Numerical Techniques 2023–2024

2. The oscillation equation and time differencing

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Previously on Numerical Techniques...

- Positioning of the course in the postgraduate program
- Discretization and finite differences
- Consistency, convergence and stability
- Von Neumann analysis and Courant number $\mu = c\frac{\Delta t}{\Delta x}$, linking spatial resolution to temporal resolution
- Example of upstream scheme for 1D advection equation
- Don't worry about math too much!

Today's content...

- The oscillation equation
- Errors due to time discretization: amplitude and phase
- Concrete schemes
  - Single stage, two timelevel
    Forward, backward, trapezium
  - Multistage, two timelevel
    Heun, Matsuno, Runge-Kutta
  - Single stage, three timelevel
    Leapfrog, Adams-Bashforth
  - Filter for computational modes

The oscillation equation is given by:

$$\frac{d\psi}{dt} = i\kappa\psi$$

Although much simpler than the partial differential equations (PDE's) in atmospheric modeling, the oscillation equation is very relevant:

1. Wave-dominated hyperbolic PDE's can be decoupled in advection equations
2. The advection equation in Fourier expansion looks like the oscillation equation

From advection equation to oscillation equation

- The advection equation

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

in Fourier expansion $\left(\psi(x,t) = \sum_{k=-\infty}^{\infty} \hat{\psi}_k(t) e^{ikx}\right)$ looks like

$$\frac{d\hat{\psi}_k}{dt} = -ikc\,\hat{\psi}_k$$

which is actually the oscillation equation

$$\frac{d\psi}{dt} = i\kappa\psi$$

- The influence of the space discretization is removed by the Fourier transform, so we can now focus on the *time differencing*.

The oscillation equation: time evolution

- The exact time evolution of the solution is

$$\psi(t_0 + \Delta t) = e^{i\kappa\Delta t}\psi(t_0) \equiv A_e\psi(t_0)$$

- For an approximate (numerical) solution, $\phi^{n+1} = A\phi^n$.
- The quality of the approximation will depend on the difference between A and A_e.
- Note: we will use the exponential notation of a complex number:

$$A = |A|e^{i\theta}$$

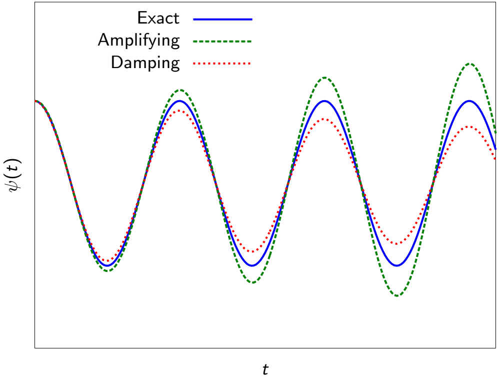
with

$$|A| = \sqrt{\mathcal{R}\{A\}^2 + \mathcal{I}\{A\}^2}$$
$$\theta = \arg(A) = \arctan\left(\frac{\mathcal{I}\{A\}}{\mathcal{R}\{A\}}\right)$$

Approximation of exact solution $A_e = e^{i\kappa\Delta t}$ by numerical solution $A = |A|e^{i\theta}$:

- Amplitude

$\|A\| > 1$	amplifying
$\|A\| = 1$	neutral
$\|A\| < 1$	damping



Approximation of exact solution $A_e = e^{i\kappa\Delta t}$ by numerical solution $A = |A|e^{i\theta}$:

- Amplitude

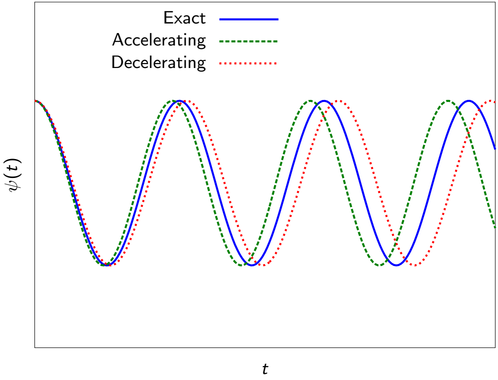
$$\begin{array}{ll} |A| > 1 & \text{amplifying} \\ |A| = 1 & \text{neutral} \\ |A| < 1 & \text{damping} \end{array}$$

- Phase speed: error is characterized by the *relative* phase change

$$R = \frac{\theta}{\kappa\Delta t}$$

Then

$$\begin{array}{ll} R > 1 & \text{accelerating} \\ R < 1 & \text{decelerating} \end{array}$$



We will now review several schemes:

- Single stage, two-time-level schemes
- Multistage schemes
- Three-time-level schemes

Single stage two-time-level schemes

- For the generic equation

$$\frac{d\psi}{dt} = F(\psi)$$

the single-stage two-time-level schemes have the form

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

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- Some terminology:

$\alpha = 1$	$\beta = 0$	forward differencing
$\alpha = 0$	$\beta = 1$	backward differencing
$\alpha = \frac{1}{2}$	$\beta = \frac{1}{2}$	trapezoidal differencing

Single stage two-time-level schemes: amplification factor

- For the oscillation equation the right-hand side is simply $F(\psi) = i\kappa\psi$, so the single-stage two-time-level schemes become

$$(1 - i\beta\kappa\Delta t)\,\phi^{n+1} = (1 + i\alpha\kappa\Delta t)\,\phi^{n}$$

- The amplification factor is then

$$A \equiv \frac{\phi^{n+1}}{\phi^{n}} = \frac{1 + i\alpha\kappa\Delta t}{1 - i\beta\kappa\Delta t}$$

Single stage two-time-level schemes: accuracy

- The order of accuracy is identified when taking the Taylor expansion of the amplification factor A:

$$A = 1 + i(\alpha + \beta)\kappa\Delta t - (\alpha + \beta)\beta(\kappa\Delta t)^2 + O(\Delta t^3)$$

  while the exact amplification factor is:

$$A_e = e^{i\kappa\Delta t} = 1 + i\kappa\Delta t - \tfrac{1}{2}(\kappa\Delta t)^2 + O(\Delta t^3)$$

  so

  - forward and backward schemes are first order accurate
  - trapezium scheme is second order accurate

Single stage two-time-level schemes: stability

- The modulus of the amplification factor is

$$|A|^2 = \frac{1 + \alpha^2 \kappa^2 \Delta t^2}{1 + \beta^2 \kappa^2 \Delta t^2}$$

- So the stability properties are:
  - Forward scheme ($\alpha = 1, \beta = 0$) $\Rightarrow$ unstable (amplifying)
  - Trapezium scheme ($\alpha = \beta = 1/2$) $\Rightarrow$ stable (neutral)
  - Backward scheme ($\alpha = 0, \beta = 1$) $\Rightarrow$ stable (damping)

Single stage two-time-level schemes: phase error

- The relative phase change is

$$R \equiv \frac{\arg(A)}{\kappa \Delta t} = \frac{1}{\kappa \Delta t} \arctan\left(\frac{(\alpha+\beta)\,\kappa \Delta t}{1-\alpha\beta\,(\kappa \Delta t)^2}\right)$$

- For the forward scheme ($\alpha = 1, \beta = 0$) and the backward scheme ($\alpha = 0, \beta = 1$),

$$R_{\text{forward}} = R_{\text{backward}} = \frac{\arctan \kappa \Delta t}{\kappa \Delta t}$$

- Using the Taylor expansion of arctan:

$$\arctan x = x - \frac{x^3}{3} + \ldots$$

it follows that for good numerical resolution ($\kappa \Delta t \ll 1$),

$$R_{\text{forward}} = R_{\text{backward}} \approx 1 - \frac{(\kappa \Delta t)^2}{3}$$

So the forward scheme and the backward scheme are decelerating.

- For the trapezium scheme ($\alpha = \beta = 1/2$),

$$
\begin{aligned}
R_{\text{trapezoidal}} &= \frac{1}{\kappa\Delta t} \arctan\left(\frac{\kappa\Delta t}{1 - \frac{\kappa^2\Delta t^2}{4}}\right) \\
&\approx 1 - \frac{(\kappa\Delta t)^2}{12}
\end{aligned}
$$

So the trapezium scheme is also decelerating, but the phase error is less than with the forward and the backward schemes.

Important remark:

For the backward and the trapezoidal scheme, $F(\phi^{n+1})$ is needed to compute ϕ^{n+1}:

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

Such schemes are called *implicit* schemes. Schemes for which only ϕ^{n} is needed, are called *explicit* schemes.

For the oscillation equation $F(\psi) = i\kappa\psi$, so the solution is trivial. For other expressions for $F(\psi)$, this will not be the case!

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Implicit schemes are much more stable, but the cost-per-timestep is higher.

Some examples of challenges for implicit schemes:

- nonlinear systems, e.g. $F(\psi) = \sin(\psi)$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{1}{2}\sin\left(\phi^n\right) + \frac{1}{2}\sin\left(\phi^{n+1}\right)$$

  This usually has to be solved iteratively.

Implicit versus explicit schemes

Some examples of challenges for implicit schemes:

- nonlinear systems
- systems with multiple variables become *coupled*, e.g. shallow water equations with 2 variables u and h (cfr. Lesson 5):

$$\frac{u^{n+1} - u^n}{\Delta t} = -g \frac{\partial}{\partial x}\left(h^n + h^{n+1}\right)$$
$$\frac{h^{n+1} - h^n}{\Delta t} = -H \frac{\partial}{\partial x}\left(u^n + u^{n+1}\right)$$

  A linear system has to be solved.

Implicit versus explicit schemes

Some examples of challenges for implicit schemes:

- nonlinear systems
- systems with multiple variables become *coupled*
- for systems involving spatial derivatives, the gridpoints become coupled, e.g. advection equation:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = -\frac{c}{2}\left(\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} + \frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x}\right)$$

A (LARGE!) tridiagonal system has to be solved.

Multistage methods: Heun scheme

Multistage methods evaluate the RHS $F(\phi)$ several times instead of one single time.

Example: Heun scheme (also called Runge-Kutta-2) which replaces ϕ^{n+1} in the RHS of the trapezium scheme by a forward estimate:

$$\tilde{\phi}^{n+1} = \phi^n + \Delta t F(\phi^n) \qquad \text{forward estimate of } \phi^{n+1}$$

$$\phi^{n+1} = \phi^n + \frac{\Delta t}{2}\left[F(\phi^n) + F(\tilde{\phi}^{n+1})\right] \qquad \text{trapezium-like timestep}$$

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Exercise: what is the amplification factor of the Heun scheme applied to the oscillation equation $F(\psi) = i\kappa\psi$?

Substituting $F(\psi) = i\kappa\psi$ in the Heun scheme gives:

$$\tilde{\phi} = (1 + i\kappa\Delta t)\phi^n$$
$$\phi^{n+1} = \phi^n + \frac{i\kappa\Delta t}{2}\left(\phi^n + \tilde{\phi}\right)$$

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Substituting $\tilde{\phi}$ in the second equation gives

$$\phi^{n+1} = \left(1 + i\kappa\Delta t - \frac{(\kappa\Delta t)^2}{2}\right)\phi^n$$

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So the amplification factor is

$$A = \frac{\phi^{n+1}}{\phi^n} = 1 + i\kappa\Delta t - \frac{1}{2}(\kappa\Delta t)^2$$

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So the amplification factor is

$$A = \frac{\phi^{n+1}}{\phi^n} = 1 + i\kappa\Delta t - \frac{1}{2}(\kappa\Delta t)^2$$

which is second-order accurate (compare with Taylor expansion of exact amplification factor).

Multistage methods: Heun scheme

The modulus is

$$|A|^2 = 1 + \frac{1}{4}(\kappa \Delta t)^4 > 1$$

So the Heun scheme is unconditionally unstable!

The Matsuno scheme combines a forward estimate with a backward step:

$$\tilde{\phi}^{n+1} = \phi^n + \Delta t F(\phi^n) \qquad \text{forward estimate of } \phi^{n+1}$$
$$\phi^{n+1} = \phi^n + \Delta t F(\tilde{\phi}^{n+1}) \qquad \text{backward-like timestep}$$

The amplification factor is

$$A = 1 + i\kappa\Delta t - (\kappa\Delta t)^2$$

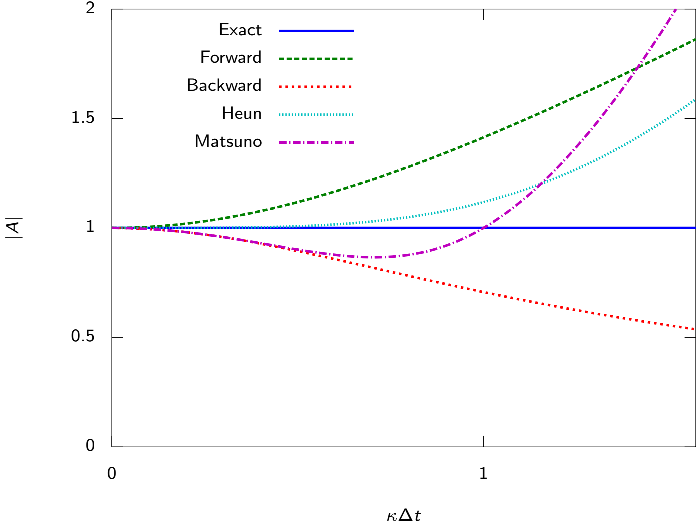
which is first-order accurate.

The modulus is

$$|A|^2 = 1 - (\kappa\Delta t)^2 + (\kappa\Delta t)^4$$

So the Matsuno scheme is conditionally stable: $\kappa\Delta t < 1$

Multistage methods: amplification

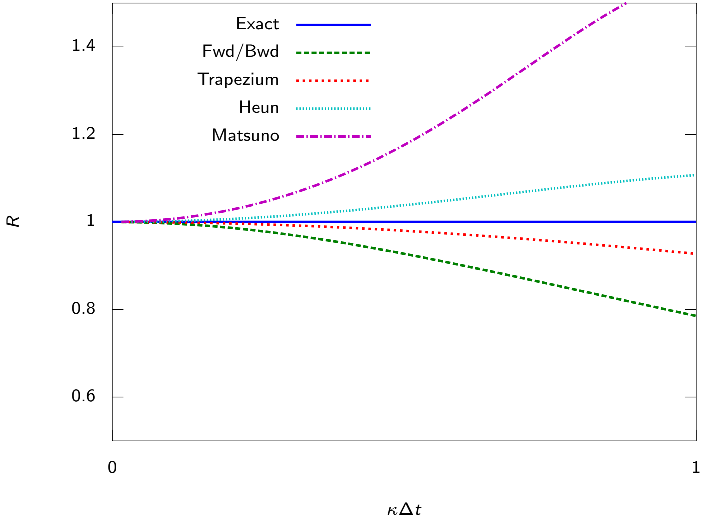


Approximated for $\kappa\Delta t \ll 1$,

$$R_{\mathrm{Heun}} \approx 1 + \tfrac{1}{6}\left(\kappa\Delta t\right)^2$$
$$R_{\mathrm{Matsuno}} \approx 1 + \tfrac{2}{3}\left(\kappa\Delta t\right)^2$$

So the Heun scheme has less phase change than the Matsuno scheme.

Multistage methods: phase change



The following scheme is quite popular because it's 4th order accurate:

$$
\begin{aligned}
q_1 &= \Delta t F(\phi^n) \\
q_2 &= \Delta t F(\phi^n + q_1/2) \\
q_3 &= \Delta t F(\phi^n + q_2/2) \\
q_4 &= \Delta t F(\phi^n + q_3) \\
\phi^{n+1} &= \phi^n + \tfrac{1}{6}\left(q_1 + 2q_2 + 2q_3 + q_4\right)
\end{aligned}
$$

This scheme is conditionally stable ($|\kappa \Delta t| < 2.828$).

The drawback of multistage methods is that the right hand side $F(\psi)$ needs to be evaluated several times. This makes them suitable for toy-models, but not for operational 3D NWP models.

It is possible to reuse information from the previous timestep ϕ^{n-1}:

$$\phi^{n+1} = \alpha_1 \phi^n + \alpha_2 \phi^{n-1} + \beta_1 \Delta t F(\phi^n) + \beta_2 \Delta t F(\phi^{n-1})$$

Such a scheme will be at least second-order if

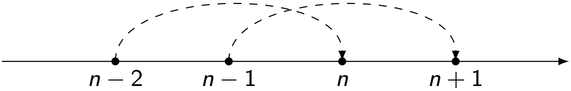
$$\alpha_1 = 1 - \alpha_2 \qquad \beta_1 = \tfrac{1}{2}(\alpha_2 + 3) \qquad \beta_2 = \tfrac{1}{2}(\alpha_2 - 1)$$

We limit ourselves to the following (second order) schemes:

	α_1	α_2	β_1	β_2
Leapfrog	0	1	2	0
Adams-Bashforth	1	0	$\frac{3}{2}$	$-\frac{1}{2}$

The leapfrog scheme for the oscillation equation:

$$\phi^{n+1} = \phi^{n-1} + 2i\kappa\Delta t\phi^{n}$$



The amplification factor satisfies

$$A^2 - 2i\kappa\Delta t A - 1 = 0$$

so

$$A_{\pm} = i\kappa\Delta t \pm \sqrt{1-\kappa^2\Delta t^2}$$

which is second-order accurate.

There are 2 solutions corresponding to 2 'modes'. If $\kappa\Delta t \to 0$ then $A_+ \to 1$ and $A_- \to -1$. Therefore,

$$\begin{aligned} A_+ &\sim \text{physical mode} \\ A_- &\sim \text{purely artificial `computational' mode} \end{aligned}$$

- If $|\kappa\Delta t| \leq 1$, $|A_+| = |A_-| = 1$ so the scheme is stable.
- If $\kappa\Delta t > 1$

$$|A_+| = \left| i\kappa\Delta t + i\sqrt{(\kappa^2\Delta t^2 - 1)} \right| > |i\kappa\Delta t| > 1$$

  So the scheme is unstable.

- If $\kappa\Delta t < -1$ then $|A_-| > 1$ so the computational mode is unstable.

The computational mode is easy to analyse in the case $\kappa = 0$:

$$\phi^{n+1} = \phi^{n-1}$$

and the roots are $A_+ = 1, A_- = -1$
For the initial condition $\phi^0 = C$:

$$\phi^2 = \phi^4 = \phi^6 = \cdots = C$$

ϕ^1 is usually determined by another two-time-level scheme: $\phi^1 = C + \epsilon$ with ϵ some error. Then

$$\phi(t) = \{\, C\,,\ C+\epsilon\,,\ C\,,\ C+\epsilon\,,\ C\,,\ C+\epsilon\ \ldots \}$$

So the error ϵ stays in the solution.

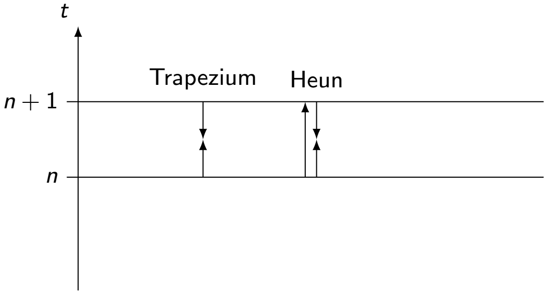
The relative phase change of the physical mode of the leapfrog scheme is given by

$$
\begin{aligned}
R_{\text{leapfrog}} &= \frac{1}{\kappa\Delta t}\arctan\left(\frac{\kappa\Delta t}{\sqrt{1-\kappa^2\Delta t^2}}\right) \\
&\approx 1 + \tfrac{1}{6}\left(\kappa\Delta t\right)^2
\end{aligned}
$$

So the leapfrog scheme is accelerating.

The trapezium scheme is very attractive (neutral, 2nd order, small phase error), but it is implicit: it requires $F(\phi^{n+1})$ to determine ϕ^{n+1}.

The Heun scheme attempts to approximate the trapezium scheme by using a forward estimate in the RHS:



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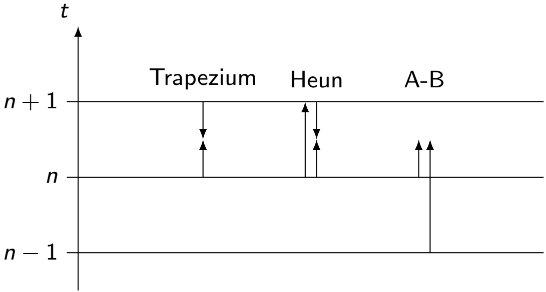

The Adams-Bashforth scheme estimates $F\left(\phi^{n+\frac{1}{2}}\right)$ by extrapolating from $F\left(\phi^{n}\right)$ and $F\left(\phi^{n-1}\right)$.

The Adams-Bashforth scheme writes:

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

For the oscillation equation, the amplification factor satisfies

$$A^2 - \left(1 + \tfrac{3}{2}i\kappa\Delta t\right)A + \tfrac{1}{2}i\kappa\Delta t = 0$$

with two modes,

$$A_{\pm} = \tfrac{1}{2}\left[1 + \tfrac{3}{2}i\kappa\Delta t \pm \sqrt{1 - \tfrac{9}{4}\left(\kappa\Delta t\right)^2 + i\kappa\Delta t}\right]$$

For good temporal resolution $\kappa\Delta \leq 1$,

$$
\begin{aligned}
|A_+|_{\text{A-B2}} &\approx 1 + \tfrac{1}{4}\left(\kappa\Delta t\right)^4 \\
|A_-|_{\text{A-B2}} &\approx \tfrac{1}{2}\kappa\Delta t \\
R_{\text{A-B2}} &\approx 1 + \tfrac{5}{12}\left(\kappa\Delta t\right)^2
\end{aligned}
$$

In NWP application we want strict stability, so this weak instability makes Adams-Bashforth unattractive.

In contrast, the leapfrog mode contains the artificial computational mode. However, this mode can be controlled by a Robert-Asselin filter.

The Robert-Asselin filter

We modify the leapfrog-scheme by adding a filter step:

$$\phi^{n+1} = \overline{\phi^{n-1}} + 2\Delta t F(\phi^n) \qquad \text{normal leapfrog}$$

$$\overline{\phi^n} = \phi^n + \gamma\left(\overline{\phi^{n-1}} - 2\phi^n + \phi^{n+1}\right) \qquad \text{apply filter}$$

where typically $\gamma = 0.06$ in meteorological models.

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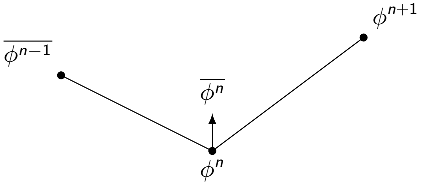
where typically $\gamma = 0.06$ in meteorological models.

The term $\overline{\phi^{n-1}} - 2\phi^n + \phi^{n+1}$ can be interpreted as a temporal filter that damps the high frequencies (esp. the $2\Delta t$-mode): if $\overline{\phi^{n-1}} > \phi^n$ and $\phi^{n+1} > \phi^n$, then $\overline{\phi^n}$ will be increased:



Amplification of Asselin-leapfrog:

$$A_{\pm} = \gamma + i\kappa\Delta t \pm \sqrt{(1-\gamma)^2 - \kappa^2\Delta t^2}$$

For small $\kappa\Delta t$,

$$A_{+} \approx 1 + i\kappa\Delta t - \frac{(\kappa\Delta t)^2}{2(1-\gamma)}$$

$$A_{-} \approx -1 + 2\gamma + i\kappa\Delta t + \frac{(\kappa\Delta t)^2}{2(1-\gamma)}$$

while expansion of the exact solution is:

$$A_e = e^{i\kappa\Delta t} = 1 + i\kappa\Delta t - \tfrac{1}{2}(\kappa\Delta t)^2 - i\tfrac{1}{6}(\kappa\Delta t)^3 + O[(\kappa\Delta t)^4]$$

So the Robert-Asselin filter degrades the accuracy of the scheme from 2nd order to 1st order.

The modulus of the amplification factor becomes:

$$|A_+| \approx 1 - \frac{\gamma}{2(1-\gamma)}(\kappa\Delta t)^2$$

$$|A_-| \approx (1-2\gamma) + \frac{\gamma}{2-6\gamma+4\gamma^2}(\kappa\Delta t)^2$$

Note that the computational mode is (slightly) damped.

The relative phase change becomes:

$$R_+ \approx 1 + \frac{1+2\gamma}{6(1-\gamma)}(\kappa\Delta t)^2$$

Summary

- We work on the *oscillation equation*, to focus on the time differencing aspect
- A scheme is characterized by
  - amplitude: amplifying, neutral or damping
  - relative phase change: accelerating or decelerating
  - explicitness or implicitness
  - order of accuracy
- Concrete examples:
  - Two time-level schemes: forward, backward, **trapezium**
  - Multistage schemes: Heun, Matsuno, **Runge-Kutta-4**
  - Three time-level schemes: **leapfrog** and Adams-Bashforth
    $\Rightarrow$ computational mode, filter
- There is no 'best' scheme: every scheme has disadvantages.
- What matters is methodology!