Wave Propagation Workshop – Extra Notes

12th November 2019

1 The 1D Wave Equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Where u is a function of space and time, i.e: $u(x,t)$

Also, potentially $c(x)$ – but we'll begin with c constant for normal mode solutions at first...

1.0.1 Use 'separation of variables' to find solution as normal modes

Assume we can write: $u(x,t) = X(x)\,T(t)$

Then we have: $X\frac{\partial^2 T}{\partial t^2} = c^2\,\frac{\partial^2 X}{\partial x^2}T$

Divide through by X and T: $\frac{1}{T(t)}\frac{\partial^2 T(t)}{\partial t^2} = c^2\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2}$

But LHS is function of time only, while RHS is function of space only. Therefore both sides must be constant –let's call it β:

$$c^2\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} = \beta \qquad \text{i.e: } \frac{\partial^2 X(x)}{\partial x^2} = \frac{\beta}{c^2}X(x)$$

$$\frac{1}{T(t)}\frac{\partial^2 T(t)}{\partial t^2} = \beta \qquad \text{i.e: } \frac{\partial^2 T(t)}{\partial t^2} = \beta\,T(t)$$

$$\frac{\partial^2 X(x)}{\partial x^2} = \frac{\beta}{c^2}X(x) \quad \Rightarrow \quad X(x) = X_0\,e^{\pm\sqrt{\beta}\frac{x}{c}}$$

$$\frac{\partial^2 T(t)}{\partial t^2} = \beta\,T(t) \quad \Rightarrow \quad T(t) = T_0\,e^{\pm\sqrt{\beta}\,t}$$

Everything remains real for the case of β positive. But it also grows or decays exponentially in time and space, so seems like not quite what we would want...
Instead, consider the case where the constant factor is negative, so let's replace β by $-\beta$.
Real-valued solutions have the form:

$$\frac{\partial^2 X(x)}{\partial x^2} = -\frac{\beta}{c^2} X(x) \quad \Rightarrow \quad X(x) = X_0 \sin\left(\omega \tfrac{x}{c} + \theta_X\right)$$

$$\frac{\partial^2 T(t)}{\partial t^2} = -\beta\, T(t) \quad \Rightarrow \quad T(t) = T_0 \sin\left(\omega t + \theta_T\right)$$

where: $\omega = \pm\sqrt{\beta}$ and the above are clearly oscillatory, with ω as angular frequency: $\omega = 2\pi f$

So we can write the solution as: $u(x,t) = A_0 \sin(\pm\frac{\omega}{c}x + \theta_X)\ \sin(\pm\omega t + \theta_T)$ where $A_0 = X_0 T_0$ is the amplitude

By considering all four cases for the $\pm$ (and we might also allow negative A_0) they can all be written in the form:

$$u(x,t) = A_0 \sin(\tfrac{\omega}{c}x + \theta_X)\ \sin(\omega t + \theta_T)$$

Recall that wavelength is $\lambda = \dfrac{c}{f}$

Also, (angular) wavenumber is $k = \dfrac{\omega}{c} = \dfrac{2\pi}{\lambda}$

So we can see how k is to x as ω is to t: $u(x,t) = A_0 \sin(kx + \theta_X)\ \sin(\omega t + \theta_T)$

Alternatively, we can solve it all in the complex domain, which leads to:

$$X(x) = X_0\, e^{\pm\frac{i\omega x}{c} + i\phi_X} \quad \text{and} \quad T(t) = T_0\, e^{\pm i\omega t + i\phi_T}$$

$$\text{So:} \quad u(x,t) = A_0\, e^{\pm i\omega\,(\frac{x}{c} \pm t) + i\phi}$$

$$\text{where:} \quad A_0 = X_0\, T_0 \quad \text{and} \quad \phi = \phi_X + \phi_T$$

More generally, the wave-eqn is linear, so sums of above also work: $u(x,t) = \sum_m A_m\, e^{i\omega_m\,(\frac{x}{c} \pm t) + i\phi_m}$

$$\text{Or, just taking the real part:} \quad u(x,t) = \sum_m A_m \cos\left(\omega_m(\tfrac{x}{c} \pm t) + \phi_m\right)$$

$$= \sum_m A_m \sin\left(\omega_m(\tfrac{x}{c} \pm t) + \theta_m\right) \quad \text{where: } \theta_m = \phi_m - \pi/2$$

The general solution could be written as sum of (complex) waves of varying frequencies:

$$u(x,t) = \sum_m u_m(x)\, e^{-i\omega_m t} \quad \text{where the } u_m\text{'s are complex}$$

>>> Quick exercise: demonstrate above summed solutions (both real and complex) do satisfy the 1d wave equation.

1.0.2 Normal modes: e.g. solutions with zero boundary condition at ends

We want to find solutions which have $u(x,t)$=0 at x=0 and x=L for all time, and $u(x,t)$ is some initial shape at zero time.

$$\text{i.e:} \quad u(0,t) = u(L,t) = 0 \quad \forall t \quad \text{and} \quad u(x,0) = u_0(x) \quad (\text{ which also means that } u_0(0)=u_0(L)=0\text{ })$$

$$\text{Write in separated form: } u(x,t) = \sum_m A_m \sin(\tfrac{\omega_m}{c} x + \alpha_m) \ \sin(\omega_m t + \beta_m)$$

$$\text{So:} \quad u(0,t) = \sum_m A_m \sin(\alpha_m) \ \sin(\pm\omega_m t + \beta_m) = 0 \quad \forall t$$

$$\text{Also:} \quad u(L,t) = \sum_m A_m \sin(k_m L + \alpha_m) \ \sin(\omega_m t + \beta_m) = 0 \quad \forall t$$

Assuming the amplitudes, A_m, are not zero, one possibility for the first condition is that α_m=0 for all m.
This leads to the possibility for the second condition that $k_m L$ is some multiple of π.
–In fact, we might as well put k_m= $m\pi/L$, which tells us that ω_m= $mc\pi/L$ (and remember we can have negative m, too).

$$\text{We can write our solution so far as:} \quad u(x,t) \ = \ \sum_m A_m \sin(m\pi\tfrac{x}{L}) \ \sin(m\pi\tfrac{ct}{L} + \beta_m)$$

We also want to satisfy the initial condition at t=0:

$$\text{i.e:} \quad \sum_m A_m \sin(m\pi\tfrac{x}{L}) \ \sin(\beta_m) = u_0(x) \quad \text{for } x = 0 \text{ to } L$$

We know from Fourier analysis that we can form any shape in the interval 0 to L as a sum of harmonics using sine and cosine waves. More specifically, if it has zero at both ends, then it only needs to be a sum of sine waves.
–So we could just put β_m=$\pi/2$ for all m, and use Fourier analysis to find the A_m's.
Recall that $\sin(\theta+\pi/2)$ is just $\cos(\theta)$ –and cosine is an even function, so we could drop the $\pm$ at this point instead, if we want.

$$\text{We can write our final solution as:} \quad u(x,t) = \sum_m A_m \sin(m\pi\tfrac{x}{L}) \ \cos(m\pi\tfrac{ct}{L})$$

$$\text{where:} \quad \sum_m A_m \sin(m\pi\tfrac{x}{L}) = u_0(x) \quad \text{and we find } A_m \text{ for all } m \text{ by Fourier analysis of } u_0(x).$$

If we choose to look at initial conditions where $u_0(x)$ is a sine wave of the form $\sin(n\pi\frac{x}{L})$, then we just have the solution:

$$u(x,t) = \sin(n\pi\tfrac{x}{L}) \ \cos(n\pi\tfrac{ct}{L})$$

>>> Quick exercise: check above satisfies the 1d wave equation...

$$\frac{\partial u}{\partial t} \ = \ -n\pi\tfrac{c}{L} \ \sin(n\pi\tfrac{x}{L}) \ \sin(n\pi\tfrac{ct}{L})$$

$$\frac{\partial^2 u}{\partial t^2} \ = \ -(n\pi\tfrac{c}{L})^2 \ \sin(n\pi\tfrac{x}{L}) \ \cos(n\pi\tfrac{ct}{L})$$

$$\frac{\partial u}{\partial x} = n\pi\tfrac{1}{L}\ \cos(n\pi\tfrac{x}{L})\ \cos(n\pi\tfrac{ct}{L})$$

$$\frac{\partial^2 u}{\partial x^2} = -(n\pi\tfrac{1}{L})^2\ \sin(n\pi\tfrac{x}{L})\ \cos(n\pi\tfrac{ct}{L}) = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

What about propagating waves...? So far, we've not seen anything that looks like waves moving through space, so where are they?

Consider a solution in terms of fixed-shape functions, travelling along x with speed $\pm c$: $u(x,t) = f(x+ct)+$

Put $s = x + ct$ and $s' = x - ct$: $\dfrac{\partial u}{\partial t} = \dfrac{\partial f}{\partial s}\dfrac{\partial s}{\partial t} + \dfrac{\partial g}{\partial s'}\dfrac{\partial s'}{\partial t} = c\dfrac{\partial f}{\partial s} - c\dfrac{\partial g}{\partial s'}$ (Note: we're assuming c constant)

And: $$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(c\frac{\partial f}{\partial s} - c\frac{\partial g}{\partial s'}\right) = c\frac{\partial^2 f}{\partial s^2}\frac{\partial s}{\partial t} - c\frac{\partial^2 g}{\partial s'^2}\frac{\partial s'}{\partial t} = c^2\frac{\partial^2 f}{\partial s^2} + c^2\frac{\partial^2 g}{\partial s'^2}$$

Similarly, for RHS of wave equation: $$\frac{\partial u}{\partial x} = \frac{\partial f}{\partial s}\frac{\partial s}{\partial x} + \frac{\partial g}{\partial s'}\frac{\partial s'}{\partial x} = \frac{\partial f}{\partial s} + \frac{\partial g}{\partial s'}$$

And: $$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial t}\left(\frac{\partial f}{\partial s} + \frac{\partial g}{\partial s'}\right) = \frac{\partial^2 f}{\partial s^2}\frac{\partial s}{\partial t} + \frac{\partial^2 g}{\partial s'^2}\frac{\partial s'}{\partial t} = \frac{\partial^2 f}{\partial s^2} + \frac{\partial^2 g}{\partial s'^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

Splitting 2nd-order 1d wave equation into two first-order equations (For interest...)

Note that $g(x-ct)$ satisfies 1st-order PDE: $\dfrac{\partial u}{\partial t} = c\dfrac{\partial u}{\partial x}$ i.e: $\left(\dfrac{\partial}{\partial t} - c\dfrac{\partial}{\partial x}\right)u = 0$

Also, $f(x+ct)$ satisfies 1st-order PDE: $\dfrac{\partial u}{\partial t} = -c\dfrac{\partial u}{\partial x}$ i.e: $\left(\dfrac{\partial}{\partial t} + c\dfrac{\partial}{\partial x}\right)u = 0$

Multiply the two operators in brackets together and we get: $$\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u = 0$$

Multiplying that out gives our 1d wave equation: $$\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial^2 u}{\partial x^2} = 0$$

In other words, we can 'factorise' the second-order PDE into two parts, each being a first-order PDE. And each of these corresponds to a fixed-shape function travelling in each direction – and that matches what we found above!

1.1 Discretisation of 1D wave equation using 2nd-order finite-difference

$$\text{Taylor series:} \quad f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$

$$f(x_0+\delta x) = f(x_0) + \frac{f'(x_0)}{1!}\delta x + \frac{f''(x_0)}{2!}\delta x^2 + \frac{f'''(x_0)}{3!}\delta x^3 + O(\delta x^4)$$

$$f(x_0-\delta x) = f(x_0) - \frac{f'(x_0)}{1!}\delta x + \frac{f''(x_0)}{2!}\delta x^2 - \frac{f'''(x_0)}{3!}\delta x^3 + O(\delta x^4)$$

$$\text{So:} \quad f(x_0+\delta x) + f(x_0-\delta x) = 2f(x_0) + f''(x_0)\delta x^2 + O(\delta x^4)$$

$$\text{i.e:} \quad \underline{f''(x_0) = \frac{f(x_0+\delta x) + f(x_0-\delta x) - 2f(x_0)}{\delta x^2} + O(\delta x^2)}$$

Putting that into LHS of wave equation, to discretise time:

$$\frac{u(x,t+\delta t) - 2u(x,t) + u(x,t-\delta t)}{\delta t^2} + O(\delta t^2) \;=\; c(x)^2\,\frac{\partial^2 u(x,t)}{\partial x^2}$$

Leading to <u>time-stepping equation</u> (using <u>τ</u> for the <u>time index</u>):

$$u^{\tau+1}(x) \;\approx\; \delta t^2 c(x)^2\,\frac{\partial^2 u^{\tau}(x)}{\partial x^2} + 2u^{\tau}(x) - u^{\tau-1}(x)$$

Same for RHS, and in spatial dimension (using ξ for x-position index):

$$u_{\xi}^{\tau+1} \;\approx\; \delta t^2 c_{\xi}^2 \left(\frac{u_{\xi+1}^{\tau} - 2u_{\xi}^{\tau} + u_{\xi-1}^{\tau}}{\delta x^2}\right) + 2u_{\xi}^{\tau} - u_{\xi}^{\tau-1}$$

Turning that into some form of (pseudo-)code might look something like:

```
nx = ?  # number of discretisation points in space
nt = ?  # number of discretisation points in time

dx = ?  # distance between spatial discretisation points - i.e. grid-spacing
dt = ?  # time between temporal discretisation points - i.e. time-step

set up c[nx]  # i.e. speeds of waves at each point in spatial grid

initialise u_prv[nx] and u_cur[nx]  # i.e. initial conditions across space at t=0
declare u_nxt[nx]  # as a third wavefield that we will write into at each step


# start the time-stepping...

loop t = 0 to nt-1:  # i.e. over time
```

```
loop ix = 0 to nx-1:  # i.e. over space
    u_nxt[ix] = ( u_cur[ix+1] - 2*u_cur[ix] + u_cur[ix-1] ) * (c[ix]*dt/dx)**2 \
                                            + 2*u_cur[ix] - u_prv[ix]

# Must 'cycle' wavefields, so current goes into prev, and next into current:
u_prv[:] = u_cur[:]
u_cur[:] = u_nxt[:]
```

Is there a problem with the pseudo-code above...?
Yes! –We can't fill in start and end-points (i.e. u_nxt[ix] for ix=0 and ix=nx-1) since u_cur[-1] & u_cur[nx] are out of bounds.
But that's fine for the case of zero boundary-conditions (i.e. ends are fixed at zero): we can just loop over all the 'internal' points (ix=1 to nx-2) and leave the end ones.
–Since we want the boundary points to be zero anyway (in this simulation), then as long as we don't touch them during the simulation, everything should satisfy the equations as we want.

1.1.1 Absorbing layer (in 1d)...

We want the wave to 'fade away' over time. So start from a constant frequency complex wave:

$$u(x,t) \;=\; u_0(x)\, e^{-i\omega t}$$

To make it fade away we can add an extra real term in the exponent: $u(x,t) \;=\; u_0(x)\, e^{-i\omega t-\alpha c t}$

That should cause it to decay by factor $e^{-\alpha c t}$ as it travels distance ct from time zero to t.

Let's see how this affects the wave equation...

$$\frac{\partial u}{\partial t} \;=\; -u_0(x)\,(i\omega+\alpha c)\, e^{-i\omega t-\alpha c t} \;=\; -i\omega\, u \;-\; \alpha c\, u$$

$$\frac{\partial^2 u}{\partial t^2} \;=\; u_0(x)\,(i\omega+\alpha c)^2\, e^{-i\omega t-\alpha c t} \;=\; -\omega^2\, u \;+\; \alpha^2 c^2\, u \;+\; 2i\omega\alpha c\, u$$

But we can re-arrange the first equation for $\frac{\partial u}{\partial t}$ to give: $i\omega\, u \;=\; -\alpha c\, u - \frac{\partial u}{\partial t}$

So we have: $$\frac{\partial^2 u}{\partial t^2} \;=\; -\omega^2\, u \;+\; \alpha^2 c^2\, u \;-\; 2\alpha^2 c^2\, u \;-\; 2\alpha c \frac{\partial u}{\partial t}$$

If we assume RHS of wave equation is unchanged (we only decayed with time), so $\frac{\partial^2 u}{\partial t^2}$ is still $-\omega^2 u$, then:

$$\frac{\partial^2 u}{\partial t^2} \;=\; c^2 \frac{\partial^2 u}{\partial x^2} \;-\; \alpha^2 c^2\, u \;-\; 2\alpha c \frac{\partial u}{\partial t}$$

Let's discretise the final term above in time as: $$\left.\frac{\partial u}{\partial t}\right|_{t_\tau} \approx \frac{u^{\tau+1}(x) - u^{\tau-1}(x)}{2\delta t}$$

Recall that our time-stepping equation before was: $u^{\tau+1}(x) \approx \delta t^2 c(x)^2 \dfrac{\partial^2 u^\tau(x)}{\partial x^2} + 2u^\tau(x) - u^{\tau-1}(x)$

With the modification, it becomes: $(1+q)\, u^{\tau+1}(x) \approx \delta t^2 c(x)^2 \dfrac{\partial^2 u^\tau(x)}{\partial x^2} + (2-q^2)\, u^\tau(x) - (1-q)\, u^{\tau-1}(x)$

Where: $q = \alpha c \delta t$ (note that it collapses back to previous for q=0, as we would expect)

A remaining question is how to gain some sense about the magnitude of α...
The answer to this is to consider what we're trying to do – which is that we want to make the wavefield 'fade away' over time, as it propagates through an absorbing region.
In particular, let's say that we'd like the magnitude of a wave to fall by a factor of 20 as it travels through an absorbing region. –In other words, we would like to have $e^{-\alpha c t} = 0.05$ for t being the time it takes to cross the absorbing region.
If that absorbing region has a thickness d then the time it takes to cross it, travelling at speed c, is d/c, meaning we have: $e^{-\alpha d} = 0.05$
Converting distance d so it's in terms of number of grid-points across the absorbing region width ($d = n_{absorb}\delta x$) gives us an expression for α in terms of our chosen decay factor of 1/20th:

$$\alpha = -\frac{ln(0.05)}{n_{absorb}\delta x} \approx \frac{3}{n_{absorb}\delta x} \qquad \text{i.e:} \quad q \approx \frac{3}{n_{absorb}} \frac{c\delta t}{\delta x}$$

For the worksheet examples, we've often used an absorbing boundary of around 60 grid-points.

$$\text{So this works out as:} \quad q \approx 0.05 \frac{c\delta t}{\delta x}$$

This should (hopefully) give some insight into the values used for `absfct` in the worksheets (i.e. somewhere in the region of 0.05).
In practice, though, we've made lots of somewhat invalid assumptions in this derivation (e.g. that adding this decay in time doesn't affect the wavefield in space – it clearly does!), so it's really only a rough guide to the expected magnitude, and we need to tweak it somewhat by hand to make it behave well.

Modifying our (pseudo-)code might then look something like:

```
nx = ?  # number of discretisation points in space
nt = ?  # number of discretisation points in time

dx = ?  # distance between spatial discretisation points - i.e. grid-spacing
dt = ?  # time between temporal discretisation points - i.e. time-step

set up c[nx]  # i.e. speeds of waves at each point in spatial grid
somehow(??) set up q[nx]  # i.e. our absorbing layers at each end of the domain

initialise u_prv[nx] and u_cur[nx]  # i.e. initial conditions across space at t=0
declare u_nxt[nx]  # as a third wavefield that we will write into at each step

# start the time-stepping...
```

```
loop t = 0 to nt-1:  # i.e. over time

    loop ix = 0 to nx-1:  # i.e. over space
        u_nxt[ix] = ( ( u_cur[ix+1] - 2*u_cur[ix] + u_cur[ix-1] ) * (c[ix]*dt/dx)**2 \
                    + (2-q[ix]**2)*u_cur[ix] - (1-q[ix])*u_prv[ix] ) / (1+q[ix])

    # Must 'shift' wavefields along so current goes into prev, and next into current:
    u_prv[:] = u_cur[:]
    u_cur[:] = u_nxt[:]
```

1.1.2 Predictive absorbing boundary (in 1d)...

This works by predicting what the value will be at the edge point(s) at the next time-step, because we know what the current value is at that point, and at the point just inside, and we know the speed that the wave should be propagating out of the domain (since we know the model properties).
By joining the edge point and the point just inside with a simple linear relation, and 'shifting' that line across by the crossing factor (i.e. how far the wave should move during the step), we can 'predict' what the new value will be at the edge point on the next time-step.

This looks like: $u(0, t+\delta t) \;\approx\; (1-C_0)\, u(0,t) \;+\; C_0\, u(\delta x, t)$ where: $C_0 = \dfrac{c(0)\ \delta t}{\delta x}$ is 'crossing factor' near x=0

And for other edge: $u(L, t+\delta t) \;\approx\; (1-C_L)\, u(L,t) \;+\; C_L\, u(L-\delta x, t)$ where: $C_L = \dfrac{c(L)\ \delta t}{\delta x}$ (i.e. near x=L)

1.1.3 Some optimisations...

1. Replacing loop over space with 'vectorised' versions. (This will be important for speed when it comes to 2d.)
   So instead of using `for ix in range(1,nx-1)` with `u_nxt[ix] = ...` to loop over (almost) the whole array, we'll just use a single line that works on (almost) the whole array on one go: `u_nxt[1:-1] = ...`

(A couple more for you to consider trying...)

2. **>>> Optimisation: reduce to two wavefields instead of three**
   (i.e. avoid having both of `u_prv` and `u_nxt` by overwriting into `u_prv`)

3. **>>> More optimisation: avoid copying between wavefields by alternating**
   (e.g. define propagation step as a function that takes two wavefields, and alternate order for each step)

1.1.4 Fourth order stencil (in space)

(Just for interest...)

$$f(x_0+\delta x) = f(x_0) + \tfrac{f'(x_0)}{1!}\delta x + \tfrac{f''(x_0)}{2!}\delta x^2 + \tfrac{f'''(x_0)}{3!}\delta x^3 + \tfrac{f''''(x_0)}{4!}\delta x^4 + \tfrac{f'''''(x_0)}{5!}\delta x^5 + O(\delta x^6)$$

$$f(x_0-\delta x) = f(x_0) - \tfrac{f'(x_0)}{1!}\delta x + \tfrac{f''(x_0)}{2!}\delta x^2 - \tfrac{f'''(x_0)}{3!}\delta x^3 + \tfrac{f''''(x_0)}{4!}\delta x^4 + \tfrac{f'''''(x_0)}{5!}\delta x^5 + O(\delta x^6)$$

$$f(x_0+2\delta x) = f(x_0) + \tfrac{f'(x_0)}{1!}(2\delta x) + \tfrac{f''(x_0)}{2!}(2\delta x)^2 + \tfrac{f'''(x_0)}{3!}(2\delta x)^3 + \tfrac{f''''(x_0)}{4!}(2\delta x)^4 + \tfrac{f'''''(x_0)}{5!}(2\delta x)^5 + O(\delta x^6)$$

$$f(x_0-2\delta x) = f(x_0) - \tfrac{f'(x_0)}{1!}(2\delta x) + \tfrac{f''(x_0)}{2!}(2\delta x)^2 - \tfrac{f'''(x_0)}{3!}(2\delta x)^3 + \tfrac{f''''(x_0)}{4!}(2\delta x)^4 - \tfrac{f'''''(x_0)}{5!}(2\delta x)^5 + O(\delta x^6)$$

So: $f(x_0+\delta x) + f(x_0-\delta x) = 2f(x_0) + f''(x_0)\delta x^2 + \frac{1}{12}f''''(x_0)\delta x^4 + O(\delta x^6)$

And: $f(x_0+2\delta x) + f(x_0-2\delta x) = 2f(x_0) + 4f''(x_0)\delta x^2 + \frac{4}{3}f''''(x_0)\delta x^4 + O(\delta x^6)$

Eliminate $f''''(x_0)\delta x^4$: $16\,[f(x_0+\delta x) + f(x_0-\delta x)] - [f(x_0+2\delta x) + f(x_0-2\delta x)] =$
$(32-2)f(x_0) + (16-4)f''(x_0)\delta x^2 + O(\delta x^6)$

To give: $$f''(x_0) = \frac{-f(x_0-2\delta x) + 16f(x_0-\delta x) - 30f(x_0) + 16f(x_0+\delta x) - f(x_0+2\delta x)}{12\delta x^2} + O(\delta x^4)$$

We can now use that to replace the $\dfrac{\partial^2 u^\tau(x)}{\partial x^2}$ term in the time-stepping equation we found earlier:

$$(1{+}q)\; u^{\tau+1}(x) \approx \delta t^2 c(x)^2\; \frac{-u^\tau(x{-}2\delta x) + 16u^\tau(x{-}\delta x) - 30u^\tau(x) + 16u^\tau(x{+}\delta x) - u^\tau(x{+}2\delta x)}{12\delta x^2}$$
$$+\;(2-q^2)\; u^\tau(x) - (1{-}q)\; u^{\tau-1}(x)$$

i.e. our fourth-order space-time discretisation finally becomes:

$$(1+q)\; u_\xi^{\tau+1} = \delta t^2 c_\xi^2\; \frac{-u_{\xi-2}^\tau + 16u_{\xi-1}^\tau - 30u_\xi^\tau + 16u_{\xi+1}^\tau - u_{\xi+2}^\tau}{12\delta x^2} + (2-q^2)\; u_\xi^\tau - (1-q)\; u_\xi^{\tau-1}$$

>>> What will be a new issue here for discretisation at edges of domain?
– for both reflective and 'predictive' boundary conditions?

Answer: We had the loop over x-gridpoints (ξ above) range from 1 to nx-2 because the 2nd-order stencil refers to ξ-1 and ξ+1.
But the 4th-order one also refers to ξ-2 and ξ+2, so we can now only loop from 2 to nx-3, which means there are *two* points on each side that don't get evaluated during a propagation step (not just one on each side).
Concentrating on just one side for now (the x=0 side), this leads to questions about the values to set for one of these two points on this side, since we only have a specific value (zero) at one point, x=0.
–Should we add an extra point at $x=-\delta x$ on this left side (and $x=L+\delta x$ on the other)? And then what do we set for that point's value at each step?
It also means we need to do 'prediction' for two gridpoints (rather than just one) on each side that has a predictive boundary.

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2 The Isotropic 3D Elastic Wave Equation

Start with equation of motion: $\rho \dfrac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma}$

$\boldsymbol{\sigma}$ is the Cauchy stress tensor: $\sigma_{ij} = C_{ijkl}\, e_{kl}$ (Hooke's Law, using summation convention)

$\mathbf{e}$ is strain tensor: $e_{ij} = \frac{1}{2}\left(\nabla_i u_j + \nabla_j u_i\right)$ (for small displacements $\mathbf{u}$)

For the isotropic case: $\sigma_{ij} = \lambda\, e_{kk}\, \delta_{ij} + 2\mu\, e_{ij}$ (note: $K = \lambda + \frac{2}{3}\mu$ is bulk modulus)

Where λ and μ are the Lamé parameters, and $e_{kk} = \frac{1}{2}\left(\nabla_k u_k + \nabla_k u_k\right) = \nabla \cdot \mathbf{u}$ (which we'll call θ)

So equation of motion becomes: $\rho \dfrac{\partial^2 u_i}{\partial t^2} = \nabla_j\, \sigma_{ij} = \nabla_j(\lambda\, \theta\, \delta_{ij}) + \nabla_j(\mu(\nabla_i u_j + \nabla_j u_i))$

So: $\rho \dfrac{\partial^2 u_i}{\partial t^2} = (\nabla_i \lambda)\theta + \lambda \nabla_i \theta + (\nabla_j \mu)(\nabla_i u_j + \nabla_j u_i) + \mu(\nabla_j \nabla_i u_j + \nabla_j \nabla_j u_i)$

Turning this back into vector notation shows we have:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\nabla \cdot \mathbf{u})\,(\nabla\lambda) + \lambda\, \nabla(\nabla \cdot \mathbf{u}) + (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\,(\nabla \mu) + \mu\left(\nabla(\nabla \cdot \mathbf{u}) + \nabla^2 \mathbf{u}\right)$$

Note: it's worth stopping for a moment to consider the various parts of above, thinking what type of mathematical object each is. For example, $\nabla \cdot \mathbf{u}$ is a scalar, $\nabla\lambda$ is a vector, while $\nabla \mathbf{u}$ is a tensor (hence we can add its transpose to itself as above).

Use the identity $\nabla^2 \mathbf{a} \equiv \nabla(\nabla \cdot \mathbf{a}) - \nabla \times \nabla \times \mathbf{a}$ to lead to the 3d elastic, isotropic wave equation:

$$\begin{aligned}\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} &= (\nabla \cdot \mathbf{u})\,(\nabla\lambda) + \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)(\nabla \mu) \\ &\quad + (\lambda + 2\mu)\, \nabla(\nabla \cdot \mathbf{u}) - \mu\, \nabla \times \nabla \times \mathbf{u}\end{aligned}$$

In the case that λ and μ vary slowly in space (homogeneous), we can ignore the top two terms on RHS:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + 2\mu)\, \nabla(\nabla \cdot \mathbf{u}) - \mu\, \nabla \times \nabla \times \mathbf{u}$$

This doesn't look so much like a wave equation – however, see the next two sections...

2.0.1 Relate the 3d elastic wave equation back to the 3d acoustic wave equation...

For the acoustic case, $\mu = 0$, so: $\rho \dfrac{\partial^2 \mathbf{u}}{\partial t^2} = (\nabla\lambda)\,(\nabla \cdot \mathbf{u}) + \lambda\,\nabla(\nabla \cdot \mathbf{u}) = \nabla\,(\,\lambda\,\nabla \cdot \mathbf{u}\,)$

But force follows negative pressure gradient, so we also have: $\rho \dfrac{\partial^2 \mathbf{u}}{\partial t^2} = -\nabla p$ where p is acoustic pressure

This implies: $p = -\lambda\,\nabla \cdot \mathbf{u}$ i.e. $\nabla \cdot \mathbf{u} = -\dfrac{1}{\rho c^2} p$ (since $\lambda = \rho c^2$ in acoustic case)

(You may recall seeing that we can decompose σ_{ij} into $-p\delta_{ij} + \sigma'_{ij}$)

Now, divide the equation of motion by density, and apply divergence on both sides...

This leads to the 3d acoustic wave equation: $\dfrac{1}{\rho c^2}\dfrac{\partial^2 p}{\partial t^2} = \nabla \cdot \left(\dfrac{1}{\rho}\nabla p\right)$

Also note that density cancels out if it varies slowly enough in space (i.e. it's near enough constant).

This leads back to the standard isotropic 3D wave equation: $\dfrac{1}{c^2}\dfrac{\partial^2 p}{\partial t^2} = \nabla^2 p$

2.0.2 Showing elastic wave equation supports both P-waves and S-waves...

Go back to isotropic homogeneous 3d elastic wave equation: $\rho \dfrac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + 2\mu)\,\nabla(\nabla \cdot \mathbf{u}) - \mu\,\nabla \times \nabla \times \mathbf{u}$

Separate $\mathbf{u}$ into two parts, one part having no curl (i.e. rotation) since it is the gradient of a scalar potential Φ, and one with no divergence since it is the curl of a vector potential $\boldsymbol{\Psi}$.

$$\text{i.e:} \quad \mathbf{u} = \nabla\Phi + \nabla \times \boldsymbol{\Psi}$$

And then put this expression into the isotropic 3d (homogeneous) elastic wave equation, and use the following three identities:

$$\nabla \times (\nabla b) \equiv \mathbf{0}\,, \quad \nabla \cdot (\nabla \times \mathbf{a}) \equiv 0\,, \quad \nabla \times \nabla \times \mathbf{a} \equiv \nabla\,(\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a}$$

...to rearrange the equation such that Φ is on one side and $\boldsymbol{\Psi}$ on the other (similar to separation of variables).

Assume there exists a solution where both sides are constant, and equal to zero.

This produces two independent 3d wave equations, one for each of $\nabla\Phi$ and $\nabla \times \boldsymbol{\Psi}$. The first corresponds to the acoustic wave equation we derived above, i.e. pressure waves. The other corresponds to shear waves.

These two separated wave equations also show the propagation speed for each type of wave (in terms of properties of the medium, i.e. ρ, λ, μ) – acoustic waves travel at speed $\sqrt{(\lambda + 2\mu)\;/\;\rho}$, shear waves travel at $\sqrt{\mu\;/\;\rho}$.

In practice these two types can convert from one to the other, so they don't actually separate in the neat way forced above (caused by assuming both sides of the split equation are constant and zero).

2.0.3 Plane wave solution of 3d isotropic homogeneous wave equation...

Assume pressure, p, is a function of $s = \mathbf{r} \cdot \hat{\mathbf{n}} - ct$, where $\mathbf{r}$ is position vector (x, y, z) and $\hat{\mathbf{n}}$ is unit vector (n_x, n_y, n_z).

$$\text{Then:} \quad \frac{\partial p}{\partial t} = \frac{\partial p}{\partial s}\frac{\partial s}{\partial t} \; = -c\frac{\partial p}{\partial s} \quad \text{(Note: we're assuming } c \text{ constant)}$$

$$\text{And:} \quad \frac{\partial^2 p}{\partial t^2} \; = \; -c\frac{\partial^2 p}{\partial s \partial t} \; = \; -c\frac{\partial^2 p}{\partial s^2}\frac{\partial s}{\partial t} \; = \; c^2\frac{\partial^2 p}{\partial s^2}$$

$$\text{Similarly:} \quad \frac{\partial p}{\partial x} = \frac{\partial p}{\partial s}\frac{\partial s}{\partial x} \; = \; n_x\frac{\partial p}{\partial s}$$

$$\text{And:} \quad \frac{\partial^2 p}{\partial x^2} \; = \; n_x\frac{\partial^2 p}{\partial s \partial x} \; = \; n_x\frac{\partial^2 p}{\partial s^2}\frac{\partial s}{\partial x} \; = \; n_x^2\frac{\partial^2 p}{\partial s^2}$$

$$\text{So:} \quad \nabla^2 p \; = \; \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} \; = \; n_x^2\frac{\partial^2 p}{\partial s^2} + n_y^2\frac{\partial^2 p}{\partial s^2} + n_z^2\frac{\partial^2 p}{\partial s^2} \; = \; \frac{\partial^2 p}{\partial s^2} \; = \; \frac{1}{c^2}\frac{\partial^2 p}{\partial t^2}$$

Since the wave equation is linear, we can sum planar functions moving in different directions:

$$p \; = \; \sum_m p_m(\mathbf{r} \cdot \hat{\mathbf{n}}_m - ct)$$

Can also express it in terms of sum of waves with different frequencies & amplitudes (just as we did in 1d):

$$p \; = \; \sum_m p_m e^{i\omega_m\left(\frac{\mathbf{r}\cdot\hat{\mathbf{n}}_m}{c} - t\right) + i\phi_m}$$

These are (complex) plane waves, each acting just like our 1d case, all moving at speed c, but with (potentially) different directions in 3d space.

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3 Adding a Source Term to the Wave Equation

In all the code written so far, we have introduced the source function in time as some kind of 'forced' boundary condition on the pressure (or whatever the oscillating function may be), by actually setting the pressure, at a point(s) in space over all time, to some specified value(s).
Quite often, this is not how a source is injected when modelling the real world. Instead, it's an extra term which is *added* to the RHS of the wave equation. When running a simulation, this means it gets injected by *adding* it to the new wavefield at each step.
We can demonstrate how this works in the equations by including an extra force vector in the equation of motion (here done only for the simpler acoustic case)...

$$\text{Start from equation of motion, but add an 'external' force, } \mathbf{f}\text{:} \quad \rho\,\frac{\partial^2 \mathbf{u}}{\partial t^2} \; = \; -\nabla p \; + \; \mathbf{f}$$

$$\text{Continue as before, using:} \quad \nabla \cdot \mathbf{u} \; = -\frac{1}{\rho c^2} p$$

This leads to the 3D acoustic wave equation with source term: $$\frac{1}{\rho c^2}\frac{\partial^2 p}{\partial t^2} \;=\; \nabla\cdot\left(\frac{1}{\rho}\nabla p\right) \;+\; S$$

Where: $S \;=\; -\nabla\cdot(\,\mathbf{f}\,/\,\rho\,)$

For the case of constant background density: $$\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} \;=\; \nabla^2 p \;-\; \nabla\cdot\mathbf{f}$$

So we just have that the effective source, S, in the 3D isotropic wave equation (with constant density) is the negative divergence of the force **f**.

For interest...
Consider an 'explosive' source, which gets 'switched on' at time t=0, as a force which exists all around the surface of a spherical shell with radius a, with constant magnitude, f, and with direction pointing outward from the shell:
– What is the behaviour over time of the integral of acoustic pressure, p, inside the spherical shell?
– What is the behaviour over time of the acoustic pressure just outside the spherical shell?