19 The Lax-Wendroff Method and Conservation Equations

One explicit method which attempts to get the second order terms correct is due to Lax and Wendroff. We know that

$$\frac{u_n^{j+1}-u_n^j}{k} = [u_t + \tfrac{1}{2}ku_{tt}]_n^j + O(k^2)\ . \tag{19.1}$$

So if $u_t = -cu_x$ with c constant, then $u_{tt} = -cu_{xt} = c^2u_{xx}$, and we may write

$$\frac{u_n^{j+1}-u_n^j}{k} = -c\frac{\Delta u_n^j}{2h} + \frac{kc^2}{2h^2}\delta^2 u_n^j + O(k^2,\, h^2) \tag{19.2}$$

This leads to the centred scheme (**Scheme F**) in §15.2.

$$U_n^{j+1} = U_n^j - \tfrac{1}{2}q\Delta U_n^j + \tfrac{1}{2}q^2\delta^2 U_n^j \tag{19.3}$$

Note that this formula requires c to be constant.

However, a similar result can be derived for the **conservation** equation: $u_t + [f(u,\, x)]_x = 0$.

19.1 Simultaneous conservation equations

More generally, let $\mathbf{u}$ and $\mathbf{f}[\mathbf{u}]$ be p-vectors satisfying

$$\mathbf{u}_t + (\mathbf{f}[\mathbf{u}])_x = 0 \tag{19.4}$$

Equation (19.4) represents the conservation of p physical quantities. Ideally, we would like our FDM to conserve them also. For example, we could write

$$\mathbf{U}_n^{j+1} - \mathbf{U}_n^j = -\tfrac{1}{2}s\Delta\mathbf{F}_n^j \qquad \text{where} \quad \mathbf{F}_n^j = \mathbf{f}\left[\mathbf{U}_n^j\right] \quad \text{and} \quad s = k/h. \tag{19.5}$$

This scheme is **conservative** because if we sum over all values of n the right-hand-side all cancel (apart possibly from boundary terms if we are on a finite region of x), so that $\sum_n \mathbf{U}_n^{j+1} = \sum_n \mathbf{U}_n^j$. However, we have seen that (19.5) may be unstable. Alternatively we might rewrite (19.4) in the form

$$\left[\frac{\partial(u_l)}{\partial t}\right] + \sum_{m=1}^{p} A_{lm}\left[\frac{\partial(u_m)}{\partial x}\right] = 0 \qquad \text{for} \quad l = 1\ldots p \qquad \text{where} \quad A_{lm} = \frac{\partial(f_l)}{\partial(u_m)}\ , \tag{19.6}$$

and u_m is the m-th component of $\mathbf{u}$. If $A[\mathbf{u}]$ is the matrix whose (l,m)'th element is A_{lm}, we could then approximate

$$\mathbf{U}_n^{j+1} - \mathbf{U}_n^j = -\tfrac{1}{2}sA\left(\Delta\mathbf{U}_n^j\right) \tag{19.7}$$

but this would **not** be conservative unless A is constant. The Lax-Wendroff idea applied to (19.4) gives

$$\mathbf{u}_{tt} = -(\mathbf{f}[\mathbf{u}])_{xt} = -(A\mathbf{u}_t)_x = (A(\mathbf{f})_x)_x$$

so that

$$\left.\begin{aligned}(\mathbf{u}_{tt})_n^j &= \tfrac{1}{h}\left[A_{n+1/2}^j\left(\mathbf{f}_x\right)_{n+1/2}^j - A_{n-1/2}^j\left(\mathbf{f}_x\right)_{n-1/2}^j\right] + O(h^2)\\ &= \tfrac{1}{h^2}\left[A_{n+1/2}^j\left(\mathbf{f}_{n+1}^j - \mathbf{f}_n^j\right) - A_{n-1/2}^j\left(\mathbf{f}_n^j - \mathbf{f}_{n-1}^j\right)\right] + O(h^2)\end{aligned}\right]\ . \tag{19.8}$$

In the above, to the same order of accuracy we can approximate

$$A^j_{n+1/2} \equiv A[\mathbf{u}^j_{n+1/2}] = A\left[\tfrac{1}{2}(\mathbf{u}^j_{n+1} + \mathbf{u}^j_n)\right] + O(h^2)\,.$$

Using the estimate (19.8) for $\mathbf{u}_{tt}$, we obtain

$$\mathbf{U}^{j+1}_n = \mathbf{U}^j_n - \tfrac{1}{2}s\Delta\mathbf{F}^j_n + \tfrac{1}{2}s^2\Big[A^j_{n+1/2}\left(\mathbf{F}^j_{n+1} - \mathbf{F}^j_n\right) - A^j_{n-1/2}\left(\mathbf{F}^j_n - \mathbf{F}^j_{n-1}\right)\Big]\,. \tag{19.9}$$

However while (19.9) is a second order scheme, it is still non-conservative if A depends on $\mathbf{u}$, and moreover it is necessary to calculate $A^j_{n+1/2}$. A superior two-step version of the Lax-Wendroff scheme is due to Richtmyer. The system

$$\left.\begin{array}{ll} \mathbf{U}^{j+1/2}_{n+1/2} & = \frac{1}{2}\left(\mathbf{U}^j_n + \mathbf{U}^j_{n+1}\right) - \frac{1}{2}s\left(\mathbf{F}^j_{n+1} - \mathbf{F}^j_n\right) \\ \mathbf{U}^{j+1}_n & = \mathbf{U}^j_n - s\left(\mathbf{F}^{j+1/2}_{n+1/2} - \mathbf{F}^{j+1/2}_{n-1/2}\right) \end{array}\right]\,. \tag{19.10}$$

has truncation error $O(k^2 + h^2)$, is **conservative** and stable if the Courant condition holds. When A is constant, so that $\mathbf{F} = A\mathbf{U}$, it reduces to (19.9). For the one-dimensional case $p = 1$, with $f = cu$, we obtain the two-step scheme (**Scheme D**) with a different step-size.

19.2 Finite volume method in two-dimensions

Suppose the flux function in 2D is $\mathbf{F}(u) = (f(u), g(u))$, then it follows the conservation law has the form

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} + \frac{\partial g(u)}{\partial y} = 0.$$

Hence

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial g}{\partial u}\frac{\partial u}{\partial y} = 0,$$

with (f_u, g_u) representing the wave speed of the 2D system in the (x, y) directions – the advection speed vector $\mathbf{v}$ is thus given by

$$\mathbf{v} = f_u\,\mathbf{i} + g_u\,\mathbf{j}.$$

Averaging the value of u over a now 2D finite-volume cell as depicted in Fig. 19.1, we obtain the general form of an explicit FV method, namely

$$\frac{u^{j+1}_{m,n} - u^j_{m,n}}{\Delta t} + \frac{f^*(u^j_{m,n}, u^j_{m+1,n}) - f^*(u^j_{m-1,n}, u^j_{m,n})}{\Delta x} + \frac{g^*(u^j_{m,n}, u^j_{m,n+1}) - g^*(u^j_{m,n-1}, u^j_{m,n})}{\Delta y} = 0,$$

hence defining intermediate fluxes

$$f^{*j}_{m+1/2,n} = f^*(u^j_{m,n}, u^j_{m+1,n}) \;\text{ and }\; g^{*j}_{m,n+1/2} = g^*(u^j_{m,n}, u^j_{m,n+1}).$$

It follows we may write, noting expressions 17.49, 17.52 and 18.6,

$$\frac{u^{j+1}_{m,n} - u^j_{m,n}}{\Delta t} + \frac{f^{*j}_{m+1/2,n} - f^{*j}_{m-1/2,n}}{\Delta x} + \frac{g^{*j}_{m,n+1/2} - g^{*j}_{m,n-1/2}}{\Delta y} = 0.$$

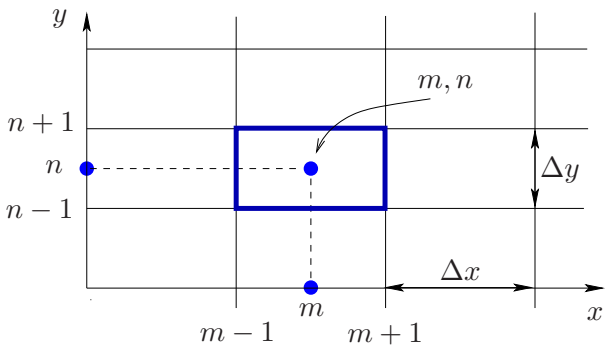

Figure 19.1: 2D flux

Lax Wendroff in two-dimensions :

The two-step Lax-Wendroff scheme (19.10) may be thus be extended to two space dimensions without difficulty. Consider the equation for $\mathbf{u}(x,\, y,\, t)$, with $\mathbf{u}$ representing a system of coupled hyperbolic PDEs in conservation form

$$\mathbf{u}_t + \mathbf{f}_x + \mathbf{g}_y = 0 \qquad \text{and take} \quad \Delta x = \Delta y = h.$$

We define $\mathbf{U}$ at the half time-levels for $(p,\, q) = (m,\, n + 1/2)$ or $(m + 1/2,\, n)$ by

$$\mathbf{U}_{pq}^{j+1/2} = \tfrac{1}{4}\left[\mathbf{U}_{p+,q}^{j} + \mathbf{U}_{p-,q}^{j} + \mathbf{U}_{p,q+}^{j} + \mathbf{U}_{p,q-}^{j}\right] - \tfrac{1}{2}s\left[\mathbf{F}_{p+,q}^{j} - \mathbf{F}_{p-,q}^{j} + \mathbf{G}_{p,q+}^{j} - \mathbf{G}_{p,q-}^{j}\right] \ ,$$

where $p\pm$ denotes $p \pm 1/2$ and similarly $q\pm$. At the integer time levels, for $(p,\, q) = (m,\, n)$ or $(m + 1/2,\, n + 1/2)$,

$$\mathbf{U}_{pq}^{j+1} = \mathbf{U}_{pq}^{j} - s\left[\mathbf{F}_{p+,q}^{j+1/2} - \mathbf{F}_{p-,q}^{j+1/2} + \mathbf{G}_{p,q+}^{j+1/2} - \mathbf{G}_{p,q-}^{j+1/2}\right] \ .$$

The resulting scheme is second order and conservative.

20 The 2D Wave Equation

We return now to pure Hyperbolic equations, such as the one-dimensional wave equation for $u(x,t)$,

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad \text{with} \quad u(x,0) \quad \text{and} \quad u_t(x,0) \quad \text{given.} \tag{20.1}$$

We know we could write this as two first order equations, but suppose we treat it directly, introducing a grid (h,k) and seek an approximation U_n^j to $u(nh,jk)$ in the familiar way. Using explicit centred differences in time and space we have the two-step second-order accurate in space and time scheme

$$U_n^{j+1} - 2U_n^j + U_n^{j-1} = q^2(U_{n+1}^j - 2U_n^j + U_{n-1}^j). \quad \text{where } q = \frac{ck}{h}. \tag{20.2}$$

The scheme is often referred to as the **leapfrog scheme**.

It being a second order equation in t, we need two initial conditions on U_n^0 and U_n^1 and then we can easily step to find U_n^{j+1} . We analyse the stability with Fourier methods, namely looking at solutions of the form

$$U_n^j = (\lambda)^j exp(in\xi)$$

and we find

$$\lambda^2 - 2\lambda + 1 = \lambda q^2(2\cos(\xi) - 2) \tag{20.3}$$

or

$$\lambda^2 - \left(2 - 4q^2\sin^2(\frac{\xi}{2})\right)\lambda + 1 = 0. \tag{20.4}$$

We need $|\lambda| \leq 1$ for stability (note Fig. 20.1). Now without calculating λ explicitly, we can see from the constant term that the two roots have product 1. If the roots are real and distinct this means that one of the roots will have modulus greater than 1, and so the scheme will be unstable. Thus we require complex or double roots, or

$$\left(2 - 4q^2\sin^2(\frac{\xi}{2})\right)^2 \leq 4 \quad \rightarrow \quad -2 \leq \left[2 - 4q^2\sin^2(\frac{\xi}{2})\right] \leq 2 \tag{20.5}$$

As usual, the worst case is $\xi = \pi$ and we require the **Courant-Friedrichs-Lewy** condition $q \leq 1$ for stability, as we might have expected. The scheme (20.2) is conservative and

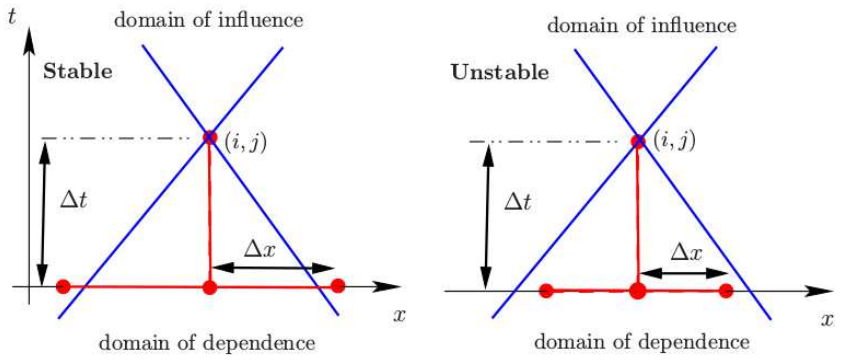

Figure 20.1: Domains of dependence and influence, CFL-condition. Stable configuration (left), unstable configuration (right).

models left and right travelling waves, $u = f(x-ct)+g(x+ct)$. If we have a boundary, say at $x = 0$, where we impose $u = 0$, then we must have $f = g$. Thus if a leftwards travelling wave encounters such a boundary, it will reflect, giving rise to a rightwards travelling wave. So if we want to have a **non-reflecting** boundary, we would need to impose the condition

$$cu_x = +u_t, \quad \text{on} \quad x = 0.$$

This is easy enough to implement. We can combine (20.2) on the boundary $n = 0$ with

$$q(U_1^j - U_{-1}^j) = U_n^{j+1} - U_n^{j-1}$$

to eliminate the ghost points at $n = -1$, keeping 2^{nd} order accuracy. Can we extend this scheme to two and three dimensions?

20.1 2D Wave equation: non reflecting boundary conditions

Suppose now $u(x, y, t)$ satisfies

$$\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = c^2\,\nabla^2 u \tag{20.6}$$

We can model this explicitly on a rectangular grid (h_x, h_y) by

$$\frac{U_{mn}^{j+1} - 2U_{mn}^j + U_{mn}^{j-1}}{c^2k^2} = \frac{1}{h_x^2}\delta_x^2 U_{mn}^j + \frac{1}{h_y^2}\delta_y^2 U_{mn}^j.$$

For simplicity, we take $h_x = h_y = h$. We analyse the stability with

$$U_{mn}^j = (\lambda)^j exp(im\xi + in\eta)$$

and as before we find stability provided λ is complex for all ξ and η, which requires

$$q \le 1/\sqrt{2}.$$

Similarly, in 3-dimensions, the CFL condition would be $q \le 1/\sqrt{3}$.

In 2 or 3 dimensions it is quite likely that we will want to include artificial boundaries to the computational domain which do not reflect waves, but this is harder to do. Suppose we are in $y > 0$ with a boundary at $y = 0$. Taking Fourier transforms, the general solution to (20.6) can be written as a superposition of the waves $\exp(ilx + imy + i\omega t)$, where l, m and ω are related by

$$c^2(l^2 + m^2) = \omega^2.$$

On $y = 0$, we wish to impose that only waves travelling in the negative y direction are permitted, in other words, assuming $\omega > 0$ then we must have $m > 0$, so that

$$mc = +\omega - \frac{c^2 l^2}{2\omega}.$$

This is equivalent to the unusual boundary condition

$$cu_{yt} = u_{tt} - \frac{1}{2}c^2 u_{xx}, \quad \text{on} \quad y = 0. \tag{20.7}$$

This can be implemented on the boundary and greatly reduces unwanted reflections.

This boundary condition is somewhat more difficult to implement but results in a much improved outflow boundary condition. This type of boundary condition is the most commonly used, due to its relative ease of implementation and its efficiency in substantially reducing backscatter. This type of outflow boundary conditions has been implemented, and the results are shown in Fig. 20.2.

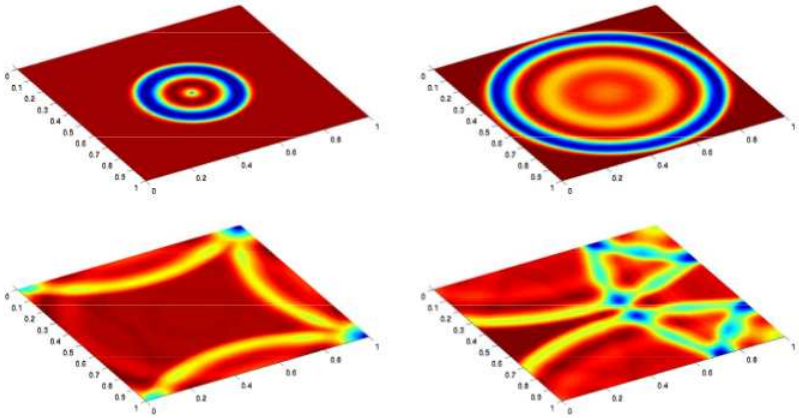

Figure 20.2: Propagation of a localised disturbance. Three reflecting and one non-reflecting boundaries based on Eqn. (20.7).

An even simpler outgoing boundary condition based on the linear advection equation for this problem is shown in Fig. 20.3.

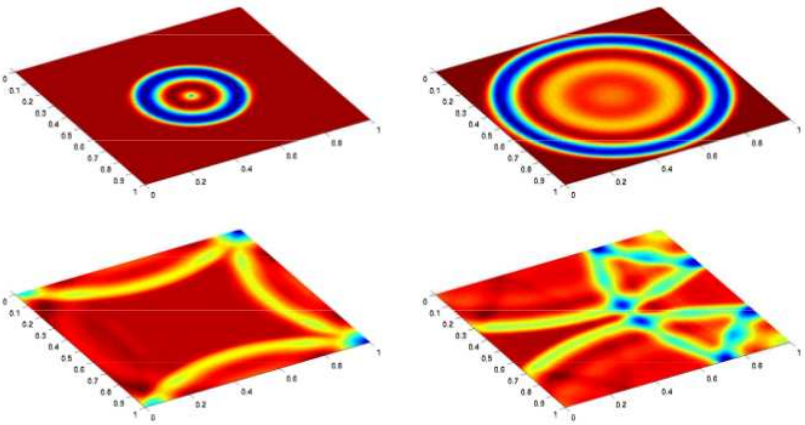

Figure 20.3: Propagation of a localised disturbance. Three reflecting and one non-reflecting boundaries based on the linear advection equation $u_t = cu_x$

But still it is imperfect. An important technique for avoiding unphysical reflections is known as **PML**, which stands for **Perfectly Matched Layer**.

21 Perfectly Matched Layers

Solutions of the wave equation can move large distances without dissipating. As a result, correct treatment of "*infinity*" is crucial – if outgoing waves are allowed to reflect back towards the region of interest, they may eventually completely invalidate the solution. Last lecture we derived an approximate boundary condition which greatly reduced spurious reflections at the edge of the computational domain, but we would like to do better.

How can we accurately impose non-reflecting boundary conditions? In real life we might clad a concert hall ceiling with absorbing material – curtains and carpets are well known to muffle echoes in houses. So imagine cladding the domain in which we are interested with a region which causes waves to decay. The difficulty is to do this in a manner which does not encourage reflections. Waves may bounce off many inhomogeneities (think of mirages, for example). Techniques to model the waves behaviour at the boundaries of a finite domain can be dealt with by attempting to solve or approximate the exact dispersion relation for waves in the far-field and impose the corresponding conditions on the boundary of the computational domain such that this boundary appears transparent to outgoing waves.

We are familiar with acoustic waves, the need also arises in quantum mechanics. Consider the 1D Schrodinger equation

$$\begin{aligned} i\frac{\partial u}{\partial t} &= -\frac{\partial^2 u}{\partial x^2} + V(x,t)u, \quad x \in \Re, t > 0, \\ \lim_{|x|\to\infty} u(x,t) &= 0, \\ u(x,0) &= u_I(x), \end{aligned} \qquad .$$

Here, V denotes a given real potential. The equation arises in quantum semiconductors, electromagnetic wave propagation, seismic propagation, underwater acoustics among others*.

Techniques which **artificially** manipulate the waves behaviour at the boundaries of a finite domain is an alternative means to avoid issues with reflections at the boundaries. In this, the idea is to surround the computational domain by additional grid points on which a highly dissipative equation can be solved that damps the outgoing waves. A switching function is used to blend from the equations governing the flow evolution on the inside of the domain (*i.e.*, the physically relevant domain) to the equations causing the dissipation of the flow in the absorbing layer. Even though this is a simple and appealing concept, the proper implementation in a numerical simulation is far from trivial.

Specifically, on a boundary at, say $x = 0$, we want a solution which behaves like

$$e^{ik(x-ct)}$$

in $x < 0$, to match with something which decays exponentially with x in $x > 0$. One way of doing that is to add an imaginary part to x. We may think of this as following the same solution along a contour in the complex x-plane other than the x-axis. Consider a variable

$$X = x + if(x),$$

*Antoine *et al.* Commun. Comput. Phys., Vol 4(4) pp729-796, 2008

where $f(x) > 0$ for $x > 0$, and $f(x) = 0$ for $x < 0$. Then the derivatives transform as

$$\frac{\partial}{\partial X} = \frac{1}{1 + if'(x)} \frac{\partial}{\partial x}$$

The idea is to solve the equation in X-space and hope that the resultant solution has the desired decaying properties in x-space.

Waves in homogeneous medium : explanation

Generally, in a homogeneous medium in infinite space, we assume that propagating waves form a superposition of linear plane-waves, namely in a simple 1-D reference frame, we may assume

$$p(x,t) = p_o e^{i(\alpha x - \omega t)},$$

where ω/α is the phase velocity. Next let us add an additional term to the above,

$$p(x,t) = p_o e^{i(\alpha(x + i\gamma x) - \omega t)},$$

with γ some *real positive* quantity. This may be re-written

$$p(x,t) = p_o e^{i(\alpha x - \omega t)}\ e^{-\gamma \alpha x},$$

that is the solution decays exponentially provided $(\gamma\alpha)$ is real and positive. Choosing where $\gamma \neq 0$, we have effectively there, introduced a *complex material* with *absorbing or dampening* properties.

The basic idea is, for unbounded domain problems, far away from the field of interest we can devise a modified set of PDEs with additional terms, which damp out the outwardly propagating waves. With hope that the wave amplitude has been effectively reduced to zero by the time it reaches the final computational boundary point, **within** the PML regions. In the non-PML regions the additional tems are zero, and so we solve the precise PDE that we **do** want to solve.

21.1 A more general wave equation

A generalised form of the wave equation for $p(\mathbf{x}, t)$ is

$$p_{tt} = b\ \nabla \cdot\ (a \nabla p), \tag{21.1}$$

where $a(\mathbf{x})$ and $b(\mathbf{x})$ are given, positive functions of position, and can represent an inhomogeneous medium through which the waves travel. We assume they do not vary with x at the boundary $x = 0$, though they may do elsewhere. If both a and b are constant, we have the standard wave equation. Now (21.1) can be written as a system of first order equations if we introduce the vector $\mathbf{v}$ such that

$$\mathbf{v}_t = a\ \nabla p, \quad \text{and} \quad p_t = b\ \nabla \cdot \mathbf{v}. \tag{21.2}$$

We will start with the 1-D wave equation in terms of X and t, so that

$$v_t = a\ p_X, \quad \text{and} \quad p_t = b\ v_X.$$

Assuming an $\exp(-i\omega t)$ behaviour and transforming from X to x, we have

$$-i\omega v \equiv v_t = \frac{a\ p_x}{1+if'(x)} \quad \text{and} \quad -i\omega p \equiv p_t = \frac{b\ v_x}{1+if'(x)}$$

or multiplying up

$$-i\omega p + \omega f' p = b\ v_x \quad \text{and} \quad -i\omega v + \omega f' v = a\ p_x.$$

If we introduce $\sigma(x) = \omega f'$ and re-insert the time derivatives, we have the system

$$p_t = b\ v_x - \sigma p \quad \text{and} \quad v_t = a\ p_x - \sigma v.$$

We can choose a function $\sigma(x)$ which is zero for $x < 0$ and implement this scheme easily. Common choices for $\sigma(x)$ range from piece-wise constant functions to piece-wise linear functions to smooth, monotonically increasing functions. An assortment of the most commonly used is given in Fig. 21.1.

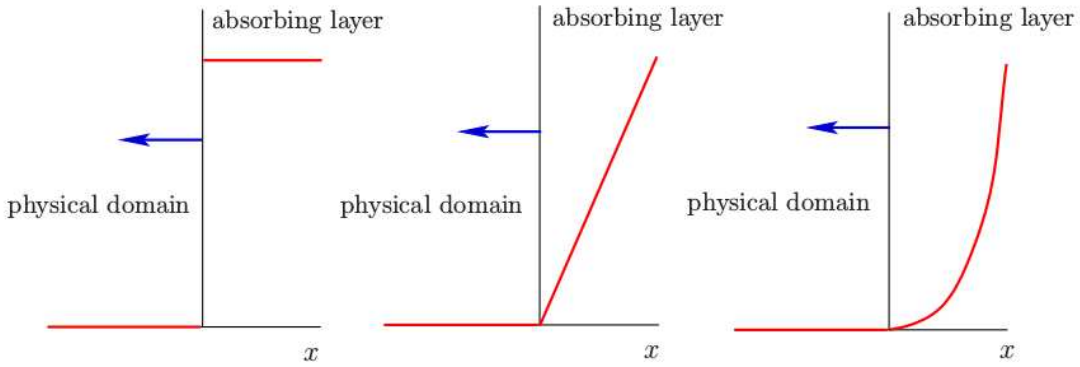

Figure 21.1: Choices for the absorption coefficient $\sigma(x)$.

At the interface between the PML and normal region, a *perfectly devised layer* should have the key feature of not causing any internal reflections back into the region of interest, to corrupt the solution. The interface is not reflection-free, but by careful choice of how the strength of $\sigma(x)$ varies (generally increasing) as one goes more and more deeper into the PML an optimal solution can usually be found, with a few iterations or fine-tuning of the $\sigma(x)$ function and observing its impact.

For the 1-D problem σ appears in a simple manner. But we saw last time there is no difficulty in imposing a non-reflecting boundary condition for the 1-D problem. In 2D we developed an approximate condition, see Eqn. (20.7), but it would clearly be useful to devise a better more general approach.

21.2 A perfectly matched layer in 2D

Now let's write $\mathbf{v} = (v, w)$. Our system takes the form

$$-i\omega p \equiv p_t = b\ \nabla \cdot \mathbf{v} \equiv b\ v_X + b\ w_y, \tag{21.3}$$

$$-i\omega v \equiv v_t = a\ p_X \quad \text{and} \quad -i\omega w \equiv w_t = a\ p_y. \tag{21.4}$$

Now the second equation in (21.4) does not involve X. Substituting for X into the first equation in (21.4) and in (21.3) and multiplying up by $(1 + i\sigma/\omega)$, we have

$$b\, v_x + b\, w_y(1 + i\sigma/\omega) = -i\omega p + \sigma p, \tag{21.5}$$

$$a\, p_x = -i\omega v + \sigma v. \tag{21.6}$$

Equation (21.6) easily translates to time derivatives, but (21.5) involves $1/(i\omega)$ which corresponds to time integration rather than differentiation. So we introduce a function $\psi(x, y, t)$, such that

$$-i\omega\psi = b\, \sigma\, w_y \text{ with } \psi = 0 \text{ at } t = 0.$$

Then (21.5) reads

$$b\, v_x + b\, w_y + \psi = -i\omega p + \sigma p,$$

and we can write the system as The obvious generalisation to three dimensions would be

$$\left.\begin{aligned} p_t &= b\, \nabla \cdot \mathbf{v} - \sigma p + \psi \\ v_t &= a\, p_x - \sigma v \\ w_t &= a\, p_y \\ \psi_t &= b\, \sigma\, w_y \end{aligned}\right\} \tag{21.7}$$

Where $\sigma = 0$ these equations reduce to (21.2). In the layer where $\sigma > 0$, we have decay with no reflection. We can place a boundary a little distance into the layer, secure in the knowledge that any reflections from this boundary will have decayed exponentially and should not cause significant errors in the region of computational interest. Naturally, it is easy to modify these equations for other boundaries.