Stabilization of NH dynamics - some underlying ideas

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1. Introduction

Common goal of NWP models is to predict evolution of atmosphere given by set of nonlinear partial differential equations. However, it is not possible to work with continuous representation. Models have to be discretised both in space and time. Aim of this short article is to illustrate some basic ideas and assumptions which are used in effort to stabilize NH dynamics.

Three different temporal schemes will be described: leapfrog, semi-implicit (SI) and fully implicit, known also as predictor--corrector (PC). Current effort in ALADIN non-hydrostatic dynamics is to implement PC scheme. It was shown experimentally that SI correction, which works well in hydrostatic model, is not sufficient for NH dynamics. Instability of NH model was partially reduced by implicit treatment of complete 3D divergence, not only its linear part. This treatment requires iterations (`NSITER` scheme). Positive impact on stability indicates that implicit treatment of complete nonlinear model might stabilize NH dynamics. Recently it was recognized that change of prognostic variables can have strong impact on model stability. This opened a new way which can contribute to stabilization of NH dynamics.

Symbolical notation will be used. Spatially discretised state of atmosphere can be represented by column vector $\mathbf{x} \in \mathbf{R}^n$. In finite difference model vector $\mathbf{x}$ contains grid point values of all prognostic fields. In spectral model it contains spectral coefficients instead of gridpoint values. All admissible vectors $\mathbf{x}$ form the phase space. Temporal evolution is described by phase trajectory $\mathbf{x}(t)$. It is determined by equation:

$$\frac{d\mathbf{x}(t)}{dt} = M(\mathbf{x}(t)) \qquad (1)$$

$$\mathbf{x}(t_0) = \mathbf{x}_0$$

Vector $\mathbf{x}_0$ represents initial state. Operator $M : \mathbf{R}^n \to \mathbf{R}^n$ is nonlinear. For autonomous systems it does not depend on t. It can be interpreted as a vector field on phase space. Integral curves of this field are phase trajectories.

2. Temporal discretisation - from leapfrog to fully implicit

Equation (1) still have to be discretised in time. Standard notation will be used for this purpose:

$$\mathbf{x}^+ = \mathbf{x}(t+\Delta t) \qquad \mathbf{x}^0 = \mathbf{x}(t) \qquad \mathbf{x}^- = \mathbf{x}(t-\Delta t)$$

One common scheme used in NWP is leapfrog:

$$\frac{\mathbf{x}^+ - \mathbf{x}^-}{2\,\Delta t} = M(\mathbf{x}^0) \qquad (2)$$

It is an explicit 3-time-level scheme. The state $\mathbf{x}^+$ can be expressed as:

$$\mathbf{x}^+ = \mathbf{x}^- + 2\,\Delta t\; M(\mathbf{x}^0) \qquad (3)$$

Another scheme is fully implicit scheme. It can be obtained from equation (2) by time averaging the right hand side:

$$\frac{\mathbf{x}^+ - \mathbf{x}^-}{2\,\Delta t} = \frac{M(\mathbf{x}^+) + M(\mathbf{x}^-)}{2} \tag{4}$$

Fully implicit scheme is a 2-time-level scheme, because $\mathbf{x}^0$ disappeared from equation (4). It can be rearranged into the form:

$$(\mathbf{I} - \Delta t\, M)\, \mathbf{x}^+ = (\mathbf{I} + \Delta t\, M)\, \mathbf{x}^- \tag{5}$$

It can be seen from equation (5) that evaluation of $\mathbf{x}^+$ requires inversion of operator $(\mathbf{I} - \Delta t\, M)$. But since operator M is nonlinear, equation (5) must be solved iteratively. This can be done using predictor--corrector algorithm.

A step between leapfrog and fully implicit scheme is so-called semi-implicit scheme (SI). Basic idea is to linearize operator M at suitably chosen stationary state $\mathbf{x}^*$ and split right hand side of (2) into linear part and nonlinear residual. Linear part is treated implicitly, nonlinear residual explicitly:

$$\mathbf{L} = M'(\mathbf{x}^*) \qquad M(\mathbf{x}^*) = 0$$

$$\frac{\mathbf{x}^+ - \mathbf{x}^-}{2\,\Delta t} = \frac{\mathbf{L}\mathbf{x}^+ + \mathbf{L}\mathbf{x}^-}{2} + (M - \mathbf{L})\mathbf{x}^0 \tag{6}$$

Equation (6) can be manipulated into the form:

$$(\mathbf{I} - \Delta t\, \mathbf{L})\, \mathbf{x}^+ = (\mathbf{I} + \Delta t\, \mathbf{L})\, \mathbf{x}^- + 2\,\Delta t\, (M - \mathbf{L})\, \mathbf{x}^0 \tag{7}$$

Evaluation of $\mathbf{x}^+$ from equation (7) requires inversion of matrix $(\mathbf{I} - \Delta t\, \mathbf{L})$. If operator M was linear, it would be equal to its linearization $\mathbf{L}$ and equations (5), (7) would be identical. It means that in linear case SI scheme is equivalent to fully implicit scheme.

As was mentioned in introduction, results from numerical experiments indicate that fully implicit scheme is better than SI scheme which is better than leapfrog. All three schemes are of second order accuracy, so where does this difference comes from ? Answer is far from trivial, because considered system is nonlinear. At least some indication can be obtained by examination of linear system:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{L}\mathbf{x}(t) \tag{8}$$

However, in this case there are only 2 different schemes to study because SI scheme is identical to fully implicit scheme. Analysis of linear system leads to following results:

- If system (8) has a neutral mode, corresponding modes of leapfrog scheme and fully implicit scheme are also neutral. (For leapfrog this is true only conditionally, Δt must be smaller than some critical value.) Both schemes introduce only phase error for such mode. Leapfrog scheme is accelerating, fully implicit scheme is decelerating (figure 1) .
- Since leapfrog is a 3-time-level scheme, computational mode exists. For practical usability time filter must be applied. It strongly damps computational mode, but introduces some damping also for physical mode. This violates desirable property from previous point.

  Fully implicit scheme is a 2-time-level scheme, so only physical mode exists. Time filter is not needed.
- If there exists a quadratic invariant for system (8), i.e. such non-zero symmetric matrix $\mathbf{G}$ that

  $$\frac{d}{dt}\left[\mathbf{x}^{\mathrm{T}}(t)\ \mathbf{G}\ \mathbf{x}(t)\right] = 0,$$

  this invariant is conserved by fully implicit scheme.

It can be seen from given points that at least in linear case there are some advantages of fully implicit scheme over leapfrog scheme.

3. Choice of prognostic variables -- impact to stability

Evolution of atmosphere as a dynamical system has geometric nature. It does not depend on choice of prognostic variables. These variables plays a role of coordinates in phase space and can be chosen in infinitely many ways.

Situation changes when continuous system is discretised and approximate solution is constructed. Same numerical scheme applied in different coordinates can lead to different results. Choice of prognostic variables can affect qualitative behaviour of approximate solution. This can be illustrated on simple example. Consider following continuous system (phase space is $\mathbf{R}^2$):

$$\begin{aligned} \partial_t x &= -\omega y \\ \partial_t y &= \omega x \\ \omega &\neq 0 \end{aligned} \tag{9}$$

It can be verified easily that distance from origin $r \equiv \sqrt{(x^2+y^2)}$ is conserved during system's evolution. Phase trajectories are circles centred at origin. Application of leapfrog scheme to equations (9) gives:

$$\begin{aligned} x^+ &= x^- - 2\omega\Delta t\, y^0 \\ y^+ &= y^- + 2\omega\Delta t\, x^0 \\ \Delta t &> 0 \end{aligned} \tag{10}$$

System (10) can be analysed using standard techniques. There are 2 physical and 2 computational modes. Final form of physical solution is :

$$\mathbf{x}^+ = \mathbf{R}\mathbf{x}^0 \qquad \mathbf{x}^0 = \mathbf{R}\mathbf{x}^-$$

$$\mathbf{x} \equiv \begin{pmatrix} x \\ y \end{pmatrix} \qquad \mathbf{R} = \begin{pmatrix} \sqrt{1-(\omega\Delta t)^2} & -\omega\Delta t \\ \omega\Delta t & \sqrt{1-(\omega\Delta t)^2} \end{pmatrix} \tag{11}$$

$$\left|\omega\Delta t\right| \leq 1$$

Matrix $\mathbf{R}$ is orthogonal ($\mathbf{R}^{\mathrm{T}}\mathbf{R} = 0$), it corresponds to rotation by angle $\theta = \arcsin(\omega\Delta t)$. Distance from origin r is therefore conserved by system (10) :

$$r^2 = x^2 + y^2 = \mathbf{x}^{\mathrm{T}}\mathbf{x}$$

$$(\mathbf{x}^+)^{\mathrm{T}}\mathbf{x}^+ = (\mathbf{R}\mathbf{x}^0)^{\mathrm{T}}\mathbf{R}\mathbf{x}^0 = (\mathbf{x}^0)^{\mathrm{T}}\mathbf{R}^{\mathrm{T}}\mathbf{R}\mathbf{x}^0 = (\mathbf{x}^0)^{\mathrm{T}}\mathbf{x}^0$$

$$r^+ = r^0 \tag{12}$$

It is clear from equation (12) that leapfrog scheme applied in coordinates *(x , y)* is neutral, so it reproduces qualitative behaviour of continuous system (10). There is only phase error introduced, scheme is accelerating with factor $\arcsin(\omega\Delta t) / (\omega\Delta t)$ (figure 2).

New coordinates (ρ, θ) can be introduced now. They are defined on $\mathbf{R}^2$ without half-line "$y = 0, x \geq 0$" :

$$\begin{aligned} x &= \rho e^{\theta} \cos\theta & \rho &> 0 \\ y &= \rho e^{\theta} \sin\theta & \theta &\in [0,2\pi] \\ r &= \sqrt{x^2+y^2} = \rho e^{\theta} \end{aligned}$$

System (9) rewritten into coordinates (ρ, θ) has the form:

$$\partial_t \rho = -\omega\rho$$
$$\partial_t \theta = \omega \tag{13}$$

Application of leapfrog scheme to equations (13) gives :

$$\rho^+ = \rho^- - 2\omega\Delta t\, \rho^0 \tag{14}$$

$$\theta^+ = \theta^- + 2\omega\Delta t \tag{15}$$

Equations (14), (15) are uncoupled, so they can be analysed independently. Modes of equation (14) will be find first :

$$\rho^+ = \lambda\rho^0 \qquad \rho^0 = \lambda\rho^-$$

$$\lambda^2 + 2\omega\Delta t\, \lambda - 1 = 0$$

$$\lambda_{1,2} = \pm\sqrt{1 + (\omega\Delta t)^2} - \omega\Delta t \tag{16}$$

Root λ_1 represents physical mode ($\lambda_1 \to 1$ for $\Delta t \to 0$), root λ_2 represents computational mode ($\lambda_2 \to -1$ for $\Delta t \to 0$).

As for equation (15), solution on even time levels (t, $t+2\Delta t$, $t+4\Delta t$, ...) is completely separated from solution on odd time levels ($t+\Delta t$, $t+3\Delta t$, $t+5\Delta t$, ...). For physical mode separation between θ^+ and θ^0 is the same as between θ^0 and θ^- :

$$\theta^+ - \theta^0 = \theta^0 - \theta^-$$

$$\theta^0 = \tfrac{1}{2}(\theta^+ + \theta^-)$$

In conjunction with (15) this gives :

$$\theta^+ = \theta^0 + \omega\Delta t \tag{17}$$

Combination of relations (16), (17) leads to following result for physical mode :

$$r^+ = \rho^+ e^{\theta^+} = \lambda_1\, \rho^0 e^{\theta^0 + \omega\Delta t} = \lambda_1\, \rho^0 e^{\theta^0} e^{\omega\Delta t} = \lambda_1 e^{\omega\Delta t}\, r^0$$

$$r^+ = \left(\sqrt{1 + (\omega\Delta t)^2} - \omega\Delta t\right) e^{\omega\Delta t}\, r^0 \tag{18}$$

Amplification factor (18) is less than one for $\omega\Delta t < 0$ and greater than one for $\omega\Delta t > 0$ (figure 3). This means that application of leapfrog scheme in coordinates (ρ, θ) leads to damping for $\omega < 0$ and to unstable behaviour for $\omega > 0$.

It can be concluded from given example that choice of prognostic variables can influence qualitative behaviour of numerical scheme. However instability introduced by variables (ρ, θ) is very weak. Power expansion of amplification factor in equation (18) for small Δt gives :

$$r^+ = \left(1 + \frac{(\omega\Delta t)^3}{6} + \dots\right) r^0 \tag{19}$$

It means that pathological behaviour for studied second order accurate scheme occurred at third order terms in Δt. This is not a problem for NWP, where correct behaviour up to second order terms is sufficient. However, studied system was too simple. In more complicated systems like Eulerian equations pathological behaviour can occur at second order terms. It might be caused by improperly chosen prognostic variables. Effort to find more stable NH prognostic variables is based on this fact. First experimental results indicate that there might be some better candidates than original pair.

5. Conclusions

Following facts have been illustrated:

- In linear case fully implicit scheme has some advantages over leapfrog scheme. It is believed that it could perform better also in nonlinear case, but it is not easy to give theoretical arguments for this.
- Nonlinear transformation of prognostic variables does not commute with temporal discretisation. Choice of variables can affect qualitative behaviour of discretised system. It was shown on elementary example that neutral behaviour can be changed to damping or unstable, but for second-order accurate scheme the amplification error is of third order, which is not interesting in NWP context. However, in more complicated systems instability due to choice of variables can occur at second order terms. So there is some chance that suitably chosen prognostic variables might stabilize (at least partially) NH dynamics.

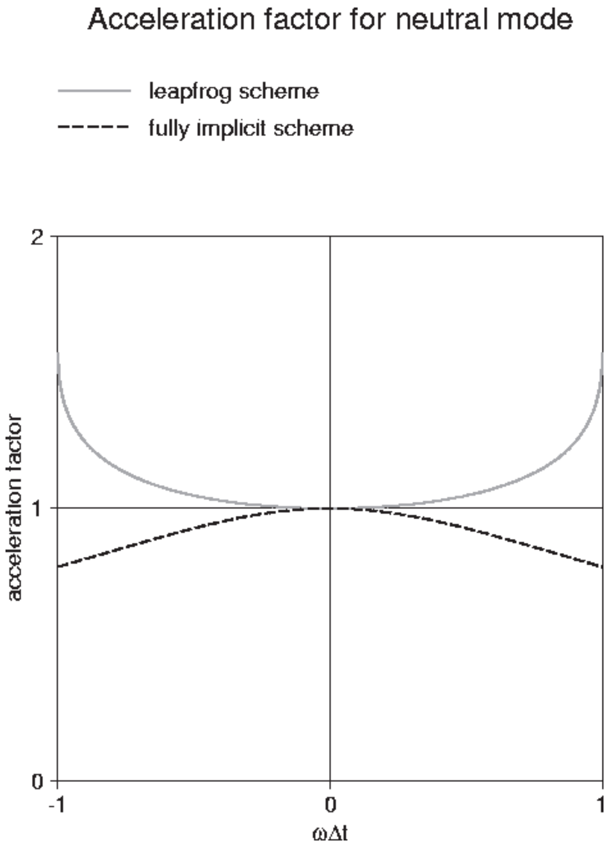

Figure 1.

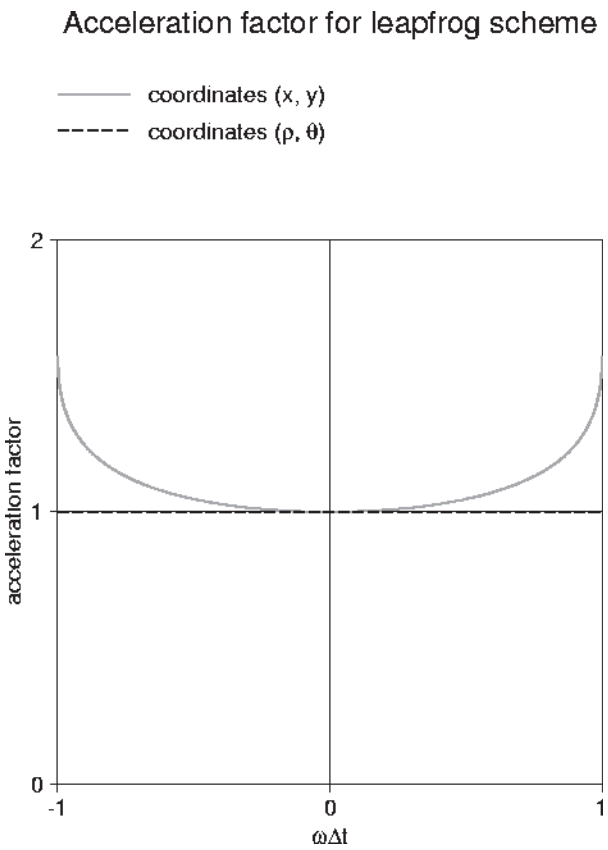

Figure 2

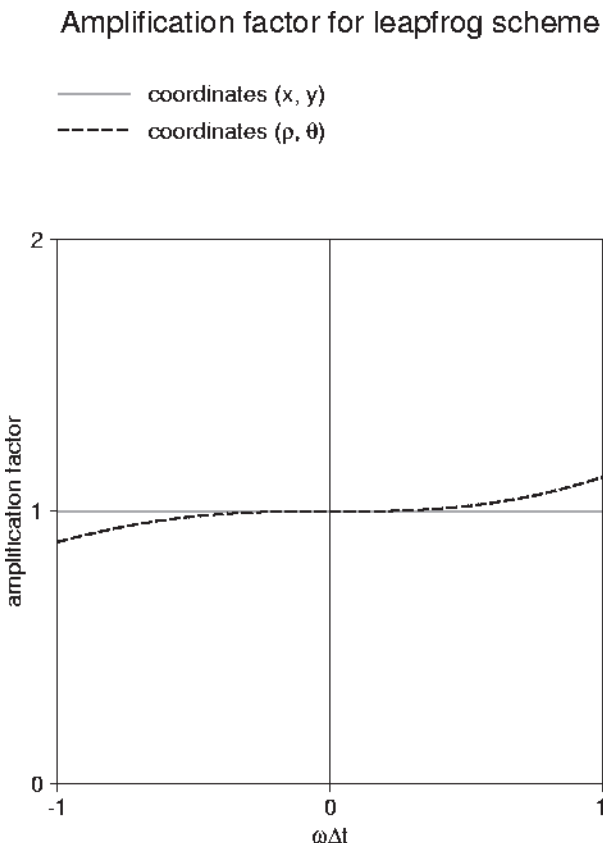

Figure 3