Monotonic Higher Order Numerical Diffusion

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1. Introduction

High-order numerical diffusion schemes are used in most NWP models to control small-scale noise, but have unwanted side effects:

(i) they are in general not monotonic and thus can introduce negative values on fields that are positive definite as, e.g., the cloud water content or specific humidity;

(ii) they introduce noise by themselves on the resolvable scales via the so-called Gibbs phenomenon.

The ideas on a monotonic higher order diffusion scheme presented in this paper refer to Dr. Ming Xue's work in the ARPS/CAPS group at the University of Oklahoma, USA (pers. comm. at a visit in spring 2000). A corresponding paper by M. Xue (Xue, 2000) will appear in Monthly Weather Review in autumn this year.

2. The Need for Numerical Smoothing

Numerical weather prediction models as well as other simulation models of atmospheric flow often apply numerical or computational diffusion (sometimes also called horizontal diffusion) to control small scale noise at or near the two grid interval wavelength. Numerical noise of such type is continuously generated by

- numerical dispersion (especially within the Leapfrog time integration using centred difference operators for advection as, e.g., in the current LM),
- weak nonlinear numerical instabilities,
- physical processes (which in general act discontinuous at single grid points and thus always introduce noise at the $2\Delta x$-scale),
- forcing from topography and surface inhomogeneities.

Computational diffusion is mostly realized by introducing an additional operator to the right hand side of the prognostic equations:

$$\frac{\partial \psi}{\partial t} = S(\psi) + (-1)^{n/2+1} \alpha_n \nabla^n \psi \,, \tag{1}$$

where ψ is one of the prognostic variables and S represents all physical and dynamical source terms for ψ. The last term in Eq.(1) is the added linear diffusion term where n ($n = 2, 4, 6, \cdots$) denotes the (even) order of computational diffusion and α_n is the corresponding diffusion coefficient of order n.

The higher the order of the diffusion operator, the more scale selectively wavelength components are damped. Figure 1 shows the amplification factor (here: damping factor) for a one dimensional version of Eq.(1) using a forward in time and centred in space finite difference scheme for integration, plotted against the normalized wavelength $k\Delta x$ where k is the wavenumber and Δx is the grid spacing. For each of the second, fourth and sixth order schemes the corresponding diffusion coefficient α_n is chosen so that the shortest waves representable on a discrete grid ($2\Delta x$, i.e. $k\Delta x = \pi$) are damped completely within one integration time step.

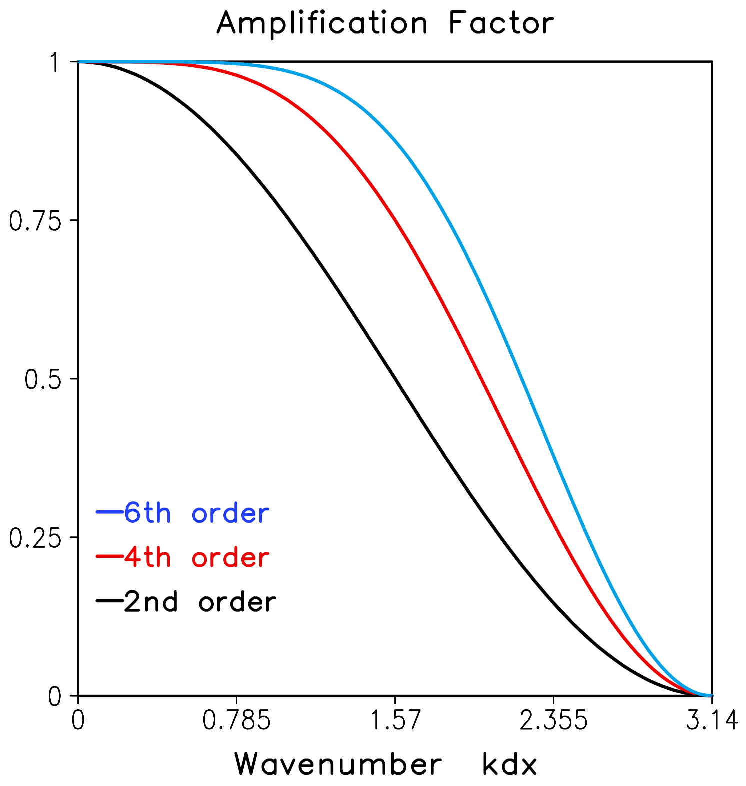

Figure 1: *Amplification factor plotted against the normalized wavenumber*

As can be seen from Fig. 1, all schemes damp not only the two grid interval wavelength, but also longer wave components in a wave spectrum. For example, the amplitude of a $4\Delta x$ wave is reduced by a factor of 0.5 in the second order scheme, and longer waves are also damped significantly. The fourth and sixth order scheme have much less damping for these longer waves, which contain physical meaningful information in a simulation and should not be affected by a numerical filter. Clearly, higher order schemes provide a more scale selective damping.

Many models use the 4th order linear computational diffusion scheme because of its relative computational efficiency compared to the 6th order scheme and of its superior damping properties compared to the second order scheme. Schemes of higher than 2nd order, however, have unwanted side effects. The 2n order scheme has a Laplacian form and thus is always monotonic: by transferring higher values of the field into regions with smaller values no new minima or maxima can be created. This is not the case for the 4th, 6th and even higher order schemes, where spatial oscillations are introduced (Gibbs phenomenon), as can be seen in Fig. 2.

Figure 2 shows the one dimensional numerical solution of Eq.(1) (with $S = 0$) for 2nd, 4th and 6th order diffusion applied to an initial rectangular structure. The second order scheme (left) is strongly diffusive even for this large scale structure. At the end of the integration ($t = 100$) the amplitude of the entire square wave is significantly reduced. The 4th (middle) and 6th order (right) schemes retain the initial structure much better, and at the lateral edges, where short wavelengths components dominate, the sharp gradients are maintained in the solution (somewhat better by using the 6th order scheme).

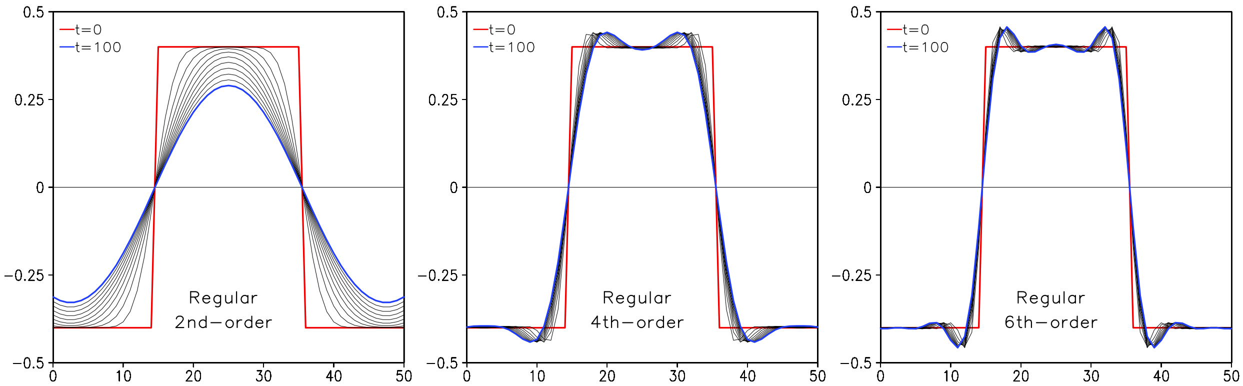

Figure 2: *1-D numerical solution of Eq.(1) for an initial square wave (red, $t = 0$) in case of 2nd (left), 4th (middle) and 6th order (right) linear diffusion. The domain has 51 grid points with a grid spacing of 1/50 m and the time step is 1 sec. The diffusion coefficients are chosen such that there is full damping of a $2\Delta x$ wave within one time step, i.e. $\alpha_n = (\Delta x/2)^n/\Delta t$. The solutions are plotted at 10 timestep intervals.*

However, over- and undershoots are generated by the numerical solution. The amplitude of this unphysical, both positive and negative spatial oscillations is increased by increasing the order of the diffusion operator. That is, going to higher than 4th order diffusion will not cure this side effect. Obviously, the $2\Delta x$ waves are removed from the solution, but at the cost of *introducing new noise on the resolvable scales.* In the context of a full simulation model these oscillations will interact nonlinearly with the physics as well as with the dynamics (as they are on the resolvable scales) and thus can result in unforseeable effects. Moreover, negative oscillations are unacceptable for positive definite fields such as cloud water content or specific humidity.

3. Monotonic Diffusion Operators

This section describes two types of monotonic diffusion schemes. One is based on a Zalesak-type flux correction, similar to that used in many advection schemes, and the other is based on a simple flux limiter proposed by M. Xue (pers. comm.).

The basic pre-requisite to apply these schemes is to rewrite the diffusion operator in Eq.(1) in a flux form. Omitting the source term S, the diffusive tendency then reads

$$\frac{\partial \psi}{\partial t} = (-1)^{n/2+1} \alpha_n \nabla^n \psi = -\nabla \cdot \mathbf{F} \,, \tag{2}$$

where $\mathbf{F}$ denotes the diffusive flux being defined by

$$\mathbf{F} \equiv (-1)^{n/2} \alpha_n \nabla (\nabla^{n-2} \psi) \,. \tag{3}$$

(a) Zalesak-type Flux Correction

Using the notations in Eqs.(2) and (3) the numerical scheme to integrate the 1-D version of the diffusion equation (the extension to more than one dimension is readily adopted) using a forward in time and centred in space scheme reads

$$\psi_i^{n+1} = \psi_i^n - (A_{i+1/2}^n - A_{i-1/2}^n), \tag{4}$$

where n denotes the time level, i is the gridpoint index and

$$A_{i+1/2}^n \equiv F_{i+1/2}^n \Delta t / \Delta x \tag{5}$$

denotes the normalized diffusive flux. Following the flux correction idea of Zalesak (1979, J. Comp. Phys., 31, 335-362), that was applied to the advection equation, Xue proposed a flux corrected scheme based on the combination of a low-order and a high-order diffusion scheme. The time integration scheme (4) is rewritten as

$$\begin{aligned} \psi_i^* &= \psi_i^n - (A_{i+1/2}^L - A_{i-1/2}^L)\,, \\ \psi_i^{n+1} &= \psi_i^* - (C_{i+1/2}A_{i+1/2}^{HL} - C_{i-1/2}A_{i-1/2}^{HL})\,. \end{aligned} \tag{6}$$

Here, A^L is the low order diffusive flux which is chosen to be of second order and thus guarantees monotonicity. A^{HL} denotes the difference between a high order diffusive flux A^H and the 2nd order one, i.e.

$$A^{HL} = A^H - A^L. \tag{7}$$

The factor C is called the flux correction coefficient or flux limiter, where $0 \leq C \leq 1$. When $C = 0$, the integration scheme (6) reduces to the 2nd order scheme, and when $C = 1$ it becomes purely high order. The idea is to use the high order scheme to the maximum extend possible, i.e. to reduce the fluxes by a factor C (to be determined for each grid interval interface) only when the monotonicity constraint is not met.

Since the diffusion process should not generate new minima or maxima by stepping from the current time level n to the future time level $n + 1$, the monotonicity constraint is chosen to be

$$\psi_i^{min} \leq \psi_i^{n+1} \leq \psi_i^{max}, \tag{8}$$

where ψ_i^{min} and ψ_i^{max} are the minimum and the maximum of ψ at the gridpoint and the adjacent points at the current time level n:

$$\psi_i^{min} = \min(\psi_{i-1}^n, \psi_i^n, \psi_{i+1}^n)\,, \quad \psi_i^{max} = \max(\psi_{i-1}^n, \psi_i^n, \psi_{i+1}^n)\,. \tag{9}$$

Following Zalesak, a flux limiter satisfying condition (8) can be defined as

$$C_{i+1/2} = \begin{cases} \min(1, R_{i+1}^+, R_i^-) & \text{if } \mathrm{A}_{i+1/2}^{HL} \geq 0 \\ \min(1, R_i^+, R_{i+1}^-) & \text{if } \mathrm{A}_{i+1/2}^{HL} < 0\,, \end{cases} \tag{10}$$

where

$$\begin{aligned} R_i^+ &= (\psi_i^{max} - \psi_i^*)/(A_i^{in} + \epsilon)\,, \\ R_i^- &= (\psi_i^{min} - \psi_i^*)/(A_i^{out} + \epsilon)\,. \end{aligned} \tag{11}$$

Here, ϵ is a small positive number to avoid division by zero. A_i^{in} and A_i^{out} are, respectively, the sum of all incoming and outgoing corrective fluxes A^{HL} of a grid box.

(b) The Xue Flux-Limiter

The monotonic scheme described above guarantees monotonicity, the computational costs, however, appear to be quite high. Xue pointed out that diffusive fluxes in high order schemes are not necessarily downgradient (as they are in the monotonic second order scheme) because they are no longer related to the local gradient of the diffused variable ψ. Updradient fluxes can result in unphysical solutions and explain the over- and undershoots when applying high order schemes.

As a simple way to prevent upgradient fluxes to occur, Xue proposed to set the diffusive fluxes to zero whenever they have the same sign as the gradient of ψ:

$$\tilde{F}_{i+1/2} = -F_{i+1/2} \min[0, \mathrm{sign}(F_{i+1/2}\delta_x\psi)] \, . \tag{12}$$

The application of this simple flux limiter in higher order diffusion schemes prevents over- and undershoots and thus ensures monotonicity of the solution. Obviously, the Xue-limiter (12) if far more efficient than the Zalesak-type flux corrected scheme since the extra computational costs are very small.

4. Results from Simplified Tests

The solutions of the one dimensional square waves test using 4th and 6th order regular diffusion and the simple flux limited scheme (12) are shown in Figure 3.

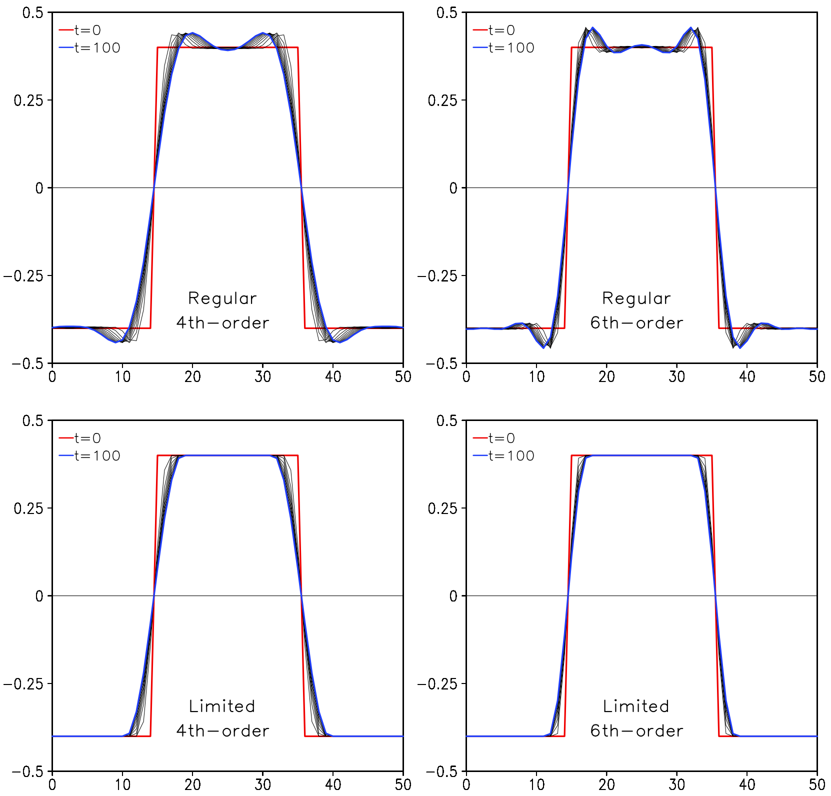

Figure 3: *As in Fig. 2, but for 4th (left) and 6th order (right) linear regular diffusion (upper panel) and Xue flux-limited monotonic diffusion (lower panel).*

Obviously, the unwanted numerical effects associated with the Gibbs phenomena are no longer present when using the simple Xue limiter, but the smoothing characteristic is maintained. The solution obtained with the Zalesak limiter are very similar (not shown), but require more CPU time.

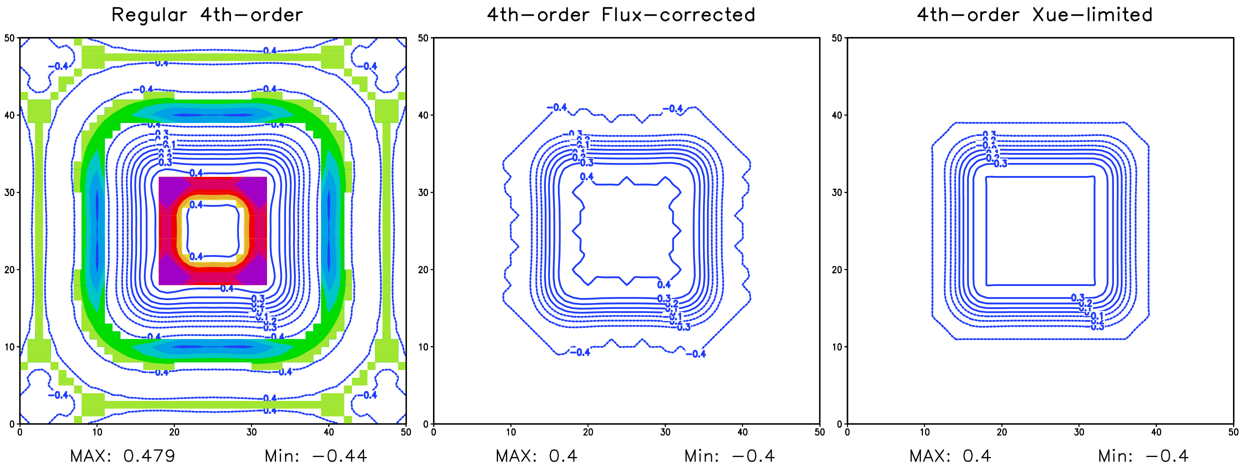

Figure 4: *2-D numerical solution of Eq.(1) for an initial square wave after 100 time steps. Left: 4th order regular diffusion, middle: 4th order flux limited, right: 4th order using the Xue flux limiter. Red shading indicates regions of overshoots, green shading regions of undershoots. The contour interval is 0.1.*

The extension of the monotonic schemes described in Section 3 to more than one dimension is straightforward. Fig. 4 shows the solution obtained after 100 time steps for the 2-D square wave test, where initially a block of 20 by 20 gridlines with a field value of 0.4 is placed in a background field having a value of -0.4. All parameters are the same as in the 1-D test, except that the diffusion coefficient for maximal damping has been adopted for the twodimensional case. The regular 4th order linear diffusion suffers significantly from the Gibbs phenomenon, with overshoots of the order of 10% and undershoots of the order of 5% of the initial amplitude. This effect is completely avoided by applying the Zalesak limiter or the Xue limiter. The maxima and minima values of the field are exactly 0.4 and -0.4, respectively, and a somewhat better gradient is maintained by the monotonic schemes. The noisy appearance of the 0.4 and -0.4 contour line in the solution by the Zalesak scheme is due to roundoff errors which, however, have no detrimental impact. Compared to the regular 4th order diffusion, the computation time ratio of the Zalesak flux correction scheme is 3.1, but only 1.3 for applying the simple Xue limiter (on an SGI Octane workstation).

5. First Results from LM Simulations

As a first test, the Xue limiter was applied to all prognostic variables for a randomly chosen real case from 18 September 2000. Figure 5 shows the vertically integrated cloud water content of a 12h-forecast starting at 00 UTC. Concerning the structure of the two cloud bands over Denmark and over the Northern Sea, no apparent differences between the reference run using regular 4th order diffusion and the model version with monotonic diffusion can be noticed. However, the area mean value of the integrated cloud water content is slightly reduced from 41 to 38 gm^{-2}.

This can also be noticed from the scatter diagram (Figure 5, right), where the gridpoint values of the integrated cloud water content of the reference run (y-axis) are plotted against those from the experiment (x-axis). Obviously, the values obtained from the reference are on average somewhat larger than those resulting from the run with monotonic diffusion. The same type of impact can also be noticed in the precipitation amount, which is slightly smaller in the experiment (not shown). One could attribute this to the removal of overshoots from the solution for the cloud water field. In a complex nonlinear model, however, such a clear assignment of cause and effect is not possible. Due to the noticeable effect on the cloud water content, a more thorough evaluation is necessary to assess the impact of the monotonic diffusion scheme on the cloud-radiation interactions.

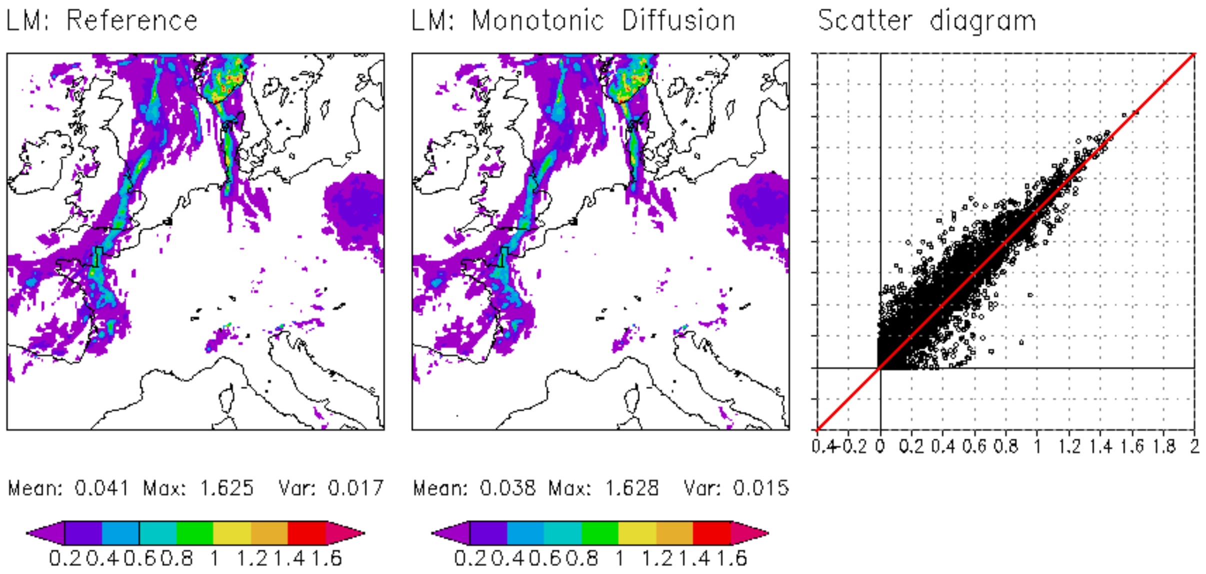

Figure 5: *Vertically integrated cloud water (kg/m^2) content of a 12-h LM forecast starting at 18 September 2000 00 UTC. Left: reference solution with 4th oder regular diffusion; middle solution from a run with monotonic Xue limited diffusion; right: Scatter diagram of values form the reference (y-axis) viz. experiment (x-axis) runs.*

6. Summary

Most NWP models require numerical smoothing to damp small-scale (2 grid interval) noise being related to stepwise or singular signals which are permanently generated in a nonlinear model. However, regular high order linear diffusions tends to introduce unphysical solutions on the resolvable scales. The Xue-limiter is an numerically efficient method to achieve monotonic higher order diffusion, i.e. not to create new noise on the resolvable scales.

In the test cases considered so far, there is only a relatively small impact from using monotonic 4th order diffusion with a tendency for lower vertically integrated cloud water and smaller peak precipitation amounts. Larger impact has been found in nonlinear convection experiments (rising dry bubble tests, Ming Xue, pers. comm.).

In LM, the scheme should replace the regular 4th order diffusion. Furthermore, the scheme offers the opportunity to apply additional limiters, e.g. in case of steep topography. This will be considered in future.