On coordinate transformations for summation-by-parts operators.

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Abstract

High order finite difference methods obeying a summation-by-parts (SBP) rule are developed for equidistant grids. With curvilinear grids, a coordinate transformation operator that does not destroy the SBP property must be used. We show that it is impossible to construct such an operator without decreasing the order of accuracy of the method.

1 Introduction.

Many problems in computational fluid dynamics (CFD) and computational aero acoustics (CAA) require very accurate spatial resolution to correctly model high frequency phenomena. We will examine properties of a special class of such high order finite difference operators obeying a summation-by-parts rule (SBP-operators) developed by Kreiss and Scherer, [1] and [2]. These norms are of a non-diagonal form. The main advantage of SBP-operators is that they simplify the procedure to obtain energy estimates.

To accurately model the influence of realistic geometries, it is essential to be able to use the SBP-operators on curvilinear grids. In this work accurate coordinate transformation operators are analyzed using the linear advection equation as a model problem.

The contents of this report are divided as follows; in section 2 the linear advection equation is considered and an energy estimate is derived; the equation is discretized on a non-equidistant grid. A general coordinate transformation operator is analyzed in section 3 which also contains numerical experiments. In section 4, conclusions are drawn.

2 The continuous and semi-discrete problem.

Let $\xi(x)$ be a transformation between the x-coordinate and ξ-coordinate and let $x(\xi)$ be the inverse transformation. Then the advection equation,

$$v_t + v_x = 0, \qquad t \geq 0, \qquad a \leq x \leq b, \tag{1}$$

can be written as,

$$x_\xi v_t + v_\xi \;\; = \;\; 0 \quad t \geq 0, \quad 0 \leq \xi \leq 1, \tag{2}$$

since $\xi_x^{-1} = x_\xi$ and $\xi(a) = 0$, $\xi(b) = 1$.

The energy-rate for equation (1) is obtained by multiplying by $v$and integrating over x,

$$\frac{d}{dt}||v||^2 = (v(a,t))^2 - (v(b,t))^2. \tag{3}$$

Equation (2) is discretized on $[0,1]$ with $n+1$ equidistant points indexed from 0 to n. Let the matrix X_ξ^d be such that, $(X_\xi^d)_{ii} = x_\xi(i\Delta\xi), \quad i = 0...n$, on the diagonal and 0 elsewhere. Let u be the approximate solution to v in each grid point, $u(t) = [u_0(t), u_1(t), ..., u_n(t)]^T$. Then the discretized version of equation (2) becomes,

$$X_\xi^d u_t + P^{-1}Qu = 0, \tag{4}$$

where $P^{-1}Q$ is the difference operator on an equidistant grid. P is a norm, i.e. P is a positive definite symmetric $(n+1) \times (n+1)$ matrix and Q, with $Q + Q^T = diag(-1, 0...0, 1)$, is almost skew-symmetric.

In the same manner as in the continuous case, equation (4) is multiplied by $u^T P$ to acquire,

$$u^T P X_\xi^d u_t + u^T Q u = 0.$$

Adding the transpose yields,

$$u^T P X_\xi^d u_t + u_t^T (P X_\xi^d)^T u + u^T (Q + Q^T) u = 0. \tag{5}$$

In general, PX_ξ^d is not a norm since PX_ξ^d is neither positive definite nor symmetric. Thus (5) does not lead to an energy estimate. If PX_ξ^d could be modified to a norm, PX_ξ, equation (5) would be,

$$\frac{d}{dt}(u^T P X_\xi u) + u^T (Q + Q^T) u = 0, \quad or \quad \frac{d}{dt}||u||^2_{PX_\xi} = u_0^2 - u_n^2. \tag{6}$$

i.e. an equation similar to eq (3). Note that if P is diagonal matrix, PX_ξ^d would indeed be a norm since a valid coordinate transformation X_ξ^d is positive definite and diagonal by construction.

3 Analysis.

A general result by Gustafsson (see [3] and [4]), is that in a $\tau + 1$ order approximation, a finite number of points with order of accuracy τ is allowed.

Assume that the accuracy in the interior is $\tau + 1$ and the boundaries are closed with l points at the accuracy of τ. Kreiss and Scherer,[1], [2], showed that for SBP-operators, P can be chosen to be diagonal except at the upper left and lower right corners where blocks, at least of size $l \times l$ are situated. To make equation (6) valid (and make sure that PX_ξ can be used to define a norm) the following conditions must be fulfilled,

$$\begin{aligned} X_\xi &= X_\xi^d + \mathcal{O}(\Delta\xi^p), && (7)\\ v^T P X_\xi v &\geq 0, \quad \text{for all } v \in \mathbf{R}^{n+1} && (8)\\ (PX_\xi)^T &= PX_\xi, && (9) \end{aligned}$$

where $p = \tau$ at s points near the boundaries and $p = \tau + 1$ in the interior.

3.1 Accuracy conditions.

The accuracy conditions (7) are acquired from Taylor expansions. Let X_ξ with components ξ_{ij} be the unknown accurate representation of the diagonal matrix X_ξ^d with components ξ_{ii}^d. X_ξ is diagonal except at the corners where $(s \times s)$ blocks are situated. The diagonal part, being the same as X_ξ^d, automatically satisfies conditions (7)-(9). Thus, only the upper left block will be considered since similar reasoning will directly be applicable to the lower right corner. The upper left block will be indexed $i = 0...s-1, j = 0...s-1$. The grid point considered will be denoted $p \in \{0...s-1\}$. Finally, $\tau + 1$ is the interior accuracy and τ the boundary accuracy.

The accuracy conditions for a point p obtained from Taylor expansion are,

$$\begin{aligned} \sum_{i=0}^{s-1} \xi_{pi}(i-p)^0 &= \xi_p^d && (10)\\ \sum_{i=0}^{s-1} \xi_{pi}(i-p)^1 &= 0 && (11) \end{aligned}$$

$$\sum_{i=0}^{s-1} \xi_{pi}(i-p)^2 = 0 \tag{12}$$

$$\vdots$$

$$\sum_{i=0}^{s-1} \xi_{pi}(i-p)^{\tau-1} = 0. \tag{13}$$

The conditions (10)-(13) can be rewritten to resemble the conditions for $p = 0$ for all p, i.e. we aim for a formulation with p and ξ_p^d on the right hand side and all the unknowns ξ_{pi} on the left hand side. Equation (10) remains unchanged,

$$\sum_{i=0}^{s-1} \xi_{pi} = \xi_p^d. \tag{14}$$

Using (14), equation (11) yields,

$$\sum_{i=0}^{s-1} \xi_{pi}(i-p)^1 = 0 \Rightarrow \sum_{i=0}^{s-1} \xi_{pi} i = \sum_{i=0}^{s-1} \xi_{pi} p = p\xi_p^d. \tag{15}$$

In the same manner, using the two previous results, equation (12) leads to,

$$\sum_{i=0}^{s-1} \xi_{pi} i^2 = -\sum_{i=0}^{s-1} \xi_{pi}(p^2 - 2pi) = -p^2\xi_p^d + 2p \cdot p\xi_p^d = p^2\xi_p^d. \tag{16}$$

Note that the exponent of p is the same as the exponent of i in expressions (14),(15) and (16) which suggests that the accuracy conditions (10) to (13) can be written as,

$$\sum_{i=0}^{s-1} \xi_{pi} i^r = p^r \xi_p^d, \quad r = 0...\tau - 1 \quad \text{for all} \quad p \in \{0...s-1\}. \tag{17}$$

The following lemma states that this is indeed the case for accuracy conditions of arbitrary order.

Lemma 3.1 *Let e_r be the $(n \times 1)$-vector $e_r = (0^r, 1^r, 2^r, ..., (s-1)^r, 0, ..., 0)^T$, where $0^0 = 1$ is taken as a definition. Then, the accuracy conditions (10) to (13) can be written*

$$X_\xi e_r = X_\xi^d e_r, \quad r = 0...\tau - 1, \tag{18}$$

where X_ξ, X_ξ^d are defined at the beginning of the present subsection.

Proof We begin by showing that (17) is true for arbitrary τ. The first two steps are already shown in equations (14)-(16). Then by induction we will show that (17) holds for $k = r + 1$, if it is true for $k = 0...r$. Beginning with an arbitrary point, p, and the $r+1$:th accuracy condition, the following holds,

$$\begin{aligned}
0 &= \sum_{i=0}^{s-1} \xi_{pi}(i-p)^{r+1} = \\
&= \sum_{i=0}^{s-1} \xi_{pi} \sum_{k=0}^{r+1} \binom{r+1}{k} i^{r+1-k}(-p)^k = \\
&= \sum_{i=0}^{s-1} \xi_{pi} \binom{r+1}{0} i^{r+1}(-p)^0 + \sum_{i=0}^{s-1} \xi_{pi} \sum_{k=1}^{r+1} \binom{r+1}{k} i^{r+1-k}(-p)^k = \\
&= \sum_{i=0}^{s-1} \xi_{pi} i^{r+1} + \sum_{i=0}^{s-1} \sum_{k=1}^{r+1} \xi_{pi} \binom{r+1}{k} i^{r+1-k}(-p)^k. \qquad (19)
\end{aligned}$$

Using a standard binomial formula, $\sum_{k=0}^{n} \binom{n}{k}(-1)^k = 0$, which can be restated as $0 = \binom{n}{0} + \sum_{k=1}^{n} \binom{n}{k}(-1)^k$ or $\sum_{k=1}^{n} \binom{n}{k}(-1)^k = -1$ and the induction hypothesis, the last term in (19) can be rewritten as,

$$\begin{aligned}
\sum_{i=0}^{s-1} \sum_{k=1}^{r+1} \xi_{pi} \binom{r+1}{k} i^{r+1-k}(-p)^k &= \sum_{k=1}^{r+1} \xi_p^d p^{r+1-k} \binom{r+1}{k} (-1)^k p^k = \\
&= \xi_p^d p^{r+1} \sum_{k=1}^{r+1} \binom{r+1}{k} (-1)^k = \xi_p^d p^{r+1}(-1). \qquad (20)
\end{aligned}$$

Inserting (20) in (19) shows that (17) holds. The accuracy conditions (17) can by denoting the vector with components $\xi_{pi}, \quad i = 0...s-1$ by (ξ_p) be stated as,

$$(\xi_p)e_r = \xi_p^d p^r, \quad r = 0...\tau - 1, \quad p = 0...s-1. \qquad (21)$$

Since ξ_p^d are the diagonal components of X_ξ^d, equation (18) follows. ∎

The relation (18) refers to the s boundary points but it can naturally be extended to the whole domain since in the interior the modified and the original transformation operators are identical. Thus, by changing the definition of e_r to $e_r = (0^r, 1^r, 2^r, ..., (s-1)^r, 1, 1, ..., 1, (s-1)^r, ..., 2^r, 1^r, 0^r)^T$ equation (18) is valid for the entire domain.

3.2 Observation on coordinate transformations.

The main result of this report is stated in the following theorem.

Theorem 3.2 *It is not possible to construct a coordinate transformation operator X_ξ such that PX_ξ can be used to define a norm and keep the order of accuracy for $\tau + 1 \geq 3$ with a non-constant X_ξ^d.*

Observe that for $\tau + 1 \leq 2$ there are SBP-operators with diagonal norms. Thus $X_\xi = X_\xi^d$ with values only on the diagonal will satisfy all conditions.

For $\tau + 1 \geq 3$, blocks are needed in P to obtain the desired accuracy according to Kreiss and Scherer ([1], [2]). Let $\rho_{ij} = e_i^T P X_\xi e_j$ be the components of the matrix $R = E^T P X_\xi E$ where $E = (e_0 \quad e_1 \quad ... \quad e_{\tau-1})$. In the proof below, symmetry properties of the auxiliary matrix R is examined to obtain a contradiction.

Proof Suppose that $PX_\xi = (PX_\xi)^T$ then

$$\rho_{ij} = e_i^T P X_\xi e_j = e_i^T (P X_\xi)^T e_j = e_j^T P X_\xi e_i = \rho_{ji}. \tag{22}$$

That is, for PX_ξ symmetric, R is also symmetric. Next note that for a block norm P, $PX_\xi^d \neq (PX_\xi^d)^T$ for a non-constant X_ξ^d, since the commutator $[PX_\xi^d - (PX_\xi^d)^T]_{ij} = P_{ij}(\xi_i^d - \xi_j^d) \neq 0$ for $i \neq j$. Using the accuracy condition in lemma 3.1 leads to,

$$\rho_{ij} = e_i^T P X_\xi e_j = [(18)] = e_i^T P X_\xi^d e_j \neq \rho_{ji} = e_j^T P X_\xi^d e_i, \tag{23}$$

i.e. R is not symmetric which means that the accuracy result (23), contradicts the symmetry result (22). ∎

Corollary 3.3 *PX_ξ is a norm if and only if P is diagonal. Then, X_ξ^d can be used as X_ξ.*

Proof If P is diagonal then P commutes with X_ξ^d in (23) such that $\rho_{ij} = \rho_{ji}$. Further, if $X_\xi = X_\xi^d$, the conditions (7)-(9) are satisfied. If PX_ξ is a norm then the commutator $[PX_\xi^d - (PX_\xi^d)^T]_{ij} = P_{ij}(\xi_i^d - \xi_j^d) = 0$. Thus, $P_{ij} = 0$ for $i \neq j$. ∎

3.3 Numerical examination of eigenvalues.

The absence of an energy estimate does not necessarily mean that the scheme is unstable, in fact, for long times the location of the eigenvalues are more

important. Consider the following system for $u(x,t)$ and $v(x,t)$,

$$\begin{aligned} u_t + \xi_x u_\xi = 0, \quad & 0 < x < L, \quad u(0,t) = v(1,t), \\ v_t + \xi_x v_\xi = 0, \quad & 0 < x < L, \quad v(0,t) = u(1,t), \\ u(x,0) = f(x), \quad & v(x,0) = g(x). \end{aligned} \tag{24}$$

The eigenvalues of (24) can be acquired using the Laplace transform technique (cf [5]). After Laplace transformation of (24) with homogeneous initial conditions and $L = 1$ we get,

$$\begin{aligned} s\hat{u} + \hat{u}_x = 0, \quad \hat{u}(0) = \hat{v}(1) \\ s\hat{v} + \hat{v}_x = 0, \quad \hat{v}(0) = \hat{u}(1) \end{aligned} \tag{25}$$

The ansatz $\hat{u} = c_1 e^{\kappa_1 x}$, $\hat{v} = c_2 e^{\kappa_2 x}$ yields, $\kappa_1 = \kappa_2 = -s$. Inserting the ansatz in the boundary conditions leads to,

$$\begin{pmatrix} 1 & -e^{-s} \\ e^{-s} & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{26}$$

The only non-trivial solutions are $e^{-2s} = 1$, yielding, $s = n\pi i$, $n \in \mathbf{N}$. Since $Re(s) = 0$, the solution should neither increase nor decrease.

In the computations below the boundaries will be treated with the penalty method, see [6], [7]. The discrete counterpart of (24), where $u(t)$ and $v(t)$ are the vectors corresponding to $u(x,t)$ and $v(x,t)$, is,

$$u_t + X_\xi^{-1} P^{-1} Q u = \sigma_1 P^{-1}(e_0(u_0 - v_n), \tag{27}$$

$$v_t + X_\xi^{-1} P^{-1} Q v = \sigma_2 P^{-1}(e_0(v_0 - u_n)), \tag{28}$$

where the right hand side are the penalty terms and $e_0 = (1, 0...0)$. Since PX_ξ is not a norm, the analysis has to be carried out for an equidistant grid. Applying the energy method to this problem with $X_\xi = I$, is done by multiplying (27) and (28) by $u^T P$ and $v^T P$ respectively, yielding,

$$u^T P u_t + u^T Q u = \sigma_1 u^T (e_0(u_0 - v_n), \tag{29}$$

$$v^T P v_t + v^T Q v = \sigma_2 v^T (e_0(v_0 - u_n)). \tag{30}$$

Add to each equation its transpose and rearrange the terms,

$$\frac{d}{dt}||u||_P^2 = -u_n^2 + (\sigma_1 + 1)u_0^2 + \sigma_1(u_0 - v_n)^2 - \sigma_1 v_n^2, \tag{31}$$

$$\frac{d}{dt}||v||_P^2 = -v_n^2 + (\sigma_2 + 1)v_0^2 + \sigma_2(v_0 - u_n)^2 - \sigma_2 u_n^2. \tag{32}$$

Adding the two equations, yields,

$$\frac{d}{dt}||u||_P^2 + \frac{d}{dt}||v||_P^2 = \begin{pmatrix} u_0 & v_n \end{pmatrix} \begin{pmatrix} 2\sigma_1 + 1 & -\sigma_1 \\ -\sigma_1 & -1 \end{pmatrix} \begin{pmatrix} u_0 \\ v_n \end{pmatrix} + \begin{pmatrix} v_0 & u_n \end{pmatrix} \begin{pmatrix} 2\sigma_2 + 1 & -\sigma_2 \\ -\sigma_2 & -1 \end{pmatrix} \begin{pmatrix} v_0 \\ u_n \end{pmatrix} \tag{33}$$

Both matrices should be negative semi-definite for stability. Thus, the only solution is $\sigma_{1,2} = -1$. Next, reformulate (27) and (28) as, $w_t = Gw$, where $w = (u^T \quad v^T)^T$.

We will examine a quadratic polynomial coordinate transformation for $\xi \in [0, 1]$. Let $x(\xi) = c_0 + c_1\xi + c_2\xi^2$, then $x'(\xi) = c_1 + 2c_2\xi$. To avoid the rescaling of σ_1 and σ_2, $x_\xi^{-1}(0) = 1$ has been chosen, see equations (27) and (28). Note that $x'(0) = 1$ gives $c_1 = 1$.

Further, c_2 is obtained by considering the first few points. The choice, $\Delta x_2 = 1.1\Delta x_1$ or $x(\xi_2) - x(\xi_1) = 1.1(x(\xi_1) - x(\xi_0))$ is a reasonable stretching for a grid around an airfoil. This condition gives $c_2 = \frac{0.1}{1.9\Delta\xi}$ where $\Delta\xi$ is the step size on the ξ-grid. These coefficients have been used in G together with a fourth order accurate block norm difference operator, $P^{-1}Q$, displayed in Appendix I. The eigenvalues of G, $\lambda(G)$, are shown in table 1 ($n + 1$ refers to the number of grid points.). The eigenvalues of the continuous problem have zero real part so the eigenvalues of G are expected to be non-positive.

$n+1$	$max(Re(\lambda(G)))$	number of positive eigenvalues
20	$3.2 \cdot 10^{-4}$	5
50	$2.4 \cdot 10^{-4}$	12
100	$7.2 \cdot 10^{-5}$	16

Table 1: Grid transformation with 10% initial stretching.

Next a fixed grid transformation with $c_2 = 1$ is considered and more points are added, see table 2.

$n+1$	c_2	$max(Re(\lambda(G)))$	number of positive eigenvalues
20	1	$3.6 \cdot 10^{-4}$	6
100	1	$5.0 \cdot 10^{-5}$	25
150	1	$1.9 \cdot 10^{-5}$	34

Table 2: Largest real part of the eigenvalues for a fixed grid transformation.

Both in table 1 and 2 there are significant positive eigenvalues. However, these eigenvalues are close to the continuous spectrum and their convergence rate are $3.7 - 4.0$. Further, the convergence rate of the maximum real part of all eigenvalues for each n is approximately 2 for $n + 1 = 50...170$. Thus, this scheme is formally strictly stable, i.e. the time growth of the discrete problem agrees with the continuous problem within an $\mathcal{O}(h)$ error, cf [5]. In table 3 the effect of increasing the stretching with n fixed is shown.

$n+1$	stretching	c_2	$max(Re(\lambda(G)))$	number of positive eigenvalues
50	4 %	1	$1.9 \cdot 10^{-4}$	15
50	18%	5	$2.4 \cdot 10^{-4}$	13
50	33%	10	$2.5 \cdot 10^{-4}$	12

Table 3: Largest real part of the eigenvalues for a grid with increasing stretching.

As a reference, table 4 shows the utmost right eigenvalue for the block norm scheme on an equidistant grid. These are zero to the order of the round off error.

$n+1$	$max(Re(\lambda(G)))$	number of positive eigenvalues
20	$1.4 \cdot 10^{-15}$	1
50	$2.4 \cdot 10^{-15}$	1
100	$3.6 \cdot 10^{-15}$	1
150	$1.2 \cdot 10^{-15}$	3

Table 4: Largest real part of the eigenvalues for the equidistant case ($c_2 = 0$).

For a diagonal norm corresponding to the third order accurate difference operator seen in Appendix II on a non-equidistant grid, the eigenvalues should be non-positive to round off errors. This is verified in table 5.

$n+1$	$max(Re(\lambda(G)))$
20	$-1.0 \cdot 10^{-15}$
50	$3.1 \cdot 10^{-15}$
100	$-6.0 \cdot 10^{-17}$
150	$3.3 \cdot 10^{-15}$

Table 5: Largest real part of the eigenvalues for a diagonal norm scheme with 10% stretching.

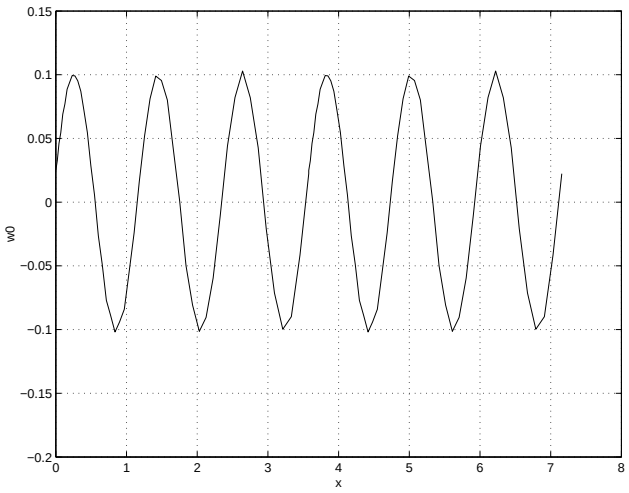

Figure 1: The initial function w0(x).

3.4 Numerical simulations.

The eigenvalue analysis indicates that in both the block norm and diagonal norm cases stability is achieved and to check this, the system (27) and (28) was implemented and integrated in time on a grid with 50 points and 10% stretching. That is, $\xi \in [0, 1]$ and $x \in [0, 3.58]$. First, a fourth order block norm scheme (see Appendix I) was used. The mode associated with the eigenvalue with the largest real part, λ is used as initial data. The initial function has been integrated using a fourth order Runge-Kutta method, until it theoretically should have increased by 20%. That is $e^{\lambda t_{end}} = 1.2$ yielding $t_{end} = ln(1.2)/\lambda$. Figure 1 shows the initial mode in the physical space $x(\xi)$. v is inserted after u on the x-axis instead of on the same interval as u (This is the case in all figures.). Figure 2 shows the solution at $t_{end} = 783$ computed with a fourth order scheme with block norm. Figure 3 shows the maximal amplitude normalized with the initial amplitude as a function of time. The amplitude has grown about 18%, ie close to the predicted 20%.

Next, the corresponding computations were made using a third order diagonal norm scheme (Appendix II). The initial data is the same as for the previous example. Figure 4 shows the solution at $t = t_{end}$ and figure 5 shows the relative amplitude for long times. The final amplitude, at $t = 2000$, in figure 5 has decreased to approximately 17% of the initial value and to about 50% at $t = 783$.

The computations using a diagonal norm are dissipative. As a reference the block norm scheme were run on an equidistant grid, with $n + 1 = 50$ points and the same initial data. Then the relative amplitude has decreased

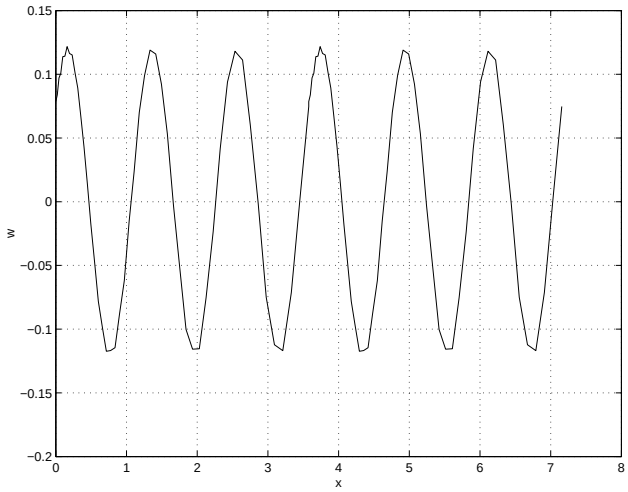

Figure 2: The solution, w, at $t = 783$ computed with a fourth order block norm scheme.

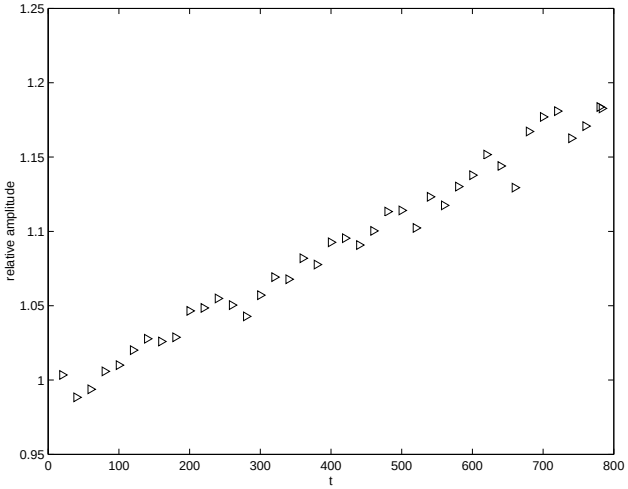

Figure 3: The relative amplitude (Normalized with the amplitude at $t = 0$.) as a function of time computed with a fourth order block norm scheme.

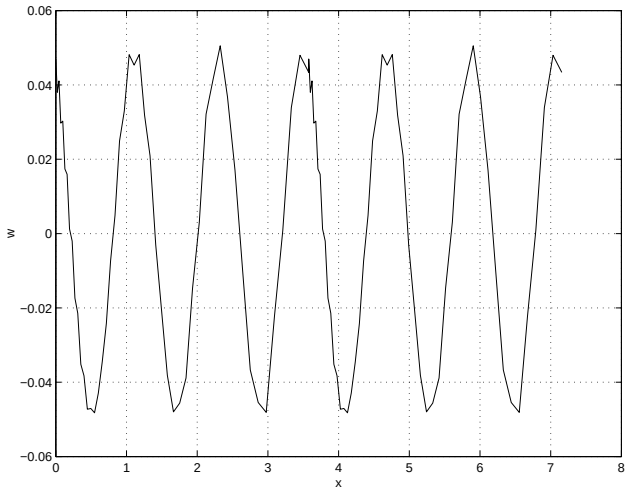

Figure 4: The solution, w, at $t = 783$ computed with a third order diagonal norm scheme.

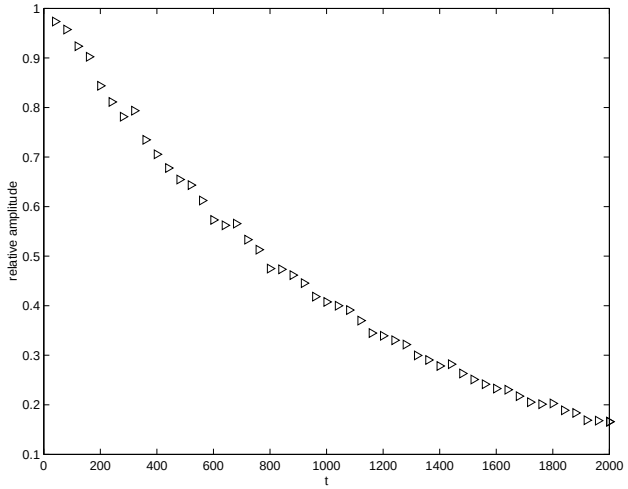

Figure 5: The relative amplitude (Normalized with the amplitude at $t = 0$.) as a function of time, computed with a third order diagonal norm scheme.

approximately 0.3% at $t = 2000$. In the cases with stretching, the grid on a part of the domain is too coarse. There, the mode is not well resolved. Adding more grid points makes the eigenvalues converge. This is verified by computations where the time growth get closer to the analytical.

4 Conclusions.

The objective of this work was to study how coordinate transformations influence high order SBP schemes and if possible, construct an accurate SBP preserving coordinate transformation operator. But, as is stated in theorem 3.2, the conditions for a sufficiently accurate SBP preserving coordinate operators are not possible to fullfil. Thus, either the stability or the accuracy conditions must be relaxed.

If the accuracy conditions are kept (using a block norm) there is no systematic way of proving stability and the location of the eigenvalues has to be checked for each problem. Further, there is nothing that guarantees stability when the number of grid points are increased.

If the accuracy conditions are relaxed, a diagonal norm scheme was shown to be the only choice that fullfil the remaining stability conditions making it possible to treat the boundaries in a stable and systematic manner.

The block norm scheme allows for an unphysical growth. In our opinion it is better that unresolved modes slowly dissipate than grow. Therefore the diagonal norm scheme is the prefered choice.

APPENDIX

I Fourth order accurate block norm operators.

The discrete norm H is,

$$H = \frac{1}{h} \begin{bmatrix} H11 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & H22 \end{bmatrix},$$

where h denotes the spatial step and,

$$H11 = \begin{bmatrix} h11 & h12 & h13 & h14 \\ h12 & h22 & h23 & h24 \\ h13 & h23 & h33 & h34 \\ h14 & h24 & h34 & h44 \end{bmatrix}$$

$$H22 = \begin{bmatrix} h44 & h34 & h24 & h14 \\ h34 & h33 & h23 & h13 \\ h24 & h23 & h22 & h12 \\ h14 & h13 & h12 & h11 \end{bmatrix}.$$

The values are,

$$
\begin{aligned}
h11 &= -\frac{1}{60}\, r2 - 1/6\, r1 + \frac{425}{2592},\\
h12 &= \frac{3}{20}\, r2 + 5/4\, r1 + \frac{89}{108},\\
h13 &= -1/20\, r2 - 1/2\, r1 - \frac{89}{288},\\
h14 &= -1/12\, r2 - \frac{7}{12}\, r1 - \frac{421}{1296},\\
h22 &= -\frac{19}{20}\, r2 - 15/2\, r1 - \frac{2245}{864},\\
h23 &= \frac{17}{20}\, r2 + \frac{27}{4}\, r1 + \frac{1459}{432},\\
h24 &= -1/20\, r2 - 1/2\, r1 - \frac{131}{864},\\
h33 &= -\frac{19}{20}\, r2 - 15/2\, r1 - \frac{2557}{864},\\
h34 &= \frac{3}{20}\, r2 + 5/4\, r1 + \frac{67}{108},\\
h44 &= -\frac{1}{60}\, r2 - 1/6\, r1 + \frac{2417}{2592},
\end{aligned}
$$

where

$$
\begin{aligned}
r1 &= -\frac{2177}{25488}\sqrt{295369} + \frac{43201}{944}\\
r2 &= \frac{7355}{11328}\sqrt{53}\sqrt{5573} - \frac{35909375}{101952}.
\end{aligned}
$$

The discrete fourth order accurate difference operator approximating the derivative is $D = H^{-1}Q$, where Q is given by,

$$
Q = \begin{bmatrix}
q11 & q12 & q13 & q14 & & & & & \\
-q12 & q22 & q23 & q24 & & & & & \\
-q13 & -q23 & q33 & q34 & -1/12 & & & & \\
-q14 & -q24 & -q34 & q44 & 2/3 & -1/12 & & & \\
 & & 1/12 & -2/3 & 0 & 2/3 & -1/12 & & \\
 & & & 1/12 & -2/3 & q44 & q34 & q24 & q14 \\
 & & & & 1/12 & -q34 & q33 & q23 & q13 \\
 & & & & & -q24 & -q23 & q22 & q12 \\
 & & & & & -q14 & -q13 & -q12 & q11,
\end{bmatrix},
$$

with the following values,

$$
\begin{aligned}
q11 &= -1/2, \\
q12 &= -1/5\, r2 - 3/2\, r1 - \frac{61}{864}, \\
q13 &= 2/5\, r2 + 3\, r1 + \frac{145}{108}, \\
q14 &= -1/5\, r2 - 3/2\, r1 - \frac{667}{864}, \\
q23 &= -3/5\, r2 - 9/2\, r1 - \frac{463}{288}, \\
q24 &= 2/5\, r2 + 3\, r1 + \frac{83}{54}, \\
q34 &= -1/5\, r2 - 3/2\, r1 - \frac{157}{864}.
\end{aligned}
$$

II Third order accurate diagonal norm operators.

The discrete norm H is given by,

$$
H = \frac{1}{h}\begin{bmatrix}
\frac{17}{48} & & & & & & & & & & \\
& \frac{59}{48} & & & & & & & & & \\
& & \frac{43}{48} & & & & & & & & \\
& & & \frac{49}{48} & & & & & & & \\
& & & & 1 & & & & & & \\
& & & & & \ddots & & & & & \\
& & & & & & 1 & & & & \\
& & & & & & & \frac{49}{48} & & & \\
& & & & & & & & \frac{43}{48} & & \\
& & & & & & & & & \frac{59}{48} & \\
& & & & & & & & & & \frac{17}{48}
\end{bmatrix},
$$

Where h denotes the spatial step.

The discrete third order accurate difference operator approximating the

derivative is $D = H^{-1}Q$, where Q is defined,

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

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