An update on research into transparent boundary conditions.

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1. Introduction.

For some years I have been engaged in a research program whose objective is to see if the treatment of the lateral boundaries in the HIRLAM can be improved. The main thrust has been to address the following question: can the boundary generation technique of Engquist and Majda (1977) be applied to the primitive meteorological equations?

Their method generates boundary conditions which render the lateral boundaries of the integration area 'transparent' to outgoing and incoming waves to a well defined order of approximation. It has two additional attractive features. First, their boundary conditions give rise to a mathematically well-posed system. Second, only a single line of externally supplied boundary data is required, in contrast to the 8-10 lines of boundary data needed for the HIRLAM relaxation scheme.

Up until now the hydrostatic assumption and grid point discretization has been central to this research project. Since in HIRLAMA we are embracing non-hydrostaticity and spectral decomposition it is unclear whether this approach is any longer relevant. Therefore this is a good time to step back and review the situation. Hence this note, whose purpose is to describe the present status of that research project, and by implication to raise the question: where do we go from here?

The background to the present situation is that tests of 'transparent' lateral boundary conditions for the shallow water equations, McDonald (2002, 2003), and the two dimensional linearized hydrostatic equations, McDonald (2005, 2006), were sufficiently encouraging to test them in the fully non-linear system of equations using the reference HIRLAM.

In section 3 is sketched the generalization of the derivation of the boundary conditions to the linearized hydrostatic primitive equations using hybrid vertical coordinates. In section 4 a 48h forecast using 'lowest order transparent' boundary conditions is compared with the reference HIRLAM 'relaxation' conditions.

2. The boundary conditions.

The linearized equations associated with the full primitive equations of motion which use hybrid coordinates in the vertical can be written as follows subsequent to vertical discretization. See eqs. (2.26), (2.27), (2.18), and (2.11), respectively, of the HIRLAM Documentation Manual, Undén et al., (2002), called HIRDOC henceforth.

$$\frac{du_l}{dt_0} + \frac{\partial G_l}{\partial x} - f_0 v_l = 0, \tag{2.1}$$

$$\frac{dv_l}{dt_0} + \frac{\partial G_l}{\partial y} + f_0 u_l = 0, \tag{2.2}$$

$$\frac{dT_l}{dt_0} + (\boldsymbol{\tau D})_l = 0, \tag{2.3}$$

$$\frac{d(lnp_s)}{dt_0} + (\boldsymbol{\nu . D}) = 0, \tag{2.4}$$

where $l = 1, N$, and

$$\frac{d}{dt_0} = u_0 \frac{\partial}{\partial x} + v_0 \frac{\partial}{\partial y}, \tag{2.5}$$

$$G_l = (\boldsymbol{\gamma T})_l + R_d T_0 lnp_s, \tag{2.6}$$

and

$$D_l = \frac{\partial u_l}{\partial x} + \frac{\partial v_l}{\partial y}. \tag{2.7}$$

The notation is conventional and the variables and parameters are defined in the list in the appendix. The matrices $\boldsymbol{\gamma}$, $\boldsymbol{\tau}$, and the transpose vector $\boldsymbol{\nu}$, are functions of the 'background atmosphere' parameters (designated by the subscript '0') defined by the relationships

$$(\boldsymbol{\gamma T})_l = R_d(\alpha_0 T)_l + R_d \sum_{j=l+1}^{N} (T\Delta lnp_0)_j, \tag{2.8}$$

$$(\boldsymbol{\tau D})_l = \kappa T_0 \left[\left(\frac{\Delta lnp_0}{\Delta p_0} \right)_l \sum_{j=1}^{l-1} (D\Delta p_0)_j + (\alpha_0 D)_l \right], \tag{2.9}$$

$$(\boldsymbol{\nu . D}) = \sum_{j=1}^{N} \left(D \frac{\Delta p_0}{p_0} \right)_j , \tag{2.10}$$

where $\alpha_l = 1 - (\Delta lnp/\Delta p)_l p_{l-1/2}$.

Multiplying eq. (2.3) by γ and eq. (2.4) by $R_d T_0$ and adding results in

$$\frac{dG_l}{dt_0} + (\boldsymbol{MD})_l = 0, \tag{2.11}$$

where

$$\boldsymbol{M} = \boldsymbol{\gamma\tau} + R_d T_0 \boldsymbol{\nu}. \tag{2.12}$$

Assume there exists a matrix $\boldsymbol{E}$ which diagonalizes $\boldsymbol{M}$:

$$(\boldsymbol{E^{-1} M E})_{ml} = c_l^2 \delta_{ml} , \tag{2.13}$$

then eqs. (2.1), (2.2), and (2.11) can be re-written as a set of shallow water equations each with its own associated effective depth, H_m, defined by $gH_m = c_m^2$:

$$\frac{d\tilde{u}_m}{dt_0} + \frac{\partial \tilde{G}_m}{\partial x} - f_0 \tilde{v}_m = 0, \tag{2.14}$$

$$\frac{d\tilde{v}_m}{dt_0} + \frac{\partial \tilde{G}_m}{\partial y} + f_0 \tilde{u}_m = 0, \tag{2.15}$$

$$\frac{d\tilde{G}_m}{dt_0} + c_m^2 \tilde{D}_m = 0, \tag{2.16}$$

where $\tilde{\boldsymbol{\Psi}} = \boldsymbol{E^{-1}\Psi}$ for any vector $\boldsymbol{\Psi}$.

Having got the equations into this format it is now possible to to derive a hierarchy of lateral boundary conditions which are mathematically well-behaved and which are successively more transparent to incoming and outgoing waves; see McDonald (2006). For example, on the western boundary, to lowest order, the appropriate boundary fields are

$$\begin{array}{lllll}
(a) & u_0 > c_m > 0 & : & \tilde{G}_m^h + c_m\tilde{u}_m^h, \quad \tilde{v}_m^h, \quad \tilde{G}_m^h - c_m\tilde{u}_m^h \\
(b) & c_m > u_0 > 0 & : & \tilde{G}_m^h + c_m\tilde{u}_m^h, \quad \tilde{v}_m^h, \quad \tilde{G}_m^g - c_m\tilde{u}_m^g \\
(c) & 0 > u_0 > -c_m & : & \tilde{G}_m^h + c_m\tilde{u}_m^h, \quad \tilde{v}_m^g, \quad \tilde{G}_m^g - c_m\tilde{u}_m^g \\
(c) & 0 > -c_m > u_0 & : & \tilde{G}_m^g + c_m\tilde{u}_m^g, \quad \tilde{v}_m^g, \quad \tilde{G}_m^g - c_m\tilde{u}_m^g
\end{array} \tag{2.17}$$

The superscript 'h' designates the externally supplied 'host' model fields and the superscript 'g' designates the 'guest' model fields. Because the latter fields are unknown on the boundary they must be extrapolated from the interior. The next order accurate fields in the hierarchy are given in McDonald (2006).

These boundary conditions have been derived for a linearized atmosphere. In McDonald (2006) they were shown to work well. Our hope is that this will also be true for the full non-linear system of equations. Switching to the latter immediately creates a dilemma because u_0 is not a well defined quantity when the advective wind varies in the vertical. Therefore the essential switch in eq. (2.17), which depends on the relative size of u_0 with c_m, is impossible to implement and a compromise is necessary. In the forecasts described in section 3, on each of the four boundaries the inward pointing characteristic fields, $\tilde{G}_m^h - c_m(\tilde{v}_N)_m^h$, and the tangential velocity fields, $(\tilde{v}_T)_m^h$, are imposed via the host model, irrespective of the value of the advective wind. Here the subscripts 'N' and 'T' designate the outward pointing normal velocity and the tangential velocity, respectively.

3. Testing in the HIRLAM.

Because it is so difficult to encode any boundary condition other than periodic in the HIRLAM MPI code, the last non-MPI version of HIRLAM, that is, HIRLAM4.3.5, was used for the following tests. However, all subsequent upgrades to the dynamics were incorporated. Thus, the dynamics was 'non-MPI 7.0', and the physics '4.3.5'.

The boundary conditions were as follows. For the semi-implicit part of the integration, for which only $\tilde{G}_m$ and $(\tilde{v}_T)_m$ are required on the boundary, the fields $(\tilde{v}_T)_m^h$ and $\tilde{G}_m^h - c_m(\tilde{v}_N)_m^h$, were imposed. For the semi-Lagrangian part of the integration host values of *all fields except* $(v_N)_m$; were imposed. It is important to emphasise that no relaxation, extra filtering, or extra diffusion was used. These will be called characteristic boundaries in what follows and designated as 'CHAR'.

Only the equations for $\tilde{u}$ along the two lines of points $[\Delta x/2, j\Delta y]$ and $[(I-1/2)\Delta x, j\Delta y]$, over the range $j = 1, J$, and the equations for $\tilde{v}$ along the two lines of points $[i\Delta x, \Delta y/2]$ and $[i\Delta x, (J-1/2)\Delta y]$ over the range $i = 1, I$ are altered by these new boundary conditions. The technical details are in McDonald (2002). Unfortunately these changes rule out using the HIRLAM fast solver, which requires periodic boundary cobnditions. Thus, an SOR solver was used instead.

For the integrations each field was carried at 202×178 grid points located at the intersections of a $0.4^\circ \times 0.4^\circ$ horizontal C-grid mesh, which has been rotated along the Greenwich meridian so that the north pole is at (30N,210W). In the vertical there were 31 layers. The forecasts start from 0000UTC 13 May 1998. The time step was 720s. The host boundary fields were furnished via ECMWF analyses and were refreshed every 6h. The integration area is shown in figure 1. The rms errors of the forecasts were measured against the ECMWF analyses valid at the same time over the verification area shown in figure 2.

The 12h, 24h, and 36h forecasts using characteristic boundary conditions are as accurate as those using the reference boundary conditions: see figure 3, which shows the wind errors. The temperature errors (not shown) tell the same story. The 48h forecast is stable using characteristic boundary conditions but marginally less accurate than the reference forecast; again see figure 3. On the other hand, the rms error for surface pressure is smaller for the forecasts using characteristic boundary conditions from 24h onwards; see table 1.

	12h	24h	36h	48h
REF	1.10	2.08	2.85	3.44
CHAR	1.10	1.88	2.52	2.92
TWCH	1.10	1.86	2.49	2.97

TABLE 1. Evolution of the root mean square difference of surface pressure between the forecast and the confirming ECMWF analysis over the verification area.

Except for some minor alterations these were the results presented in McDonald (2004). As was said there, 'it is disappointing that the improved accuracy seen in the shallow water experiments did not also appear in the multi-level implementation'. It is also slightly surprising because the multi-level model is being solved as a deck of shallow water models. In order to try to understand the inability of the new boundary conditions to improve the accuracy of any of the fields except the surface pressure I made a list of the flaws and weaknesses in their implementation, and eliminated them, where possible.

1. The most obvious possible weakness is the over-specification implied by imposing host values of T_l^h and p_s^h on the boundary. This is inconsistent because $\tilde{\mathbf{G}}$ and by implication $\mathbf{G}$ is a well-defined combination of host and guest fields on the boundary. Therefore, we are not free to arbitrarily impose T_l^h and p_s^h there, but rather, we must compute them from eq. (2.6). Unfortunately, this is not possible because the equation is underdetermined. (Given N values of G_m we cannot extract N values of T_m *and* p_s). This is a well-known problem with the Lorenz (1960) grid and is the reason that T_l^h and p_s^h were imposed on the boundaries in the 'CHAR' tests above. A solution to this problem which avoids switching to the Charney-Phillips (1953) grid is described in McDonald (2006b), and named the 'tweaked' Lorenz grid. Although slightly inelegant it has the attraction that its implementation requires only minimal changes to the HIRLAM code. Because the relationship between $\mathbf{G}$, $\mathbf{T}$ and $\mathbf{p_s}$ is invertible on the 'tweaked' Lorenz grid the forecast called 'CHAR' above can be repeated *without imposing* T_l^h *and* p_s^h, but using instead the values compatible with the values of G_l. These changes resulted in scores which were not significantly different from those in the 'CHAR' experiment, but overall showed a very small improvement. See figure 4 and table 1, where this experiment is called 'TWCH' (TWeaked CHaracteristic). Obviously, this improvement is too small to claim that TWCH is significantly better than CHAR as far as the upper air scores are concerned.

2. If a linear system were being integrated with, for example, $(u_0, v_0) = (10, 1)ms^{-1}$, then the linear theory says that v_T should not be imposed on, but extrapolated from the interior to, every grid point on the northern and Eastern boundaries. Thus it can be surmised that, in the non-linear system, imposing v_T^h at every grid point means that this field is being over-specified at approximately half the grid points. An obvious way to attempt to alleviate this is to extrapolate the tangential velocity whenever the normal velocity is pointing out of the integration area. To test this the simplest possible extrapolation of copying v_T^{n+1} one line in from the boundary to the boundary at every grid point for which $v_N > 0$ was introduced. This change had essentially no impact on the forecast over the verification area. The errors (not shown) were almost indistinguishable from those in figure 4.

3. The passive tracers, instead of being specified as their host values, were extrapolated at outflow. This had no impact on the scores (not shown) in the verification area.

4. There is a third form of over-specification of the boundary fields. In the linear system if $u_0 > c_m$ then on the western boundary $\tilde{G}_m - c_m\tilde{u}_m$ should also be imposed, not extrapolated; see eq. (2.17a). Thus one may speculate that some of the slow modes will be reflected in the non-linear integration. There is no obvious ad-hoc way of reducing this over-specification.

4. Discussion.

Another possible reason, not discussed in section 3, why the 'CHAR' upper air forecasts are not better than the 'REF' forecasts is the following. For the purpose of argument consider the Western boundary, and assume $u_0 > 0$. What was demonstrated in McDonald (2006) was that, to lowest order in f/s, (a) imposing $\tilde{v}_m^h$ on that boundary injects potential vorticity waves into the guest area; (b) refraining from imposing $\tilde{G}_m^h - c_m\tilde{u}_m^h$ allows the outgoing gravity waves whose phase speed is $u_0 - c_m < 0$ to exit the area without reflections; (c) imposing $\tilde{G}_m^h + c_m\tilde{u}_m^h$, will *inject* gravity waves with phase speed $u_0 + c_m > 0$. Therefore, to avoid corrupting the forecast, it is essential that the host fields be such that $\tilde{G}_m^h + c_m\tilde{u}_m^h$ have small amplitude. In principle, this is not a problem: a well-behaved host model will have well-balanced fields, implying only small amplitude gravity waves. In practice, the host fields must be interpolated spatially and temporally, which tends to upset this delicate balance.

The most obvious lesson to be learned from the experiments described in the last section is that the relaxation scheme is hard to beat! However, there is still a chance that characteristic boundary conditions can give more accurate forecasts. This is because they introduce the possibility of refreshing the boundaries more often, and the more often this happens the more accurate will be the forecast, particularly for rapidly moving meteorological events. Ideally, the guest boundary should be refreshed at every time step of the host model. Two things prevent this even in a self-nested set-up. (a) If the boundary files are large they will consume a lot of space. (b) I/O can be computationally expensive in an MPI environment. Therefore the characteristic boundaries described in section 3 do have a potential advantage, in that they require only one line of host data, a factor of approximately ten smaller than is required by the relaxation scheme. Therefore, in principle, if the I/O is very time-consuming, their boundaries could be updated ten times as often as the relaxation boundaries. This give rise to the possibility of more accurate forecasts. However, there are three problems to be addressed first. (a) Demonstrate that the new boundaries are robust; only a single forecast has been run. (b) Write an MPI version of the code. (c) Find a Helmholtz solver which can accomodate the new boundary conditions and which is competitive with the HIRLAM reference solver. The question is: is it worth the effort since the HIRLAM dynamics is being mothballed? Even if this were not the case would speeding up the I/O of the relaxation scheme not be a viable alternative?

This completes the program laid out in my work plan. That, combined with the fact that we are switching to a spectral model, makes this a good time to discuss where the research on lateral boundary conditions should go from here.

5. Quo Vadis?

The spectral approach seems to be fundamentally incompatible with transparent boundary conditions. The reason is that the coefficients in the Helmholtz equations will no longer be of the form

$$(\Phi_{i-1}, \Phi_i, \Phi_{i+1}) = (1, -2, 1)\bar{\Phi}\Delta t^2/\Delta x^2$$

at a number of points adjacent to the boundaries, making the Fast Fourier Transform inapplicable. (If an FFT expert knows a way around this difficulty please tell me).

Thus it is possible that those within the HIRLAM group who have been encouraging me to pursue this line of research may wish to re-consider. If, on the other hand, it were the opinion of the Scientific Advisory Committee and The Management Group that I should continue with fundamental research into transparent boundary conditions here is a list of what I would do next.

(a) Returning to 'overspecification 4', see the last paragraph of section 3, what is required to overcome this flaw is to do a linear analysis of a system of equations whose advective velocities vary in the vertical, while remaining constant in the horizontal. This is what I was going to address next if this program of research were continued. It certainly seems tractable for a two-layer model, and it may also be possible to get some results for a multi-level model, although that is more debatable. (There is a potentially serious complication in that vertical shear introduces the possibility of *physical*, as well as *mathematical* instabilities).

(b) A first step toward transparent boundary conditions for non-hydrostatic models would be to examine the linearized equations of motion in two dimensions ($x - z$) with a view to deriving boundary conditions which allowed both the gravity waves *and* the sound waves to exit without reflection.

(c) Until now only analytical transparent boundary conditions have been derived. These have been discretized using 'intelligent guesses' (plus a prayer that they will be stable). A more correct approach would be to analyse the discretized equations and to use the analysis directly to derive stable transparent boundary conditions.

(d) There is a potentially serious problem with higher order transparent boundary conditions: there is a possibility for the solution to drift slowly to unphysical values, corrupting the forecast. An example was given in section 2.5 of McDonald (2006). There it was shown that if the initial guest analyzed fields on the boundary are different from the host boundary conditions valid at the same time the subsequent forecast will become unphysical. A first step toward understanding this problem would be to study it carefully using a simple linear system of equations.

Appendix: list of variables and constants.

c_{pd} : Specific heat of dry air (1004.64 J kg^{-1}K^{-1})
f : Coriolis parameter (s^{-1})
f_0 : Constant Coriolis parameter (s^{-1})
g : Acceleration due to gravity (9.80665 m s^{-2})
G : Linearised geopotential (g $\times$ height) (m^2 s^{-2})
N : Number of vertical levels
p : Pressure (Pa)
p_0 : Reference pressure for background atmosphere. (Pa)
p_s : Surface pressure (Pa)
q : Specific humidity (kg kg^{-1})
R_d : Gas constant for dry air (287.04 J kg^{-1} K^{-1})
R_v : Gas constant for water vapour (451.51 J kg^{-1} K^{-1})
t : Time (s)
T : Temperature (K)
T_0 : Constant temperature for semi-implicit scheme(K)
T_v : Virtual temperature (K)
u : Zonal velocity (m s^{-1})
v : Meridional velocity (m s^{-1})
u_0 : Constant zonal advection velocity (m s^{-1})
v_0 : Constant meridional advection velocity (m s^{-1})
κ : R_d/c_{pd}
x : Easterly distance
Φ : Geopotential (g $\times$ height) (m^2 s^{-2})
y : Northerly distance

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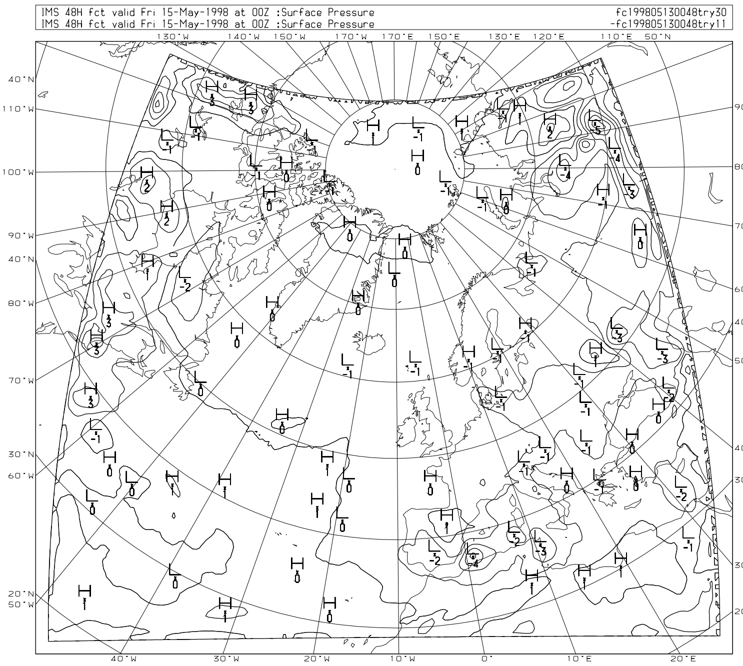

Figure 1: *The difference between the 'REF' and 'CHAR' forecasts of surface pressure at 48h displayed over the whole of the integration area.*

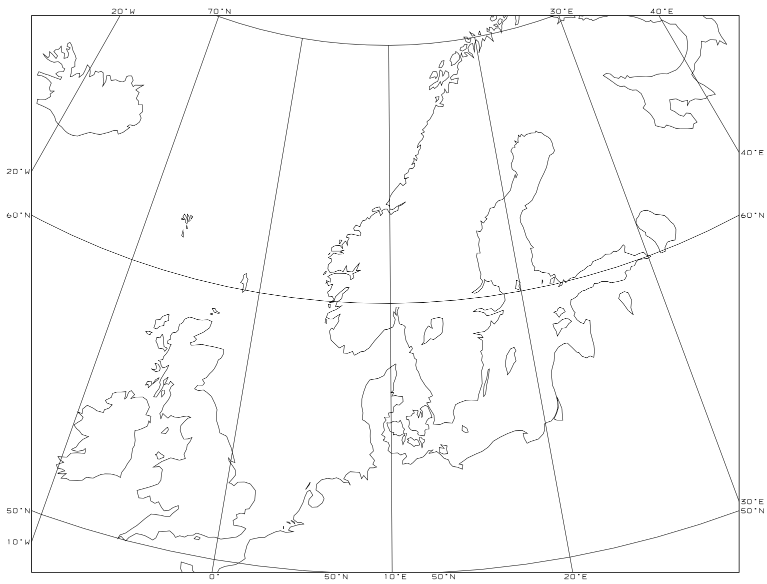

Figure 2: *The verification area.*

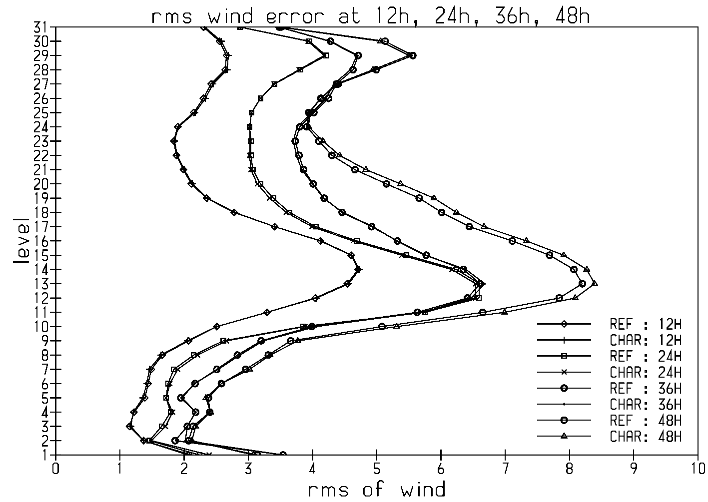

Figure 3: *The rms wind errors measured over the verification area at the model levels. CHAR refers to a forecast using characteristic boundary conditions instead of the reference HIRLAM relaxation scheme (REF).*

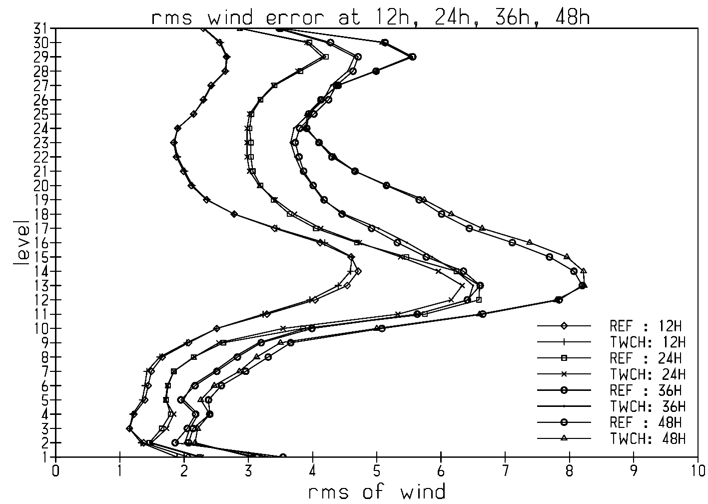

Figure 4: *Same as fig. 2, but using the 'tweaked' Lorenz grid and characteristic boundary conditions for the 'TWCH' forecast.*