Time stepping schemes for atmospheric modelling

Numerical methods for weather prediction training course
November 2024

Michail Diamantakis
michail.diamantakis@ecmwf.int

Two commonly used equation formulations in operational NWP models

Hydrostatic approximation

- Atmosphere is approximately in hydrostatic equilibrium
- Vertical motion is diagnosed from continuity equation
- Filters the very fast sound waves ⇒ no stability problems associated with very large acoustic CFL numbers in the vertical

Non-hydrostatic (NH) equation model

- Most accurate description of the atmosphere.
- More expensive equation set with often more complex and computationally demanding numerical algorithms: better use when needed i.e. high resolutions where dynamics begin to resolve convection explicitly

What motions time-stepping should resolve?

- Rossby waves & gravity waves must be resolved and transported accurately – important for good weather predictions
- Fast acoustic waves carry little energy - not important for weather but their implications must be considered: they may limit severely timestep of numerical schemes
  - To avoid such timestep restrictions, ideally an unconditionally stable numerical scheme is needed which may dissipate acoustic waves but does not dissipate other meteorologically important waves
- Using very high-orders time-stepping scheme is not practical:
  - In any model, uncertainty from model components such as parametrizations are usually large enough

Scalability: an important requirement

- Moore's law (processing power of CPU doubles every 18 months) is no longer valid but thanks to emerging accelerator technologies and communication speed improvements in massively parallel architectures time-to-solution on new supercomputers has been improving
- NWP solvers must scale well on exascale machines and able to run efficiently on heterogenous architectures with accelerators (GPU-CPU)
- Grids: regular lat/lon are not suited for high resolution global modelling:
  - Explicit timestepping: meridian convergence at poles ⇒ extremely high resolution => Δt -> 0 due to CFL limitations
  - Implicit timestepping: grid anisotropy near poles leads to poor convergence of elliptic solvers + high communication cost
- Global spectral transform models at high resolution do not scale well mainly due to the high communication cost of transpositions

Common time stepping schemes in NWP

- Schemes currently used in atmospheric modelling
  - Semi-Lagrangian, semi-implicit: unconditionally stable ⇒ large timesteps used for efficiency
  - Flux-form explicit Eulerian transport with semi-implicit time-stepping for fast forcing term integration
  - Split-explicit: "improved efficiency" explicit schemes
  - HEVI: Horizontally Explicit / Vertically Implicit
    - ➔ suitable for NH models as they use an implicit & unconditionally stable scheme in the vertical where highest CFL numbers occur
  - IMEX: implicit-explicit Runge-Kutta schemes
    - ➔ Implicit in the fast process, explicit in the slow.

Pros and Cons of Eulerian methods for NWP and climate

Eulerian methods use much shorter timesteps than SISL methods (even if implicit ..)

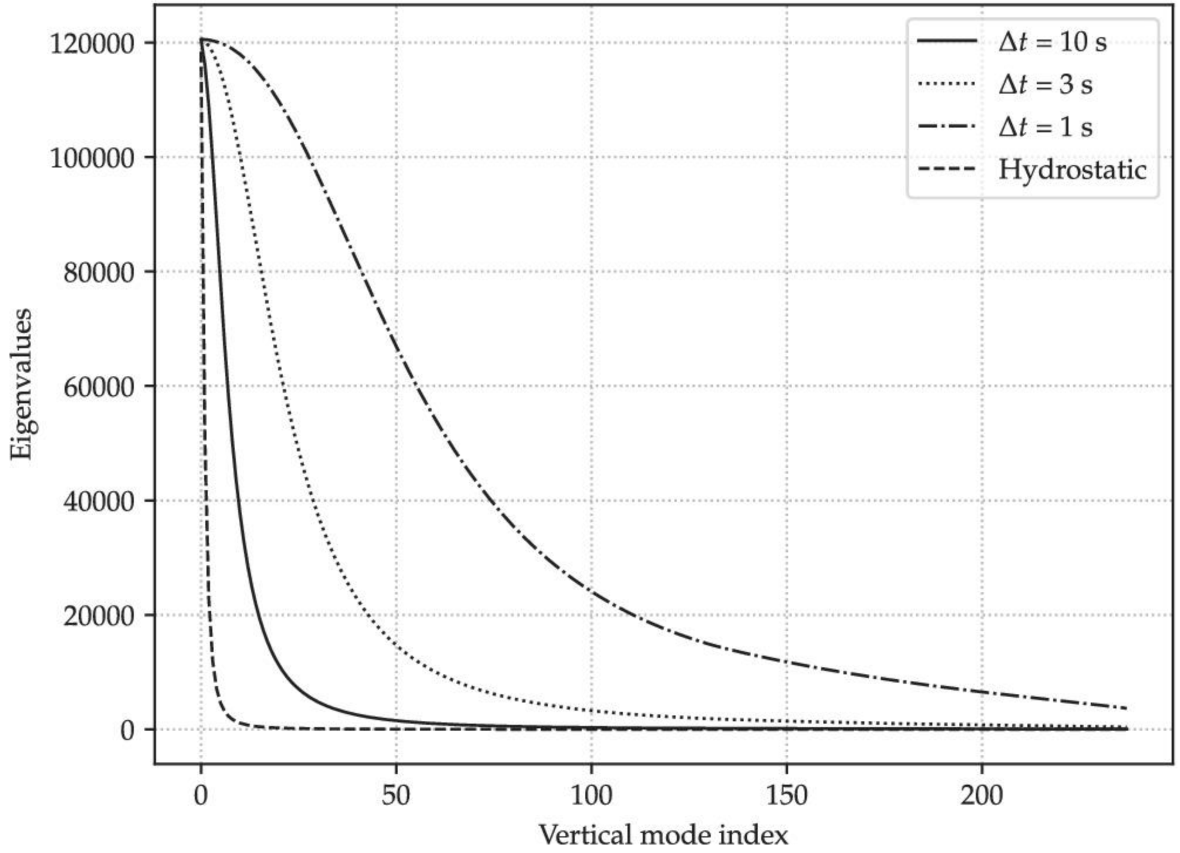
- Fully explicit methods: highly scalable, simple to implement but need very short timestep for stability
- Explicit advection combined with semi-implicit time-stepping: permit longer timesteps. Scalability depends on elliptic solver type and its implementation (Müller & Scheichl QJRMS 2013)

Mass conservation:

- With a flux-form model and Eulerian time stepping we can obtain local and global mass conservation with Finite Volume/Finite Element/Discontinuous Galerkin space discretizations

In explicit Eulerian conservative transport schemes the advective CFL must be < 1 for stability (unlike semi-Lagrangian semi-implicit which can run at CFL>1)

The problem with very long time steps and non-hydrostatic dynamics



Long time steps inhibit NH models to reach their potential in accurately representing vertical gravity wave propagation

Figure and conclusions from Burgot, Auger, Benard, QJRMS 2021

”improvements of the vertical wave propagation (especially gravity waves) sought during the implementation of an NH model in favour of an H model, are fully satisfied when the time step is small”

Eulerian advection scheme: conservative vs not conservative

Advection of a tracer with density Ψ and mixing ratio m_ψ in conservative form:

$$\frac{\partial \Psi}{\partial t}+\frac{\partial(u\Psi)}{\partial x}=0,\quad \Psi=\rho m_\psi$$

Finite difference forward in-time discretization (conservative form):

$$\Psi_j^{n+1}=\Psi_j^n+\frac{\Delta t}{\Delta x}\left[F^n_{j+1/2}-F^n_{j-1/2}\right]$$

- F is a numerical flux e.g. $F_j=(u\Psi)_{j-1/2}$
- If the numerical flux F is 'consistent' with the flux $f=u\Psi$ i.e. $F(u,u,\dots,u)=f(u)$ then the above scheme with a is conservative:

$$\sum_{j=1}^{N}\Psi_j^{n+1}\Delta x=\sum_{j=1}^{N}\Psi_j^n\Delta x,\quad \text{assuming periodic boundary condition or flux}=0$$

- If the discretization is TVD it remains stable

Equivalent non-conservative form of the advection equation for a tracer with mixing ratio m_ψ:

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

Finite difference discretization:

$$(m_\psi)_j^{n+1}=(m_\psi)_j^n+\frac{\Delta t\, u_j^n}{\Delta x}\left[(m_\psi)_j^n-(m_\psi)_{j-1}^n\right],\quad u>0\ (\text{upwinding}\ -\ \text{stable for } CFL<1)$$

⇓ Assume constant density ρ of background air and compute total mass at two consecutive timesteps

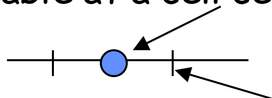
$$\sum_{j=1}^{N}(m_\psi)_j^{n+1}\rho\Delta x_j\neq\sum_{j=1}^{N}(m_\psi)_j^{n}\rho\Delta x_j$$

if resolution or velocity varies

MPDATA: 2nd order positive definite conservative advection

Smolarkiewicz & Margolin (1998) MPDATA in finite difference form:

Upstream approximation of flux equation: $\frac{\partial \Psi}{\partial t} = -\frac{\partial}{\partial x}(u\Psi),$



$$\Psi_i^{n+1} = \Psi_i^n - \left[F\left(\Psi_i^n, \Psi_{i+1}^n, U_{i+1/2}\right) - F\left(\Psi_{i-1}^n, \Psi_i^n, U_{i-1/2}\right)\right],$$

$$F(\Psi_L, \Psi_R, U) \equiv [U]^+\Psi_L + [U]^-\Psi_R \;, \quad U \equiv \frac{u\Delta t}{\Delta x} \;\; (\text{local Courant Number})$$

$$[U]^+ \equiv 0.5(U+|U|), \quad [U]^- \equiv 0.5(U-|U|).$$

MPDATA steps

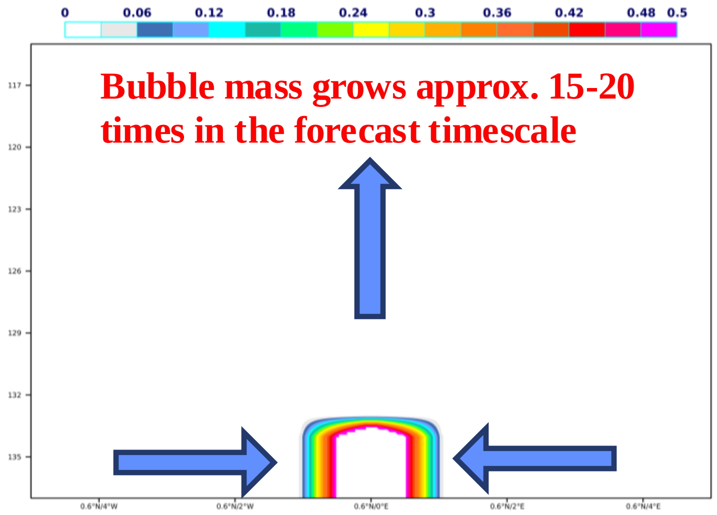
- ♦ **Compute 1st order upstream approximation** $\Psi_i^{(1)}$ **from above formula** $\Psi_i^{(1)}$
- ♦ **Subtrac** $\Psi_i^{(2)} = \Psi_i^{(1)} - \left[F\left(\Psi_i^{(1)}, \Psi_{i+1}^{(1)}, V_{i+1/2}^{(1)}\right) - F\left(\Psi_{i-1}^{(1)}, \Psi_i^{(1)}, V_{i-1/2}^{(1)}\right)\right]$ **r accuracy**

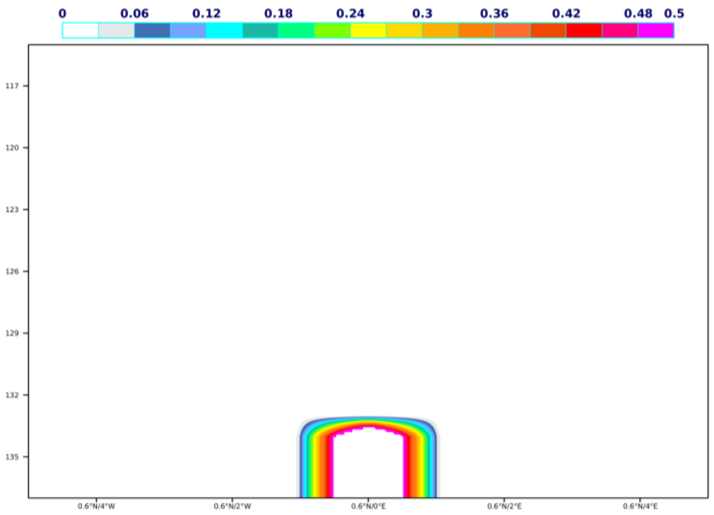
where → $V_{i+1/2}^{(1)} \equiv (|U| - U^2)\frac{\Psi_{i+1}^{(1)} - \Psi_i^{(1)}}{\Psi_{i+1}^{(1)} + \Psi_i^{(1)}} \equiv (|U| - U^2)A_{i+1/2}^{(1)}$

Pseudo-velocity

A case that makes semi-Lagrangian advection and schemes in non-conservative form break

Standard SemiLag bottom boundary condition:
mixing ratio constant between surface and atmospheric level above it





Setting mixing ratio 0 at the surface: lifts the bubble but the correct boundary condition for the general case is flux=0 rather than mix ratio=0

- An idealised case with symmetric winds converging at a point of no wind: upward motion and transfer of mass from the surface because of the boundary condition
- Very rare but elements of this problem can contribute to mass growth from the boundary in semi-Lagrangian based models
- Interpolation method COMAD in IFS (Malardel and Ricard QJRMS, 2014) can partially alleviate this
- A flux-form scheme e.g. MPDATA behaves like the right plot but for different reason which is correct: influx of 'clean' air from the east-west side of the bubble

ECMWF

A simple test model for fast process integration: 1d gravity wave equations

Linearised shallow water equations:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial \phi}{\partial x} = 0 \\ \dfrac{\partial \phi}{\partial t} + \Phi \dfrac{\partial u}{\partial x} = 0 \end{cases}$$

$$\Phi = gH$$

$$\phi = gh$$

Fluid mean depth

Perturbation from mean depth

$\partial/\partial t$ on first equation and eliminate φ to obtain the familiar equation of a 1-dimensional wave:

$$\frac{\partial^2 u}{\partial t^2} - \Phi \frac{\partial^2 u}{\partial x^2} = 0$$

propagating with speed: $c \equiv \dfrac{\omega}{k} = \pm\sqrt{\Phi} = \pm\sqrt{gH}$

Explicit Leapfrog time stepping on 1D GW eqn

Three-time-level explicit Leapfrog scheme

Leapfrog on a general problem: $$\frac{d\psi}{dt} = f(\psi) \Rightarrow \psi^{n+1} = \psi^{n-1} + 2\Delta t\ f\left(\psi^{n}\right)$$

Leapfrog on 1D GW equations:
$$\begin{cases} u_j^{n+1} = u_j^{n-1} - 2\Delta t \dfrac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} \\ \phi_j^{n+1} = \phi_j^{n-1} - 2\Delta t\ \Phi \dfrac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \end{cases}$$

Note Paul Williams (prof. in U of Reading) & associates work on high order leapfrog and high order filters for leapfrog

Neutral (no damping) + 2nd order BUT phase + dispersion errors + computational mode

Von Neuman stability: $$\Delta t \le \frac{\Delta x}{\sqrt{\Phi}} \approx \frac{\Delta x}{300}$$

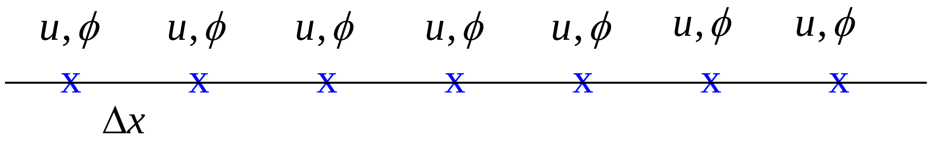
Solution is a combination of a physical and a computational mode which can be damped by use of a time filter, e.g. Asselin filter (but damps energy in long integrations)

$$\psi^{n} \leftarrow \psi^{n} + \gamma\left(\psi^{n-1} - 2\psi^{n} + \psi^{n+1}\right),\ \gamma > 0,\ \psi = u, \varphi$$

Typical value for global models: $\gamma = 0.06$

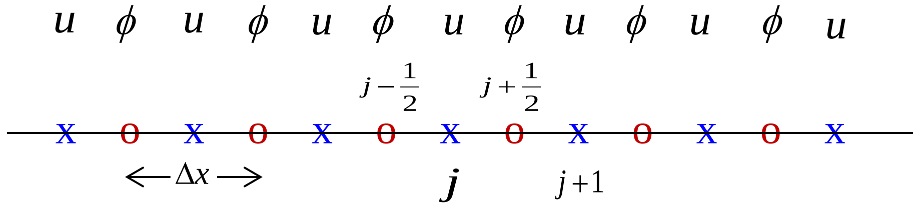
Staggering variables to improve accuracy

- The prognostic variables can be
  - On the same location on the grid, i.e. co-located



$$\begin{cases} \Delta_t u_j + \dfrac{\phi_{j+1} - \phi_{j-1}}{2\Delta x} = 0 \\ \Delta_t \phi_j + \Phi \dfrac{u_{j+1} - u_{j-1}}{2\Delta x} = 0 \end{cases}$$

  - In between (half way) each other, i.e. staggered

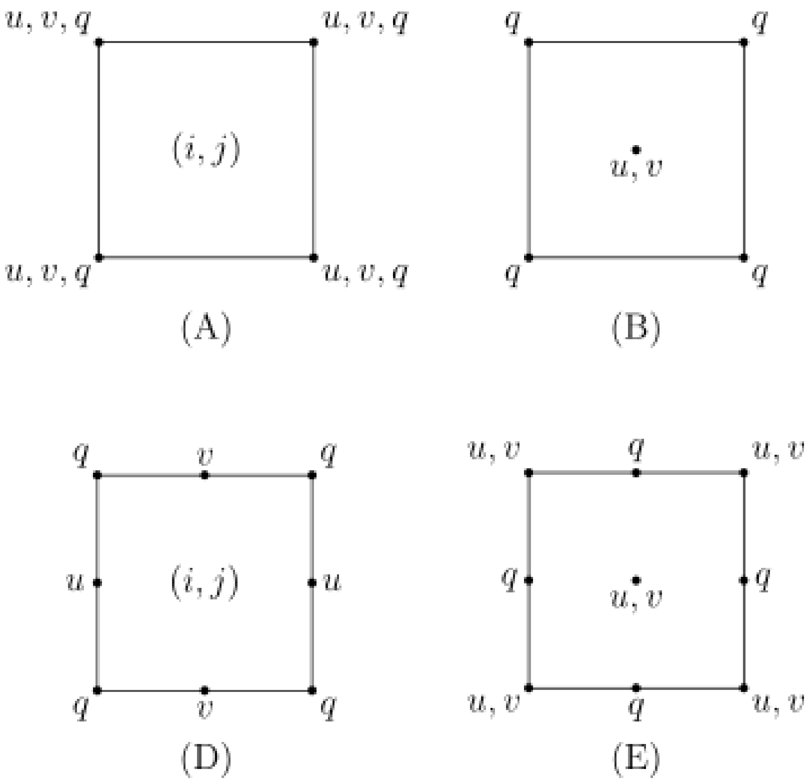


$$\begin{cases} \Delta_t u_j + \dfrac{\phi_{j+1/2} - \phi_{j-1/2}}{\Delta x} = 0 \\ \Delta_t \phi_{j+1/2} + \Phi \dfrac{u_{j+1} - u_j}{\Delta x} = 0 \end{cases}$$

→ Improved accuracy + dispersion properties

→ On explicit techniques staggering results into a more restrictive timestep e.g.: $\dfrac{c\Delta t_{\max}}{\Delta x/2} < 1$ instead of $\dfrac{c\Delta t_{\max}}{\Delta x} < 1$

Different Arakawa horizontally staggered grids



"A benefit of C-grid is that it captures well the propagation of inertio-gravity waves and hence the process of geostrophic adjustment"
Arakawa and Lamb 1977

q: geopotential or pressure

Fig source: Wikipedia By Rpnl ocn - Own work, CC BY-SA 4.0,
https://commons.wikimedia.org/w/index.php?curid=47077493

Vertical grid staggering

Lorenz staggering

- Good for energy conservation
- Presence of a computational mode

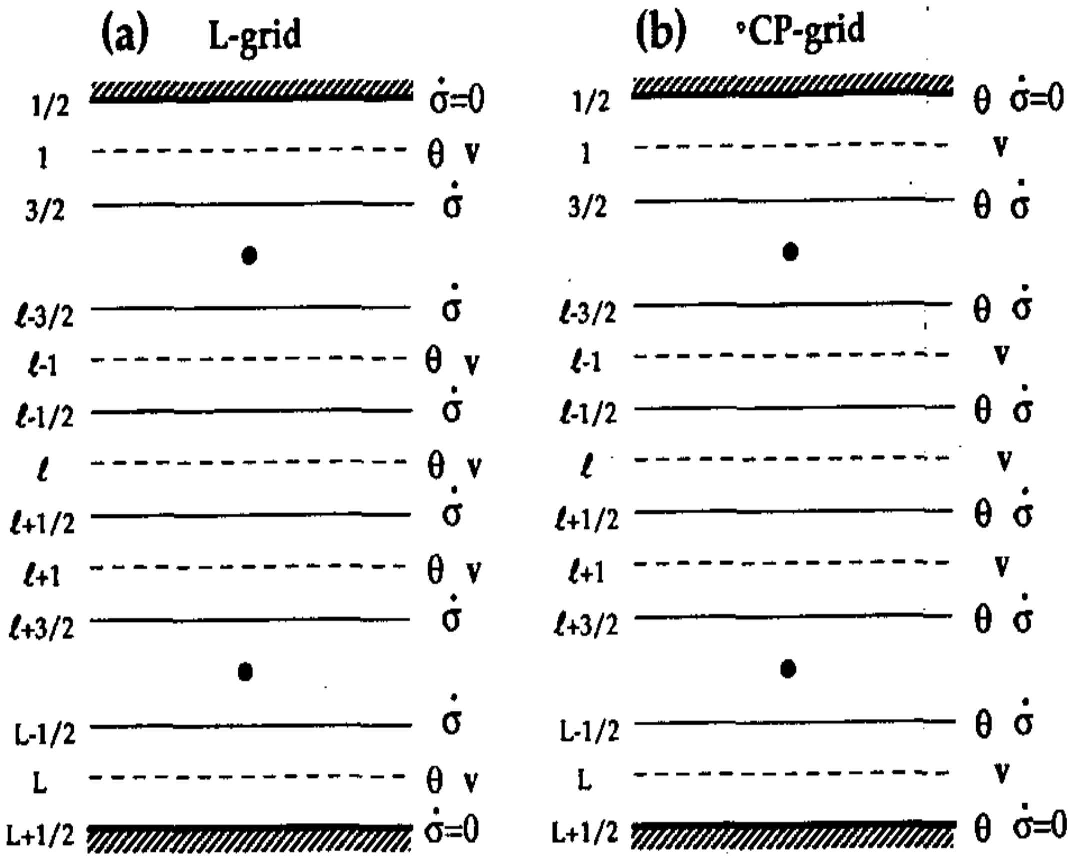


FIG. 1. An illustration of (a) the Lorenz grid and (b) the Charney–Phillips grid for a σ coordinate.

Charney-Philips staggering

- No computational mode
- Conservation of PV

ECMWF IFS:

- No staggering at all

Why is that acceptable?

- High order (spectral transform) horizontal discretization
- High order (finite-element) vertical discretization

Picture from Arakawa and Konor MWR, 1996, vol 124, 511-

Enhancing stability: forward-backward integration

- **Forward-backward** scheme: a predictor-corrector type scheme

The predictor and the corrector are applied on separate equations.

$$\begin{cases} \phi_j^{n+1} = \phi_j^n - \dfrac{\Phi \Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n) \\ u_j^{n+1} = u_j^n - \dfrac{\Delta t}{2\Delta x}(\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}) \end{cases}$$

forward

backward (pseudo-implicit)

$$\Delta t \le \frac{2\Delta x}{\sqrt{\Phi}} \approx \frac{\Delta x}{150}$$

Fwd-Bwd versus Leapfrog:

1. Wider stability region allowing twice as big timestep compared with leapfrog
2. Neutral (no damping)
3. Two-time-level scheme ⇒ no computational mode

Runge-Kutta RK3 scheme

- Runge-Kutta (Wicker & Skamarock, MWR 2002) RK3 scheme:
  - three-stage, two-time-level (2nd order) scheme from the RK family

$$Solve: \quad \frac{dY}{dt} = f(Y)$$

$$Y^{*} = Y^{n} + \frac{\Delta t}{3} f(Y^{n})$$

$$Y^{**} = Y^{n} + \frac{\Delta t}{2} f(Y^{*})$$

$$Y^{n+1} = Y^{n} + \Delta t \; f(Y^{**})$$

Applied on 1d-GW eqn:

$$Y = \begin{pmatrix} u \\ \phi \end{pmatrix}, \quad f(Y) = \begin{pmatrix} -\dfrac{\partial \phi}{\partial x} \\ -\Phi \dfrac{\partial u}{\partial x} \end{pmatrix}$$

3^{rd} or 4th order FD scheme for estimating derivatives

Compared with leapfrog almost doubles (1.62) Δt when 3^{rd} order spatial discretization used

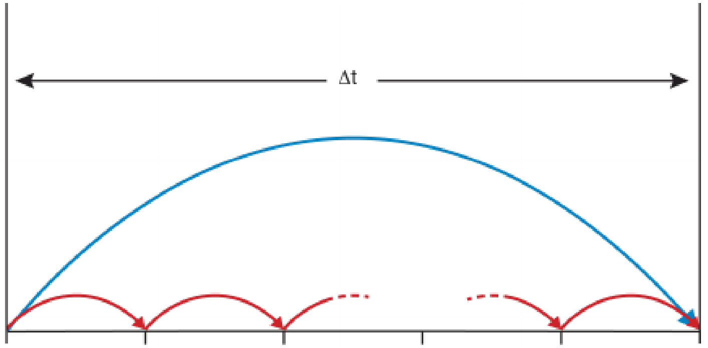
In WRF this is used in combination with time-splitting …

Splitting the time integration: the motivation

- In an atmospheric model fast and slow wave motions co-exist
  - Splitting exploits the multi-time-scale nature of the governing equations
- Explicit techniques are only conditionally stable which imposes use of very small timesteps for fast processes
  - Let Δt be the longest permissible timestep for integrating stably the slow process => Δt will be too long for stable integration of the fast process
- A practical solution is to split the integration:
  - ➔ integrate slow process with "long" Δt
  - ➔ integrate fast process with a fraction of it i.e. $\Delta t/n$

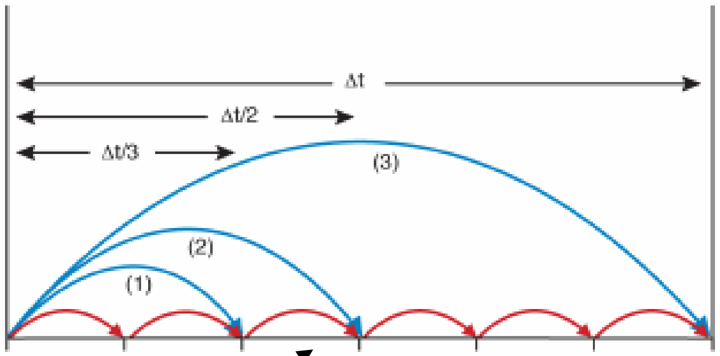
Split-explicit example in a diagram

Split-explicit Euler



Split-explicit RK3

Runge-Kutta internal step i: each approximates solution at $t+c_i\,\Delta t$ where, c_i=1/3,1/2,1 the RK3 coefficient



sub-step fast process only (with timestep Δt/n)

(Diagram from S.J. Lock, ECMWF Seminar proceedings 2013, HEVI time-stepping for NWP and climate models)

ECMWF

Split-explicit forward Euler integration

$$\frac{\partial \psi}{\partial t} = F(\psi) + S(\psi)$$

Fast forcing term   Slow forcing term

Integrate forward n_s - times with $\Delta\tau = \Delta t / n_s$ from t to $t + \Delta t$:

$$\psi^{t+m\Delta\tau} = \psi^{t+(m-1)\Delta\tau} + \Delta\tau\, F\left(\psi^{t+(m-1)\Delta\tau}\right) + \Delta\tau\, S\left(\psi^{t}\right), \quad m = 1,2,\dots n_s$$

Fast term updated   Slow term kept constant (stored)

Equivalent to :

$$\psi^{t+\Delta t} = \psi^{t} + \Delta\tau \sum_{m=1}^{n_s}\left[F\left(\psi^{t+(m-1)\Delta\tau}\right) + S\left(\psi^{t}\right)\right] = \overbrace{\psi^{t} + \Delta t\, S\left(\psi^{t}\right)}^{\text{fw Euler with big step}} + \Delta\tau \sum_{m=1}^{n_s} F\left(\psi^{t+(m-1)\Delta\tau}\right),$$

It is an efficient approach :

Store : $R\left(\psi^{t}\right) = \Delta\tau\, S\left(\psi^{t}\right)$

Integrate : $\psi^{t+m\Delta\tau} = \psi^{t+(m-1)\Delta\tau} + \Delta\tau\, F\left(\psi^{t+(m-1)\Delta\tau}\right) + R\left(\psi^{t}\right), \quad m = 1,2,\dots n_s$

$1*S + n_s*F$ evaluations
versus FW-Euler
$n_s*S + n_s*F$ evaluations

Split-explicit RK3 integration

$$\frac{\partial \psi}{\partial t} = F(\psi) + S(\psi)$$

Step 1: integrate from t to $t+\Delta t/3$ with $\Delta\tau = \Delta t/n_s$:

$$\psi^{t+m\Delta\tau} = \psi^{t+(m-1)\Delta\tau} + \Delta\tau\, F\left(\psi^{t+(m-1)\Delta\tau}\right) + \Delta\tau\, S\left(\psi^{t}\right), \quad m = 1,2,\ldots n_s/3$$

Step 2: integrate from t to $t+\Delta t/2$ with $\Delta\tau = \Delta t/n_s$:

$$S\left(\psi^{*}\right) = S\left(\psi^{t+\Delta t/3}\right), \qquad \psi^{*} \equiv \psi^{t+\Delta t/3} : \text{ final result from stage 1}$$

$$\psi^{t+m\Delta\tau} = \psi^{t+(m-1)\Delta\tau} + \Delta\tau\, F\left(\psi^{t+(m-1)\Delta\tau}\right) + \Delta\tau\, S\left(\psi^{*}\right), \quad m = 1,2,\ldots n_s/2$$

Step 3: integrate from t to $t+\Delta t$ with $\Delta\tau = \Delta t/n_s$:

$$S\left(\psi^{**}\right) = S\left(\psi^{t+\Delta t/2}\right), \qquad \psi^{**} \equiv \psi^{t+\Delta t/2} : \text{ final result from stage 2}$$

$$\psi^{t+m\Delta\tau} = \psi^{t+(m-1)\Delta\tau} + \Delta\tau\, F\left(\psi^{t+(m-1)\Delta\tau}\right) + \Delta\tau\, S\left(\psi^{**}\right), \quad m = 1,2,\ldots n_s$$

S term is evaluated only once per internal RK step and added at each sub-cycle

Leapfrog (3TL) split-explicit fw-bw example

fast/forward   slow/leapfrog

$$\begin{cases} \dfrac{\partial \psi_1}{\partial t} = F_1(\psi_2) + S_1(\psi_1, \psi_2) \\ \dfrac{\partial \psi_2}{\partial t} = F_2(\psi_1) + S_2(\psi_1, \psi_2) \end{cases}$$

backward   leapfrog

Repeated short timestep integration from t to $t + \Delta t$ $(m = 1,2,\ldots,2n_s,\ \Delta\tau = \Delta t / n_s)$:

$$\psi_1^{t-\Delta t+m\Delta\tau} = \psi_1^{t-\Delta t+(m-1)\Delta\tau} - \Delta\tau\, F_1\left(\psi_2^{t-\Delta t+(m-1)\Delta\tau}\right) - \Delta\tau\, S_1\left(\psi_1^t, \psi_2^t\right)$$

$$\psi_2^{t-\Delta t+m\Delta\tau} = \psi_2^{t-\Delta t+(m-1)\Delta\tau} - \Delta\tau\, F_2\left(\psi_1^{t-\Delta t+m\Delta\tau}\right) - \Delta\tau\, S_2\left(\psi_1^t, \psi_2^t\right)$$

fast F terms updated

Slow terms kept constant

$$\psi_1^{t+\Delta t} = \psi_1^{t-\Delta t} - 2\Delta t S_1\left(\psi_1^t, \psi_2^t\right) - \overbrace{\Delta\tau \sum_{m=1}^{2n_s} F_1\left(\psi_2^{t-\Delta t+(m-1)\Delta\tau}\right)}^{fw-Euler-small-steps}$$

$$\psi_2^{t+\Delta t} = \underbrace{\psi_2^{t-\Delta t} - 2\Delta t S_2\left(\psi_1^t, \psi_2^t\right)}_{leapfrog-large-step} - \underbrace{\Delta\tau \sum_{m=1}^{2n_s} F_2\left(\psi_1^{t-\Delta t+m\Delta\tau}\right)}_{bw-Euler-small-steps}$$

Drawbacks of the split-explicit approach

- In deep global models O(100km) there is no much benefit from split-explicit approach in the horizontal
  - Stratospheric polar jet velocities are not very far from speed of sound ➡ advective CFL number is close to acoustic CFL number
    - ➔ All processes are fast and therefore horizontal splitting will not bring significant efficiency benefit
  - Splitting needs damping for stabilization
- Other than split-explicit methods:
  - Horizontally Explicit Vertically Implicit (HEVI)
  - Implicit Explicit (IMEX) RK (unconditionally stable implicit scheme for fast processes and cheap explicit for slow)

HEVI schemes

In NH models acoustic CFL in the vertical is much larger because vertical resolution is at the order of few metres only: explicit time-stepping requires very small timesteps

$$e.g.\quad \Delta t_{\max} < \frac{\Delta z}{c} = \frac{10m}{300m/s} \approx 0.03s$$

Solution: Horizontally Explicit, Vertically Implicit schemes

- Explicit in the horizontal scheme (or split explicit) - horizontal CFL is much smaller than the vertical
- Unconditionally stable implicit scheme for the vertical to deal with high acoustic CFL numbers

Some HEVI / split-explicit models

- ICON (DWD Germany): global NWP, LAM weather and climate unified model
  - forward-backward explicit time-stepping (no splitting) in the horizontal + vertically semi-implicit (Crank-Nicolson)
- EU-COSMO: former DWD operational NH LAM
  - RK3 + split-explicit in the horizontal + semi-implicit Crank-Nicolson in the vertical
- NICAM: cloud resolving NH global model (Japan)
  - Split-explicit forward-backward in the horizontal + implicit in vertical
- WRF, MPAS (USA): LAM, Global research & operational
  - Split-explicit RK3 + vertically semi-implicit

IMEX: Blending explicit with implicit

$$\frac{d\mathbf{y}}{dt} = \underbrace{\mathbf{s}(t,\mathbf{y})}_{\text{slow process}} + \underbrace{\mathbf{f}(t,\mathbf{y})}_{\text{fast process}}$$

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b} \end{array} = \begin{array}{c|ccc} \tilde{c}_1 & \tilde{\alpha}_{11} & \cdots & \tilde{\alpha}_{1\nu} \\ \vdots & \vdots & & \vdots \\ \tilde{c}_\nu & \tilde{\alpha}_{\nu 1} & \cdots & \tilde{\alpha}_{\nu\nu} \\ \hline & \tilde{b}_1 & \cdots & \tilde{b}_\nu \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & b \end{array} = \begin{array}{c|ccc} c_1 & \alpha_{11} & \cdots & \alpha_{1\nu} \\ \vdots & \vdots & & \vdots \\ c_\nu & \alpha_{\nu 1} & \cdots & \alpha_{\nu\nu} \\ \hline & b_1 & \cdots & b_\nu \end{array}$$

$\tilde{\alpha}_{ij} = 0 \quad \forall j \geq i$ (explicit) $\qquad \alpha_{ij} = 0$ for $j > i$ (diagonally impl)

Compute RK stages $\mathbf{Y}^{(j)}$, $j = 1, \ldots, \nu$ and then new solution $\mathbf{y}^{n+1}$:

$$\mathbf{Y}^{(j)} = \mathbf{y}^n + \Delta t \sum_{\ell=1}^{j-1} \tilde{\alpha}_{j\ell} \mathbf{s}(t^n + \tilde{c}_\ell \Delta t, \mathbf{Y}^{(\ell)}) + \sum_{\ell=1}^{j} \alpha_{j\ell} \mathbf{f}(t^n + c_\ell \Delta t, \mathbf{Y}^{(\ell)})$$

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t \sum_{j=1}^{\nu} \tilde{b}_j \mathbf{s}(t^n + \tilde{c}_j \Delta t, \mathbf{Y}^{(j)}) + \sum_{j=1}^{\nu} b_j \mathbf{f}(t^n + c_j \Delta t, \mathbf{Y}^{(j)})$$

Some useful theoretical properties

- A-stability: unconditionally stability for damping & oscillatory linear problems $\frac{dy}{dt} = \lambda y, \quad \lambda = \beta + i\omega, \; \beta < 0$ and consequently for linear constant coefficient systems
  - Explicit methods cannot be A-stable (stability functions are polynomials rather than rational functions)
- L-Stability: A-stable + rapid decay for stiff problems at long timesteps i.e. $\lim_{q\Delta t \to \infty} \frac{y^{t+\Delta t}}{y^t} = 0$ for the above linear equation
- Strong Stability Preserving: SSP is a desirable property for a hyperbolic PDE $u_t = -f(u)_x$. A scheme is SSP if for a given space discretization which is Total Variation Diminishing (TVD) when combined with forward Euler time discretization, it preserves the TVD property for some norm and timestep i.e.

$$TV(u^{n+1}) \le TV(u^n), \quad TV(u) = \sum_{j=1}^{N} \left| u_{j+1} - u_j \right|$$

Example of IMEX – ARK2(2,3,2)

- **Giraldo et al SIAM J.Sci.Comp., 2013 option in NUMA NH US Navy model**

$$
\begin{array}{c|ccc}
0 & 0 & & \\
2-\sqrt{2} & 2-\sqrt{2} & 0 & \\
1 & 1-\alpha_{32} & \alpha_{32} & 0 \\
\hline
 & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 1-\frac{1}{\sqrt{2}}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & & \\
2-\sqrt{2} & 1-\frac{1}{\sqrt{2}} & 1-\frac{1}{\sqrt{2}} & \\
1 & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 1-\frac{1}{\sqrt{2}} \\
\hline
 & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 1-\frac{1}{\sqrt{2}}
\end{array}
$$

$$a_{32} = \frac{1}{6}\left(3+2\sqrt{2}\right)$$

- 2^{nd} order + L-Stable, overall very accurate and stable (Weller et al JCP 2013)

A more recent technique: exponential integrators

Split F (right hand side of space discretized system) to a linear and nonlinear part:

$$\frac{dU}{dt} = F(U), \quad F(U) = J\,U + N\,(U)$$

The linear part contains the Jacobian J while N(U) the nonlinear residual. After multiplying with an integrating factor e^{-Jt} the following exact formula is derived:

$$\frac{dU}{dt} = J\,U + N\,(U) \Rightarrow U(t_n + \Delta t) = e^{\Delta t J}\,U(t_n) + \int_0^{\Delta t} e^{(\Delta t - \tau)J}\,N\big(U\,(t_n + \tau)\big)\,d\tau$$

Clancy et al, Tellus 2013: use of exponential integration methods in atmospheric models

- Analytic solution for the stiff (fast changing) linear term expressed as the action of a matrix exponential to a vector which can be computed using truncated Taylor expansions or Krylov techniques (Niesen and Wright ACM TOMS 38(3), 2012)
- The integral can be computed using numerical quadrature U_n e.g. Runge-Kutta type formulae:

$$U_{n+1} = e^{hJ_n}U_n + h\sum_{i=1}^{s} b_i(hJ_n)N_n\big(U(t_n + c_i h)\big), \quad h \equiv \Delta t$$

$$U(t_n + c_i h) = e^{c_i hJ_n}U_n + h\sum_{j=1}^{s} a_{ij}(hJ_n)N_n\big(U(t_n + c_j h)\big)$$

Coefficients a, b are matrix functions of hJ_n and c_i are the nodes [0,1]. They are analogous to the Runge-Kutta coefficients and satisfy special order conditions.

Further reading: Luan et al, JCP Vol 376, Jan 2019, p 817-837

Exponential Integrators:

- Stable with long timesteps and thus efficient
- Accurate with fast dynamics
- They reduce unphysical oscillations

Overview

There are many choices of numerical techniques

What to choose depends on the problem you solve (mathematical formulation, resolution, domain) and the computer architecture you apply your algorithm

Nowadays mainly due to hardware requirements and interest in developing very high resolution systems there is considerable research & development activity in scalable compact stencil Eulerian techniques which are also suited for developing dynamical cores with formal conservation properties

Some references (alphabetically by author's surname)

- J. Coiffier book: Fundamentals of Numerical Weather Prediction (2011)
- Dale Durran's book: "Numerical methods for Wave Equations in Geophysical Fluid Dynamics"
- Lauritzen et al book: Numerical Techniques for Global Atmospheric Models, Springer 2011
- Mengaldo et al, Archives of Comp. Meth. in Eng. (2018): Current and Emerging Time-Integration Strategies in Global NWP
- Wicker & Skamarock (MWR 2001): "Time-Splitting Methods for Elastic Models Using Forward Time Schemes"