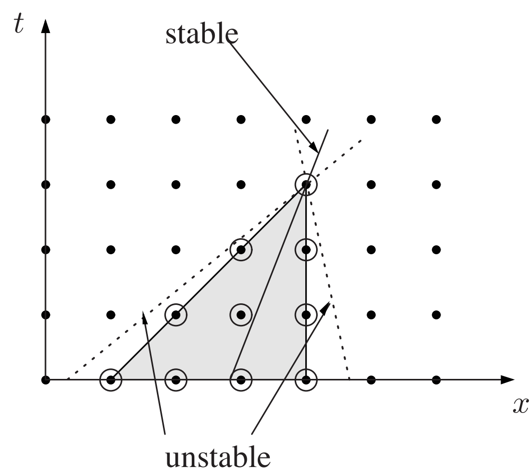
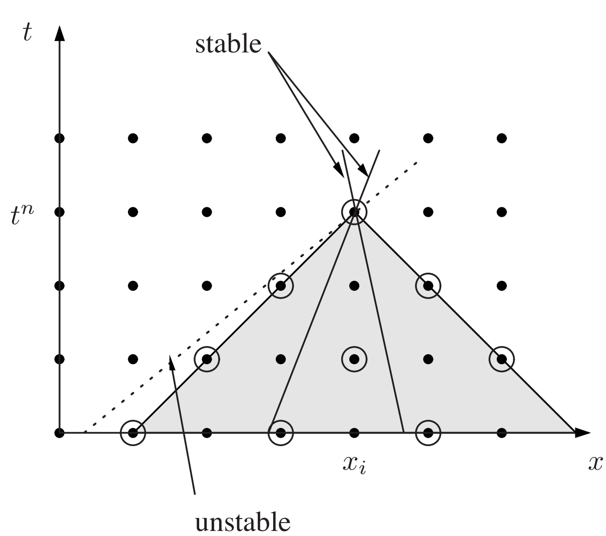
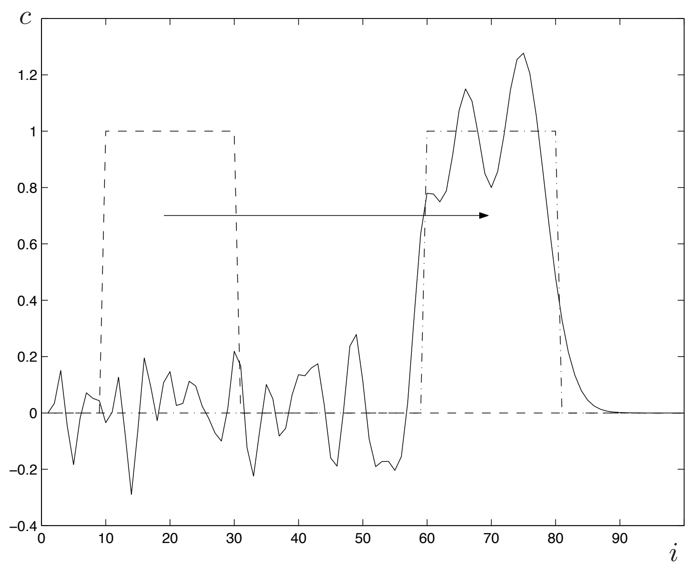


Figure 6-7 Domain of dependence of the upwind scheme. If the characteristic (dashed line) lies outside the numerical domain of dependence, unphysical behavior will be manifested as numerical instability. The necessary CFL stability condition therefore requires $0 \leq \mathsf{C} \leq 1$ so that the characteristic lies within the numerical domain of dependence (cases of solid lines). One initial condition and one upstream boundary condition are sufficient to determine the numerical solution.

recall centered scheme



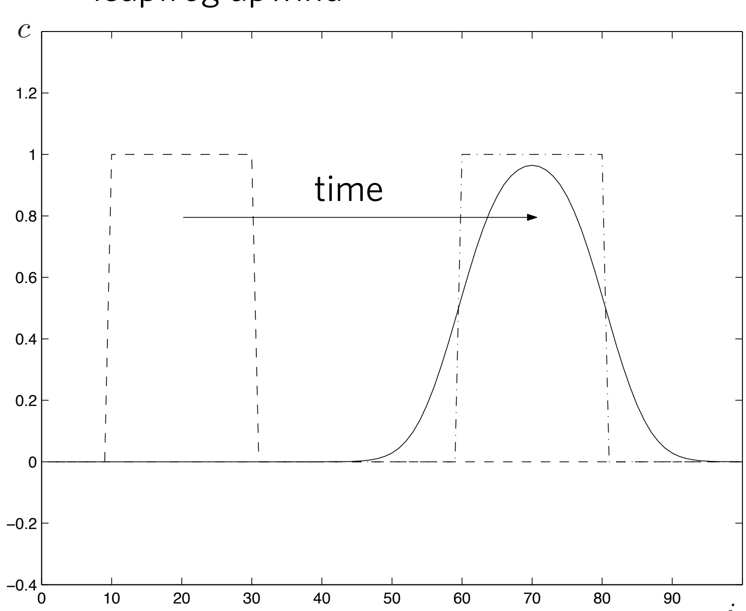
leapfrog centered



no need of BC at this boundary,
however numerical scheme needs one
(artificial boundary condition)

Figure 6-6 Leapfrog scheme applied to the advection of a "top-hat" signal with C = 0.5 for 100 times steps. The exact solution is a mere translation from the initial position (dashed curve on the left) by 50 grid points downstream (dash-dotted curve on the right). The numerical method generates a solution that is roughly similar to the exact solution, with the solution varying around the correct value.

leapfrog upwind



no need of BC at this boundary,
upwind scheme only needs upstream BC
(no artificial boundary condition)

Figure 6-8 Upwind scheme with C = 0.5 applied to the advection of a "top-hat" signal after 100 times steps. Ideally the signal should be translated without change in shape by 50 grid points, but the solution is characterized by a certain diffusion and a reduction in gradient.

this scheme diffuses signal

Understanding diffusion of the upwind scheme

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u\,\frac{c_i^n - c_{i-1}^n}{\Delta x} = 0$$

$$\frac{\partial \tilde{c}}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \tilde{c}}{\partial t^2} + \mathcal{O}\left(\Delta t^2\right) + u\left(\frac{\partial \tilde{c}}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 \tilde{c}}{\partial x^2} + \mathcal{O}\left(\Delta x^2\right)\right) = 0.$$

to eliminate second derivatives, take t and then x derivative

$$\frac{\partial^2 \tilde{c}}{\partial t^2} = u^2\,\frac{\partial^2 \tilde{c}}{\partial x^2} + \mathcal{O}\left(\Delta t, \Delta x^2\right),$$

actual equation solved by scheme

$$\frac{\partial \tilde{c}}{\partial t} + u\frac{\partial \tilde{c}}{\partial x} = \boxed{\frac{u\Delta x}{2}\left(1 - \mathsf{C}\right)\frac{\partial^2 \tilde{c}}{\partial x^2}} + \mathcal{O}\left(\Delta t^2, \Delta x^2\right)$$

actual diffusion

advection term / diffusion of scheme

$$\tilde{Pe} = 2\,\frac{UL}{U\Delta x\left(1 - \mathsf{C}\right)} \sim \frac{L}{\Delta x} \gg 1,$$

unfortunately this does not always work for GFD

Reducing diffusion of the upwind scheme

For a positive velocity the upwind (e.g. downstream)

$$\tilde{c}_i^{n+1} \;=\; \tilde{c}_i^n \;-\; \mathsf{C}\;\left(\tilde{c}_i^n - \tilde{c}_{i-1}^n\right).$$

Modify scheme and add corrections Lax-Wendroff

$$\tilde{c}_i^{n+1} = \tilde{c}_i^n - \mathsf{C}\;\left(\tilde{c}_i^n - \tilde{c}_{i-1}^n\right) - \frac{\Delta t}{\Delta x^2}(1-\mathsf{C})\frac{u\Delta x}{2}\;\left(\tilde{c}_{i+1}^n - 2\tilde{c}_i^n + \tilde{c}_{i-1}^n\right)$$

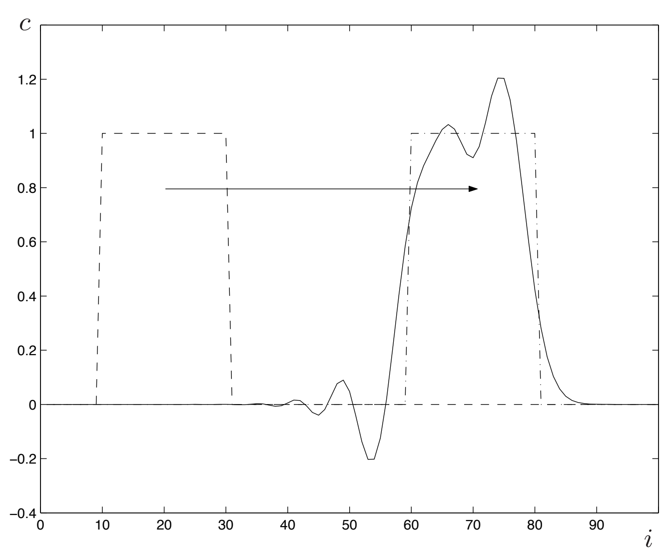


Figure 6-9 Second-order Lax-Wendroff scheme applied to the advection of a "top-hat" signal with $\mathsf{C} = 0.5$ after 100 times steps. Dispersion and non-monotonic behavior are noted.

Popular method