

Numerical Techniques 2023–2024

6. Semi-implicit semi-Lagrangian schemes

Daan Degrauwe

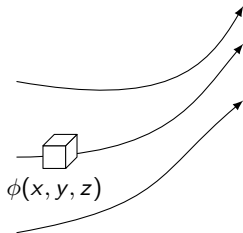
`daan.degrauwe@meteo.be`

Postgraduate Studies in Weather and Climate Modeling

Ghent University

- Introduction: Eulerian and Lagrangian schemes
- Advection equation:
 - ▶ stability
 - ▶ accuracy
 - ▶ 2D
 - ▶ nonconstant advection speed and forcings
- Shallow water equations
 - ▶ Semi-Lagrangian linearized SWE
 - ▶ Semi-implicit nonlinear SWE

Eulerian:

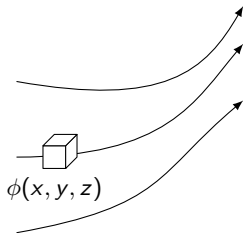


$$\delta\phi = \phi(x, y, z, t + \delta t) - \phi(x, y, z, t)$$

The derivative is the partial derivative

$$\frac{\partial\phi}{\partial t}$$

Eulerian:

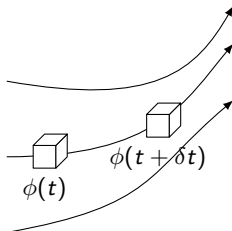


$$\delta\phi = \phi(x, y, z, t + \delta t) - \phi(x, y, z, t)$$

The derivative is the partial derivative

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Lagrangian:



$$\delta\phi = \phi(x + \delta x, y + \delta y, z + \delta z, t + \delta t) - \phi(x, y, z, t)$$

The derivative is the total derivative

$$\frac{D\phi}{Dt}$$

- The total derivative is given by

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \frac{Dx}{Dt} \frac{\partial}{\partial x} \quad \text{with} \quad \frac{Dx}{Dt} = u$$

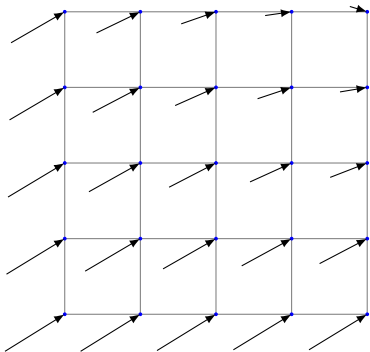
- Formulation of the advection equation in Eulerian and Lagrangian shape:

$$\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} = 0 \quad \text{or} \quad \frac{D\psi}{Dt} = 0$$

- So the time discretisation would be much simpler if we write it in a Lagrangian frame: no *nonlinear* advection term will be present.

- However, in flows that are divergent one may end up with regions that are not well represented by air particles after some time.

- However, in flows that are divergent one may end up with regions that are not well represented by air particles after some time.
- The solution: use *semi-Lagrangian* trajectories:



Choose departure points such that the trajectories arrive in the grid points of the model at the end of the time step.

The departure points are recalculated *every time step*!

- The 1D advection equation *with constant advection speed* U is discretized in the semi-Lagrangian form as

$$\frac{\phi(x_j, t^{n+1}) - \phi(\tilde{x}_j, t^n)}{\Delta t} = 0$$

with the *departure point* given by

$$\tilde{x}_j = x_j - U\Delta t$$

- Define

$$p = \left\lfloor \frac{U\Delta t}{\Delta x} \right\rfloor$$

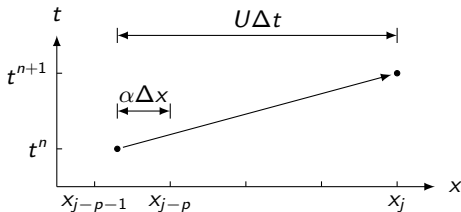
with $\lfloor z \rfloor$ the integer part of z , then

$$x_{j-p-1} \leq \tilde{x}_j \leq x_{j-p}$$

- Now, define

$$\alpha = \frac{x_{j-p} - \tilde{x}_j^n}{\Delta x}$$

- Note that by construction, $0 \leq \alpha \leq 1$, because $x_{j-p-1} \leq \tilde{x}_j^n \leq x_{j-p}$



- Next, we have to approximate ϕ in \tilde{x}_j^n , e.g. by a linear interpolation

$$\phi(\tilde{x}_j^n, t^n) = (1 - \alpha)\phi_{j-p}^n + \alpha\phi_{j-p-1}^n$$

- The advection equation then becomes

$$\frac{\phi_j^{n+1} - \phi(\tilde{x}_j^n, t^n)}{\Delta t} = 0$$

or

$$\phi_j^{n+1} = \phi(\tilde{x}_j^n, t^n) = (1 - \alpha)\phi_{j-p}^n + \alpha\phi_{j-p-1}^n$$

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- **Note 1:** this is an *explicit* scheme: values at the next timestep $n + 1$ only appear on the left-hand side.
- **Note 2:** this is very similar to the upstream scheme; even identical if $p = 0$.

- Von Neumann analysis on a solution of the form $\phi_j^n = A_k^n e^{i(kj\Delta x)}$

$$A_k = \left[1 - \alpha \left(1 - e^{-ik\Delta x} \right) \right] e^{-ikp\Delta x}$$

or

$$|A_k|^2 = 1 - 2\alpha(1 - \alpha)(1 - \cos k\Delta x)$$

then the condition for stability becomes

$$0 \leq \alpha \leq 1$$

which is **always** satisfied!

- Consider the Taylor expansion of

$$\frac{\phi_j^{n+1} - [(1 - \alpha)\phi_{j-p}^n + \alpha\phi_{j-p-1}^n]}{\Delta t} = 0$$

around the departure point (\tilde{x}_j^n, t^n) . Then

$$\frac{\psi_j^{n+1} - [(1 - \alpha)\psi_{j-p}^n + \alpha\psi_{j-p-1}^n]}{\Delta t} \approx -\frac{1}{2}\alpha(1 - \alpha)\frac{\Delta x^2}{\Delta t} \left. \frac{\partial^2 \psi}{\partial x^2} \right|_{\tilde{x}_j^n}$$

- It seems that this could not be consistent if we take the limit $\Delta t \rightarrow 0$ faster than $\Delta x^2 \rightarrow 0$.

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- It seems that this could not be consistent if we take the limit $\Delta t \rightarrow 0$ faster than $\Delta x^2 \rightarrow 0$.
- However, if the Courant number $U\Delta t/\Delta x$ becomes smaller than 1, then $\alpha = U\Delta t/\Delta x$. Using $\partial^2 \psi / \partial t^2 = U^2 \partial^2 \psi / \partial x^2$, the error becomes

$$\frac{1}{2}\Delta t \frac{\partial^2 \psi}{\partial t^2} - \frac{1}{2}U\Delta x \frac{\partial^2 \psi}{\partial x^2} \quad \text{which is first order}$$

- Quadratic interpolation:

$$\phi(\tilde{x}_j^n, t^n) = \frac{1}{2}\alpha(1 + \alpha)\phi_{j-p-1}^n + (1 - \alpha^2)\phi_{j-p}^n + \frac{1}{2}\alpha(1 - \alpha)\phi_{j-p+1}^n$$

with $p + \alpha = U\Delta t$ but p such that $|\alpha| \leq \frac{1}{2}$.

This yields $O[\Delta x^3/\Delta t]$ which gives a second-order accurate scheme.

- The cubic interpolation with $p + \alpha = U\Delta t$ and $0 \leq \alpha \leq 1$ and

$$\begin{aligned} \phi(\tilde{x}_j^n, t^n) = & -\frac{1}{6}(1 + \alpha)\alpha(1 - \alpha)\phi_{j-p-2}^n + \frac{1}{2}(1 + \alpha)\alpha(2 - \alpha)\phi_{j-p-1}^n \\ & + \frac{1}{2}(1 + \alpha)(1 - \alpha)(2 - \alpha)\phi_{j-p}^n - \frac{1}{6}\alpha(1 - \alpha)(2 - \alpha)\phi_{j-p+1}^n \end{aligned}$$

yields third-order accuracy.

- In 2 dimensions,

$$\frac{D\psi}{Dt} = \frac{\partial\psi}{\partial t} + U\frac{\partial\psi}{\partial x} + V\frac{\partial\psi}{\partial y} = 0$$

is discretized as

$$\frac{\phi(x_{j_x}, y_{j_y}, t^{n+1}) - \phi(\tilde{x}_{j_x, j_y}, \tilde{y}_{j_x, j_y}, t^n)}{\Delta t} = 0$$

with $(\tilde{x}_{j_x, j_y}, \tilde{y}_{j_x, j_y})$ the departure point and (x_{j_x}, y_{j_y}) the arrival point.

- The definition of p and α is similar to the 1D case:

$$p = \left\lfloor \frac{U\Delta t}{\Delta x} \right\rfloor \qquad \alpha = \frac{U\Delta t}{\Delta x} - p$$

$$q = \left\lfloor \frac{V\Delta t}{\Delta y} \right\rfloor \qquad \beta = \frac{V\Delta t}{\Delta y} - q$$

with $0 \leq \alpha, \beta \leq 1$

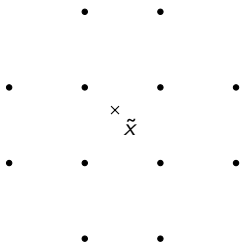
- On a quadratic *stencil*:

$$\begin{array}{ccc}
 \phi_{NW} & \phi_N & \phi_{NE} \\
 \bullet & \bullet & \bullet \\
 \phi_W & \phi_C & \phi_E \\
 \bullet & \bullet & \bullet \\
 \bullet & \bullet & \bullet \\
 \phi_{SW} & \phi_S & \phi_{SE}
 \end{array}$$

$$\begin{aligned}
 \tilde{\phi}^{n+1} = & \frac{1}{2}\alpha(1+\alpha) \left[\frac{1}{2}\beta(1+\beta)\phi_{SW}^n + (1-\beta^2)\phi_W^n - \frac{1}{2}\beta(1-\beta)\phi_{NW}^n \right] \\
 & + (1-\alpha^2) \left[\frac{1}{2}\beta(1+\beta)\phi_S^n + (1-\beta^2)\phi_C^n - \frac{1}{2}\beta(1-\beta)\phi_N^n \right] \\
 & - \frac{1}{2}\alpha(1-\alpha) \left[\frac{1}{2}\beta(1+\beta)\phi_{SE}^n + (1-\beta^2)\phi_E^n - \frac{1}{2}\beta(1-\beta)\phi_{NE}^n \right]
 \end{aligned}$$

This is second-order accurate.

- Ritchie et al. (1995): use cubic interpolation on a 12-point stencil where the corner points are neglected:



gives unconditionally stable schemes.

- If the velocity is not constant, the calculation of the departure point is no longer trivial/exact.
- The truncation error consists of two terms: an error on the departure point + an error on the interpolation:

$$\frac{1}{\Delta t} \left(\psi_j^{n+1} - \psi_d \right) + \frac{1}{\Delta t} \left(\psi_d - \sum_{k=-r}^s \beta_k \psi_{j-p+k}^n \right)$$

with $\psi_d = \psi(\tilde{x}_j^n, t^n)$ and β_k the coefficients of the interpolation.

- Suppose the departure point is computed as follows:

$$\tilde{x}_j^n = x^{n+1} - u(x^{n+1}, t^n) \Delta t$$

then one can show (Taylor expansion!) that

$$\psi_j^{n+1} = \psi_d + O[\Delta t^2]$$

- So the truncation error due to the calculation of the departure point is

$$\frac{\psi_j^{n+1} - \psi_d}{\Delta t} = O[\Delta t]$$

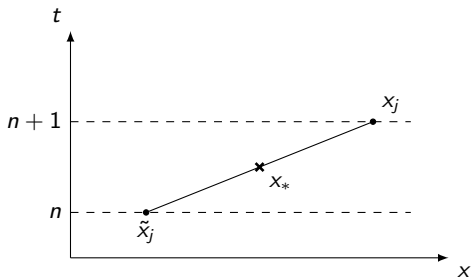
- Hence this method is first order accurate: $O[\Delta t]$.

- Estimating \tilde{x} by a midpoint method:

$$x_* = x^{n+1} - u(x^{n+1}, t^n) \Delta t / 2$$

$$\tilde{x}_j^n = x^{n+1} - u(x_*, t^{n+\frac{1}{2}}) \Delta t$$

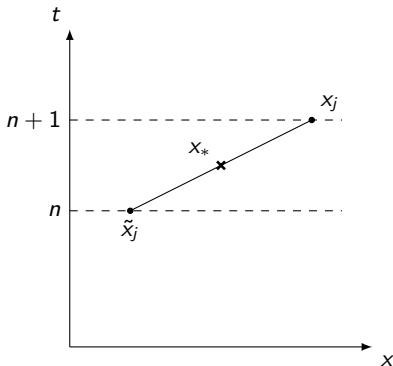
This scheme is second-order accurate.



- But how do we determine $u(x_*, t^{n+\frac{1}{2}})$?

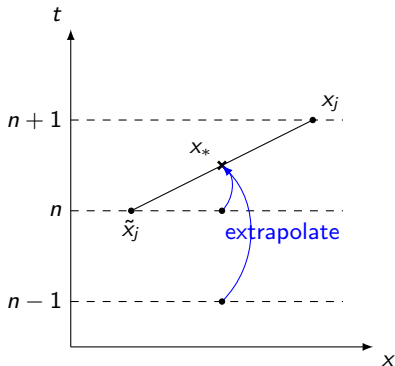
Variable velocity: midpoint method

- In fact it would be best to compute the wind at $t^{n+\frac{1}{2}}$ by interpolating between t^n and t^{n+1} .
- This is possible for passive tracers (e.g. pollutants).
- But for NWP it is not feasible: wind itself is an forecasted field, which is advected by itself!



Variable velocity: midpoint method

- In fact it would be best to compute the wind at $t^{n+\frac{1}{2}}$ by interpolating between t^n and t^{n+1} .
- This is possible for passive tracers (e.g. pollutants).
- But for NWP it is not feasible: wind itself is an forecasted field, which is advected by itself!
- Solution: *time extrapolation*



$u(x_*, t^{n+\frac{1}{2}})$ is obtained by extrapolating from t^{n-1} and t^n :

$$u(t^{n+\frac{1}{2}}) = \frac{3}{2}u(t^n) - \frac{1}{2}u(t^{n-1})$$

which is then linearly interpolated in space to x_* .

- The estimated velocity is second-order in time and in space:

$$u(x_*, t^{n+\frac{1}{2}}) = u_* + O[\Delta x^2] + O[\Delta t^2]$$

- This adds a term of order $O[\Delta t \Delta x^2] + O[\Delta t^3]$ in the estimation of the departure point.
- So there is a $O[\Delta x^2] + O[\Delta t^2]$ contribution in the semi-Lagrangian solution.

In practice the algorithm gets the following form:

- 1 estimate the midpoint

$$x_* = x^{n+1} - u(x^{n+1}, t^n) \Delta t / 2$$

- 2 linearly interpolate the current velocity and the previous velocity to this point:

$$u(t^n, x^*), \quad u(t^{n-1}, x^*)$$

- 3 compute the velocity at the midpoint by extrapolating in time

$$u_* = u(t^{n+\frac{1}{2}}, x^*) = \frac{3}{2}u(t^n, x^*) - \frac{1}{2}u(t^{n-1}, x^*)$$

- 4 compute the departure point $\tilde{x}_j^n = x^{n+1} - u_* \Delta t$
- 5 evaluate $\phi(\tilde{x}_j^n, t^n)$ using a quadratic interpolation
- 6 set ϕ_j^{n+1} equal to this.

- One may invent more accurate schemes, for instance by solving the implicit equation

$$\tilde{x}_j^n = x_j - u \left(\frac{1}{2}(x_j + \tilde{x}_j^n), t^{n+\frac{1}{2}} \right) \Delta t$$

iteratively.

- The midpoint method that we have discussed is actually an example of this.

- Let us consider the prototype problem (oscillation + diffusion)

$$\frac{D\psi}{Dt} = S = i\omega\psi + \lambda\psi \quad \text{with} \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + U \frac{\partial}{\partial x}$$

- The exact solution

$$\psi(x, t) = f(x - Ut)e^{(i\omega + \lambda)t}$$

is non amplifying for $\lambda \leq 0$.

- This can be discretized in a semi-Lagrangian way as follows:

$$\frac{\phi(x_j, t^{n+1}) - \phi(\tilde{x}_j^n, t^n)}{2\Delta t} = \frac{1}{2}S(x_j, t^{n+1}) + \frac{1}{2}S(\tilde{x}_j^n, t^n)$$

- Stability with Von Neumann analysis

$$A_k e^{ikj\Delta x} - e^{ik(j\Delta x - s)} = \frac{1}{2}(\tilde{\lambda} + i\tilde{\omega}) \left(A_k e^{ikj\Delta x} + e^{ik(j\Delta x - s)} \right)$$

with $\tilde{\lambda} = \lambda\Delta t$, $\tilde{\omega} = \omega\Delta t$ and $s = x_j - \tilde{x}_j$.

$$|A_k|^2 = \left| A_k e^{iks} \right|^2 = \frac{\left(1 + \frac{1}{2}\tilde{\lambda}\right)^2 + \frac{1}{4}\tilde{\omega}^2}{\left(1 - \frac{1}{2}\tilde{\lambda}\right)^2 + \frac{1}{4}\tilde{\omega}^2}$$

which is always smaller than 1 for $\lambda \leq 0$. Note that this is even independent of the advection U !

- Let us consider the shallow-water equations

$$\begin{aligned}\frac{Du}{Dt} &= -g \frac{\partial h}{\partial x} \\ \frac{Dh}{Dt} &= -H \frac{\partial u}{\partial x}\end{aligned}$$

- The advection is treated with a semi-Lagrangian scheme; the other terms are linearized.
- Consider a leapfrog time integration:

$$\begin{aligned}\frac{u^+ - u^-}{2\Delta t} &= -g \left(\frac{\partial h}{\partial x} \right)^0 \\ \frac{h^+ - h^-}{2\Delta t} &= -H \left(\frac{\partial u}{\partial x} \right)^0\end{aligned}$$

Note that the superscripts $+$, 0 and $-$ also mean evaluation in x_j , \tilde{x}_j and \check{x}_j

- Stability analysis with von Neumann method: difficult because it would lead to a quadratic matrix equation:
 - ▶ 3 timelevel \Rightarrow quadratic
 - ▶ system of 2 equations $\Rightarrow 2 \times 2$ amplification matrix
- However, we can reformulate the scheme as a 2-timelevel system of 4 equations.

Let

$$\mathbf{v}^t = \begin{pmatrix} u^t & h^t & u^{t-\Delta t} & h^{t-\Delta t} \end{pmatrix}^T,$$

then

$$\mathbf{v}^{t+\Delta t} = \begin{pmatrix} u^{t+\Delta t} & h^{t+\Delta t} & u^t & h^t \end{pmatrix}^T,$$

- The time-discretized system (leapfrog) then can be written as

$$\mathbf{v}^{t+\Delta t} = \begin{pmatrix} 0 & -2\Delta t g \partial/\partial x & 1 & 0 \\ -2\Delta t H \partial/\partial x & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \mathbf{v}^t$$

- Assuming a wave-shape ($\mathbf{v} \sim e^{ikj\Delta x}$) and 2nd order centered differences, the amplification matrix becomes

$$\mathbf{A} = e^{-ikU\Delta t} \begin{pmatrix} 0 & -2i\tilde{g} & 1 & 0 \\ -2i\tilde{H} & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

where $\tilde{g} = \frac{\Delta t}{\Delta x} \sin(k\Delta x)g$ and $\tilde{H} = \frac{\Delta t}{\Delta x} \sin(k\Delta x)H$.

- Stability is then determined by the eigenvalues λ of \mathbf{A} :

$$e^{-4ikU\Delta t}\lambda^4 + (4\tilde{c}^2 - 2)e^{-2ikU\Delta t}\lambda^2 + 1 = 0$$

where $\tilde{c}^2 = \tilde{g}\tilde{H}$. So

$$\tilde{\lambda}^2 = 1 - 2\tilde{c}^2 \pm 2i\tilde{c}\sqrt{1 - \tilde{c}^2}$$

where $\tilde{\lambda} = e^{-ikU\Delta t}\lambda$

- Note there are 4 solutions: 2 waves + 2 computational modes.
- The condition for stability is then:

$$|\tilde{c}| \leq 1$$

- So the stability does not depend on the mean speed U , but only on the gravity wave speed \tilde{c} .

- In the atmosphere, $c \gg U$, so there's no immediate gain in terms of stability, but
 - ▶ the accuracy is much better (phase speed error for short waves)
 - ▶ the nonlinearity is removed
- It's also possible to derive a trapezium scheme (implicit!) which is unconditionally stable.
- It's quite interesting to combine a semi-Lagrangian approach with an implicit time discretization: SL takes care of advection; the implicit scheme takes care of fast waves.

- What if we have to deal with nonlinear systems?

$$\frac{\partial \psi}{\partial t} = \mathcal{M}(\psi)$$

where \mathcal{M} is a nonlinear operator.

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$$\frac{\partial \psi}{\partial t} = \mathcal{M}(\psi)$$

where \mathcal{M} is a nonlinear operator.

- We can separate \mathcal{M} into a linear part \mathcal{L} and a nonlinear part \mathcal{N} :

$$\mathcal{M} = \mathcal{L} + \mathcal{N}$$

and treat the linear part in an implicit manner, and the nonlinear part in an explicit manner: a linear system is relatively easy to solve (esp. in spectral space!).

- For example, consider

$$\mathcal{M}(\psi) = \psi^2$$

this can be split up like

$$\mathcal{L}(\psi) = \bar{\psi}^2 + 2(\psi - \bar{\psi}) \qquad \mathcal{N}(\psi) = \psi^2 - \bar{\psi}^2 - 2(\psi - \bar{\psi})$$

If $\bar{\psi}$ is a good approximation of ψ , \mathcal{N} will be small.

- A trapezium scheme for a nonlinear problem would then look like:

$$\frac{\psi^{t+\Delta t} - \psi^t}{\Delta t} = \frac{1}{2} \left(\mathcal{L}\psi^{t+\Delta t} + \mathcal{L}\psi^t \right) + \mathcal{N}(\psi^{t+\Delta t/2})$$

where $\psi^{t+\Delta t/2}$ is extrapolated from $\psi^{t-\Delta t}$ and ψ^t .

- Let us apply this to the nonlinear shallow water model

$$\begin{aligned}\frac{Du}{Dt} &= -g \frac{\partial h}{\partial x} \\ \frac{Dh}{Dt} &= -h \frac{\partial u}{\partial x}\end{aligned}$$

Where is the nonlinearity?

- The term $h\partial u/\partial x$ is split into a linear part and a nonlinear part as follows:

$$H\partial u/\partial x + \eta(x, t)\partial u/\partial x$$

where H is a constant, and $\eta(x, t) = h(x, t) - H$.

- A semi-implicit semi-Lagrangian two-time-level (trapezium) scheme then looks like:

$$\begin{aligned}\frac{u^+ - u^0}{\Delta t} &= -\frac{g}{2} \left[\left(\frac{\partial \eta}{\partial x} \right)^+ + \left(\frac{\partial \eta}{\partial x} \right)^0 \right] \\ \frac{\eta^+ - \eta^0}{\Delta t} &= -\frac{H}{2} \left[\left(\frac{\partial u}{\partial x} \right)^+ + \left(\frac{\partial u}{\partial x} \right)^0 \right] - \frac{3}{2}\eta^0 \left(\frac{\partial u}{\partial x} \right)^0 + \frac{1}{2}\eta^- \left(\frac{\partial u}{\partial x} \right)^-\end{aligned}$$

- To check the stability of this system, we linearize u and η :

$$\begin{aligned}u &= U + u' \\ \eta &= \bar{\eta} + \eta'\end{aligned}$$

and we introduce the auxiliary variable $y^t = u^{t-\Delta t}$.

- The system then becomes

$$\begin{pmatrix} 1 & igk\Delta t/2 & 0 \\ iHk\Delta t/2 & 1 & 3i\bar{\eta}k\Delta t \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u \\ \eta \\ y \end{pmatrix}^{t+\Delta t} \\ = e^{-ikU\Delta t} \begin{pmatrix} 1 & -igk\Delta t/2 & 0 \\ -iHk\Delta t/2 & 1 & i\bar{\eta}k\Delta t \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ \eta \\ y \end{pmatrix}^t$$

- This scheme is stable (eigenvalues of amplification matrix) if

$$0 < \bar{\eta} < H$$

i.e. if the reference fluid depth always exceeds the maximum height of the actual free-surface displacement.

- Note: this stability analysis was still made for the linear part only: instability due to aliasing is not accounted for.

- This is what we do in practice:

Starting from the 3D Euler equations,

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + \frac{1}{\rho} \nabla p = -g \mathbf{k}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = 0$$

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Starting from the 3D Euler equations,

- ▶ we use *filtered* equations to remove insignificant wave solutions (see *Dynamic meteorology*)

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$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = 0$$

- This is what we do in practice:

Starting from the 3D Euler equations,

- ▶ we use *filtered* equations to remove insignificant wave solutions (see *Dynamic meteorology*)
- ▶ we control the nonlinearity of the advection with semi-Lagrangian methods

$$\frac{D\mathbf{v}}{Dt} + \frac{1}{\rho} \nabla p = -g\mathbf{k}$$

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{D\theta}{Dt} = 0$$

- This is what we do in practice:

Starting from the 3D Euler equations,

- ▶ we use *filtered* equations to remove insignificant wave solutions (see *Dynamic meteorology*)
- ▶ we control the nonlinearity of the advection with semi-Lagrangian methods
- ▶ we treat the rest with semi-implicit methods.
By cleverly choosing the nonlinear residual (or in other words choosing the reference state), one controls the stability as much as possible.

$$\frac{D\mathbf{v}}{Dt} + \frac{1}{\bar{\rho} + \rho'} \nabla p = -g\mathbf{k}$$

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{D\theta}{Dt} = 0$$

- 2TL SISL schemes are used operationally in ECMWF's IFS model and in the ACCORD model.