Numerical methods IV (time stepping)

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In part based on previous material by Mariano Hortal and Agathe Untch

What is the basis for a stable numerical implementation ?

- **A: Removal of fast - supposedly *insignificant* - external and/or internal acoustic modes (*relaxed or eliminated*), making use of infinite sound speed ($c_s \rightarrow \infty$) and/or the hydrostatic approximation from the governing equations BEFORE numerics is introduced.**
- **B: Use of the full equations WITH a *semi-implicit* numerical framework, reducing the propagation speed ($c_s \rightarrow 0$) of fast acoustic and buoyancy disturbances, retaining the slow convective-advective component (ideally) undistorted.**
- **C: *Split-explicit* integration of the full equations, since *explicit* NOT practical (~100 times slower)**

$\Rightarrow$ Determines the choice of the numerical scheme

Choices for numerical implementation

- **Avoiding the solution of an elliptic equation**

  fractional step methods (eg. split-explicit); ***Skamrock and Klemp (1992); Durran (1999)***

- **Solving an elliptic equation**

  Projection method; ***Durran (1999)***

  Semi-implicit ***Durran (1999); Cullen et. al.(1994); Benard et al. (2004); Benard (2004); Benard et al. (2005)***

  Preconditioned conjugate-residual solvers (eg. GMRES) or multigrid methods for solving the resulting Poisson or Helmholtz equations; ***Skamarock et. al. (1997); Saad (2003)***

  Direct Methods; ***Martinsson (2009)***

Split-explicit integration

Skamarock and Klemp (1992); Durran (1999); Doms and Schättler (1999);

'Slow' part of solution

$$\phi^s = F_1(\Delta t)\phi^n,$$

$$\phi^{n+1} = F_2(\Delta t)\phi^s,$$

'Fast' part of solution

$$\Rightarrow \phi^{n+1} = [F_2(\Delta t/M)]^M F_1(\Delta t)\phi^n$$

e.g. implemented in popular limited-area models: Deutschland Modell, WRF model

Semi-implicit schemes

linearised term, treated implicit

$$\frac{\delta \mathbf{X}}{\delta t} = (\mathbf{M} - \mathbf{L}^*) \cdot \mathbf{X} + \overline{\mathbf{L}^* \cdot \mathbf{X}}^t$$

non-linear term, treated explicit

(i) coefficients constant in time and horizontally (hydrostatic models *Robert et al. (1972), Benard et al. (2004), Benard (2004)* ECMWF/Arpege/Aladin NH)

(ii) coefficients constant in time *Thomas (1998); Qian, (1998); see references in Bénard (2004)*

(iii) non-constant coefficients *Skamarock et. al. (1997),* (UK Met Office NH model, EULAG model)

Design of semi-implicit methods

- Treat all terms involving the fastest propagation speeds implicitly (acoustic waves, gravity waves).
- Assume that the energy in those components is negligible.
- Consider the solvability of the resulting implicit system, which is typically an elliptic equation.

Example: Shallow water equations

Linearized:
$$\begin{cases} \dfrac{\partial u}{\partial t} + U_0 \dfrac{\partial u}{\partial x} + g \dfrac{\partial h}{\partial x} = 0 \\ \dfrac{\partial h}{\partial t} + U_0 \dfrac{\partial h}{\partial x} + H \dfrac{\partial u}{\partial x} = 0 \end{cases}$$

Linear analytic solution:

$$u(x,t) = u_0 e^{-i\omega t} e^{ikx}$$

Phase speed: $c \equiv \dfrac{\omega}{k} = U_0 \pm \sqrt{gH}$

H denotes here a mean state depth.

Shallow water equations

$$\begin{cases} \dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} + v\dfrac{\partial u}{\partial y} - fv + \dfrac{\partial \varphi}{\partial x} = 0 \\ \dfrac{\partial v}{\partial t} + u\dfrac{\partial v}{\partial x} + v\dfrac{\partial v}{\partial y} + fu + \dfrac{\partial \varphi}{\partial y} = 0 \\ \dfrac{\partial \varphi}{\partial t} + u\dfrac{\partial \varphi}{\partial x} + v\dfrac{\partial \varphi}{\partial y} + (\bar{\Phi} + \varphi)\left(\dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y}\right) = 0 \end{cases}$$

(green box) : advection

(red box) : gravity-wave (or sometimes called 'adjustment') term

In the linear version:

$$\Delta t \le \frac{\Delta s}{\sqrt{2}\sqrt{U_0^2 + V_0^2}}$$ advection

$$\Delta t \le \frac{\Delta s}{\sqrt{2}\sqrt{\bar{\Phi}}}$$ adjustment

$$\Delta t \le \frac{\Delta s}{\sqrt{2}\sqrt{U_0^2 + V_0^2 + \bar{\Phi}}}$$ combined

$$\bar{\Phi} >> U_0^2 + V_0^2$$

In the atmosphere $\sqrt{gH} = \sqrt{\bar{\Phi}} \approx 300\, m/s$

in synoptic-scale models $\Delta s < 10^5\, m$

==> $\Delta t \le 236$ sec ~ 4 min

Explicit time-stepping

- Leap-frog explicit scheme

$$
\begin{cases}
u_j^{n+1} = u_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} u_j^n - \dfrac{\Delta t}{\Delta s} \vec{\nabla}_x \varphi_j^n \\
v_j^{n+1} = v_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} v_j^n - \dfrac{\Delta t}{\Delta s} \vec{\nabla}_y \varphi_j^n \\
\varphi_j^{n+1} = \varphi_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} \varphi_j^n - \bar{\Phi} \dfrac{\Delta t}{\Delta s} \vec{\nabla} \cdot V_j^n
\end{cases}
$$

$$\bar{\Phi} = gH$$

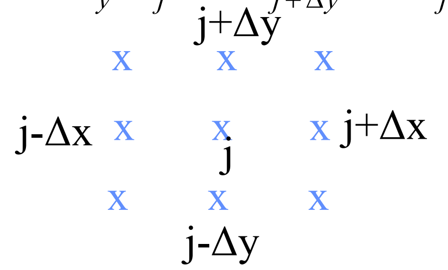
$$\Delta x = \Delta v = \Delta s$$

$$\overrightarrow{V_i} = (u_i, v_j)$$

$$\vec{\nabla} = (\nabla_x, \nabla_y)$$

$$\nabla_x A_j = A_{j+\Delta x} - A_{j-\Delta x}$$

$$\nabla_y A_j = A_{j+\Delta y} - A_{j-\Delta y}$$



Stability: $$\Delta t \le \frac{\Delta s}{\sqrt{2}\sqrt{\bar{\Phi}}}$$

If we treat implicitly the advection terms we do not get a Helmholtz equation

Increasing the allowed timestep

- Forward-backward scheme

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial \phi}{\partial x} = 0 \\ \dfrac{\partial \phi}{\partial t} + \Phi \dfrac{\partial u}{\partial x} = 0 \end{cases} \qquad \begin{cases} \phi_j^{n+1} = \phi_j^n - \dfrac{\Phi \Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n) & \text{forward} \\ u_j^{n+1} = u_j^n - \dfrac{\Delta t}{2\Delta x}(\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}) & \text{backward} \end{cases}$$

von Neumann gives $\left| \dfrac{\Delta t}{\Delta x} \sqrt{\Phi} \sin(k\Delta x) \right| \leq 2$ doubles the leapfrog timestep

- Pressure averaging

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = -\frac{1}{2\Delta x}\{(1-2\varepsilon)(\phi_{j+1}^n - \phi_{j-1}^n) + \varepsilon[(\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}) + (\phi_{j+1}^{n-1} - \phi_{j-1}^{n-1})]\}$$

if ε=0 ------> leapfrog

if ε=1/4 we get $\left| \dfrac{\Delta t}{\Delta x} \sqrt{\Phi} \sin(k\Delta x) \right| \leq 2$ doubles the leapfrog timestep

Split-explicit time-stepping

$$\begin{cases} u_j^s = u_j^{n-1} - \Delta t_s \overrightarrow{V_i^n} \cdot \vec{\nabla} u_i^n \\ v_j^s = v_j^{n-1} - \Delta t_s \overrightarrow{V_i^n} \cdot \vec{\nabla} v_i^n \\ \varphi_j^s = \varphi_j^{n-1} - \Delta t_s \overrightarrow{V_j^n} \cdot \vec{\nabla} \varphi_j^n \end{cases}$$

slow

$$\Delta t_s = M \, \Delta t_f$$

$$\begin{cases} u_j^{n+1} = u_j^s - \dfrac{\Delta t_f}{\Delta s} \vec{\nabla}_x \varphi_j^n \\ v_j^{n+1} = v_j^s - \dfrac{\Delta t_f}{\Delta s} \vec{\nabla}_y \varphi_j^n \\ \varphi_j^{n+1} = \varphi_j^s - \bar{\Phi} \dfrac{\Delta t_f}{\Delta s} \vec{\nabla} \cdot V_j^n \end{cases}$$

fast

$$\Delta t_s \leq \frac{\Delta s}{\sqrt{2}\sqrt{U_0^2 + V_0^2}}$$

Stability as before but M times a simpler problem.

$$\Delta t_f \leq \frac{\Delta s}{\sqrt{2}\sqrt{\bar{\Phi}}}$$

Potential drawbacks: splitting errors, conservation.
However recent advances for NH NWP suggested in *(Klemp et. al. 2007)*

Note: The fast solution may be computed implicitly.

Semi-implicit time-stepping

$$\begin{cases} u_j^{n+1} = u_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} u_j^n - \dfrac{\Delta t}{2\Delta s} \vec{\nabla}_x (\varphi_j^{n+1} + \varphi_j^{n-1}) \\ v_j^{n+1} = v_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} v_j^n - \dfrac{\Delta t}{2\Delta s} \vec{\nabla}_y (\varphi_j^{n+1} + \varphi_j^{n-1}) \\ \varphi_j^{n+1} = \varphi_j^{n-1} - \Delta t \overrightarrow{V_j^n} \cdot \vec{\nabla} \varphi_j^n - \Phi \dfrac{\Delta t}{2\Delta s} \vec{\nabla} \cdot (V_j^{n+1} + \overrightarrow{V_j^{n-1}}) \end{cases}$$

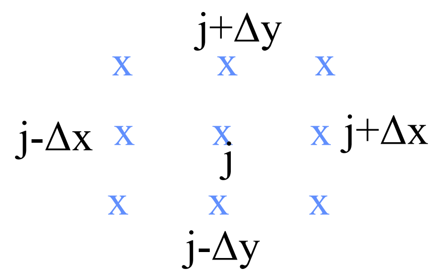
$$\Delta x = \Delta v = \Delta s$$

$$\overrightarrow{V_j} = (u_j, v_j)$$

$$\vec{\nabla} = (\nabla_x, \nabla_y)$$

$$\nabla_x A_j = A_{j+\Delta x} - A_{j-\Delta x}$$

$$\nabla_y A_j = A_{j+\Delta y} - A_{j-\Delta y}$$



Solve:

$$\nabla^2 \varphi_j^{n+1} - \frac{4(\Delta s)^2}{\overline{\Phi}(\Delta t)^2} \varphi_j^{n+1} = F^{n,n-1}$$

Helmholtz equation !

Stability: now only limited by the advection terms

Note: if we also treat the advection terms implicitly we do not get a Helmholtz equation!

Compressible Euler equations

Davies et al. (2003)

$$\frac{Du}{Dt} + c_p\theta\frac{\partial \pi}{\partial x} - fv = 0,$$

$$\frac{Dv}{Dt} + c_p\theta\frac{\partial \pi}{\partial y} + fu = 0,$$

$$\frac{Dw}{Dt} + c_p\theta\frac{\partial \pi}{\partial z} + g = 0,$$

$$\left(\frac{1-\kappa}{\kappa}\right)\frac{D\pi}{Dt} + \pi\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) = 0,$$

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

Compressible Euler equations

$$\pi^{(1-\kappa/\kappa)} = \frac{R}{p_0}\rho\theta,$$

$$\pi = \left(\frac{p}{p_0}\right)^{\kappa}, \kappa \equiv \frac{R}{c_p}, R \equiv c_p - c_V,$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}$$

A semi-Lagrangian semi-implicit solution procedure

$$u^{n+1} = u_d^n - \Delta t(1-\alpha)c_p\theta^{n+1}\left[\frac{\partial\pi}{\partial x}\right]_d^n - \Delta t\alpha c_p\theta^{n+1}\frac{\partial\pi^{n+1}}{\partial x},$$

$$v^{n+1} = v_d^n - \Delta t(1-\alpha)c_p\theta^{n+1}\left[\frac{\partial\pi}{\partial y}\right]_d^n - \Delta t\alpha c_p\theta^{n+1}\frac{\partial\pi^{n+1}}{\partial y},$$

$$w^{n+1} = w_d^n - \Delta t g - \Delta t(1-\alpha)c_p\theta^{n+1}\left[\frac{\partial\pi}{\partial z}\right]_d^n - \Delta t\alpha c_p\theta^{n+1}\frac{\partial\pi^{n+1}}{\partial z},$$

$$\theta^{n+1} = \theta_d^n,$$

(not as implemented, ***Davies et al. (2005)*** for details)

$$\rho^{n+1} = \rho_d^n\left[1+\Delta t\left(\frac{\partial u^{n+1}}{\partial x}+\frac{\partial v^{n+1}}{\partial y}+\frac{\partial w^{n+1}}{\partial z}\right)\right]^{-1},$$

$$(\pi^{n+1})^{(1-\kappa)/\kappa} = \frac{R}{p_0}\rho^{n+1}\theta^{n+1}$$

Davies et al. (1998,2005)

A semi-Lagrangian semi-implicit solution procedure

$$(\pi^{n+1})^{(1-\kappa)/\kappa}\left(1+\Delta t\nabla\cdot\mathbf{R}^n-(\Delta t)^2\alpha c_p\nabla\cdot(\theta_d^n\nabla\pi^{n+1})\right)=\frac{R}{p_0}\rho_d^n\theta_d^n$$

$$(\Delta t)^2\alpha c_p\nabla\cdot(\theta_d^n\nabla\pi^{n+1})+\frac{R}{p_0}\rho_d^n\theta_d^n\left(\frac{1}{\pi^{n+1}}\right)^{1/\kappa}\pi^{n+1}=1+\Delta t\nabla\cdot\mathbf{R}^n$$

A semi-Lagrangian semi-implicit solution procedure

$$L(\pi') - B = 0$$

Non-constant-coefficient approach!

Helmholtz equation

(solutions see e.g. Skamarock et al. 1997, Smolarkiewicz et al. 2000)

$$L(\psi) \equiv (\Delta t)^2 \alpha c_p A^{-1} \nabla \cdot (\theta_d^n \nabla \psi) - \psi,$$

$$A \equiv \frac{R}{p_0} (\pi^n)^{-1/\kappa} \rho_d^n \theta_d^n,$$

$$B \equiv \left(1 + \Delta t \nabla \cdot \mathbf{R}^n - \nabla \cdot (\theta_d^n \nabla \pi^n) - \frac{R}{p_0} \rho_d^n \theta_d^n (\pi^n)^{(\kappa-1)/\kappa} \right) A^{-1}$$

$$\pi' = \pi^{n+1} - \pi^n$$

Semi-implicit time integration in IFS

Choice of which terms in *RHS* to treat implicitly is guided by the knowledge of which waves cause instability because they are too fast (violate the CFL condition) and need to be slowed down with an implicit treatment.

In a hydrostatic model, fastest waves are horizontally propagating external gravity waves (long surface gravity waves), Lamb waves (acoustic wave not filtered out by the hydrostatic approximation) and long internal gravity waves. => implicit treatment of the adjustment terms.

L= linearization of part of RHS (i.e. terms supporting the fast modes) => good chance of obtaining a system of equations in the variables at "+" that can be solved almost analytically in a spectral model.

Two-time-level semi-Lagrangian semi-implicit time integration in the hydrostatic IFS

$$\frac{DX}{Dt} = RHS_x$$

$$\Rightarrow X^+ - 0.5\beta\Delta t L^+ = X^0 + 0.5\beta\Delta t L^0 + \Delta t RHS_x^{1/2} - \beta\Delta t L^{1/2} = X^*$$

For compact notation define:

$$\Delta_{tt} L \equiv 0.5\beta(L^+ + L^0) - \beta L^{1/2}$$

"semi-implicit correction term"

$$\Rightarrow \frac{DX}{Dt} = RHS_x^{1/2} + \Delta_{tt} L$$

Notations:
X : advected variable
RHS: right-hand side of the equation
L: part of RHS treated implicitly
Superscripts:
"0" indicates value at dep. point (t)
"1/2" indicates value at mid-point (t+0.5Δt)
"+" indicates value at arrival point (t+Δt)

L=RHS => implicit scheme

L= part of *RHS* => semi-implicit (β=1)

L=0 => explicit (β=0)

Semi-implicit time integration in IFS

$$\frac{D\vec{\mathrm{v}}_h}{Dt} + f\vec{k} \times \vec{\mathrm{v}}_h + \nabla_\eta \Phi + R_d T_v \nabla_\eta \ln p = P_\mathrm{v} + K_\mathrm{v}$$

$$\frac{DT}{Dt} - \frac{\kappa T_v \omega}{\left(1 + (\delta - 1)q\right)p} = P_\mathrm{T} + K_\mathrm{T}$$

$$\frac{\partial}{\partial t}(\ln p_s) = -\frac{1}{p_s}\int_0^1 \nabla_\eta \cdot (\vec{\mathrm{v}}_\mathrm{h} \frac{\partial p}{\partial \eta}) d\eta$$

semi-implicit corrections

$$\frac{D\vec{\mathrm{v}}_h}{Dt} = RHS_\mathrm{v} + \Delta_{tt}\left(\underline{\underline{\gamma}} \nabla_\eta T + R_d T_r \nabla_\eta \ln p_s\right)$$

$$\frac{DT}{Dt} = RHS_T + \Delta_{tt}\left(\underline{\underline{\tau}} D\right)$$

$$\frac{\partial}{\partial t}(\ln p_s) = RHS_p + \Delta_{tt}\left(\underline{\underline{\nu}} D\right)$$

semi-implicit equations

Semi-implicit time integration in IFS

$$\frac{D\vec{\mathrm{v}}_h}{Dt} = RHS_{\mathrm{v}} + \Delta_{tt}\left(\underline{\underline{\gamma}}\nabla_\eta T + R_d T_r \nabla_\eta \ln p_s\right)$$

$$\frac{DT}{Dt} = RHS_T + \Delta_{tt}\left(\underline{\underline{\tau}} D\right)$$

$$\frac{\partial}{\partial t}(\ln p_s) = RHS_p + \Delta_{tt}\left(\underline{\underline{\nu}} D\right)$$

semi-implicit equations

Reference state for linearization:

T_r ref. temperature

p_{sr} ref. surf. pressure

Where:

$$\left(\underline{\underline{\gamma}} X\right)_\eta \equiv -\int_1^\eta \frac{R_d X}{p_r}\frac{dp_r}{d\eta'}d\eta'$$

=> lin. geopotential for $X=T$

$$\left(\underline{\underline{\tau}} X\right)_\eta \equiv \frac{R_d T_r}{c_{pd} p_r}\int_0^\eta X\frac{dp_r}{d\eta'}d\eta'$$

=> lin. energy conv. term for $X=D$

$$\left(\underline{\underline{\nu}} X\right)_\eta \equiv \frac{1}{p_{sr}}\int_0^1 X\frac{dp_r}{d\eta'}d\eta'$$

Linear system to be solved

$$D^+ + 0.5\beta\Delta t\nabla^2(\gamma T^+ + R_d T_r \log(p_s{}^+)) = D^*$$

$$T^+ + 0.5\beta\Delta t\,\underline{\underline{\tau}}\,D^+ = T^*$$

$$\log(p_s{}^+) + 0.5\beta\Delta t\,\underline{\underline{\nu}}\,D^+ = P^*$$

Eliminate all variables to find also a Helmholtz equation for D^+ :

$$(1 - 0.25\beta^2\Delta t^2(\gamma\underline{\underline{\tau}} + R_d T_r \underline{\underline{\nu}})\nabla^2)D^+ = D^* - 0.5\beta\Delta t\nabla^2(\gamma T^* + R_d T_r P^*)$$

$$\Rightarrow \left(\underline{\underline{\mathrm{I}}} + \underline{\underline{\Gamma}}\,\nabla_\eta^2\right)D^+ = \widetilde{D}$$

$\underline{\underline{\Gamma}} \equiv \gamma\,\underline{\underline{\tau}} + R_d T_r \underline{\underline{\nu}}$ operator acting only on the vertical

$\underline{\underline{\mathrm{I}}}$ = unity operator

Semi-implicit time integration in IFS

$$\left(\underline{\underline{I}} + \underline{\underline{\Gamma}}\,\nabla_\eta^2\right) D^+ = \widetilde{D}$$

Vertically coupled set of Helmholtz equations. Coupling through

$$\underline{\underline{\Gamma}} \equiv \underline{\underline{\gamma}}\,\underline{\underline{\tau}} + R_d T_r \underline{\underline{\nu}}$$

Uncouple by transforming to the eigenspace of this matrix gamma (i.e. diagonalise gamma). Unity matrix "I" stays diagonal. =>

$$\left(1 + \lambda_i \nabla_\eta^2\right) D^+ = \widetilde{D}$$

One equation for each $1 \leq i \leq N_{Lev}$

In spectral space (spherical harmonics space):

$$\left(1 - \lambda_i \frac{n(n+1)}{a^2}\right) D_n^{m+} = \widetilde{D}_n^m$$

because

$$\nabla^2 Y_n^m = -\frac{n(n+1)}{a^2} Y_n^m$$

Once D^+ has been computed, it is easy to compute the other variables at "+".