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High-order symmetry-preserving discretization of convection-diffusion equations on strongly stretched grids

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1. Introduction

Many physical phenomena feature thin boundary layers, in which the solution varies much more rapidly than elsewhere in the domain of interest. A 'natural' approach is to adapt a computational grid to the variations of the solution. In this way one obtains grids with a large diversity in mesh size, i.e. the grid shows strong stretching.

'Traditional' discretization methods (based on Lagrangian interpolation) focus on minimizing local truncation error, but experience has shown that these methods prefer low grid stretching rates, e.g. [1, 8, 25, 27]. The problems arise because this approach does not take into account the properties of the discrete system matrices obtained after discretization. An alternative approach is to develop discretization schemes which mimic the properties of the system matrix - a general name for this philosophy is mimetic discretization, e.g. [21].

We have chosen to retain the symmetry properties of the operator, which in our fluid-flow application is a combination of convection and diffusion. In particular, convection is discretized such that its discrete version remains skew symmetric. An almost immediate consequence is that the system matrix remains diffusively stable (hence never can become singular) on any grid. In formula: Let the system under study be given by

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} + L\phi = 0,$$

then the evolution of the kinetic energy $||\phi||_H = \phi^* H\phi$ (where H represents the local mesh size) is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}||\phi||_H = -\phi^*((HL)^* + HL)\phi.$$

With skew-symmetric convection, the symmetric part $(HL)^* + (HL)$ of the system matrix comes only from diffusion, and the above assertion follows.

Another consequence is that the convective discretization does not produce unphysical numerical diffusion, which unavoidably will interfere with the physical diffusion. This strategy has been applied e.g. in direct numerical simulation of turbulent flow (DNS), where the small-scale balance between convection and diffusion is quite delicate [28–30]. In the paper the behaviour of second- and fourth-order symmetry-preserving finite-volume methods is demonstrated on Shishkin grids and on exponential grids. Also their performance for DNS is shown..

2. Symmetry preservation: the philosophy

As an illustration we consider a convection-diffusion equation in one space dimension (x), with a constant velocity u, and with arbitrary $k = k(x) > 0$. In conservation form it reads

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x}(u\phi) - \frac{\partial}{\partial x}\left(k\,\frac{\partial \phi}{\partial x}\right) = 0, \tag{1}$$

provided with Dirichlet boundary conditions on the unit interval (for convenience).

It is noted that analytically, ignoring influences from the boundaries, for incompressible* flow convection is a skew-symmetric operator, whereas diffusion is symmetric positive definite. A discretization that mimics these analytical properties is called *symmetry preserving* [30]. The clue to its performance follows from Bendixson's inclusion lemma, which states that all eigenvalues of a matrix lie in or on the least rectangle with sides parallel to the real and imaginary axes that contains all eigenvalues of its symmetric and skew-symmetric part, respectively [6, p. 69]. An immediate consequence hereof is the following theorem:

> *Any symmetry-preserving discretization of the convection-diffusion equation (1) leads to a positive-real† coefficient matrix. In particular, the latter cannot become singular.*

This theorem can partly explain why the use of such symmetry-preserving discretizations has been found to be very efficient in direct numerical simulation of turbulent flow on structured [28–30] as well as unstructured grids [5]; see Section 6..

3. Fourth-order space discretization

The convection-diffusion equation (1) will be discretized in a (conservative) finite-volume fashion, where the control faces are chosen halfway between the grid points (for notation see Fig. 1).

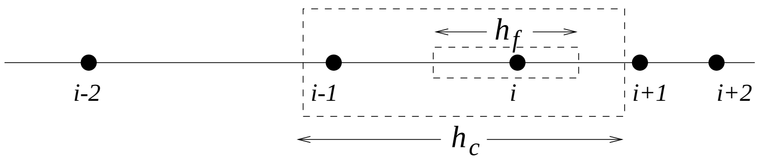

Figure 1: *Fine* (h_f) *and coarse* (h_c) *control volumes. The volume faces are located halfway the grid points* $(i, i \pm 1)$ *and* $(i, i \pm 2)$*, respectively.*

With a second-order flux in $x_{i+1/2}$ given by

$$u\frac{\phi_{i+1}+\phi_i}{2} - k\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i},$$

the semi-discrete convection-diffusion equation becomes

$$h_f\frac{\mathrm{d}\phi_i}{\mathrm{d}t} + \tfrac{1}{2}u(\phi_{i+1}-\phi_{i-1}) - k\left(\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i} - \frac{\phi_{i-1}-\phi_i}{x_{i-1}-x_i}\right) = 0. \tag{2}$$

Note that this discretization is symmetry-preserving and conservative, i.e. it conserves both energy and momentum. In an analytical formulation this combination is not possible [18], but discrete it can! Though on non-uniform grids this method may look first-order accurate, actually Manteuffel and White [14] have proven its global discretization error to be second-order accurate on any (sufficiently fine) grid; see also Hundsdorfer and Verwer [7, p. 271].

To turn this method into a fourth-order method, a similar equation on a two-times-larger control volume (Fig. 1) is written down

$$h_c\frac{\mathrm{d}\phi_i}{\mathrm{d}t} + \tfrac{1}{2}u(\phi_{i+2}-\phi_{i-2}) - \text{ diffusive terms } = 0. \tag{3}$$

The leading term in the discretization error can be removed through a Richardson extrapolation from (2) and (3). Since the errors in (2) and (3) are of third order, on a uniform grid this would

*By employing the skew-symmetric, though non-conservative, form of the flow equations the latter assumption may be dropped [18].

†A matrix is called positive real, when all eigenvalues of its symmetric part are lying in the positive half plane [32]

mean to make a combination 8*Eq. (2) - Eq. (3). On a nonuniform grid one would be tempted to tune the weights to the actual mesh sizes, but we think it important that the skew symmetry of the convective contribution is maintained. This can only be achieved when the weights are taken independent of the grid location, and hence equal to the uniform weights. In this way the discretization of the convective derivative becomes

$$H_i \frac{\mathrm{d}\phi_i}{\mathrm{d}x} \approx \tfrac{1}{2}(-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}), \tag{4}$$

where

$$H_i = 8h_f - h_c = \tfrac{1}{2}(-x_{i+2} + 8x_{i+1} - 8x_{i-1} + x_{i-2}).$$

On a uniform grid, of course, the usual fourth-order method is obtained, but on nonuniform grids the method differs considerably. In particular, the local truncation error

$$2H_i \frac{\mathrm{d}\phi}{\mathrm{d}x} = -\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2} \; + \; (h_{++}^2 - 8h_+^2 + 8h_-^2 - h_{--}^2)\phi_{xx} + \cdots$$

(where $h_{++} = x_{i+2} - x_i$, $h_+ = x_{i+1} - x_i$, etc.) does not look very promising at first sight. On irregular grids it might even behave first-order!

The diffusive term undergoes a similar treatment leading to

$$H_i \frac{\mathrm{d}^2\phi_i}{\mathrm{d}x^2} \approx 8\left(\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{\phi_{i-1} - \phi_i}{x_{i-1} - x_i}\right) - \left(\frac{\phi_{i+2} - \phi_i}{x_{i+2} - x_i} - \frac{\phi_{i-2} - \phi_i}{x_{i-2} - x_i}\right). \tag{5}$$

Remark The expressions (4) and (5) can also be derived through a coordinate transformation $x = x(\xi)$ by writing [8]

$$\frac{\mathrm{d}\phi}{\mathrm{d}x} = \frac{\mathrm{d}\phi}{\mathrm{d}\xi} / \frac{\mathrm{d}x}{\mathrm{d}\xi} \quad \text{and} \quad \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi} / \frac{\mathrm{d}x}{\mathrm{d}\xi}\right) / \frac{\mathrm{d}x}{\mathrm{d}\xi}.$$

Choose a uniform grid in ξ with mesh size Δ, then

$$\frac{\mathrm{d}\phi}{\mathrm{d}\xi} \;=\; \frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta} + O(\Delta^4),$$

and a similar expression holds for $\mathrm{d}x/\mathrm{d}\xi$. Dividing the two expressions leads to (4), and fourth-order behaviour looks obvious ...

4. Examples

We first consider the steady version of (1), for $u = 1$ and $k = 0.001$, on a so-called Shishkin grid [2, 15] consisting of two uniform subintervals separated by the point $x_s \equiv \max(0.5, 1 - ak \ln N)$, where N is the total number of grid points. Each of the two subintervals contains half of the points. The constant a is chosen such that also at small values of N reasonable resolution of the boundary layer is achieved: we set $a = 3$.

Also, some experiments on more smoothly varying exponential grids have been carried out; these grids possess a constant stretching in x. The stretch factor is chosen such that half of the grid points are lying on either side of the split point x_s of the Shishkin grid.

Figure 2 shows a comparison between the individual solutions of second- and fourth-order traditional methods and symmetry-preserving methods on the (abrupt) Shishkin grid and on the (smoothly stretched) exponential grid. Both grids contain 28 grid points. It is clearly visible that on both grids the 'traditional' fourth-order method suffers from an almost singular system matrix (an eigenvalue crosses the imaginary axis close to the origin).

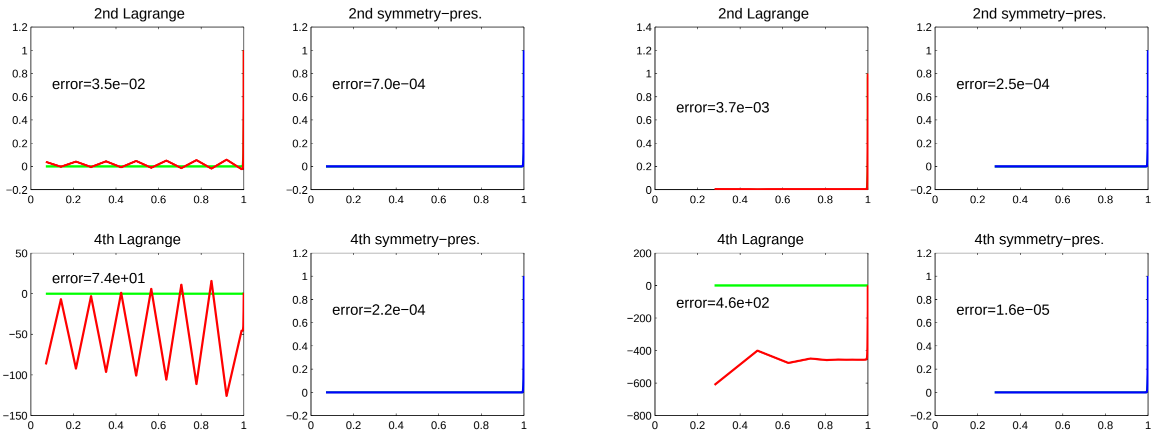

Figure 2: *Discrete solutions for $k = 0.001$ on an abrupt Shishkin grid (left) and an exponential grid (right). The 'traditional' discretization, especially the fourth-order version, has problems with the stretching of the grid.*

Figure 3 shows a systematic grid-refinement study of the second- and fourth-order traditional and symmetry-preserving methods on both typs of grids (abrupt and exponential). In order not to be bothered by special boundary conditions, for both approaches the values outside the domain have been set equal to their exact values. Some observations:

• The much more regular and forgiving character of the symmetry-preserving discretization is evident. Especially the coarser grids show a large difference in accuracy between the two discretization approaches. Note that on the abrupt Shishkin grid there is only one grid point where the symmetry-preserving discretization differs from the 'traditional' Lagrangian one. Yet this small difference is seen to have a strong influence on coarse grids.

• On exponential grids, the symmetry-preserving method seems to be constantly better than its Lagrangian counterpart. For equal accuracy, the fourth-order version can do with a roughly three times coarser grid. On Shishkin grids, both approaches show about third-order accuracy.

• Further, on the coarser grids the second-order Lagrangian method outperforms its fourth-order counterpart. Only on the finer grids the latter becomes more accurate. For the symmetry-preserving method, the fourth-order variant appears always more accurate than its second-order version (although this cannot be proven).

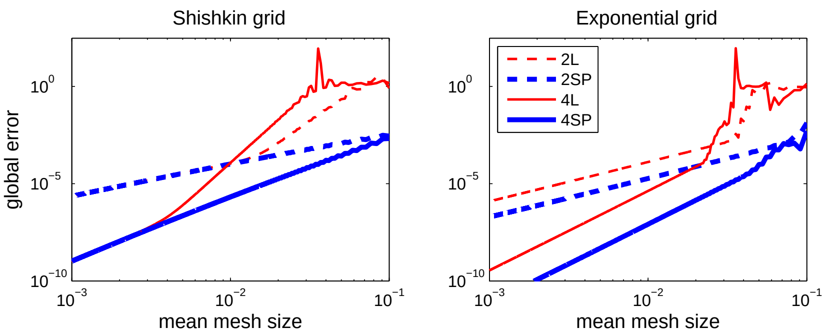

Figure 3: *The global error as a function of the mean mesh size. Half of the grid points is located in the boundary layer of thickness $1 - x_s$. Four methods are shown: 2L (second-order Lagrangian), 2SP (second-order symmetry-preserving), 4L (fourth-order Lagrangian) and 4SP (fourth-order symmetry-preserving).*

5. Application to turbulent flow

To further illustrate the accuracy of the symmetry-preserving discretization, consider a turbulent channel flow at a Reynolds number of Re=5,600. A large number of numerical results as well as experimental data is available for comparison. Figure 4 (left) shows a comparison of the mean velocity profile as obtained from the fourth-order symmetry-preserving simulation [30] with those of other direct numerical simulations. The grids used by the DNS's that we compare with have typically about 128^3 grid points, that is 16 times more grid points than our grid has. Nevertheless, the agreement is excellent.

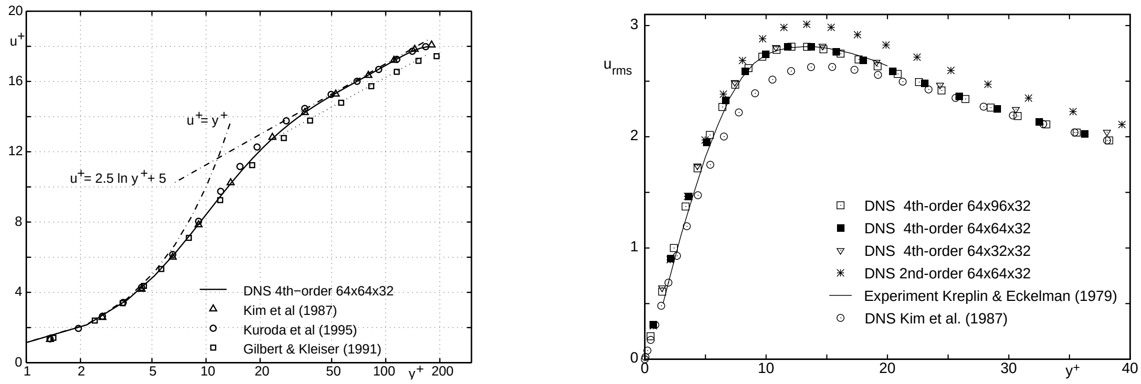

Figure 4: *Comparison of the mean streamwise velocity* u^+ *(left) and its root-mean-square (right) as function of the wall normal coordinate* y^+.

The root-mean-square of the fluctuating streamwise velocity u_{rms} near the wall ($0 < y^+ < 40$) is presented in Fig. 4 (right). The results show that the u_{rms} predicted by the fourth-order simulation fits the experiment data of Kreplin and Eckelmann [11] nicely. This holds for very coarse grids too, as can be inferred from the results computed with the fourth-order symmetry-preserving scheme with only 32 grid points in the wall-normal direction. It is interesting to compare the ratio between 'our' 32 or 64 grid points in wall-normal direction and the 128 grid points used in the reference computations [3, 9, 12]. This ratio (a factor two to four) compares quite well with the 'predicted' possible increase in grid size (a factor of three) as found in the one-dimensional test case described above.

This flow case has also been used to carry out a grid refinement study to show indeed fourth-order convergence behaviour. The skin-friction coefficient C_f has been monitored as obtained from simulations on five different grids, denoted A – E. Their spacings differ only in the direction normal to the wall, with 128 (A), 96 (B), 64 (C), 56 (D) and 48 (E) points, respectively. The first (counted from the wall) grid line varies between $y_1^+ = 0.72$ (grid A) and $y_1^+ = 1.9$ (grid E). The refinement study, as indicated in Fig. 5, clearly shows a fourth-order behaviour on the nonuniform grid. The straight line in Fig. 5 is approximately given by $C_f = 0.00836 - 0.000004(y_1^+)^4$. The extrapolated value at the crossing with the vertical axis $y_1^+ = 0$ lies in between the C_f reported by Kim et al. [9] (0.00818) and Dean's correlation $C_f = 0.073Re^{-1/4} = 0.00844$. Note that the extrapolation eliminates the (leading term of the) discretization error in the wall-normal direction, but not the other discretization errors in space and time.

The convergence of the fluctuating streamwise velocity near the wall ($0 < y^+ < 20$) is presented in Fig. 5 (right). Here, we have added results obtained on three still coarser grids (with 32, 24 and 16 points in the wall-normal direction, respectively), since the results on the grids A–E fall almost on top of each other. The coarsest grid, with only 16 points to cover the channel width is coarser than most of the grids used to perform a large-eddy simulation (LES) of this turbulent flow. Nevertheless, in the near wall region, the $64 \times 16 \times 32$ solution is not that far off the solution on finer grids.

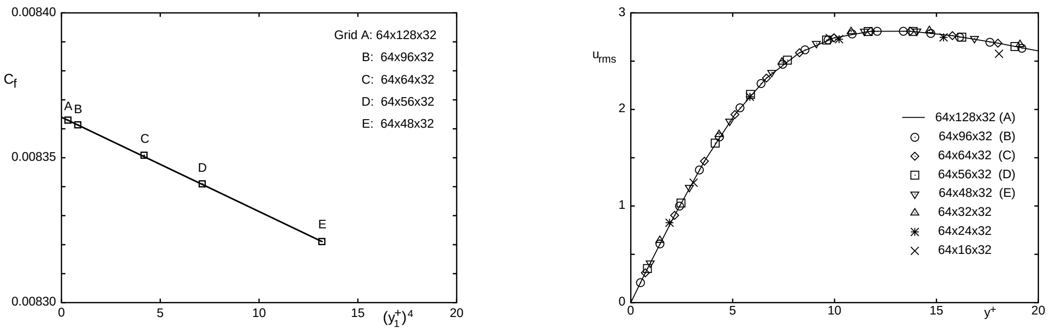

Figure 5: *Left: Convergence of the skin-friction coefficient upon grid refinement, displayed as a function of the fourth power of the cell size next to the wall. Right: The root-mean-square velocity fluctuations normalized by the wall shear velocity as a function of the wall coordinate* y^+ *on various grids for* $y^+ \leq 20$.

6. DISCUSSION

To obtain some feeling about what is going on, let's have a look at the global error between the discrete solution ϕ_h and the analytical solution ϕ_{exact}. It is given by

$$\| \phi_h - \phi_{\text{exact}} \| = L^{-1}\tau,$$

where L is the discrete coefficient matrix and τ the local truncation error. The global error is the product of the local truncation error and the inverse of the coefficient matrix. Obviously, when the coefficient matrix becomes singular it destroys the accuracy of the discrete solution. This is what happens with the traditional Lagrangian discretization methods which concentrate on minimizing τ. By using a symmetry-preserving discretization, the coefficient matrix can never become singular. Moreover, its convective part does not contribute to numerical damping. In the turbulent-flow examples this property is believed to be crucial.

The properties of the coefficient matrix have inspired many authors to design generalizations of second-order central discretization methods for non-uniform grids. Early discussions on self-adjoint (diffusive) equations can be found already in the work of Tikhonov and Samarskii [24] in the 1960's; see also [20]. Several other studies on nonuniform grids can be mentioned, e.g. [1, 8, 25]. Piacsek and Williams [18] explicitly advocated the use of a skew-symmetric analytic formulation in case of convective equations. Later, Verstappen and Veldman [28–30] showed that the same discretization can be obtained from the conservative divergence form of the equations. Closely related are the mimetic discretizations as developed by Steinberg and co-workers; see e.g. [21]. Another related criterion is the summation-by-parts property introduced by Strand [22], which achieves similar properties of the discretization.

Also, lower-order upwind discretizatios have been studied on nonuniform grids. On Shishkin grids, Miller et al. [15] and Roos [19] have analysed their convergence properties; for a recent overview we refer to [13]. However, Golub et al. [4] have warned that upwind discretization may produce some negative diffusion on expanding and contracting grids (the coefficient matrix need not be positive real, which may give problems to some iterative methods). By invoking the summation-by-parts property [16] or by using a symmetry-preserving discretization [26], the latter objection can be removed. Also, k-uniform convergence on Shishkin grids can be established [26].

Discussions of higher-order algorithms on Shishkin grids are rather rare in the literature, and seem to be restricted to Hermite discretization of reaction-diffusion equations, i.e. without convection [23, 31]. It would be interesting to analyse the current convective discretization in a similar way.

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