Numerical Techniques 2024–2025

6. Semi-implicit semi-Lagrangian schemes

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  - stability
  - accurracy
  - 2D
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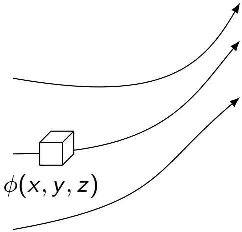
Eulerian:

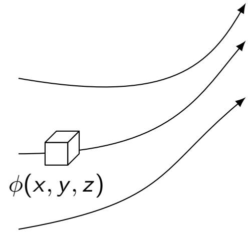


$$\delta\phi = \phi(x, y, z, t + \delta t) - \phi(x, y, z, t)$$

The derivative is the partial derivative

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

Eulerian:



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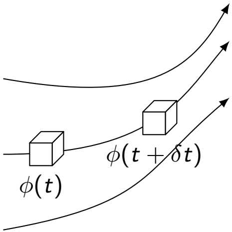
Lagrangian:



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

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:

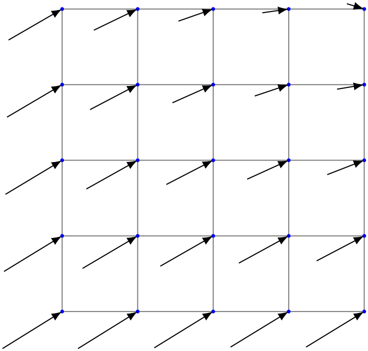
$$\frac{\partial \psi}{\partial t} + u\frac{\partial \psi}{\partial x} = 0 \qquad \text{or} \qquad \frac{D\psi}{Dt} = 0$$

- 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

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

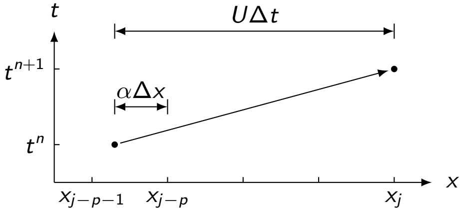
with $\lfloor z \rfloor$ the integer part of z, then

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

- 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

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

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

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

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

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

- 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

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

- Quadratic interpolation:

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

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

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

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

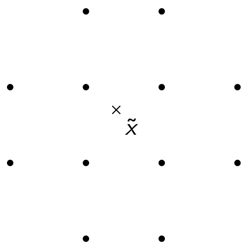
- On a quadratic *stencil*:

$$\begin{array}{ccc}
\phi_{NW} & \phi_{N} & \phi_{NE} \\
\bullet & \bullet & \bullet \\
\phi_{W} & \phi_{C} & \phi_{E} \\
\bullet & \bullet & \bullet \\
 & & \\
\bullet & \bullet & \bullet \\
\phi_{SW} & \phi_{S} & \phi_{SE}
\end{array}$$

$$\begin{aligned}
\tilde{\phi}^{n+1} &= \tfrac{1}{2}\alpha(1+\alpha)\left[\tfrac{1}{2}\beta(1+\beta)\phi^n_{SW} + (1-\beta^2)\phi^n_W - \tfrac{1}{2}\beta(1-\beta)\phi^n_{NW}\right] \\
&\quad + (1-\alpha^2)\left[\tfrac{1}{2}\beta(1+\beta)\phi^n_S + (1-\beta^2)\phi^n_C - \tfrac{1}{2}\beta(1-\beta)\phi^n_N\right] \\
&\quad - \tfrac{1}{2}\alpha(1-\alpha)\left[\tfrac{1}{2}\beta(1+\beta)\phi^n_{SE} + (1-\beta^2)\phi^n_E - \tfrac{1}{2}\beta(1-\beta)\phi^n_{NE}\right]
\end{aligned}$$

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

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

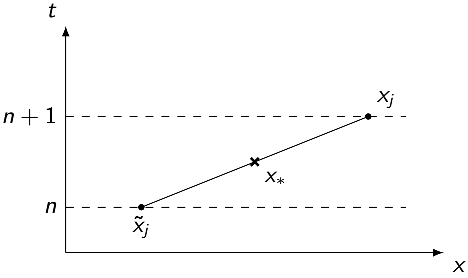
- Hence this method is first order accurate: $O[\Delta t]$.

Variable velocity: midpoint method

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

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

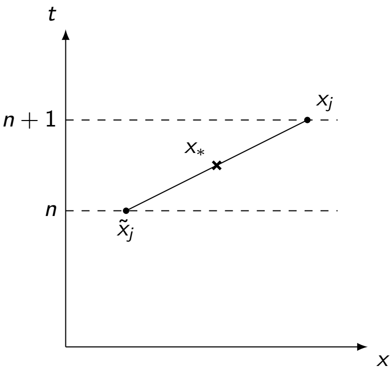
This scheme is second-order accurate.



- 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!



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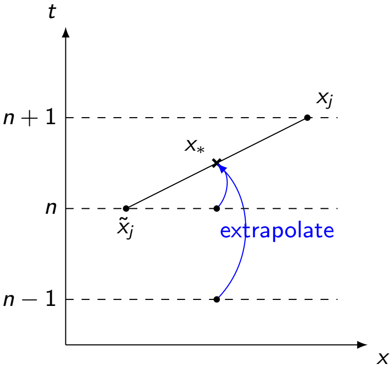
- This is possible for passive tracers (e.g. pollutants).
- But for NWP it is not feasible: wind itself is an forecasted field, which is advected by itself!
- Solution: *time extrapolation*



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

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

which is then linearly interpolated in space to x_*.

Variable velocity: midpoint method

- 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.

Variable velocity: midpoint method

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

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

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.

Forcing terms

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

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

- 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:

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

- 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

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

- The advection is treated with a semi-Lagrangian scheme; the other terms are linearized.

- Consider a leapfrog time integration:

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

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 $\Rightarrow$ 2×2 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 $\mathbf{A}$:

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

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.

Semi-implicit semi-Lagrangian (SISL) schemes

- What if we have to deal with nonlinear systems?

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

  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:

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

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

$$u = U + u'$$
$$\eta = \bar{\eta} + \eta'$$

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

Discussion

- 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.

Discussion

- This is what we do in practice:

  Starting from the 3D Euler equations,

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + \frac{1}{\rho} \nabla p = -g\mathbf{k}$$
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = 0$$

Discussion

- 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*)

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

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

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

Discussion

- 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

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

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

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

Discussion

- 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.