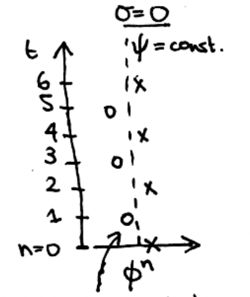
If $\sigma = 0$ $[d\psi/dt = 0]$, $a_+ = 1 = e^{\sigma \Delta t}$ as expected for the physical mode, but $a_- = -1$ $\Rightarrow$ an undamped computational mode. This reflects "even-odd" decoupling in the leapfrog scheme for $\sigma = 0$:

${}^{+1} = \phi^{n-1}$ so $\phi^0 = \phi^2 = \phi^4 \ldots$

$\phi^1 = \phi^3 = \phi^5 \ldots$



Error in initializing ϕ^1 is never damped
$\Rightarrow 2\Delta t$ oscillation = computational mode.

Now consider oscillations $\sigma = -i\omega$. Now

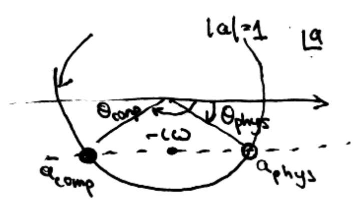
$$a_{phys} = a_+ = -i\omega\Delta t + \left(1 - (\omega\Delta t)^2\right)^{\frac{1}{2}}$$

$$\Rightarrow |a_{phys}|^2 = (\omega\Delta t)^2 + 1 - (\omega\Delta t)^2 = 1$$

$$\Rightarrow a_{phys} = e^{i\theta_{phys}} \quad \text{if } |\omega\Delta t| \le 1$$

where

$$\theta_{phys} = -\sin^{-1}[\omega\Delta t]$$



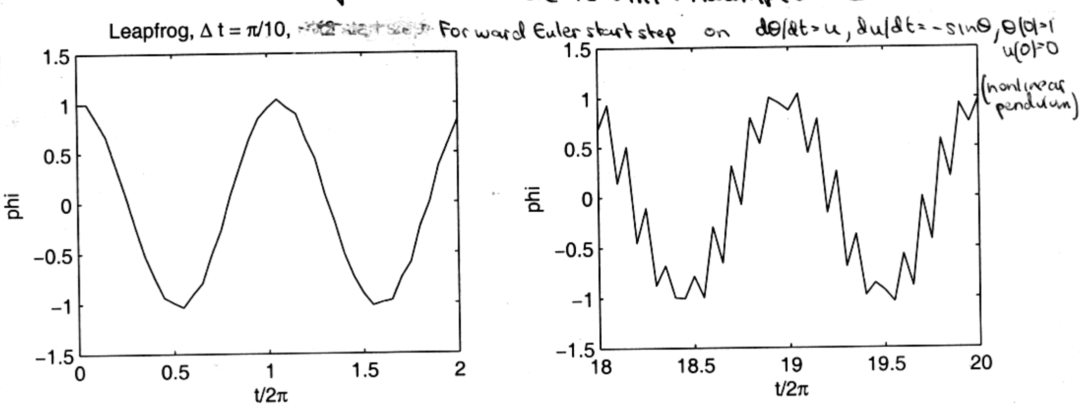
Similarly $a_{comp} = e^{i\theta_{comp}}$.
where

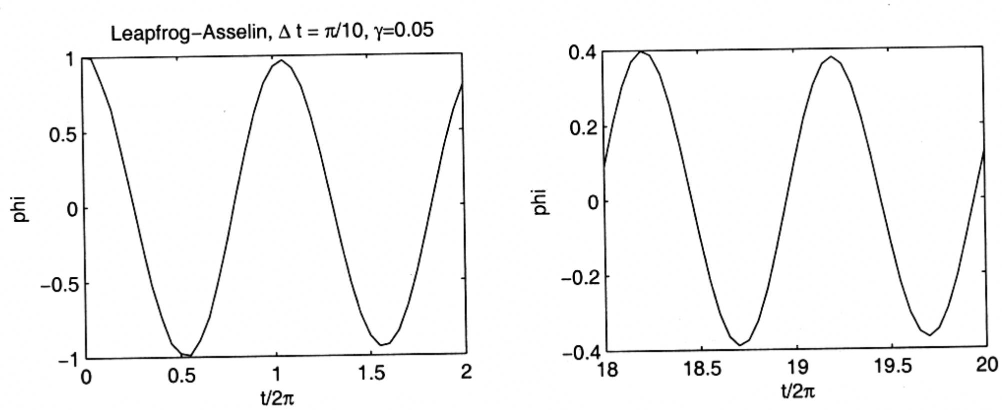
$$\theta_{comp} = -\pi - \theta_{phys}$$

As $\omega \to 0$, $\theta_{phys} \to 0$ and $\theta_{comp} \to -\pi$ ($2\Delta t$ oscillation).

Thus, the physical mode is stable for $|\omega\Delta t| \le 1$ ✓

... but the computational mode is still undamped ☹





Damping the leapfrog computational mode

Method 1: Odd-even average every N (say 100) timesteps.

$$\phi^{n+1} = \phi^{n-1} + 2\Delta t\, F(\phi^n) \quad , n = 1, \ldots, N$$

then . . .

$$\phi^{N+\frac{1}{2}} = \tfrac{1}{2}(\phi^N + \phi^{N+1})$$

$$\phi^N = \phi^{N+\frac{1}{2}} - \frac{\Delta t}{2} F(\phi^{n+\frac{1}{2}})$$

$$\phi^{N+1} = \phi^{N+\frac{1}{2}} + \frac{\Delta t}{2} F(\phi^{n+\frac{1}{2}})$$

. . . and repeat. Accuracy + stability depend on N.

This approach is still 2nd order accurate

Method 2: Asselin filter

$$\phi^{n+1} = \bar{\phi}^{n-1} + 2\Delta t\, F(\phi^n)$$

$$\bar{\phi}^n = \phi^n + \gamma(\phi^{n+1} - 2\phi^n + \bar{\phi}^{n-1})$$

(a diffusive smoother, which preferentially filters the highest frequencies).

Stability analysis ⇒

$$A_{phys} = 1 - i\omega\Delta t - \underbrace{\frac{(\omega\Delta t)^2}{2(1-\gamma)}}_{\text{not identical to } A_{ex} \text{ if } \gamma \neq 0} + O((\omega\Delta t)^4)$$

⇒ only first-order accurate!

$$A_{comp} = 1 - 2\gamma + O(\Delta t^2)$$

⇒ computational mode damped. Typically $\gamma = 0.05$ is a good compromise between minimizing truncation error and adequately damping the computational mode. However, the nonlinear pendulum example on prev. page shows there is still significant damping at $t/2\pi = 18-20$, unlike with plain leapfrog which still has undamped amplitude (though the $2\Delta t$ oscillation is clear). A RK4 scheme with the same Δt would hardly produce any numerical damping (though one with $4\Delta t$ does worse than the Asselin-Leapfrog in this case).

Lastly: The computational mode grows when $\sigma_r < 0$ (physical decay)

⇒ Don't use leapfrog when there is a damped mode!

Synopsis of time-differencing methods

Method	Order	Levels	Stages	Max $\sigma_i\Delta t$	Max $\sigma_r\Delta t$	Comments
Forward	1	2	1	0	2	Simple, poor stability
Backward	1	2	1	∞	∞	Good stability for diffusion terms. Implicit.
Trapezoidal	2	2	1	∞	∞	Accurate. Stable (but less than backward). Implicit.
Leapfrog	2	3	1	1	0	Good for waves, but must filter computational mode
AB3	3	4	1	0.71	0.56	Stable and accurate for oscillations
RK4	4	2	4	2.82	2.82	Stable, highly accurate for oscillations

Space differencing

We now return to the effect of space-differencing errors on an example PDE, the advection equation.

$$L[\psi] = \frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = 0. \qquad (*)$$

In general, if we use a p'th order accurate time-differencing scheme and an m'th order accurate space-differencing scheme, the LTE would be of the form $c_t(\Delta t)^p + c_x(\Delta x)^m$ + H.O.T. To focus on space-differencing let us assume $\Delta t \to 0$, i.e. we assume perfect time-differencing with no error (the "semi-discrete" idealization). We assume our FDA for $\frac{\partial}{\partial x}$ is

$$D[\phi_j] = \sum_{l=-l_1}^{l_2} \alpha_l \phi_{j+l} \qquad \left[\begin{array}{c}\text{to get m'th order accuracy} \\ l_2 + l_1 \geq m\end{array}\right].$$

By Taylor expansion, since $D[\psi] = \frac{\partial \psi}{\partial x} + O(\Delta x^m)$, we must have α_l's $= O\left(\frac{1}{\Delta x}\right)$ and

$$D[\psi(x_j,t)] = \sum_{l=-l_1}^{l_2} \alpha_l \left\{\psi + l\Delta x\frac{\partial \psi}{\partial x} \cdots + \frac{(l\Delta x)^{m+1}}{(m+1)!}\frac{\partial^{m+1}\psi}{\partial x^{m+1}} + \frac{(l\Delta x)^{m+2}}{(m+2)!}\frac{\partial^{m+2}\psi}{\partial x^{m+2}}\cdots\right\}_{x_j}$$

$$= \left(\frac{\partial \psi}{\partial x}\right)_j + a\,(\Delta x)^m\left(\frac{\partial^{m+1}\psi}{\partial x^{m+1}}\right)_j + b\,\Delta x^{m+1}\left(\frac{\partial^{m+2}\psi}{\partial x^{m+2}}\right)_j.$$

Thus the LTE of the semi-discrete in x-approximation to the advection eqn $(*)$ is:

$$L[\psi] = \frac{\partial \psi}{\partial t} + cD[\psi] = c\left\{a\frac{\partial^{m+1}\psi}{\partial x^{m+1}} + b\frac{\partial^{m+2}\psi}{\partial x^{m+2}}\cdots\right\}$$

and the modified equation is

$$\frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = c\left\{a\frac{\partial^{m+1}\psi}{\partial x^{m+1}} + b\frac{\partial^{m+2}\psi}{\partial x^{m+2}}\right\}$$

with dispersion relation

$$-i\omega + ick = c\left\{a(ik)^{m+1} + b(ik)^{m+2}\right\}$$

$$\omega = ck + ca\,i^{m+2}k^{m+1} + cb\,i^{m+3}k^{m+2}$$

Note that if m is <u>odd</u>, the leading error term in ω is imaginary, i.e. (for a stable method) numerical <u>dissipation</u>, with a secondary dispersion term, while...

if m is <u>even</u>, the leading error term in ω is real (numerical dispersion) with a secondary dissipation term. This is true regardless of method.