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Non-hydrostatic semi-elastic hybrid-coordinate SISL extension of HIRLAM. Part I: numerical scheme

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ABSTRACT

Two-time-level, semi-implicit, semi-Lagrangian (SISL) scheme is applied to the non-hydrostatic pressure coordinate equations, constituting a modified Miller–Pearce–White model, in hybrid-coordinate framework. Neutral background is subtracted in the initial continuous dynamics, yielding modified equations for geopotential, temperature and logarithmic surface pressure fluctuation. Implicit Lagrangian marching formulae for single time-step are derived. A disclosure scheme is presented, which results in an uncoupled diagnostic system, consisting of 3-D Poisson equation for omega velocity and 2-D Helmholtz equation for logarithmic pressure fluctuation. The model is discretized to create a non-hydrostatic extension to numerical weather prediction model HIRLAM. The discretization schemes, trajectory computation algorithms and interpolation routines, as well as the physical parametrization package are maintained from parent hydrostatic HIRLAM. For stability investigation, the derived SISL model is linearized with respect to the initial, thermally non-equilibrium resting state. Explicit residuals of the linear model prove to be sensitive to the relative departures of temperature and static stability from the reference state. Relayed on the stability study, the semi-implicit term in the vertical momentum equation is replaced to the implicit term, which results in stability increase of the model.

1. Introduction

Since the original demonstration of the efficiency advantage of the semi-implicit semi-Lagrangian (SISL) method by Robert (1981), this numerical integration scheme is being used in an increasing range of atmospheric models.

First the SISL-ideology to integrate the hydrostatic (HS) primitive equations numerically was proposed by Robert for shallow water equations (1981, 1982), encouraged by the earlier positive experience with the semi-implicit Eulerian scheme (Robert, 1969; Robert et al., 1972). Two-time-level SISL schemes were developed by Temperton and Staniforth (1987), Purser and Leslie (1988), McDonald and Bates (1989) and Côté and Staniforth (1988). Baroclinic, multilevel, HS primitive-equation SISL models soon followed: three-time-level σ-coordinate scheme by Robert et al. (1985), Tanguay et al. (1989). Two-time-level σ-coordinate versions were presented by Bates and McDonald (1982), McDonald (1986), Leslie and Purser (1991), McDonald and Haugen (1992) and Bates et al. (1993), the hybrid-coordinate version was proposed by McDonald and Haugen (1992). Non-hydrostatic (NH) versions of SISL were developed in three-time-level version by Tanguay et al. (1990) and in two-time-level realization by Golding (1992). Operationally, the two-time-level HS SISL was launched in 1995 at ECMWF (Ritchie et al., 1995), at HIRLAM (McDonald, 1995) and at Meteo-France (Bubnova et al., 1995).

In this paper, a novel two-time-level NH SISL extension to the numerical weather prediction model HIRLAM (Undén et al., 2002) is presented. The basis for NH updating is the non-hydrostatic pressure coordinate model, initially developed by Miller (1974), Miller and Pearce (1974), Miller and White (1984) and White (1989), which will be referred as the MPW model hereafter. The MPW model derivation from general elastic pressure-coordinate equations (Rõõm, 1990) is discussed also in detail by Rõõm (2001).

Roughly speaking, the MPW model is a simplest generalization of the HS pressure-coordinate primitive equations, which takes vertical acceleration into consideration, while maintaining in other respect the appearance and the main characteristics of the hydrostatic model.

In acoustic wave handling, the MPW model behaves exactly like the HS primitive-equation model does: it filters internal acoustic waves while maintains the external Lamb waves. This property gives reason to refer the model also to as 'semi-elastic' (Rõõm et al., 2006). An intercomparison of exact analytical solutions of MPW equations with 'full' elastic model was carried out by Rõõm and Männik (1999), who demonstrated that there is no difference in two models on the synoptic and shorter scale,

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including the HS and NH mesoscale domains. On shorter synoptic scale and on mesoscales the solutions of MPW equations and fully elastic set are indistinguishable. The MPW equations coincide asymptotically at horizontal scales >30 km with the HS pressure-coordinate primitive-equation (PE) model. Thus, at description of large-scale processes they are as accurate, as the HS primitive equations which are currently applied in all global NWP models.

Being the most simple and straightforward generalization of the HS primitive equations, the MPW model is in numerical realization very close to the hydrostatic model, which makes its implementation in an existing HS numerical pressure-coordinate environment rather straightforward. This closeness to the HS model along with the simplicity should also result in the robustness, stability and computational efficiency of the numerical scheme, comparable to those of the HS 'parent' dynamics. That has been the main motivation for the introduction of the MPW model rather than of the 'full' pressure-coordinate dynamics (Rõõm, 1990). The MPW model has been already applied with success in heretofore developed three-time-level, explicit-Eulerian (Männik and Rõõm, 2001) and SI Eulerian (Rõõm and Männik, 2002; Männik, 2003) schemes of HIRLAM. The aim of this paper is to present the SISL extension of these implementations.

With the aim of further enhancement of the robustness of numerical scheme, the applied equation set is modified substantially in comparison with original MPW model and also in comparison with previous SI Eulerian scheme (Rõõm and Männik, 2002; Männik et al., 2003) prior to discretization and SISL implementation. Modifications, absolutely not affecting neither the physical nor hydrodynamic nature of the model, start with partition of the temperature to a pressure-dependent reference state and a fluctuative component. The temperature partition is actually required further anyway for the separation of forcing to linear 'main' part, depending on the reference temperature, and supplementary non-linear residual, depending on the temperature fluctuations. In the current treatment, however, the separation is applied in the original continuous model, whereas the height-dependent reference temperature is used instead of the isothermal background state, common in traditional HS SISL approach. The temperature partition involves further modifications of MPW equations. A very large by value but neutral in dynamical respect (as not causing any forcing) constituent of hydrostatic geopotential is removed. The remaining fluctuative part of HS geopotential will depend on temperature and logarithmic surface pressure fluctuations. The surface pressure separates to a mean component, which includes orography, but is in hydrostatic balance with the reference temperature, and a dynamic fluctuative part, expressed by means of logarithmic surface pressure fluctuations in the role of new independent dynamic field. For this new variable, a prognostic equation is introduced instead of the common surface pressure equation, representing a modified formulation of the 'mean orography advection scheme', introduced by Ritchie and Tanguay (1996). Finally, equation for full temperature is substituted to Lagrangian transport equation for the fluctuative part of temperature with suitable modification of energy conversion term. Due to the significance for SISL approach, the applied modifications are discussed comprehensively in the introductory part of model description. Keeping in mind maximum generality and mathematical transparency of presentation, all the intrinsic SISL description is carried out in spatially continuous framework.

As the reference temperature is chosen in application as an area mean for each fixed pressure-level, it becomes time-dependent together with the reference surface pressure. This dependence is actually weak and does not cause any sophistication in computational aspect, except that the reference fields have to be recalculated from time to time; neither does it cause any instability. Thus, the model possesses adaptive reference temperature and surface pressure. As a result, the actual temperature and surface pressure deviations from the reference state become minimal in certain respect, minimizing the non-linear explicit residuals and giving rise to additional numerical stability. That is the main idea and motivation for introduction of adaptive reference states.

Due to the used modifications, especially due to application of adaptive height-dependent reference temperature, which helps to minimize the explicit non-linear residuals, the developed two time level SISL scheme proved to be numerically stable in limited area modelling (Rõõm et al., 2006). However, as the recent computation (results of which will be demonstrated in the forthcoming Part II of the paper) in conditions of extreme cross-area temperature contrasts has shown, this stability may be violated at traditional semi-implicit treatment of the forcing term in the vertical momentum equation. Instability arises, when the horizontal temperature contrasts exceed ∼30 K, and it is usually absent in a limited area model with lateral flanks not exceeding 1000–1500 km, as the temperature contrasts remain subcritical for sufficiently small areas. Even in the subcritical temperature contrast conditions, this instability source manifests itself in the time-step diminishing. It represents a variant of instability, first reported by Simmons et al. (1978, SHB78 hereafter). However, in this case, the instability source is not the non-constant reference temperature like in SHB78, but the explicit residual in the vertical forcing term of the vertical momentum equation. In this respect, the instability is more close to that, described by Benard (2003, 2004) for fully elastic model. The instability rise can be easily avoided, proceeding from the semi-implicit handling of vertical forcing to the fully implicit treatment. Both variants of numerical model, with semi-implicit (SVF) and implicit (IVF) vertical forcing handling, are introduced in following. Though the IVF is preferable in computations as the more stable one, the SVF scheme is illuminating for comparative stability study. The model stability is subject to numerical experimentation with non-linear, complete SISL scheme, which will be carried out in the forthcoming Part 2 of the paper. However, due to the

importance of the stability properties to the model general quality, a linearized subcase of the MPW model is especially derived in Section 4, suited for further theoretical stability treatment. The linearization is carried out with respect to a resting but thermally non-equilibrium initial state, thus following the SHB78 ideology. Important point in linearization is the proper handling of the Lagrangian finite time differencing formula in the vicinity of resting state. The linearized model presents a SISL approximation of normal-mode equations with analytic presentation of explicit linear thermal residuals. Coefficients in these residuals depend on the reference state and are proportional to the initial temperature departure. Though a detailed study of the linear stability is not in scope of this paper, some preliminary speculation on the role of these coefficients for available time-step size is made, which shall be proved in the Part II.

2. Continuous model

2.1. Coordinate system and integration area

The η-coordinate system, introduced by Simmons and Burridge (1981), is a convenient tool for introduction of a terrain-following coordinate system for equations, initially formulated in isobaric coordinates. Pressure presents in η-coordinates

$$p = A(\eta) + B(\eta)p_s(x, y, t), \tag{1}$$

where $p_s(x, y, t)$ is the surface pressure. Transformation coefficients A and B can be in more detail presented as

$$A(\eta) = \eta[1 - q(\eta)]p_s^0, \quad B(\eta) = \eta q(\eta), \tag{2}$$

where $p_s^0 = p_s^0(t)$ is the area-mean surface pressure. Commonly, p_s^0 is chosen a standard constant mean seal level pressure (101 326 Pa in the case of HS HIRLAM, for instance). However, in our case with the time-dependent adaptive reference temperature (introduced further), the area mean surface pressure becomes time-dependent; a detailed definition of $p_s^0(t)$ will be given further.

Function $q(\eta)$, satisfying conditions $0 \le q(\eta) \le 1$, is the weight of the terrain-following pressure component on level η, $1 - q(\eta)$ is the weight of the 'pure' pressure coordinate component. For $q = 0$ we get isobaric coordinate representation, while $q = 1$ yields a native σ-coordinate system with η in the role of the σ-coordinate. The pressure-coordinate for optional q follows also in the 'water planet case', when $p_s = p_s^0$. Choosing $q(\eta)$ monotonically decreasing with height from $q(1) = 1$ on the surface to $q(\eta) = 0$ in the stratosphere, the hybrid coordinate will behave like a σ-coordinate near surface, transforming steadily to the pressure-coordinate near the top.

Horizontally the spherical geometry is considered, thus x, y are local geographical coordinates on the mean sea level pressure surface. The area of integration is

$$-L_x < x = r_0 \cos\theta\lambda < L_x, \quad -L_y < y = r_0\theta < L_y,$$

with r_0 as the mean radius of earth and with λ, θ as the polar coordinates in a suitably chosen spherical coordinate system.

2.2. Primary modifications

The MPW model equations we will apply are in essence the White extension of Miller and Pearce model, presented in (White, 1989) as eqs (27)–(31). However, some prior modifications, not affecting the physical nature of the model, are required in formal presentation of these equations, conditioned by hybrid coordinates and by SISL approach requirements. The main modification, obligatory for a discrete SISL approximation anyway, but applied here in the continuous case prior to any discretization, consist in separation of the temperature to the main, horizontally homogeneous in pressure coordinates, that is, barotropic component $T^0(p)$ and fluctuative part T'

$$T = T^0 + T'. \tag{3}$$

Choice of $T^0(p)$ is somewhat optional with exception that it should approximate the real temperature distribution at time t. In applications, a good choice is to specify T^0 as the area-mean over isobaric surface p:

$$T^0(p) = \frac{\int_S T(x, y, p, t)\,\mathrm{d}x\,\mathrm{d}y}{\int_S \mathrm{d}x\,\mathrm{d}y}. \tag{4}$$

At such choice, the reference temperature is in general time dependent. However, we will treat T^0 locally in time as a constant field. First, (4) is applied not necessarily at every time-step, but from time to time. Second, if the reference field T^0 is recalculated anew on some time level t, then T' is modified in (3) in the way that the total field $T(x, y, \eta, t)$ remains unchanged. Similar approach is applied with regard to all reference fields in this paper. This prevents from the further arrival of local tendencies like $\partial T^0/\partial t$ in the explicit residuals of SISL scheme, simplifying the model both formally and in application.

The complete geopotential $\Phi = gz(x, y, \eta, t)$, where g is gravitational acceleration and $z(x, y, \eta, t)$ is the height of a material air particle with coordinates x, y, η at time t, can be presented as the sum of hydrostatic geopotential φ^s and non-hydrostatic residual ϕ,

$$\Phi = \varphi^s + \phi,$$

where

$$\varphi^s = gh + \int_p^{p_s} RTd(\ln p') = gh + \int_\eta^1 \frac{RT}{p} m d\eta,$$

$h(x, y)$ is the surface elevation, R is the gas constant of moist air, and

$$m = \frac{\partial p}{\partial \eta} \tag{5}$$

represents the η-coordinate 'density'. Further, the hydrostatic geopotential φ^s can be split with the help of (3) to the neutral

background geopotential $\hat{\varphi}$, baric fluctuation φ^p, and thermal part φ^T: and deviation φ:

$$\varphi^s = \hat{\varphi}(p) + \varphi^p(x, y, t) + \varphi^T(x, y, \eta, t), \tag{6}$$

where

$$\hat{\varphi} = gh + R^0 \int_p^{\hat{p}_s} T^0 \, \mathrm{d}(\ln p'), \tag{7a}$$

$$\varphi^p = R^0 \int_{\hat{p}_s}^{p_s} T^0 \, \mathrm{d}(\ln p'), \tag{7b}$$

$$\varphi^T = \int_p^{p_s} (RT)' \, \mathrm{d}(\ln p') = \int_\eta^1 (RT)' m \frac{\mathrm{d}\eta'}{p}, \tag{7c}$$

R^0 is the gas constant for dry air, $(RT)' = RT - R^0 T^0$, and $\hat{p}_s(x, y)$ is the reference pressure on the surface. If $\hat{p}_s$ is chosen to satisfy condition (which represents an implicit barometric formula for reference surface pressure)

$$R^0 \int_{\hat{p}_s}^{p_s^0} T^0 \, \mathrm{d}(\ln p') = gh(x, y), \tag{7d}$$

then $\nabla_p \hat{\varphi} = 0$, that is, $\hat{\varphi}$ does not cause forcing and may be safely left out from geopotential composition. Thus, a rather large but dynamically passive part of geopotential can be removed, improving the smoothness of isobaric gradient $\nabla_p \varphi = \nabla_p \varphi^s$ and giving rise to numerical accuracy of the final discrete scheme. Analogous temperature separation is partially applied already in the original MPW model by Miller (1974) and White (1989), and it is also used in some numerical schemes (Girard et al., 2005).

The thermal geopotential φ^T cannot be simplified further, except that in the numerical implementation it will be substituted by a finite sum over discrete vertical levels. Due to closeness of p_s to $\hat{p}_s$, it is advantageous to evaluate the baric geopotential φ^p analytically, rather than numerically, using the smoothness of T^0 and representing it near surface as $T^0(p) = T^0(\hat{p}_s) + (\mathrm{d}T^0/\mathrm{d}p)_{\hat{p}_s} (p - \hat{p}_s)$:

$$\varphi^p = C^2[\chi + 2\gamma(\mathrm{e}^\chi - 1 - \chi)], \tag{8}$$

where

$$\chi = \ln(p_s/\hat{p}_s), \tag{9}$$

and

$$C^2 = R^0 T^0[\hat{p}_s(x, y, t)], \quad \gamma = \left(\frac{p}{2T^0} \frac{\partial T^0}{\partial p} \right)_{p=\hat{p}_s(x,y,t)}.$$

Due to the smallness of χ ($|\chi| < 5 \times 10^{-2}$ even in the most strong cyclones) and $|\gamma| < 0.1$, (8) can be approximated as

$$\varphi^p \approx C^2 \chi \, (1 + \gamma \chi) \approx C^2 \chi, \tag{8'}$$

the first approximation being valid within relative error $\sim|\gamma| \, \chi^2/3 < 10^{-4}$ and the second within relative error $\sim|\gamma| \, \chi < 5 \times 10^{-3}$. In the particular case of isothermal stratification if $\gamma = 0$, (8) simplifies to $\varphi^p = C^2 \chi$, and thus, the second approximation in (8′) becomes exact. That is, in baric geopotential computations, the error due to isothermal approximation $\gamma = 0$ does not exceed 0.5%.

Further, for hydrostatic geopotential fluctuation will be used notation

$$\varphi = \varphi^p + \varphi^T, \tag{10}$$

with φ^p and φ^T defined as (8) and (7c), consequently.

This fluctuative part is small, when measured in C^2 units: the amplitude of φ^p/C^2 is about 1/100, whereas the amplitude of φ^T/C^2 is about 1/10.

As φ is a function of χ, it is advantageous to derive a prognostic equation for χ instead of equation for total surface pressure p_s. The vertically integrated mass balance equation

$$\frac{\partial p_s}{\partial t} = -\nabla \cdot \int_0^1 \mathbf{v} \, m \, d\eta,$$

where $\nabla\cdot$ and $\mathbf{v}$ are the horizontal divergence operator and wind vector on the sphere, can be presented with the help of (1) and (5) in the form

$$\frac{\mathrm{d}_B p_s}{\mathrm{d}t} = -\int_0^1 \nabla \cdot \mathbf{v} \, m \, d\eta,$$

where

$$\frac{\mathrm{d}_B}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v}_B \nabla, \quad \mathbf{v}_B = \int_0^1 B' \mathbf{v} d\eta. \tag{11}$$

Equation for log-pressure fluctuation χ becomes with the help of these relationships

$$\frac{\mathrm{d}_B \chi}{\mathrm{d}t} = -\frac{1}{p_s} \int_0^1 \nabla \cdot \mathbf{v} \, m \, \mathrm{d}\eta - \mathbf{v}_B \cdot \nabla \ln \hat{p}_s \equiv \mathcal{F}_\chi, \tag{12a}$$

representing a modified formulation of the 'mean orography advection scheme' of Ritchie and Tanguay (1996) and constituting the first equation in the modified MPW model.

2.3. Semi-elastic equations in hybrid-coordinates

The surface pressure eq. (12a) is not incorporated into the MPW equations (Miller, 1974; White, 1989) explicitly. Remaining relationships present, however, the White extension of Miller and Pearce model (White, 1989, eqs 27–31), rewritten here for variables ω, $\mathbf{v}$, T', φ, ϕ, in hybrid-coordinates, as the vertical momentum, horizontal momentum, fluctuative temperature and continuity equations:

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = -\frac{p^2}{mH^2} \frac{\partial \phi}{\partial \eta} + \omega \left(\frac{c_v \omega}{c_p p} - \frac{A_T}{T} - \frac{\mathrm{d} \ln R}{\mathrm{d}t} \right) + A_\omega \equiv \mathcal{F}_\omega, \tag{12b}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\nabla_p(\varphi + \phi) - f\mathbf{k} \times \mathbf{v} + \mathbf{A}_\mathbf{v} \equiv \mathcal{F}_\mathbf{v}, \tag{12c}$$

$$\frac{\mathrm{d}T'}{\mathrm{d}t} = S\omega + A_T \equiv \mathcal{F}_T, \tag{12d}$$

$$\nabla_p \cdot \mathbf{v} + \frac{1}{m}\frac{\partial \omega}{\partial \eta} = 0, \tag{12e}$$

where

$$\nabla_p = \nabla - \frac{\nabla p}{m}\frac{\partial}{\partial \eta}$$

and ∇ presents the horizontal (in η-coordinates) gradient and divergence over a sphere with the mean radius of the Earth. The Lagrangian material derivative is

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \dot{\eta}\frac{\partial}{\partial \eta} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_p + \frac{\omega}{m}\frac{\partial}{\partial \eta},$$
$$\dot{\eta} = \frac{\omega - \mathbf{v}\cdot\nabla p}{m},$$

and the energy conversion coefficient in (12d) is

$$S = \left(\kappa\frac{T}{p} - \frac{\mathrm{d}T^0}{\mathrm{d}p}\right).$$

In eqs (12), the HS geopotential fluctuation φ is defined as (10), $\omega = \mathrm{d}p/\mathrm{d}t$ and $\dot{\eta} = \mathrm{d}\eta/\mathrm{d}t$ are the pressure-coordinate and η-coordinate vertical material velocities, ϕ is the non-hydrostatic geopotential perturbation, $H = RT/g$ is the scale height. Terms $\mathbf{A_v}$, A_T and A_ω are general notation for diabatic forcing and spectral smoothing, the last arriving in discrete case only. Coriolis parameter f is a given function of geographical latitude, $\mathbf{k}$ is a unit vector in local vertical of geographical location $\mathbf{x}$; $\varkappa = R/c_p$, c_p and $c_v = c_p - R$ are the isochoric and isobaric specific heats of moist air. They depend in general on the water content of air, due to which time derivative $d\ln R/dt$ arrives in the right hand side of (12b).

Model (12) is actually a 'mixed representation': η-coordinates are used throughout the model, though in the role of vertical momentum equation stands (12b) for ω rather than for $\dot{\eta}$. Equation (12b) is preferred for consistency with the continuity eq. (12e). The non-hydrostatic geopotential ϕ is caused by the departure of the atmosphere from hydrostatic equilibrium. There is no closed formula for it, like the integral (7c) for thermal geopotential or formula (8) for baric geopotential are. It can be specified from the continuity condition (12e), which will yield an elliptic equation for it (Rõõm et al., 2006). Another option, used in this paper, is to derive such an elliptic equation first for the omega velocity, and then calculate ϕ via ω. This procedure is in detail described further in the Section 3.4.

3. SISL scheme

3.1. General principles

The SISL modification of system (12) is based on the application of the two-time-level, semi-implicit, semi-Lagrangian scheme (McDonald and Haugen, 1992, 1993; McDonald, 1995, 1998, 1999). We use for the evolution eqs (12a)–(12d) general notation $\mathrm{d}\psi/\mathrm{d}t = \mathcal{F}(\psi)$ and separate the right hand side forcing to the linear main part $\mathcal{L}\psi$ and non-linear residual $\mathcal{N} = \mathcal{N}(\psi) = \mathcal{F}(\psi) - \mathcal{L}\psi$:

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = \mathcal{L}\psi + \mathcal{N}.$$

The semi-Lagrangian approach to this equation is based on integration along a short piece of trajectory for every material particle (in discrete case—for every particle, who's end of trajectory is a grid node). Denoting the departure point (initial point of the trajectory sequence) coordinate of such a particle at time t via $\mathbf{x}_* = \mathbf{x}(t) = \{x(t), y(t), \eta(t)\}$, and the corresponding destination point (end-point) coordinate at time $t + \Delta t$ via $\mathbf{x} = \mathbf{x}(t + \Delta t) = \{x(t + \Delta t), y(t + \Delta t), \eta(t + \Delta t)\}$, the semi-implicit, discrete in time, semi-Lagrangean approximation of this equation in point $\mathbf{x}$ reads

$$D_t\psi = \overline{\mathcal{L}\psi} + \langle\mathcal{N}\rangle, \tag{13}$$

where the Lagrangean differencing operator D_t is

$$D_t\psi = \frac{\psi(\mathbf{x}, t + \Delta t) - \psi(\mathbf{x}_*, t)}{\Delta t},$$

whereas

$$\overline{\mathcal{L}\psi} = \frac{1}{2}\left[(1+\varepsilon)\mathcal{L}\psi(\mathbf{x}, t + \Delta t) + (1-\varepsilon)\mathcal{L}\psi(\mathbf{x}_*, t)\right],$$
$$\langle\mathcal{N}\rangle = \frac{1}{2}\left[(1+\varepsilon)\mathcal{N}(\mathbf{x}, t + \Delta t/2) + (1-\varepsilon)\mathcal{N}(\mathbf{x}_*, t + \Delta t/2)\right]$$

are the implicit and explicit averaging operators along trajectory. The optional small parameter ε ($0 \le \varepsilon \le 0.05$) is introduced to increase the weight of the final point in forcing formation. Equation (13) can be alternatively presented as

$$(1 - \Delta t_+\mathcal{L})\psi(\mathbf{x}, t + \Delta t) = [(1 + \Delta t_-\mathcal{L})\psi](\mathbf{x}_*, t) + \Delta t\,\langle\mathcal{N}\rangle, \tag{14}$$

where $\Delta t_\pm = (1 \pm \varepsilon)\Delta t/2$. This equation is still implicit with respect to $\psi(\mathbf{x}, t + \Delta t)$. For disclosure, operator $1 - \Delta t_+\mathcal{L}$ has to be inverted:

$$\psi^{t+\Delta t} = (1 - \Delta t_+\mathcal{L})^{-1}\left\{[(1 + \Delta t_-\mathcal{L})\psi](\mathbf{x}_*, t) + \Delta t\,\langle\mathcal{N}\rangle\right\}.$$

The disclosure is not a trivial operation in our 5-D state vector case, yet it can be solved numerically rather reliably.

The linear part of forcing is assumed to correspond to a reference sate with temperature $T^0(p)$ and uniform surface p_0^s. If using for the forcing-vector notation $\mathcal{F} = \mathcal{F}(\psi; T^0, \hat{p}_s)$, the linear part and non-linear residual are

$$\mathcal{L}\psi = \left(\frac{\delta\mathcal{F}(\psi; T^0, p_s^0)}{\delta\psi}\right)_{\psi=0}\psi, \quad \mathcal{N} = \mathcal{F}(\psi; T^0, \hat{p}_s) - \mathcal{L}\psi,$$

where $\delta F/\delta\psi$ is the functional derivative—ordinary partial derivative, if F is an ordinary function, and an operator, if F presents an operator upon ψ. As an instance, $\delta(\partial\phi/\partial\eta)/\delta\phi = \partial/\partial\eta$.

The uniform mean surface pressure p_s^0 can be chosen—like the mean temperature—as the area-mean actual surface pressure

$$p_s^0 = \frac{\int_S p_s(x, y, t)\,\mathrm{d}x\,\mathrm{d}y}{\int_S \mathrm{d}x\,\mathrm{d}y},$$

and can differ in general from the mean sea level pressure.

The pressure and density distributions, corresponding to p_s^0, are in accordance with (2)

$$p^0 = A(\eta) + B(\eta)p_s^0 = p_s^0\,\eta,$$

$$m^0 = \frac{\partial p^0}{\partial \eta} = A' + B' p_s^0 = p_s^0.$$

3.2. Linear forcing and non-linear residuals

As numerical investigation with ideal fronts shows (examples of which will be presented in Part II), SISL scheme can become unstable for large cross-area temperature gradients, if the geopotential term $p^2/(H^2 m)\partial\phi/\partial\eta$ in vertical forcing (12b) is separated according to the above-described traditional manner to the linear main part $p_s^0\eta^2/(H^0)^2\ \partial\phi/\partial\eta$ and non-linear residual. Instability can be avoided, if this forcing is treated completely as the implicit one. Thus, in parallel with traditional presentation, denoted in following as SVF, also a modification with full implicit treatment of term $p^2/(H^2 m)\partial\phi/\partial\eta$ (IVF) is considered where appropriate. The application of both variants in parallel permits to show and check that the main potential instability source in the SISL MPW model is just maintenance of the explicit residual in vertical forcing. Thus, the main linear (except $\mathcal{L}_\omega$, which becomes non-linear in IVF case) parts of the forcing on the right hand side of (12a)–(12d) are

$$\mathcal{L}_\chi = \int_0^1 \overline{\nabla}\cdot\mathbf{v}\,\mathrm{d}\eta, \quad \mathcal{L}_\omega = \begin{cases} \frac{p_s^0\eta^2}{(H^0)^2}\frac{\partial\phi}{\partial\eta}, & SVF \\ \frac{p^2}{H^2 m}\frac{\partial\phi}{\partial\eta}, & IVF \end{cases}$$

$$\mathcal{L}_\mathbf{v} = \nabla(\phi+\varphi^0) \quad \mathcal{L}_T = S^0\omega,$$

whereas the main part of continuity eq. (12e) is

$$\mathcal{L}_D = \overline{\nabla}\cdot\mathbf{v} + \frac{1}{p_s^0}\frac{\partial\omega}{\partial\eta}.$$

In these formulae operator $\overline{\nabla}\cdot$ presents the 'plane' divergence, in which the planet's sphericity is disregarded,

$$\overline{\nabla}\cdot\mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y},$$

as the linear dynamics is assumed to be planar, while the effects due to sphericity are considered as non-linear perturbations. This is justified, if the flank of integration area does not exceed 4000 km.

The reference scale-height and stability parameters are

$$H^0 = R^0 T^0/g, \quad S^0 = \left(\kappa^0\frac{T^0}{p} - \frac{\mathrm{d}T^0}{\mathrm{d}p}\right)_{p=p^0},$$

while φ^0 is the HS geopotential fluctuation (10) in reference pressure state $p^0(\eta)$

$$\varphi^0 = C_0^2\chi + \int_\eta^1 R^0 T' \frac{\mathrm{d}\eta'}{\eta'}, \tag{15}$$

with $C_0 = \sqrt{R^0 T^0(p_s^0)}$ as isochoric sound speed on the mean surface p_s^0.

The consequent explicit residuals of (12a)–(12d) are

$$\mathcal{N}_\chi = \int_0^1 \overline{\nabla}\cdot\mathbf{v}\,\mathrm{d}\eta - \frac{1}{p_s}\int_0^1 \nabla\cdot\mathbf{v}\,m\,\mathrm{d}\eta - \mathbf{v}_B\cdot\nabla\ln\hat{p}_s,$$

$$\mathcal{N}_\omega = \begin{cases} \frac{p_s^0\eta^2}{(H^0)^2}\frac{\partial\Phi}{\partial\eta} - \frac{p^2}{mH^2}\frac{\partial\Phi}{\partial\eta} + \omega\left(\frac{c_v\omega}{c_p p} - \frac{A_T}{T} - \frac{\mathrm{d}\ln R}{\mathrm{d}t}\right) + A_\omega, & SVF \\ \omega\left(\frac{c_v\omega}{c_p p} - \frac{A_T}{T} - \frac{\mathrm{d}\ln R}{\mathrm{d}t}\right) + A_\omega, & IVF \end{cases}$$

$$\mathcal{N}_\mathbf{v} = \nabla(\varphi^0+\phi) - \nabla_p(\phi+\varphi) - f\mathbf{k}\times\mathbf{v} + \mathbf{A}_\mathbf{v}\,.$$

$$\mathcal{N}_T = (S - S^0)\omega + A_T,$$

whereas the explicit part of (12e) is

$$\mathcal{N}_D = \nabla\cdot\mathbf{v} + \frac{1}{m}\frac{\partial\omega}{\partial\eta} - \left(\overline{\nabla}\cdot\mathbf{v} + \frac{1}{p_s^0}\frac{\partial\omega}{\partial\eta}\right).$$

3.3. SISL equations

The SISL equations in the form (13) are

$$D_t\omega + \overline{\mathcal{L}_\omega} = \langle\mathcal{N}_\omega\rangle\,, \tag{16a}$$

$$D_t\mathbf{v} + \overline{\nabla(\phi+\varphi^0)} = \langle\mathcal{N}_\mathbf{v}\rangle\,, \tag{16b}$$

$$D_t T' - \overline{S^0\omega} = \langle\mathcal{N}_T\rangle \tag{16c}$$

$$D_B\chi + \overline{\int_0^1 \overline{\nabla}\cdot\mathbf{v}d\eta}^{B} = \langle\mathcal{N}_\chi\rangle^B, \tag{16d}$$

$$\overline{\left(\overline{\nabla}\cdot\mathbf{v} + \frac{1}{p_s^0}\frac{\partial\omega}{\partial\eta}\right)} = -\langle\mathcal{N}_D\rangle\,. \tag{16e}$$

The 2-D difference operator D_t^B and averaging operators $\overline{(\psi)}^B$, $\langle\psi\rangle^B$ are applied on the 2-D trajectories, corresponding to velocity field $\mathbf{v}_B$ (11).

The presented form of SISL equations, matching most closely the initial set of equations, is suitable for theoretical investigation (as an example, for further linearization, as applied later below). However, for numerical application and for disclosure, more convenient is presentation in the form (14):

$$\omega + \Delta t_+\mathcal{L}_\omega = \hat{\omega} \tag{17a}$$

$$\mathbf{v} + \Delta t_+\nabla(\phi+\varphi^0) = \hat{\mathbf{v}}, \tag{17b}$$

$$T' - \Delta t_+ S^0\omega = \hat{T} \tag{17c}$$

$$\chi + \Delta t_+\int_0^1 \overline{\nabla}\cdot\mathbf{v}\,\mathrm{d}\eta = \hat{\chi}, \tag{17d}$$

$$\overline{\nabla}\cdot\mathbf{v} + \frac{1}{p_s^0}\frac{\partial\omega}{\partial\eta} = -\hat{\mathcal{D}}. \tag{17e}$$

The quest quantities $\chi = \chi(\mathbf{x}, t + \Delta t), \ldots . T' = T'(\mathbf{x}, t + \Delta t)$ are concentrated on the left hand side, while on the right are quantities, specified via known fields on time levels t and $t + \Delta t/2$:

$$\hat{\omega} = (\omega - \Delta t_- \mathcal{L}_\omega)^t_* + \Delta t \, \langle \mathcal{N}_\omega \rangle \,, \tag{18a}$$

$$\hat{\mathbf{v}} = [\mathbf{v} - \Delta t_- \nabla(\varphi^0 + \phi)]^t_* + \Delta t \, \langle \mathcal{N}_\mathbf{v} \rangle \,, \tag{18b}$$

$$\hat{T} = (T' + \Delta t_- S^0 \omega)^t_* + \Delta t \, \langle \mathcal{N}_T \rangle \,, \tag{18c}$$

$$\hat{\chi} = \left(\chi - \Delta t_- \int_0^1 \overline{\nabla} \cdot \mathbf{v} d\eta \right)^t_{*B} + \Delta t \, \langle \mathcal{N}_\chi \rangle^B \,, \tag{18d}$$

$$\hat{\mathcal{D}} = \frac{1-\varepsilon}{1+\varepsilon} \left(\overline{\nabla} \cdot \mathbf{v} + \frac{1}{p_s^0} \frac{\partial \omega}{\partial \eta} \right)^t_* + \frac{2}{1+\varepsilon} \, \langle \mathcal{N}_D \rangle \,. \tag{18e}$$

3.4. Disclosure

To get prognostic quantities explicitly, system (17) has to be solved with respect to left side quantities ω, $\mathbf{v}$, T', and χ. This task can be accomplished, developing a diagnostic equation for $\omega = \omega(\mathbf{x}, t + \Delta t)$, solution of which then enables successive step-by-step disclosure of remaining prognostic quantities.

First, some auxiliary relationships are required. Considering (15) on time level $t + \Delta t$ and using formulae (17c), (17a) for successive elimination of T' and ω, the total geopotential fluctuation on time level $t + \Delta t$ can be presented as a sum of explicit part Q and implicit contribution ξ

$$(\phi + \varphi^0) = Q + \xi, \tag{19}$$

$$Q = R^0 \int_\eta^1 (\hat{T} + \Delta t_+ S^0 \hat{\omega}) \frac{\mathrm{d}\eta'}{\eta'} \tag{20}$$

$$\xi = C_0^2 \chi^{t+\Delta t} + \phi^{t+\Delta t} - (\Delta t_+)^2 \int_\eta^1 N^2 \frac{\partial \phi^{t+\Delta t}}{\partial \eta'} \, \mathrm{d}\eta', \tag{21}$$

where

$$N^2 = \begin{cases} R^0 \frac{p^0 S^0}{(H^0)^2}, & SVF \\ R^0 \frac{p^2 S^0}{\eta m H^2}, & IVF \end{cases}$$

is the reference state Brunt-Väisälä frequency in the cases of semi-implicit and implicit treatment of the NH vertical forcing term.

Using (19), the horizontal wind formula (17b) modifies to

$$\mathbf{v} = \hat{\mathbf{v}} - \nabla Q - \Delta t_+ \nabla \xi \tag{22}$$

from which the 'plane' wind divergence is

$$(\overline{\nabla} \cdot \mathbf{v}) = \overline{\nabla} \cdot (\hat{\mathbf{v}} - \nabla Q) - \Delta t_+ \overline{\nabla}^2 \xi. \tag{23}$$

Application of $\partial/\partial\eta$ to (17e) with subsequent implementation of (23) and (21) gives an elliptic equation for $\omega(\mathbf{x}, t + \Delta t)$

$$\left(\frac{\partial}{\partial \eta} \right)^2 \omega + \overline{\nabla}^2 (W^2 \omega) = \mathcal{A}, \tag{24}$$

$$\mathcal{A} = \overline{\nabla}^2 (W^2 \hat{\omega}) - p_s^0 \frac{\partial}{\partial \eta} [\hat{\mathcal{D}} + \overline{\nabla} \cdot (\hat{\mathbf{v}} - \overline{\nabla} Q)],$$

where

$$W^2 = \begin{cases} \frac{1 + \Delta t_+^2 N^2}{\eta^2} (H^0)^2 \;, & SVF, \\ \frac{1 + \Delta t_+^2 N^2}{p^2} p_s^0 m H^2, & IVF. \end{cases}$$

This equation must be solved upon upper and lower boundary conditions

$$\omega|_{\eta=0} = 0, \quad \omega|_{\eta=1} = 0. \tag{25}$$

Note that in the IVF case, W^2 is a function of η and horizontal coordinates via H and p, whereas in SVF case, it is solely an η function. Meanwhile, the SVF includes additional explicit residuals in $\widehat{\mathcal{D}}$, absent in the IVF case.

In an earlier version (Rõõm et al., 2006), a similar to (24) equation was derived for the auxiliary potential $\xi - C^2 \chi$. However, due to the significant role of boundary conditions (25) in numerical stability provision, in recent applications, the preference is given to the omega-equation (24) and boundary conditions (25).

Solution of eq. (24) accomplishes the one-step Lagrangian marching. The non-hydrostatic geopotential $\phi(\mathbf{x}, t + \Delta t)$ can be subsequently specified, integrating (17a) in vertical

$$\phi = \frac{1}{\Delta t_+} \begin{cases} \int_\eta^1 (\omega - \hat{\omega}) \frac{(H^0)^2}{p_s^0 \eta^2} \, d\eta, & SVF \\ \int_\eta^1 (\omega - \hat{\omega}) \frac{H^2 m}{p^2} \, d\eta, & IVF \end{cases}$$

whereas $T'(\mathbf{x}, t + \Delta t)$ is determined from (17c). To solve $\chi(x, y, t + \Delta t)$, the following Helmholtz equation applies

$$\left(1 - \Delta t_+^2 C_0^2 \overline{\nabla}^2\right) \chi = \hat{\chi} +$$

$$\Delta t_+^2 \overline{\nabla}^2 \int_0^1 \left(\phi + \Delta t_+^2 N^2 \eta \frac{\partial \phi}{\partial \eta} \right) \mathrm{d}\eta - \Delta t_+ \int_0^1 \overline{\nabla} \cdot \hat{\mathbf{v}} \, \mathrm{d}\eta, \tag{26}$$

which follows with help of some algebra from (17d), (23) and (21). The hydrostatic geopotential $\varphi^0(\mathbf{x}, t + \Delta t)$ is then calculated from (15), and finally, horizontal wind vector $\mathbf{v}(\mathbf{x}, t + \Delta t)$ is found from (22).

4. Linearized SISL for stability study

4.1. General treatment

Linearization in SISL equations is essential for stability study. As shown in SHB78, numerical SISL model can become unstable, if the initial thermal fluctuation

$$\widetilde{T}(x, y, \eta) = (T - T^0)^{\text{init}}$$

becomes large, and the reference profile T^0 is non-constant. Thus, the choice of proper reference profile $T^0(p)$ can be crucial for model stability. The instability can arrive due to large explicit thermal residuals, and can become evident in an resting yet thermally non-equilibrium initial state already, when dynamics becomes linear in vicinity of this initial state.

It is illuminating to linearize the general eq. (13) first. Choosing the state vector $\psi = \{\chi, \omega, \mathbf{v}, \widetilde{T} + T', \phi\}$ as the sum of the initial state and infinitesimal fluctuation

$$\psi = \widetilde{\psi} + \psi', \quad \widetilde{\psi} = \{0, 0, 0, \widetilde{T}, 0\},$$

$$\psi' = \{\chi, \omega, \mathbf{v}, T', \phi\} \Rightarrow 0,$$

eq. (13) becomes

$$D_t(\widetilde{\psi} + \psi') = \overline{\mathcal{L}(\widetilde{\psi} + \psi')} + \langle \mathcal{N}(\widetilde{\psi} + \psi') \rangle. \tag{27}$$

The left-hand side presents as

$$D_t(\widetilde{\psi} + \psi') = \frac{(\widetilde{\psi} + \psi')(\overline{\mathbf{x}} + \langle \mathbf{u} \rangle \, \Delta t/2, t + \Delta t) - (\widetilde{\psi} + \psi')(\overline{\mathbf{x}} - \langle \mathbf{u} \rangle \, \Delta t/2, t)}{\Delta t},$$

$$\overline{\mathbf{x}} = \frac{1}{2} \left[\mathbf{x}(t + \Delta t) + \mathbf{x}_*(t) \right],$$

$$\langle \mathbf{u} \rangle = \frac{1}{2} \left[\mathbf{u}(\mathbf{x}, t + \Delta t/2) + \mathbf{u}(\mathbf{x}_*, t + \Delta t/2) \right],$$

where $\mathbf{u}$ is the 3-D velocity with components $\{v_x, v_y, \dot{\eta}\}$. As $\mathbf{u} \to 0$, this expression linearizes to the form

$$D_t(\widetilde{\psi} + \psi') = \langle u_i \rangle \frac{\partial \widetilde{\psi}}{\partial x_i} + \delta_t(\psi'),$$

field $\widetilde{\psi}$, while the second-term presents Eulerian differencing of ψ' in the fixed point $\mathbf{x}$:

$$\delta_t(\psi') = \frac{\psi'(\mathbf{x}, t + \Delta t) - \psi'(\mathbf{x}, t)}{\Delta t}.$$

Linearizing also the right-hand side in (27), we get

$$\delta_t(\psi') = A(\widetilde{\psi}) + \overline{\mathcal{L}(\psi')} + \left(\frac{\delta \mathcal{N}(\psi)}{\delta \psi} \right)_{\widetilde{\psi}} \langle \psi' \rangle - \langle u_i \rangle \frac{\partial \widetilde{\psi}}{\partial x_i}, \tag{28}$$

where the steady source

$$A(\widetilde{\psi}) = \overline{\mathcal{L}(\widetilde{\psi})} + \langle \mathcal{N}(\widetilde{\psi}) \rangle = \mathcal{L}(\widetilde{\psi}) + \mathcal{N}(\widetilde{\psi})$$

appears when the initial sate is unbalanced. Main conclusions from the general treatment of SISL equation linearization with respect to resting, unbalanced initial state are:

(1) There is no difference between Lagrangean and Eulerian two-time-level approach in this (resting atmosphere) case.

(2) The solution of (28) has linear drift from the rest state due to steady source A. To avoid such drift, the source must be nullified. Resulting linear system is a SISL approximation of normal mode equations.

(3) The implicit term remains implicit in linear regime, too.

(4) Two explicit terms arrive in the linear model, the first one as a result of linearization of the explicit non-linear residual, the other due to explicit advection of the initial state. This second-term can become large, if the initial field fluctuation $\widetilde{\psi}$ has large gradient, and disappears, if $\widetilde{\psi}$ becomes constant.

4.2. Linearized SISL equations

Applying described linearization technique to the eqs (16a) in the simplest case of uniform ground ($\hat{p}_s = p_s^0$, $\hat{p} = \eta p_s^0$, $\hat{m} = p_s^0$) we obtain

$$\delta_t \omega = -p_s^0 \frac{\eta^2}{(H^0)^2} \left(\frac{\partial \overline{\phi}}{\partial \eta} + \varepsilon_\phi \frac{\partial \langle \phi \rangle}{\partial \eta} \right), \tag{29a}$$

$$\delta_t \mathbf{v} = -\overline{\nabla} \left[\overline{\phi} + C^2 (\overline{\chi} + \varepsilon_\chi \langle \chi \rangle) + R \int_\eta^1 \overline{T'} \, \frac{\mathrm{d}\eta'}{\eta'} \right] + \mathbf{F}, \tag{29b}$$

$$\delta_t T' = S(p^0)(\overline{\omega} + \varepsilon_\omega \langle \omega \rangle), \tag{29c}$$

$$\delta_t \chi = -\int_0^1 \frac{\partial D}{\partial \eta} d\eta, \tag{29d}$$

$$\overline{\nabla} \cdot \mathbf{v} + \frac{1}{p_s^0} \frac{\partial \omega}{\partial \eta} = 0. \tag{29e}$$

The Coriolis term is omitted as having no relevance to numerical stability in the resting atmosphere. Forcing $\mathbf{F}$ arrives due to initial temperature fluctuation

$$\mathbf{F} = -R \nabla \int_\eta^1 \widetilde{T} \, \frac{d\eta'}{\eta'}.$$

The ε-coefficients in explicit terms of equations (29) are

$$\varepsilon_\phi = \begin{cases} \left(\frac{T^0}{T^0 + T} \right)^2 - 1 \approx -2 \frac{\widetilde{T}(x,y,\eta)}{T^0(\eta p_s^0)}, & SVF \\ 0 \qquad\qquad\qquad\qquad , & IVF \end{cases} \tag{30a}$$

$$\varepsilon_\chi = \frac{\widetilde{T}(x, y, 1)}{T^0(p_s^0)}, \tag{30b}$$

$$\varepsilon_\omega = \frac{\kappa \widetilde{T} - \eta \partial \widetilde{T}/\partial \eta}{\kappa T^0 - \eta \partial T^0/\partial \eta}. \tag{30c}$$

Coefficient ε_ϕ settles the explicit residual amplitude in vertical forcing. The important quality ε_ϕ, having decisive role in stability provision, is that it turns zero in IVF case, which means absence of the explicit residual in the non-linear SISL scheme. Coefficient ε_ω determines the explicit residual amplitude in the temperature equation. With the help of the 'static stability temperature'

$$T_* = \kappa T - \eta \frac{\partial T}{\partial \eta},$$

it can be presented also as

$$\varepsilon_\omega = \frac{\widetilde{T}_*}{T_*^0} = \frac{T_*^{\mathrm{init}} - T_*^0}{T_*^0},$$

where T_*^0, T_*^{init} and $\widetilde{T}_*$ are the static stability temperatures of reference state, initial state and fluctuative initial state, respectively.

Solution of (29) consists of the special non-homogeneous solution due to steady forcing $\mathbf{F}$, describing the drift of ψ' from the initial state of rest, and a general solution of homogeneous (i.e. corresponding to $\mathbf{F} = 0$) equations, describing free normal-mode evolution of the perturbation field ψ' from a non-zero initial state. In the actual numerical model, initial perturbations are always present in the form of a numerical noise. For a unsuitable explicit residual choice, some normal modes can behave unstably, having complex eigenfrequencies and growing exponentially in time, which leads to exponential growth of initially small perturbations and presents a numerical instability. Instability is more likely to arrive, if the ε-coefficients (30) become substantial, and vice versa, instability due to explicit residuals vanishes with (29) becoming zero, which happens, if the initial steady temperature perturbation $\widetilde{T}$ disappears.

The stability analysis does not draw back to mere ε-coefficient analysis but requires a detailed investigation of normal mode equations with respect to the eigenfrequencies, which is not in the scope of this paper. However, as a preliminary result, which will strictly proved elsewhere, we present next properties of the linear model (29). The linear model is defined conditionally stable, if there exists a positive maximum time step $\Delta t_{\max}$ such that the eigenfrequencies of (29) are all real for time steps $\Delta t < \Delta t_{\max}$ and (some of them) become complex for $\Delta t > \Delta t_{\max}$. Vice versa, the model proves to be numerically unstable, if such limit does not exist and $\Delta t_{\max} = 0$. In these terms, the linear model (29) proves to be conditionally stable, if the reference state $T^0(p)$ is statically stable, that is, $T^0_* > 0$, and $|\varepsilon_\phi|, |\varepsilon_\omega| < 1$. At that, the maximum time step is unlimited in special case $|\varepsilon_\phi| = 0$. Concerning ε_χ, the model is stable with respect to the size of this parameter so far the condition $T^0(p_s) + \widetilde{T}|_{\eta=1} > 0$ holds.

Numerical simulations in real conditions show, that the most influential coefficient with respect to the numerical stability is ε_ϕ. In the non-linear case, instability can arrive already at $|\varepsilon_\phi| \sim 0.1$, which is far below the linear theory limit $|\varepsilon_\phi| = 1$, and which forces to introduce the IVF approach for situations with large initial temperature fluctuation $\widetilde{T}$.

5. Numerical algorithm

The described NH scheme is an extension of the HS parent HIRLAM and makes use of HIRLAM discretization schemes, interpolation facilities and departure point calculation routines. Vast components of the numerics are the tools for departure point evaluation. As these routines do not depend on physical nature of dynamical system, all the trajectory calculus, initially developed for HS dynamics, is applicable without changes also in the NH model. For calculation of dynamic fields ψ at intermediate time level $t + \Delta t/2$ the Adams-Bashford extrapolation scheme is used:

$$\psi^{t+\Delta t/2} = 1.5\psi^t - 0.5\psi^{t-\Delta t}.$$

The departure point evaluation is based on the non-linear equation

$$\mathbf{x} - \mathbf{x}_* = \Delta t \mathbf{u}[(\mathbf{x} + \mathbf{x}_*)/2, t + \Delta t/2].$$

Initially, HIRLAM solved this equation iteratively (McDonald and Haugen, 1993; McDonald, 1995). Later, McDonald introduced a non-iterative algorithm (McDonald, 1998, 1999; Undén et al., 2002), representing a generalization of the approach by Temperton and Staniforth (1987):

$$\begin{aligned}
&\mathbf{x} - \mathbf{x}_* = \Delta t \mathbf{U},\\
&\mathbf{U} = a\mathbf{u}^t_{\mathbf{x}} + c\mathbf{u}^t_{\mathbf{x}-\mathbf{u}^t_{\mathbf{x}}\Delta t} + e\mathbf{u}^t_{\mathbf{x}-2\mathbf{u}^t_{\mathbf{x}}\Delta t} + b\mathbf{u}^{t-\Delta t}_{\mathbf{x}} + d\mathbf{u}^{t-\Delta t}_{\mathbf{x}-\mathbf{u}^t_{\mathbf{x}}\Delta t}\\
&\quad + f\mathbf{u}^{t-\Delta t}_{\mathbf{x}-2\mathbf{u}^t_{\mathbf{x}}\Delta t}
\end{aligned} \tag{31}$$

with constants $a = -0.25$, $b = 0$, $c = 1.50$, $d = 0.5$, $e = 0.25$, $f = -1.0$.

The above-described two-time level SISL was derived in spatially continuous form and the destination point $\mathbf{x}(t + \Delta t)$ is principally optional inside the domain of integration. However, for obvious computational reasons it is inevitable to introduce some spatial discretization. The destination points are then all grid-points, while the corresponding departure points are located, in common, in the intergrid space and the fields in departure points are interpolated from their grid-point values at time level t or $t + \Delta t/2$. The grid applied is the 3-D staggered (Arakawa C) grid. Interpolation routines are cubic spline interpolations in horizontal and linear in vertical (so more rigorous routines can be applied). In the discrete case, the horizontal and vertical differential operators are approximated by relevant difference formulae and vertical integrals, like in (7c), (12a), (15), (21), (26), are replaced by numerical quadratures:

$$\int_\eta^1 f(\eta')\, m d\eta' \to \sum_{k'=k}^{k_{\max}} f_{k'} \Delta p_{k'},$$

etc., though more complicated and probably more precise (but certainly computationally more expensive) approximations could be applied.

For reference temperature and reference pressure calculations, the boundary fields, extracted from the nesting model, are used. Let t_j and t_{j+1} are the two successive boundary field updating times (typically $t_{j+1} - t_j = 1$, 3 or 6 hours). Let the extracted boundary fields of temperature are $T^B_j(x, y, \eta)$, $T^B_{j+1}(x, y, \eta)$. The 'boundary' reference temperature fields $T^0_j(p)$, $T^0_{j+1}(p)$ are then calculated from T^B_j and T^B_{j+1} in accordance with (4), while the corresponding 'boundary' reference surface pressure fields $\hat{p}_{sj}$, $\hat{p}_{s(j+1)}$ are found solving the barotropic eq. (7d) with T^0_j and T^0_{j+1}. The actual reference fields are then linearly interpolated for each time level t ($t_j < t \le t_{j+1}$):

$$T^0(p) = (1 - \alpha)T^0_j(p) + \alpha T^0_{j+1}(p),$$

$$\hat{p}_s(x, y) = (1 - \alpha)\hat{p}_{sj}(x, y) + \alpha \hat{p}_{s(j+1)}(x, y),$$

$$\alpha = \frac{t - t_j}{t_{j+1} - t_j}.$$

Thus, the reference field handling is rather economical and takes little time.

In the numerical implementation, the central diagnostic eqs (24) and (26) are solved, using the fast cosine-Fourier transformation in horizontal coordinates. In the case of SVF approach, when W is independent of horizontal coordinates, (24) draws for each horizontal wavenumber back to an independent, 1-D, vertically discrete second order difference equation, whish is solved either using discrete eigen-vectors (Männik and Rõõm, 2001; Rõõm and Männik, 2002), or the direct Gaussian solver (Rõõm et al., 2006).

In the IVF case, (24) is resolved first to horizontally homogeneous part and non-homogeneous residual, using

$$W = W_0(\eta) + W'(x, y, \eta),$$

and the resulting equation is then treated iteratively, solving at ith iteration equation

$$\left(\frac{\partial}{\partial \eta}\right)^2 \omega^{(i)} + W_0^2 \overline{\nabla}^2 \omega^{(i)} = \mathcal{A} + \overline{\nabla}^2 \left[\left(W_0^2 - W^2\right)\omega^{(i-1)}\right].$$

The number of required iterations is typically three, though five iterations can be required in the very beginning of time-stepping. The same iterative scheme with implicit treatment of non-linear vertical forcing term was in principal applied already in the former SI Eulerian scheme (Männik et al., 2003).

Main model is the IVF scheme. The SVF, which was formerly applied in pre-operational weather forecast (Rõõm et al., 2006), is optional, its main purpose is to provide reference for 'mild' temperature contrast cases and for stability study. The IVF scheme consumes in adiabatic mode in comparison with SVF case approximately 1.5 times more computational time per single time-step, but this superfluous time-consumption is in full compensated by the gain in available time-step size and robustness of the computational scheme.

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