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A stable and conservative method for locally adapting the design order of finite difference schemes

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Abstract

A procedure to locally change the order of accuracy of finite difference schemes is developed. The development is based on existing Summation-By-Parts operators and a weak interface treatment. The resulting scheme is proven to be accurate and stable.

Numerical experiments verify the theoretical accuracy for smooth solutions. In addition, shock calculations are performed, using a scheme where the developed switching procedure is combined with the MUSCL technique.

Key words: Finite difference methods, high order accuracy, shock calculations, conservation, stability, summation-by-parts

1. Introduction

The most common and perhaps most intuitive way of imposing boundary condition is to use strong implementation, also called injection. Then the numerical solution has exactly the same value at the boundary as the continuous solution, by construction.

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Weakly implemented boundary conditions mean that the numerical solution does not necessarily equal the data at the boundary but is allowed to deviate somewhat. The deviation from the boundary data decreases with increased resolution, so that the design order of the scheme is preserved. The deviation should not be interpreted as a drawback, on the contrary it can serve as an error estimate for the solution in the interior. However, the most important advantage of weak boundary treatment is that combined with the Summation-By-Parts (SBP) operators, it yields stability [1, 2, 3, 4, 5, 6].

The technique of using penalty terms to make the solution fulfill the boundary conditions can be generalized to also hold for block interfaces, although instead of data the solution in the other block is used, see [7, 8, 9, 10, 11, 12, 13]. Block interfaces are useful when generating grids for complex geometries, or as in our case, to change the properties of the scheme from one computational domain to another.

The problem with changing schemes has been studied by others. In [14] coupled schemes were analyzed using the Kreiss theory [15, 16]. Other efforts to couple different schemes (e.g. shock capturing schemes and linear difference schemes) have been done [17, 18, 19]. It proves to be unexpectedly difficult to show stability and conservation for a coupled scheme, even though both ingoing schemes have these properties separately.

Coupled schemes can be used when the order of a numerical scheme has to be lowered in a small region, e.g. at a discontinuity. Another possible application is to increase the order of the scheme in regions of interest, for example when following a propagating wave.

When using the penalty technique, the grid points come in pairs of two

at a block interface. This has the benefit of producing two solution values at the same position (the difference between the two solutions can be used to estimate the error of the solution). However, if one needs to move the interface, e.g. to keep track of a moving shock, one can use the multi-valued interface treatment as a basic procedure, merge the double points into single ones, and obtain a sliding interface treatment. This will be the procedure used in this paper.

2. Interface treatment for a hyperbolic problem

2.1. The continuous formulation

To explain our technique we consider the scalar advection equation

$$u_t + au_x = 0, \quad -1 \leq x \leq 1. \quad (1)$$

We introduce an interface at $x = 0$, such that $u_t^L + au_x^L = 0$ holds in the left domain ($-1 \leq x \leq 0$) and $u_t^R + au_x^R = 0$ holds in the right domain ($0 \leq x \leq 1$). The interface condition is $u^L(0, t) = u^R(0, t)$.

Since we have the same equation in both domains the interface is just an imaginary barrier. When the equation is multiplied by a smooth function $\Phi(x, t)$ and integrated over each domain we obtain

$$\begin{aligned} \int_{-1}^0 \Phi u_t^L dx + \int_0^1 \Phi u_t^R dx &= a \int_{-1}^0 \Phi_x u^L dx - a \Phi u^L|_{-1}^0 + a \int_0^1 \Phi_x u^R dx - a \Phi u^R|_0^1 \\ &= a \int_{-1}^0 \Phi_x u^L dx + a \int_0^1 \Phi_x u^R dx + BT \end{aligned} \quad (2)$$

which is exactly what we would get if there was no interface. We want this conservation property to hold also for our numerical scheme. Here BT stands for boundary terms, these terms are dealt with using outer boundary conditions and are neglected in this paper.

2.2. Numerical interface treatment using penalty terms

We want to mimic the continuous case above numerically, and start by describing the original multi-valued interface treatment. Let $v^{L,R}$ denote the semi-discrete vector representations of $u^{L,R}$, such that $v_i^{L,R}(t)$ corresponds to $u^{L,R}(x_i, t)$. The grid points have indices $i = 0, 1, \dots, N_L - 1, N_L$ in the left domain and $i = 0, 1, \dots, N_R - 1, N_R$ in the right domain. For simplicity we use v_N^L as notation for the N_L th element of v^L , and in the same way v_0^R denotes the 0th element of v^R .

The interface condition $u^L(0, t) = u^R(0, t)$ will be imposed weakly, such that $v_N^L - v_0^R$ is small (goes to zero with decreased grid spacing). The differential operator d/dx is represented by the difference operator on matrix form $D_L = P_L^{-1}Q_L$ in the left domain and $D_R = P_R^{-1}Q_R$ in the right domain. The operators $D_{L,R}$ are on Summation-By-Parts form, given that $P_{L,R}$ and $Q_{L,R}$ fulfill

$$P = P^T > 0 \quad Q + Q^T = e_N e_N^T - e_0 e_0^T = \begin{bmatrix} -1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 1 \end{bmatrix} \quad (3)$$

where $e_N = [0, \dots, 0, 1]^T$ and $e_0 = [1, 0, \dots, 0]^T$ are $(N_{L,R} + 1) \times 1$ vectors. The operators D_L and D_R can be designed to have the order of accuracy 2, 4, 6 or 8 in the interior and 1, 2, 3 or 4 at the boundary. This will lead to a global order of accuracy of 2, 3, 4 or 5, see [1, 2, 20, 21]. Examples of $P_{L,R}$ and $Q_{L,R}$ can be found in A.

The resulting numerical approximation of (1) is

$$\begin{aligned} v_t^L + aD_L v^L &= \tau_L P_L^{-1} e_N (v_N^L - v_0^R) \\ v_t^R + aD_R v^R &= \tau_R P_R^{-1} e_0 (v_0^R - v_N^L) \end{aligned} \quad (4)$$

in the left and right domain, respectively. As usual we ignore the outer boundary conditions. The right-hand-sides of (4) enforce the interface condition weakly, where the vectors e_N and e_0 ensure that the penalty terms including the penalty parameters $\tau_{L,R}$ correct the scheme where they should.

First we make sure that the formulation is conservative, in the sense that it mimics (2). We multiply the two rows in (4) by $\Phi_L^T P_L$ and $\Phi_R^T P_R$, respectively, where $\Phi_{L,R}$ is a smooth function represented by a vector in each domain. This is the discrete equivalence of multiplying (1) by $\Phi(x, t)$ and integrating. This leads to

$$\begin{aligned} \Phi_L^T P_L v_t^L + a \Phi_L^T Q_L v^L &= \tau_L \Phi_L^N (v_N^L - v_0^R) \\ \Phi_R^T P_R v_t^R + a \Phi_R^T Q_R v^R &= \tau_R \Phi_R^0 (v_0^R - v_N^L) . \end{aligned} \quad (5)$$

Next, we use that $\Phi_L^N = \Phi_R^0 = \Phi_I$ and add the two rows in (5). Through the SBP property $Q + Q^T = e_N e_N^T - e_0 e_0^T$ we obtain

$$\begin{aligned} \Phi_L^T P_L v_t^L + \Phi_R^T P_R v_t^R &= a(D_L \Phi_L)^T P_L v^L + a(D_R \Phi_R)^T P_R v^R \\ &\quad + \Phi_I (v_N^L - v_0^R) (\tau_L - \tau_R - a) . \end{aligned} \quad (6)$$

We see that if we choose τ_L, τ_R such that $\tau_L - \tau_R - a = 0$, the interface terms in (6) vanish and (4) will be conservative. This requirement is fulfilled by letting $\tau_L = (a - \theta)/2$ and $\tau_R = (-a - \theta)/2$, where θ is a free parameter.

After assuring conservation we check the stability properties. The energy estimate is formed by replacing Φ_L by v^L and Φ_R by v^R in (6) and adding

the transpose. Defining $\|v\|_P^2 \equiv v^T P v$ and using the SBP properties yields

$$(\|v^L\|_{P_L}^2 + \|v^R\|_{P_R}^2)_t = -\theta \begin{bmatrix} v_N^L \\ v_0^R \end{bmatrix}^T \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} v_N^L \\ v_0^R \end{bmatrix}$$

which is stable if $\theta \geq 0$. The choice $\theta = |a|$ will give a fully up-wind implementation of the interface condition. Note again that we have omitted the outer boundaries, only taking the terms at the interface into consideration.

2.3. Transformation to a scheme with single-valued interface

We can rewrite the equations in (4) as

$$V_t + a\bar{P}^{-1}\bar{Q}V = \bar{P}^{-1}\bar{T}V \quad (7)$$

where we have defined

$$V = \begin{bmatrix} v^L \\ v^R \end{bmatrix} \quad \bar{P} = \begin{bmatrix} P_L & 0 \\ 0 & P_R \end{bmatrix} \quad \bar{Q} = \begin{bmatrix} Q_L & 0 \\ 0 & Q_R \end{bmatrix} \quad \bar{T} = \begin{bmatrix} \tau_L e_N e_N^T & -\tau_L e_N e_0^T \\ -\tau_R e_0 e_N^T & \tau_R e_0 e_0^T \end{bmatrix}. \quad (8)$$

The matrices $\bar{P}$, $\bar{Q}$ and $\bar{T}$ have dimensions $(N_L + N_R + 2) \times (N_L + N_R + 2)$.

Note that v_N^L and v_0^R are both approximations of the same continuous solution value, i.e. $u(x = 0, t)$. Now our ambition is to be able to move the interface, and hence we need to modify the scheme such that it operates without double grid points at the interface.

The new scheme will be based on the scheme in (7). The transformation to a scheme with single-valued interface will require the introduction of a new discrete solution vector. We denote this vector W , and it will be one element shorter than the vector V , i.e. W is an $(N_L + N_R + 1) \times 1$ vector. The merged solution value right at the interface is denoted W_I and is a mixture

between the values at the two old points, such that $W_I = \alpha v_N^L + (1 - \alpha)v_0^R$.

Thus $W = \tilde{K}V$, where

$$W = \begin{bmatrix} v_0^L \\ \vdots \\ v_{N-1}^L \\ W_I \\ v_1^R \\ \vdots \\ v_N^R \end{bmatrix} \quad \tilde{K} = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & 0 & 0 & 0 \\ & & 0 & \alpha & (1-\alpha) & 0 \\ & & 0 & 0 & 0 & 1 \\ & & & & & \ddots \\ & & & & & & 1 \end{bmatrix} \quad V = \begin{bmatrix} v_0^L \\ \vdots \\ v_{N-1}^L \\ v_N^L \\ v_0^R \\ v_1^R \\ \vdots \\ v_N^R \end{bmatrix}.$$

Next, we make the (bold) assumption that $v_N^L \equiv v_0^R$. Then the relation $V = \tilde{I}^T \tilde{K} V$ will hold, where $\tilde{I}$ and $\tilde{I}^T \tilde{K}$ are given below.

$$\tilde{I} = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & 0 & 0 & 0 \\ & & 0 & 1 & 1 & 0 \\ & & 0 & 0 & 0 & 1 \\ & & & & & \ddots \\ & & & & & & 1 \end{bmatrix} \quad \tilde{I}^T \tilde{K} = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & 0 & 0 & 0 \\ & & 0 & \alpha & 1-\alpha & 0 \\ & & 0 & \alpha & 1-\alpha & 0 \\ & & 0 & 0 & 0 & 1 \\ & & & & & \ddots \\ & & & & & & 1 \end{bmatrix}. \quad (9)$$

$\tilde{K}$ and $\tilde{I}$ are similar to the identity matrix, except they have dimensions $(N_L + N_R + 1) \times (N_L + N_R + 2)$ and are slightly modified in the interior.

Remark: As discussed earlier, it is in general not true that $v_N^L = v_0^R$ for weakly imposed interfaces. However, this assumption is merely a step in the derivation and will not lead to restrictions on the final scheme.

If $v_N^L = v_0^R$ holds, the right-hand-side of (7) is zero (as can be seen from (4)). With this in mind, we multiply equation (7) by $\tilde{K}$, and since $V = \tilde{I}^T \tilde{K} V$ we can insert $\tilde{I}^T \tilde{K}$ in front of V . We get

$$\tilde{K} V_t + a \tilde{K} \tilde{P}^{-1} \tilde{Q} \tilde{I}^T \tilde{K} V = 0.$$

Next, we choose $\alpha = P_L^N / \beta$ and $(1 - \alpha) = P_R^0 / \beta$. This specific choice of α and $1 - \alpha$ gives the relation $\tilde{K} \tilde{P}^{-1} = \tilde{P}^{-1} \tilde{I}$, where

$$\tilde{K} \tilde{P}^{-1} = \begin{bmatrix} 1/P_L^0 & & & & & & \\ & \ddots & & & & & \\ & & 1/P_L^{N-1} & 0 & 0 & 0 & \\ & & 0 & 1/\beta & 1/\beta & 0 & \\ & & 0 & 0 & 0 & 1/P_R^1 & \\ & & & & & & \ddots & \\ & & & & & & & 1/P_R^N \end{bmatrix} = \tilde{P}^{-1} \tilde{I}$$

and $\tilde{P} = \text{diag}(P_L^0, \dots, P_L^{N-1}, \beta, P_R^1, \dots, P_R^N)$. From $\alpha + (1 - \alpha) = 1$ we see that $\beta = P_L^N + P_R^0$. Using these particular values of α and β , and recalling that $\tilde{K} V = W$, we obtain

$$W_t + a \tilde{P}^{-1} \tilde{I} \tilde{Q} \tilde{I}^T W = 0.$$

Finally we define the new difference matrix $\tilde{Q}$ as

$$\tilde{Q} \equiv \tilde{I} \tilde{Q} \tilde{I}^T = \begin{bmatrix} \ddots & & \vdots & & \vdots & & \\ \dots & Q_L^{N-1, N-1} & & Q_L^{N-1, N} & & & \\ \dots & Q_L^{N, N-1} & & Q_L^{N, N} + Q_R^{0, 0} & Q_R^{0, 1} & \dots & \\ & & & Q_R^{1, 0} & Q_R^{1, 1} & \dots & \\ & & & \vdots & \vdots & \ddots & \end{bmatrix}.$$

This concludes the derivation and at this point we can ignore our first assumption ($v_N^L \equiv v_0^R$), since we now have a new scheme, independent of the original one. The derived scheme is

$$W_t + a\tilde{P}^{-1}\tilde{Q}W = 0. \quad (10)$$

where $\tilde{P} = \tilde{P}^T > 0$. Moreover, we see that $\tilde{Q}$ is skew-symmetric in the interior just as Q_L and Q_R , since $Q_L^{N,N} + Q_R^{0,0} = 1/2 - 1/2 = 0$. Hence the new scheme possesses the SBP properties, given in (3), which automatically leads to a conservative and stable scheme. It is also consistent since

$$(W_I)_t = -a \frac{e_N^T Q_L W_L + e_0^T Q_R W_R}{\beta} = -a (\alpha(P_L^{-1} Q_L W_L)_N + (1 - \alpha)(P_R^{-1} Q_R W_R)_0),$$

where $W_{L,R}$ refer to the left part of W (including W_I) and the right part of W (including W_I), respectively. Hence the scheme in the point W_I is nothing but two one-sided operators added together. If we denote the inner order of accuracy L in the left domain and R in the right domain, the accuracy right at the interface will be $\min(L/2, R/2)$. In total this will give an accuracy of at least $\min(L/2, R/2) + 1$.

We summarize our results in the following proposition:

Proposition 2.1. *Consider equation (1). The scheme (10) with the differential operator $\tilde{D} = \tilde{P}^{-1}\tilde{Q}$ has design order L in the left part of the computational domain and design order R in the right part of the computational domain and order $\min(L/2, R/2)$ at the interface. The scheme is on SBP form, and hence it is conservative and stable.*

Remark: The scheme in (10) is based on the scheme in (7). To be precise $\tilde{Q} \equiv \tilde{I}\bar{Q}\tilde{I}^T$ and $\tilde{P} \equiv \tilde{I}\bar{P}\tilde{I}^T$, where $\bar{Q}$ and $\bar{P}$ are given in (8) and $\tilde{I}$ is defined in (9).

Remark: Note that in the procedure presented above the orders of accuracy L and R are arbitrary (L, R can be 2, 4, 6 or 8). In addition, by modifying $\bar{Q}$, $\bar{P}$ and $\tilde{I}$ the scheme can be designed to switch order several times instead of just once.

Examples of the new operators, when having second order in one domain and fourth or sixth order in the other domain, are given in A.

2.4. A time-dependent norm

The stability analysis above is based on the energy method, where the norm $\tilde{P}$ is assumed to be constant. This is suitable for problems with an interface fixed in space. However, for a problem with a moving interface the norm will in fact not be constant over time. It will be

$$\begin{aligned}\tilde{P} &= \tilde{P}_0 + \sum_{i=1}^n H(t_i)(\tilde{P}_i - \tilde{P}_{i-1}) \\ \tilde{P}_t &= \sum_{i=1}^n \delta(t_i)(\tilde{P}_i - \tilde{P}_{i-1})\end{aligned}\tag{11}$$

where $H(t)$ is the unit step function and $\delta(t)$ the Dirac function. At the times t_i we instantly change the scheme, and thereby also the norm, from $\tilde{P}_{i-1}$ to $\tilde{P}_i$. Multiplying (10) by $W^T \tilde{P}$ from the left and adding the transpose yields $W^T \tilde{P} W_t + W_t^T \tilde{P} W = aW_0^2 - aW_N^2$, and hence we can write

$$\frac{d}{dt} (W^T \tilde{P} W) = aW_0^2 - aW_N^2 + W^T \tilde{P}_t W.\tag{12}$$

By integrating (12) in time and ignoring the outer boundary terms we get

$$W^T \tilde{P} W - W(t_0)^T \tilde{P}_0 W(t_0) \leq \int_0^T W^T \tilde{P}_t W dt.\tag{13}$$

In (13), $W(t_0)$ is the initial data and $0 = t_0 < t_1 < t_2 < \dots < t_n < T$. From (11) we have that $\tilde{P}_t = \sum_{i=1}^n \delta(t_i)(\tilde{P}_i - \tilde{P}_{i-1})$. Using the general rule

$\int \delta(a)F(t)dt = F(a)$ we rewrite (13) and find that

$$W^T \tilde{P} W + \sum_{i=1}^n W(t_i)^T \tilde{P}_{i-1} W(t_i) \leq \sum_{i=0}^n W(t_i)^T \tilde{P}_i W(t_i). \quad (14)$$

Assume $t_0 \leq t < t_1$. Then $\tilde{P} = \tilde{P}_0$, $n = 0$ and (14) reduces to

$$W^T \tilde{P}_0 W \leq W(t_0)^T \tilde{P}_0 W(t_0). \quad (15)$$

Now assume $t = t_1$. Then $\tilde{P} = \tilde{P}_1$, $n = 1$ and (14) reduces to

$$\begin{aligned} W(t)^T \tilde{P}_1 W(t) + W(t_1)^T \tilde{P}_0 W(t_1) &\leq W(t_0)^T \tilde{P}_0 W(t_0) + W(t_1)^T \tilde{P}_1 W(t_1) \\ W(t_1)^T \tilde{P}_0 W(t_1) &\leq W(t_0)^T \tilde{P}_0 W(t_0) \end{aligned}$$

and hence (15) also holds for the closed domain $t_0 \leq t \leq t_1$. Now we imagine that every time the scheme is changed one starts over with a new initial condition and a new norm. The procedure can be repeated, and consequently

$$W(t_i)^T \tilde{P}_{i-1} W(t_i) \leq W(t_{i-1})^T \tilde{P}_{i-1} W(t_{i-1}), \quad i = 1, 2, \dots, n.$$

Hence the growth of the solution is bounded locally in time. We summarize the result in the following proposition:

Proposition 2.2. *Consider the scheme (10) with a time-dependent norm $\tilde{P}(t)$. Assume that for the time interval $t_{i-1} \leq t < t_i$ the norm will be $\tilde{P}_{i-1}$. Then the solution $W(t)$ for $t_{i-1} \leq t \leq t_i$ will be bounded by the solution at time $t = t_{i-1}$.*

Remark: Proposition 2.2 bounds the solution growth locally in every time interval. A strict bound of $W(t)$ in terms of $W(t_0)$ will be non-sharp. The calculations shown below indicate that the local bound is indeed good enough.

3. Verification of the steady adaptive scheme

After having derived the adaptive scheme, we need to validate it. First we will present simulations verifying the theory, and thereafter show results from shock calculations to demonstrate applicability. Consider the domain $0 \leq x \leq 1$, and let $N + 1$ be the total amount of grid points, indexed from $i = 0$ to $i = N$. At the locations $i = i_L$ and $i = i_R$ we switch the order of the scheme, from fourth order to second order, and back again.

Consider the time-independent problem $u_x = S(x)$ with boundary condition $u(0) = g_0$, having $u(x) = \sin(7x) - \cos(4x)$ as the manufactured solution. We solve this equation using the adjustable scheme

$$\tilde{P}^{-1}\tilde{Q}v = S + \tau\tilde{P}^{-1}e_0(v_0 - g_0) \quad (16)$$

where $e_0 = [1, 0, \dots, 0]^T$ and S is the discrete representation of $S(x)$ such that $S_i \equiv S(x_i)$. As penalty parameter we use $\tau = -1$ (the time-dependent problem is stable for $\tau \leq -1/2$). The scheme in (16) changes order at $i_L = N/4$ and $i_R = 3N/4$. Hence it will be second order for $0.25 < x < 0.75$ and fourth order outside this interval. The resulting solution and error (using $N = 32$ and $N = 64$) are shown in Figure 1. From Figure 1(b) it is clear that the scheme changes at $x \approx 0.25$ and $x \approx 0.75$.

Figure 1: For $0.25 \lesssim x \lesssim 0.75$ the scheme is 2nd order accurate, while it is 4th order accurate outside.

Remark: In Figure 1 we see that the solution is second order accurate in the whole domain. To understand this, we rewrite (16) as $\mathcal{D}v = \mathcal{S}$, where $\mathcal{D} = \tilde{P}^{-1} \left(\tilde{Q} - \tau e_0 e_0^T \right)$ and $\mathcal{S} = S - \tau \tilde{P}^{-1} e_0 g_0$. The truncation error T_e is obtained by inserting the exact solution u into the numerical scheme, as $\mathcal{D}u = \mathcal{S} + T_e$. Now the solution error becomes $e = v - u = -\mathcal{D}^{-1}T_e$. By construction T_e has different order of accuracy in different regions, but when T_e is multiplied by $\mathcal{D}^{-1}$ the errors will in most cases not stay localized. For a purely second order accurate scheme $\mathcal{D}^{-1}$ can be found analytically, see [22].

The simulations in Figure 1 were done for various number of grid points N . First we used $i_L = N/4$ and $i_R = 3N/4$ (as in Figure 1) and then $i_L = N/2 - 8$ and $i_R = N/2 + 8$, such that the number of lower order points in the scheme remains constant as the mesh is refined. Two cases were considered, 2nd order in the interior and 4th order outside, and in addition 2nd order in the interior and 6th order outside.

In Figure 2 the errors from these simulations are visualized. If the proportions of lower (2nd) and higher (4th or 6th) order points in the scheme do not change, the overall order of accuracy will be the lower (2nd) one. If the number of 2nd order points in the scheme remains constant as the mesh is refined we obtain third order accuracy, for both the 4th and 6th order schemes. Both these results coincide with theory, see [2]. The errors in the 6th order case are just slightly smaller than the error in the 4th order case. This is due to the fact that for such a smooth solution most of the errors come from the second order part in the interior.

Figure 2: The L_2 norm of the error as a function of the number of grid points, N . The amount of lower order points in the scheme is either increasing with N or held constant.

4. Verification of the time-dependent adaptive scheme

As discussed earlier the solution obtained by the adaptive scheme is bounded piecewise in time. That is, as long as we do not change the scheme

the solution does not grow. For a better understanding of the stability of the time-dependent scheme we compare the solution obtained using a varying $\tilde{P}$ and $\tilde{Q}$ to the solution obtained by a stationary scheme.

Consider the advection equation

$$u_t + au_x = 0 \quad 0 \leq x \leq 1$$

where $a = 2$, and with initial data $u(x, 0) = \sin(2\pi x)$ and boundary condition $u(0, t) = \sin(2\pi(x - at))$. For the fixed scheme we switch the order of accuracy from 4th order to 2nd order at $i_L = N/8$ and back again at $i_R = N/4$. We let the simulation run to time $t = 100$ and measure the error in the $\tilde{P}$ -norm. The results, using $N = 80$, $N = 160$ and $N = 320$, are shown in Figure 3. We see that the errors are kept on constant levels as predicted. Moreover, as expected, the error decreases approximately by a factor of four each time the number of mesh points is doubled.

Figure 3: Error from the adaptive scheme, keeping the norm fixed. Top line: $N = 80$, middle line: $N = 160$ and bottom line: $N = 320$.

For the time-dependent scheme we start by having $i_L(t_0) = N/8$ and

$i_R(t_0) = N/4$, just as in the previous simulations. Then we let the second order region slide with a speed of 0.005 such that at time $t = 100$ it has moved to $i_L(t_{end}) = 5N/8$ and $i_R(t_{end}) = 3N/4$. Again we do simulations using $N = 80$, $N = 160$ and $N = 320$. This means that the scheme will change 40, 80 and 160 times, respectively, during the simulations. The resulting errors are shown in Figure 4. From Figure 4(a) it is apparent that the error makes a small jump every time the scheme and hence the norm change. However, we see that the error growth is limited. As for the case when the norm is fixed the error decreases approximately by a factor of four every time the number of mesh points is doubled.

Figure 4: Error from the adaptive scheme, when the norm is time-dependent. Top line: $N = 80$, middle line: $N = 160$ and bottom line: $N = 320$.

5. The adaptive scheme applied to a system of equations

Consider the coupled system of equations

$$U_t + AU_x = 0, \quad 0 \leq x \leq 1 \quad (17)$$

where A and U are specified below.

$$U = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad A = a \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad a = 1/2 > 0.$$

The characteristic variables of the system are $c_+ = \frac{1}{\sqrt{2}}(u_1 + u_2)$ (right-going) and $c_- = \frac{1}{\sqrt{2}}(u_1 - u_2)$ (left-going). If boundary data is given as $c_+ = r_0 c_-$ at $x = 0$, and as $c_- = r_N c_+$ at $x = 1$, then the energy estimate becomes $\|U\|_t^2 = a [c_-^2(0, t)(r_0^2 - 1) + c_+^2(1, t)(r_N^2 - 1)]$. This gives well-posedness as long as $|r_{0,N}| \leq 1$. In our case we use $r_0 = 1$ and $r_N = -1$ which yields the boundary conditions $u_2(0, t) = 0$ and $u_1(1, t) = 0$. Note that this is a very sensitive problem since it, using these boundary conditions, is completely undamped (the energy estimate is $\|U\|_t^2 = 0$).

Let V be the semi-discrete version of U , sorted as $V = [V_0^T \ V_1^T \ \dots \ V_N^T]^T$ where $V_i = [(v_1)_i \ (v_2)_i]^T$, such that $V_i(t) \approx U(x_i, t)$. The discrete correspondence to (17) can now be written

$$V_t + (\tilde{D} \otimes A)V = (\tilde{P}^{-1}e_0 \otimes \tau_0)(v_2)_0 + (\tilde{P}^{-1}e_N \otimes \tau_N)(v_1)_N.$$

where $\tilde{D} = \tilde{P}^{-1}\tilde{Q}$ is the operator of mixed order of accuracy mimicking d/dx . By choosing the penalty parameters as $\tau_0 = -a[1, 1]^T$ and $\tau_N = -a[1, -1]^T$, we obtain the energy estimate

$$\frac{d}{dt}\|V\|_{\tilde{P}}^2 = -2a(v_2)_0^2 - 2a(v_1)_N^2 \leq 0,$$

where $(v_2)_0 \approx u_2(0, t) = 0$ and $(v_1)_N \approx u_1(1, t) = 0$. That is, the discrete energy estimate is slightly damped, but the damping goes to zero as the mesh is refined.

As initial condition in our numerical simulations we use a narrow Gaussian shaped function $u_1(x, 0) = e^{-625(x-0.5)^2}$, $u_2(x, 0) = 0$. As time passes,

this will result in two wave pulses, one traveling left and one right. At the pulses the scheme will have high order (4th or 6th), whereas it will be second order accurate elsewhere. The higher order regions follow the waves as they propagate through the domain.

(a) Start, $t=0$. The scheme is 2-6-2.

(b) Waves split up, still 2-6-2.

(c) Waves separated, still 2-6-2

(d) End, $t=0.5$. The scheme is 2-6-2-6-2.

Figure 5: The solutions $u_{1,2}$, $v_{1,2}$ starts centered in $x = 0.5$ and ends at time $t = 0.5$ centered in $x = 0.5 \pm 0.25$. This example is done using $N = 64$ and $dt = 1/80$.

In Figure 5 we show the exact solutions $u_{1,2}$ versus the numerical ones $v_{1,2}$ at different times. The number of grid points is $N = 64$ and the time step used is $\Delta t = 1/80$. In addition the time-dependent norm $\tilde{P}$ is indicated.

The rates of convergence are shown in Figure 6. Note that the rates of convergence for the schemes of mixed order at first appears to be the same as for the schemes of pure higher order. The accuracy does not become second order until the errors become so small that the contribution from outside the waves comes into play.

Figure 6: L_2 -errors of $e_1 = v_1 - u_1$ at time $t = 0.5$ using mixed order scheme ((2-4-2) and (2-6-2)), respectively. Compared with pure 4th and 6th order scheme.

We have changed the scheme and followed the pulses in the following way. If x_S is the analytical center of the pulse, then the center of the higher order region will have index $i_S = n_S \text{Round}(Nx_S/n_S)$, where $n_S = N/64$ and where the function $\text{Round}(x)$ rounds a number x to the nearest integer. The actual switching take place in $i_L = i_S - w$ and $i_R = i_S + w$. The parameter w specifies the width of the higher order region. For the simulations showed in Figure 6 we have used $w = 4N/32$ for the 2-4-2 scheme and $w = 5N/32$ for the 2-6-2 scheme.

6. The adaptive scheme applied to problems with discontinuities

The most obvious application for this methodology is simulations on problems with discontinuous solutions. When differentiating over discontinuities special shock-capturing techniques can be used, for example the MUSCL scheme [23]. For scalar one-dimensional conservation laws ($u_t + F_x = 0$), we have the MUSCL scheme converted into SBP-form, see [19],

$$v_t + P^{-1}QF = -P^{-1}D_1^T B_M D_1 v. \quad (18)$$

D_1 is a first order undivided difference operator and $B_M = \text{diag}(b_0, b_1, \dots, b_N)$ is a diagonal matrix constructed such that (18) is equivalent to the standard MUSCL formulation. The terms involving B_M will be referred to as the MUSCL dissipation. The MUSCL scheme is second order accurate in smooth regions and goes to first order near a discontinuity or shock to avoid non-physical oscillations.

Since the MUSCL scheme in equation (18) is on SBP-form, it can be coupled to the adaptive scheme derived above. In the vicinity of a discontinuity, the scheme is first turned from 4th to 2nd order in the way described above. Next, we add the MUSCL treatment in form of a dissipative term close to the discontinuity. This yields

$$v_t + \tilde{P}^{-1}\tilde{Q}F = -\tilde{P}^{-1}D_1^T \tilde{B}_M D_1 v$$

which we will refer to as the Hybrid scheme. Here $\tilde{B}_M = \Phi B_M$. We have constructed a matrix Φ which limits the MUSCL dissipation, so that it is applied only in the 2nd order regions. In this paper we have used that we have a priori knowledge of the shock position to determine Φ .

Recall that the norm $\tilde{P}$ differs from the standard norm P , and for the (4-2-4)th-order switching it is visualized in Figure 7. The limiter Φ is also shown.

Figure 7: $\tilde{P}$ (normalized with grid size) for a (4-2-4)th-order switching with $N = 40$, $i_L = 20$ and $i_R = 30$. The role of the discrete function Φ is also depicted.

First, we locate the discontinuity/shock at grid index i_S , and switch scheme from 4th order to 2nd order at index $i_L = i_S - w$ and back at $i_R = i_S + w$. This leads to a scheme with $2w + 1$ grid points with first to second order accuracy around the shock (at i_L and i_R it is first order). Thereafter we activate the MUSCL dissipation in the domain from $i_S - w_M$ up to $i_S + w_M$, where $w_M < w$. In this way we make sure that the MUSCL dissipation is always disabled outside the second order region. The variables w and w_M can be varied, and in Figure 7 we have used $w = 5$ and $w_M = 2$.

In addition to Φ , which we use in the Hybrid scheme to turn the MUSCL dissipation on/off, the MUSCL scheme has a standard limiter ϕ . This limiter determines where the MUSCL scheme should be 2nd order and where it should be 1st order. Here the MUSCL scheme is based on a minmod limiter,

see [19].

In summary: In the Hybrid scheme the MUSCL dissipation is turned on in regions with discontinuities leading to a standard MUSCL scheme, and it is turned off in the smooth region leading to a higher order scheme.

To demonstrate the benefits of the new methodology we compare the Hybrid scheme to the MUSCL scheme and the third order WENO scheme, see [24]. For all computations we use the classical 4th-order Runge-Kutta method for time integration.

6.1. The linear problem

We study the advection equation

$$\begin{aligned} u_t + u_x &= 0, & 0 \leq x \leq 1 \\ u(0, t) &= g_0(t), & u(x, 0) = u_0(x) \end{aligned}$$

with boundary condition $g_0(t)$ and initial condition $u_0(x)$. We consider a combination of a Gaussian pulse and a step function as the initial solution, i.e.

$$u_0(x) = \begin{cases} e^{-100(x-0.2)^2} + 1, & 0 \leq x \leq 0.6 \\ 0.5, & 0.6 < x \leq 1. \end{cases}$$

This means that the solution has both smooth and discontinuous parts. In Figure 8 the solutions and errors from the Hybrid scheme are compared to the ones from the WENO and MUSCL schemes. We observe that both the MUSCL scheme and the WENO scheme cut the top of the Gaussian pulse. The Hybrid scheme does not. Close to the discontinuity, the solutions for all three schemes are similar. Note that the Hybrid and MUSCL schemes are identical in that region.

(a) Solution

(b) Error

Figure 8: Solution and error. Comparison between the WENO scheme, the MUSCL scheme and the Hybrid scheme. $N = 80$ and $t = 0.15$.

The L_2 -norm of the errors in Figure 8 are 0.0350 for the WENO scheme, 0.0367 for the MUSCL scheme and 0.0350 for the Hybrid scheme. However, the dominating error contribution comes from the discontinuity, and if we instead just consider the domain $0 \leq x \leq 0.5$ the L_2 -errors will be 0.0147 for the WENO scheme, 0.0157 for the MUSCL scheme and 0.0002 for the Hybrid scheme.

6.2. The non-linear problem

Next we consider the Burgers' equation, i.e.

$$u_t + (u^2/2)_x = 0, \quad 0 \leq x \leq 1,$$

with a sine wave as initial condition, $u_0(x) = \sin(2\pi x)$. An analytical solution is computed using a Newton iteration method [25]. Numerically, we start by computing the solutions until time $t = 0.1$, which is just before a shock has formed. Since no shock has yet formed, the Hybrid scheme will be identical to the 4th order scheme. It can be seen in Figure 9 that the solution obtained using the Hybrid scheme is significantly more accurate than the ones from the MUSCL scheme and the WENO scheme.

As soon as the slope of the solution at $x = 0.5$ is too steep to be resolved by the 4th order scheme, we activate the MUSCL dissipation in the Hybrid scheme. We turn the MUSCL dissipation on at time $t = 0.16$. In Figure 10 the simulations at time $t = 0.2$ are shown. This is after a shock has formed. Again the Hybrid scheme produces a solution that is more accurate than the ones from the MUSCL scheme and the WENO scheme.

(a) Solution

(b) Error

Figure 9: Solution and error from the WENO scheme, the MUSCL scheme and the Hybrid scheme. At this point the Hybrid scheme is identical with the 4th order scheme. Time $t = 0.1$ and $N = 80$.

(a) Solution

(b) Error

Figure 10: Solution and error from the WENO scheme, the MUSCL scheme and the Hybrid scheme. After time $t = 0.16$ the MUSCL dissipation is turned on in the Hybrid scheme, with $w = 10, w_M = 8$. Time $t = 0.2$ and $N = 80$.

(a) Solution

(b) Error

Figure 11: Solution and error from the WENO scheme, the MUSCL scheme and the Hybrid scheme. Time $t = 0.5$ and $N = 80$.

In Figure 11 the simulations at time $t = 0.5$ are shown. By this time the solution is composed by almost straight lines and thus the errors away from the shock are small. The benefits from the Hybrid scheme compared to the MUSCL and WENO schemes are therefore less distinct than before.

The L_2 -norm of the errors in Figure 9 are 0.0022 for the WENO scheme, 0.0027 for the MUSCL scheme and 0.0001 for the Hybrid scheme. In Figure 10, at time $t = 0.2$, the L_2 -errors are 0.0164 for the WENO scheme, 0.0057 for the MUSCL scheme and 0.0022 for the Hybrid scheme, and at time $t = 0.5$ the L_2 -errors are 0.0093 for the WENO scheme, 0.0014 for the MUSCL scheme and 0.0014 for the Hybrid scheme.

As mentioned above the parameters w, w_M can be varied as long as $w_M < w$. In all simulations using the Hybrid scheme we have used $w = 10, w_M = 8$. We have not investigated which is the optimal parameter choice, as long as the MUSCL domain is wide enough to avoid oscillations the choice is not essential.

7. Summary and conclusions

We have developed a stable and conservative way of locally changing the order of a finite difference scheme. The resulting scheme has at least the same overall accuracy as the lowest included scheme.

This procedure serves as a very efficient way of doing accurate calculations even in the presence of shocks. We combine our adaptive accuracy scheme with the MUSCL shock capturing technique and compare the results with the ones obtained using only the MUSCL scheme. We also make a comparison with the results obtained using the third order WENO scheme.

The procedure described in this paper is completely general and can be used on all SBP schemes that have a diagonal norm. The extension to multi-dimensional problems is trivial since the equations are discretized separately in each dimension. By the use of kronecker products, the stability and implementation of the schemes are easily handled. The extension to parabolic equations such as the heat equation can be done, and will be presented in a future paper.

A. The new operators expressed explicitly

The stability requirements on general Summation-By-Parts operators P and Q are given in (3). P_p and Q_p can be designed such that the differential operator $D_p = P_p^{-1}Q_p$ gives p th order of accuracy in the interior and $(p/2)$ th order of accuracy at the boundaries.

Below we present the 2nd, 4th and 6th order Summation-By-Parts operators. First the upper left corner of the norms P_p is shown

$$P_2 = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \end{bmatrix}, \quad P_4 = \Delta x \begin{bmatrix} \frac{17}{48} & & & & & \\ & \frac{59}{48} & & & & \\ & & \frac{43}{48} & & & \\ & & & \frac{49}{48} & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix},$$

$$P_6 = \Delta x \operatorname{diag} \left(\frac{13649}{43200} \quad \frac{12013}{8640} \quad \frac{2711}{4320} \quad \frac{5359}{4320} \quad \frac{7877}{8640} \quad \frac{43801}{43200} \quad 1 \quad \dots \right).$$

The interior of P_p consists of Δx 's and the lower right corner is just a mirror image of the upper left corner.

The upper left corner of the difference operators Q_p is presented below. The interior of the second order scheme is $[-1/2, 0, 1/2]$ in each row on the diagonal and for the fourth order scheme it is $[1/12, -2/3, 0, 2/3, -1/12]$. For the sixth order scheme it is $[-1/60, 3/20, -3/4, 0, 3/4, -3/20, 1/60]$.

$$Q_2 = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & \\ & -\frac{1}{2} & 0 & \ddots \\ & & \ddots & \ddots \end{bmatrix}, \quad Q_4 = \begin{bmatrix} -\frac{1}{2} & \frac{59}{96} & -\frac{1}{12} & -\frac{1}{32} & & \\ -\frac{59}{96} & 0 & \frac{59}{96} & 0 & & \\ \frac{1}{12} & -\frac{59}{96} & 0 & \frac{59}{96} & -\frac{1}{12} & \\ \frac{1}{32} & 0 & -\frac{59}{96} & 0 & \frac{2}{3} & \ddots \\ & \frac{1}{12} & -\frac{2}{3} & 0 & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

$$Q_6 = \begin{bmatrix} -\frac{1}{2} & \frac{104009}{172800} & \frac{30443}{259200} & -\frac{33311}{86400} & \frac{16863}{86400} & -\frac{15025}{518400} & & \\ -\frac{104009}{172800} & 0 & -\frac{311}{51840} & \frac{20229}{17280} & -\frac{24337}{34560} & \frac{36661}{259200} & & \\ -\frac{30443}{259200} & \frac{311}{51840} & 0 & -\frac{11155}{25920} & \frac{41287}{51840} & -\frac{21999}{86400} & & \\ \frac{33311}{86400} & -\frac{20229}{17280} & \frac{11155}{25920} & 0 & \frac{4147}{17280} & \frac{25427}{259200} & \frac{1}{60} & \\ -\frac{16863}{86400} & \frac{24337}{34560} & -\frac{41287}{51840} & -\frac{4147}{17280} & 0 & \frac{342523}{518400} & -\frac{3}{20} & \ddots \\ \frac{15025}{518400} & -\frac{36661}{259200} & \frac{21999}{86400} & -\frac{25427}{259200} & -\frac{342523}{518400} & 0 & \frac{3}{4} & \ddots \\ & & & -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \ddots \\ & & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

The lower right corner of Q_p is a mirror image of the upper left corner but with reversed sign. When applying the procedure developed in this paper we get the adaptive scheme, where the interior of the norm $\tilde{P}_{24}$ looks like

$$\tilde{P}_{24} = \Delta x \operatorname{diag} \left(\begin{bmatrix} \dots & 1 & 1 & \frac{41}{48} & \frac{59}{48} & \frac{43}{48} & \frac{49}{48} & 1 & \dots \end{bmatrix} \right)$$

where $\beta = 41/48 = 1/2 + 17/48 = P_2^N + P_4^0$. The interior of the difference

matrix $\tilde{Q}_{24}$ is

$$\tilde{Q}_{24} = \begin{bmatrix} \ddots & & \ddots & & & & & & & \\ & \ddots & & 0 & \frac{1}{2} & & & & & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} & & & & & \\ & & & -\frac{1}{2} & 0 & \frac{59}{96} & -\frac{1}{12} & -\frac{1}{32} & & \\ & & & & -\frac{59}{96} & 0 & \frac{59}{96} & 0 & & \\ & & & & \frac{1}{12} & -\frac{59}{96} & 0 & \frac{59}{96} & -\frac{1}{12} & \\ & & & & \frac{1}{32} & 0 & -\frac{59}{96} & 0 & \frac{2}{3} & \ddots \\ & & & & & & \frac{1}{12} & -\frac{2}{3} & 0 & \ddots \\ & & & & & & & & \ddots & \ddots & \ddots \end{bmatrix}$$

and the final differential operator becomes

$$\tilde{D}_{24} = \frac{1}{\Delta x} \begin{bmatrix} \ddots & & \ddots & & & & & & & \\ & \ddots & & 0 & \frac{1}{2} & & & & & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} & & & & & \\ & & & -\frac{24}{41} & 0 & \frac{59}{82} & -\frac{4}{41} & -\frac{3}{82} & & \\ & & & & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ & & & & \frac{4}{43} & -\frac{59}{86} & 0 & \frac{59}{86} & -\frac{4}{43} & \\ & & & & \frac{3}{98} & 0 & -\frac{59}{98} & 0 & \frac{32}{49} & -\frac{4}{49} \\ & & & & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & \ddots \\ & & & & & & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

As a second example we show the operators when switching from 6th order to 2nd order. Then the interior of the norm $\tilde{P}_{62}$ looks like

$$\tilde{P}_{62} = \Delta x \operatorname{diag} \left(\left[\dots \quad 1 \quad \frac{43801}{43200} \quad \frac{7877}{8640} \quad \frac{5359}{4320} \quad \frac{2711}{4320} \quad \frac{12013}{8640} \quad \frac{35249}{43200} \quad 1 \quad \dots \right] \right)$$

where $\beta = 35249/43200 = 13649/43200 + 1/2 = P_6^N + P_2^0$. The interior of

the difference matrix $\tilde{Q}_{62}$ is

$$\tilde{Q}_{62} = \begin{bmatrix} \ddots & \ddots & \ddots & \ddots & & & & & \\ \ddots & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} & & & & \\ \ddots & -\frac{3}{4} & 0 & \frac{342523}{518400} & \frac{25427}{259200} & -\frac{21999}{86400} & \frac{36661}{259200} & -\frac{15025}{518400} & \\ \ddots & \frac{3}{20} & -\frac{342523}{518400} & 0 & \frac{4147}{17280} & \frac{41287}{51840} & -\frac{24337}{34560} & \frac{16863}{86400} & \\ & -\frac{1}{60} & -\frac{25427}{259200} & -\frac{4147}{17280} & 0 & -\frac{11155}{25920} & \frac{20229}{17280} & -\frac{33311}{86400} & \\ & & \frac{21999}{86400} & -\frac{41287}{51840} & \frac{11155}{25920} & 0 & -\frac{311}{51840} & \frac{30443}{259200} & \\ & & -\frac{36661}{259200} & \frac{24337}{34560} & -\frac{20229}{17280} & \frac{311}{51840} & 0 & \frac{104009}{172800} & \\ & & \frac{15025}{518400} & -\frac{16863}{86400} & \frac{33311}{86400} & -\frac{30443}{259200} & -\frac{104009}{172800} & 0 & \frac{1}{2} \\ & & & & & & & -\frac{1}{2} & 0 & \ddots \\ & & & & & & & & \ddots & \ddots \end{bmatrix}.$$

The final operator $\tilde{D}_{62}$ is easily obtained by $\tilde{D}_{62} = \tilde{P}_{62}^{-1} \tilde{Q}_{62}$.

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