Stable and high-order accurate finite difference schemes on singular grids

By M. Svärd and E. van der Weide

1. Motivation and objectives

The use of finite difference methods on curvilinear grids is an established computational method and the technique has been thoroughly analyzed with respect to accuracy and stability. However, coordinate mappings are usually assumed to be smooth and topology conserving, such that a smooth mapping to a square grid exists. For practical applications it is not always possible to construct grids with these properties and singularities are sometimes present in the metric coefficients. Yet, it is desirable to have a robust computational method on such grids and obtain high-quality solutions.

In particular, we will study the grid shown in Figure 1, which we will refer to as the circle segment. The circle segment can be viewed as the mapping from a Cartesian grid where one side is collapsed into a point.

We will use a certain kind of finite difference schemes satisfying a summation-by-parts (SBP) rule. In combination with the Simultaneous Approximation Term technique (SAT), these schemes can be proven stable using energy estimates. The SAT technique use penalty terms to impose the boundary conditions weakly. (For SBP-SAT theory see Carpenter et al. 1994; Carpenter & Nordström 1999; Kreiss & Scherer 1974; Mattsson et al. 2006; Nordström & Carpenter 1999; Strand 1994; Svärd 2004; Svärd & Mattsson 2005; Svärd & Nordström 2006.) For such schemes, we will propose two different ways to recover design order accuracy despite singularities in the grid. The first is designed for SBP-SAT schemes and can be used at boundaries where boundary conditions are supplied. The other can be applied to any boundary and any stable finite difference scheme.

2. Summation-by-parts discretization

Before studying singular grid transformations, we introduce the basic concepts of SBP-SAT schemes. Discretize $0 \leq x \leq 1$ using $N+1$ evenly distributed grid points with spacing $h$. Introduce the scalar grid function $v(t) = (v_0(t), \ldots, v_N(t))^T$. Then the first derivative is approximated by $P^{-1}Qv$, where $P$ is a positive definite (symmetric) matrix. $P$ is used to define a discrete $l_2$ equivalent norm, $\|v\|^2_P = v^TPv$. In our particular schemes $P$ is diagonal, which is a necessary requirement for stability on curvilinear grids. (See Svärd 2004.) $Q$ is skew-symmetric almost everywhere and $Q + Q^T = diag(-1, 0, \ldots, 0, 1) = B$. In two space dimensions, we use a subscript $x$ or $y$ to distinguish between operators in the respective directions.

As a model problem for the non-linear two-dimensional Euler equations, we consider,

$$u_t + a(x,y)u_x + b(x,y)u_y = 0, \quad 0 \leq x, y \leq 1, \quad t \geq 0,$$

where $a(x,y), b(x,y) > 0$. The equation is subject to the following boundary conditions,

$$u(0,y,t) = g_1(y,t), \quad u(x,0,t) = g_2(x,t).$$
We discretize the equation using $N$ points in the x-direction and $M$ in the y-direction. We denote the grid sizes by $h_x = 1/N$ and $h_y = 1/M$. Let $v_{ij}(t)$ be the approximate solution of $u(x_i, y_j, t)$ and $v$ be the vector $v = (v_{00}, v_{20}, ..., v_{NM})$. Define $a_{ij} = a(x_i, y_j)$ and $b_{ij} = b(x_i, y_j)$ and distribute $a_{ij}$ and $b_{ij}$ on the diagonal of a matrix in the same way $v_{ij}$ was distributed. Denote the resulting matrices $A$ and $B$. The discretization of (2.1) can be written.

$$v_t + A(I \otimes D_x)v + B(D_y \otimes I)v = 0$$

(2.2)

where $E_{0y} = (v_{0,0}, ..., v_{N,0})^T$, $E_{0x} = (v_{0,0}, 0, 0, ..., v_{0,M}, 0, 0)$. The symbol $\otimes$ denotes the Kronecker product. Moreover, $G_1$ and $G_2$ are vectors with $(G_1)_{0j} = g_1(y_j, t)$ and $(G_2)_{0j} = g_2(x_i, t)$ and 0 elsewhere.

To prove stability, we freeze the coefficients in $A$ and $B$ (and denote the respective scalars by $a$ and $b$) and apply the energy method by multiplying by $v^T(P_y \otimes P_x)$,

$$\tau_1(I \otimes P^{-1}E_{0x})(v - G_1) + \tau_2(P^{-1}E_{0y} \otimes I)(v - G_2)$$

(2.3)

In (2.3) we have introduced the norm $\|v\|_{P_{xy}}^2 = v^T(P_y \otimes P_x)v$. Assuming homogeneous data, $\tau_1 \leq -a/2$ and $\tau_2 \leq b/2$ guarantees stability.

In this article, we will use two different schemes. The first is the commonly used central second-order stencil with a first order boundary closure. We will refer to this schemes as the 2-1 method. The other is the standard central difference fourth-order accurate scheme with a specific second-order boundary closure that enforces the SBP property. This scheme is called the 4-2 method. In both cases the norm $P$ is diagonal and the precise form of operators ($P$ and $Q$) can be found in Strand (1994).
Consider,

\[ u_t + au_x + bu_y = 0. \quad (2.4) \]

Assume \(0 \leq a \leq 1\) and \(b = -\sqrt{1-a^2}\). The exact solution is, \(u(x,t) = \sin(ax + by - t)\). Introduce \(x = x(\xi, \eta), y = y(\xi, \eta)\). Then (2.4) can be written as,

\[ u_t + a(\xi_x u_\xi + \eta_x u_\eta) + b(\xi_y u_\xi + \eta_y u_\eta) = 0 \quad (2.5) \]

We define \(J = (x_\xi y_\eta - x_\eta y_\xi)\) and obtain,

\[ J\xi_x = y_\eta, \quad J\xi_y = -x_\eta, \quad J\eta_x = -y_\xi, \quad J\eta_y = x_\xi, \quad J = (\xi_\xi \eta_\eta - \xi_\eta \eta_\xi)^{-1}. \]

In the case of the circle segment (Figure 1) we have \(\xi\) and \(\eta\) being the polar coordinates \(r\) and \(\theta\) with the transformation \((x,y) = (r\cos(\theta) + 0.5, r\sin(\theta))\), \(r = [0,1], \theta = [0, \pi/4]\). In this case, \(\frac{\partial r}{\partial \xi} \sim 1, \frac{\partial r}{\partial \eta} \sim 1, \frac{\partial \theta}{\partial \xi} \sim \frac{1}{r}, \frac{\partial \theta}{\partial \eta} \sim \frac{1}{r}\). We rewrite equation (2.5),

\[ u_t + \hat{a}u_\xi + \hat{b}u_\eta = 0, \quad \hat{a} = a\xi_x + b\xi_y, \quad \hat{b} = a\eta_x + b\eta_y. \quad (2.6) \]

Equation (2.6) is now a variable coefficient problem in \(\xi, \eta\)-space and we wish to employ the same discretization technique as for (2.1). However, \(\hat{a}\) and \(\hat{b}\) may now be singular.

We will study the effect of the following approximation. At the singular point, approximate the indefinite metric coefficients with the coefficients of non-singular neighbors. This is a first-order approximation of the metrics and the truncation error of the approximation of the equation reduces to first order at that point.

For the circle segment (Figure 1), we note that the transformation from the square makes \(x = 0.5, y = 0\) a multi-valued point, since all the points on that side collapse to one. Let \((x(i,j), y(i,j)), i = 0...N, j = 0...M\) be a grid point. Then \((x(0,j), y(0,j)) = (x(0,k), y(0,k))\) for any valid combination \(j, k\). With that notation, we choose,

\[ y_\eta(x(0,j), y(0,j)) = y_\eta(x(1,j), y(1,j)), \quad x_\eta(x(0,j), y(0,j)) = x_\eta(x(1,j), y(1,j)). \]

3. Analysis

To study the basic mechanisms of singular coordinate transformations, we consider the one-dimensional problem,

\[ u_t + u_x = 0, \quad t \geq 0, \quad 0 \leq x \leq \infty. \quad (3.1) \]

Introduce a coordinate transformation \(x = \xi(x)\) such that,

\[ u_t + \xi_x u_\xi = 0, \quad t \geq 0, \quad 0 \leq \xi \leq 2. \quad (3.2) \]

Let \(x = \xi^2/2\) such that \(\xi_x = \xi\). Furthermore, \(\xi_x = \xi^{-1} = \frac{1}{\xi}\). This motivates the study of the following problem,

\[ u_t + \frac{1}{x} u_x = 0, \quad t \geq 0, \quad 0 \leq x \leq \infty. \quad (3.3) \]

In this case the coefficient in front of \(u_x\) becomes singular as \(x \to 0\). However, in the circle segment case it is the coefficient in front of the \(u_\eta\) that becomes singular as \(r \to 0\). This fact suggests that also the following model problem is relevant to analyze.

\[ u_t + \frac{1}{y} u_x = 0, \quad t \geq 0, \quad 0 \leq x, y \leq \infty. \quad (3.4) \]
We will also study,

\[ u_t + au_x = 0, \quad t \geq 0, \quad 0 \leq x \leq \infty, \quad a > 0, \quad (3.5) \]

which will give us insight in the properties of the penalty imposition of boundary conditions. Equation (3.5) will be referred to as Model Problem 1, since it is the simplest to analyze. Moreover, (3.3) is denoted Model Problem 2 and (3.4) Model Problem 3.

3.1. Model problem 1

Consider (3.5) and assume that \( u \to 0 \) sufficiently fast as \( x \to \infty \). We use the exact solution \( u(x,t) = \sin(ax-t) \) to provide initial and boundary data. We discretize using the SBP-SAT methodology.

\[ v_t + aP^{-1}Qv = \tau P^{-1}E_0(v-g) \quad (3.6) \]

where \( E_0 = \text{diag}(1,0,...,0) \). Assuming homogeneous data, the energy estimate becomes,

\[ (\|v\|^2_{P^0})_t - av_0^2 + av_0^2 = 2\tau v_0^2. \quad (3.7) \]

For \( \tau \leq -a/2 \) the scheme is stable. The 2-1 scheme can be proven to have a globally second-order convergence rate and the 4-2 third order. (See Gustafsson 1975, 1981; Svärd & Nordström 2006.) We define the convergence rate, \( q = \|\log(e_1/e_2)/\log(h_1/h_2)\| \) where \( e_1 \) and \( e_2 \) are the errors (in an appropriate norm) on two different grids with grid sizes \( h_1 \) and \( h_2 \). The numerical solution using the two different schemes are computed using the standard fourth-order explicit Runge-Kutta scheme in time, with a time step small enough for the temporal errors to be negligible. (Correct convergence rates have been shown for these schemes.) Our proposed remedy, for the coordinate singularity was to make a first-order approximation of the metric coefficients, i.e. to lower the accuracy of the approximation of the partial differential equations at that point. To model that, we add an order 1 error (a constant \( c \)) to the equations at the boundary point. The stability properties are not changed by the addition of a lower order term. According to classical theory Gustafsson (1975, 1981), the resulting order of accuracy should be 1.

We will now analyze this case in detail. Let \( u \) be the exact solution and define the error \( e_k(t) = u(x_k,t) - v_k(t) \) and the vector \( e = (e_1,e_2,...)^T \). Then the error equation is,

\[ e_t + aP^{-1}Qe = \tau P^{-1}E_0(e-0) + T, \]

where \( T \) is the truncation-error vector with the constant \( c \) at the boundary point included. Hence, \( T = (O(1),O(h^2),...)^T \). Next, we split the truncation error into two parts, \( T = T_i + T_b \), where \( T_i = (O(1),0,...)^T, T_b = (0,O(h^2),...)^T \). Correspondingly, we let \( e = e_i + e_b \) and split the problem into,

\[ (e_i)_t + aP^{-1}Qe_i = \tau P^{-1}E_0(e_i-0) + T_i, \quad (3.8) \]

\[ (e_b)_t + aP^{-1}Qe_b = \tau P^{-1}E_0(e_b-0) + T_b, \quad (3.9) \]

Note that, \( e_i \) and \( e_b \) are in general non-zero everywhere since there is usually a strong coupling between the interior and the boundary. It follows directly from the energy estimate of (3.8) that \( e_i \) is of order \( T_i \), i.e. second-order in this case. Let \( (P^{-1})_{00} = (hp)^{-1} \) where \( p \) is a constant. (\( p = 1/2 \) for the 2-1 scheme and \( p = 17/48 \) for the 4-2 scheme.)
Table 1. Errors and convergence rates at $t = 0.1$ for the 2-1 discretization of the advection equation with $a = 1$ and zeroth-order boundary error.

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<th>$N$</th>
<th>$l_2$-error</th>
<th>$q_2$</th>
<th>$l_{\infty}$-error</th>
<th>$q_{\infty}$</th>
<th>$l_2$-error</th>
<th>$q_2$</th>
<th>$l_{\infty}$-error</th>
<th>$q_{\infty}$</th>
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For $\hat{e}_b$ we proceed by Laplace transforming (3.9).

\[
\begin{align*}
  s(\hat{e}_b)_i + a \frac{(\hat{e}_b)_{i+1} - (\hat{e}_b)_{i-1}}{2h} &= (\hat{T}_b)_i = 0, \quad i \geq 1 \\
  s(\hat{e}_b)_0 + a \frac{(\hat{e}_b)_1 - (\hat{e}_b)_0}{h} &= \tau \frac{(\hat{e}_b)_0}{ph} + (\hat{T}_b)_0, 
\end{align*}
\]

(3.10)

We make the following ansatz, $(\hat{e}_b)_i = \sigma \kappa^i$ and define $\hat{s} = sh/a$. At the left boundary all $\kappa$ with $|\kappa| < 1$ for $Re \hat{s} > 0$ should be supplied with boundary conditions. If $\sigma$ is bounded for $Re \hat{s} \geq 0$ the scheme is stable. (See Gustafsson et al. 1995.) We use the ansatz in (3.10) and obtain $\kappa = -\frac{\hat{s}}{a} \pm \sqrt{\frac{\hat{s}^2}{a^2} + 1}$ It can be shown that $\kappa_1 = -\frac{\hat{s}}{a} + \sqrt{\frac{\hat{s}^2}{a^2} + 1} < 1$, for $Re \hat{s} > 0$. We use the definition that the square root denotes the value with positive real part. (In this case $\sigma_2 = 0$ corresponding to $\kappa_2$ due to the fall-off condition of $u$. Otherwise, it is bounded by the right boundary condition.) We insert $(\hat{e}_b)_i = \sigma_1 \kappa_1^i$ in (3.11), and use the expression for $\kappa_1$,

\[
\sigma_1 (\sqrt{\frac{\hat{s}^2}{a^2} + 1} - 1 - \frac{\tau}{ap}) = \frac{h(\hat{T}_b)_0}{a}.
\]

Denote the resolvent $R = (\sqrt{\frac{\hat{s}^2}{a^2} + 1} - 1 - \frac{\tau}{ap})$. For $Re \hat{s} \geq 0$ we have that $Re \sqrt{\frac{\hat{s}^2}{a^2} + 1} \geq 0$. Hence, $\sigma_1 \neq 0$ if $-1 - \frac{\tau}{ap} > 0$, i.e. $\tau < -a/2$. This is in full agreement with the stability analysis using the energy estimate. Choosing $\tau = constant < -a/2$ implies that $R$ is of order 1 and $\sigma_1 \sim \frac{h(\hat{T}_b)_0}{a}$. If $(\hat{T}_b)_0$ is of order $h$ we have $\sigma_1 \sim h^2$. Hence, $\hat{e}_b \sim h^2$. Transforming back using Parseval’s relation, we obtain that $\hat{e}_b$ is second-order accurate. This is the classical result that a scheme is allowed to be closed with 1 order less accuracy at the boundary without degrading the global accuracy. (See Gustafsson 1975, 1981 and also Svärd & Nordström 2006.)

In our example, $(\hat{T}_b)_0 \sim 1$ implying that $\hat{e}_b$ and consequently $e_b$ is $O(h)$. In Table 2 this case is computed, corroborating the expected first-order convergence rate. We use $c = 0.1$ as the order 1 error, $a = 1$, $\tau = -a$.

Next, we consider the case $\tau = -a/(h^p) < -a$. Now, $R \sim 1/(h^p)$ and $\sigma \sim h^{p+1}(\hat{T}_b)_0$. In our case with zeroth-order boundary closure and $p = 1$ we recover second-order global accuracy, see Table 1. Of course, there is little to gain by choosing a larger $p$ since the global order of accuracy is also limited by the interior accuracy. To show that these conclusions carry over to high-order finite difference methods, we compute a similar
example using the 4-2 scheme. For the 4-2 scheme, we add, 0.1h to the first point in the
scheme, i.e. a first-order error, and compute the solution with different scalings of the
penalty term, see Table 2. As expected the convergence rate drops to 2 with τ = a.
Third-order convergence it recovered for τ = a/h.

3.2. Model problem 2
The previous example shows a fundamental phenomenon that order of accuracy may be
increased via a stronger enforcement of the penalty boundary conditions. However, we
assumed that a(x) = a and we may only claim that the analysis holds for a case where
a(x) is smooth. But, in the coordinate transformation case the a(x) becomes singular.
Hence, we continue our analysis and consider Model Problem 2 (3.3) and observe that

\begin{equation}
\frac{\partial u}{\partial t} + AP^{-1}Qv = \tau P^{-1}E_0(v - g)
\end{equation}

Since A^{-1} and P are diagonal and positive definite, we can define a norm \( \|v\|^2 = v^T A^{-1}Pv \). Then we use the energy method with homogenous data and arrive at,

\begin{equation}
\|v\|^2_t - v_0^2 + v_N^2 = 2\tau a^{-1}(x_0)v_0^2
\end{equation}

The scheme is stable if \( \tau \leq -1/(2a^{-1}(x_0)) \). Since \( a^{-1}(x_0) = x_1 = h \) we have, \( \tau \leq -1/(2h) \). This stability limit is easily verified in computations and is valid for both the
2-1 method and 4-2 method. In the 2-1 case the first-order closure of A is sufficient for
globally second-order convergence. However, in the 4-2 case the convergence drops from
third to second order, see Table 3. Note also that the stability limit of \( \tau \) is dependent
on the strength of the singularity. In this case \( a(x) = 1/x \) implies that \( \tau \sim 1/h \). But, if
\( a(x) = 1/\sqrt{x} \) we would obtain \( \tau \sim 1/\sqrt{h} \), and so on.

Next, we consider the possibility to raise the order of accuracy at the boundary by
increasing the strength of \( \tau \) as a function of \( h \). Again, we consider the boundary portion
of the error equation for the quarter-space problem. (The interior can readily be shown
to give the correct convergence rate via the energy estimate.)

\begin{equation}
(e_i)_t + \frac{1}{x_i} \frac{e_{i+1} - e_{i-1}}{2h} = 0, \quad i > 1, \quad (e_0)_t + \frac{1}{x_1} \frac{e_1 - e_0}{h} = \frac{\tau}{ph} e_0 + T_0, \quad i = 0,
\end{equation}
\[
\begin{array}{cccccc}
\tau & -1/h & -1/h & -1/h^2 & -1/h^2 \\
N & l_2\text{-error} & q & l_2\text{-error} & q \\
10 & 0.0025 & - & 2.7040e-04 & - \\
20 & 6.1073e-04 & 2.0333 & 3.0940e-05 & 2.7921 \\
40 & 1.4964e-04 & 2.0290 & 4.7133e-06 & 3.0501 \\
80 & 3.7125e-05 & 2.0110 & 6.2343e-07 & 2.9184 \\
\end{array}
\]

Table 3. Errors and convergence rates at \( t = 0.1 \) for the 4-2 scheme with \( a = 1/x \) and first-order approximation of metrics at \( x = 0 \).

Laplace transform the first equation in (3.14) results in \( \kappa(i) = -\bar{s}x_i \pm \sqrt{(\bar{s}x_i)^2 + 1} \).

Again, \( |\kappa_1| = |-\bar{s}x_i + \sqrt{(\bar{s}x_i)^2 + 1}| < 1 \) and \( \Re \sqrt{(\bar{s}x_i)^2 + 1} > 0 \), since \( x_1 > 0 \). We note that according to our approximation \( x_0 = x_1 = h_0 \). Laplace transforming equation (3.14) and using the explicit expression for \( \kappa_1 \) yield,

\[
\sigma \left( \frac{\sqrt{(\bar{s}h)^2 + 1}}{h} - \frac{\tau}{\rho} \right) = h\mathcal{T}_0, \quad \tau = 0, \quad t \geq 0
\]

For stability, we demand that the resolvent, \( \mathcal{R} = \left( \frac{\sqrt{(\bar{s}h)^2 + 1}}{h} - \frac{\tau}{\rho} \right) > 0 \), for \( \Re \bar{s} \geq 0, \ h \geq 0 \). Since \( \Re \sqrt{(\bar{s}h)^2 + 1} \geq 0 \) we must require that, \( -\frac{1}{\rho} - \frac{\tau}{\rho} > 0 \) and obtain \( \tau < -p/h = -1/(2h) \). With \( \tau \sim 1/h \) we have \( \mathcal{R} \sim 1 \) and \( \sigma \sim h\mathcal{T}_0 \). Using Parseval’s relation, we also obtain that \( e_b \sim h\mathcal{T}_0 \).

As in the constant coefficient case we may choose \( \tau \sim 1/h^p \) to obtain \( e_b \sim h^{p+1}\mathcal{T}_0 \). With \( \tau = -1 \) the scheme is unstable as predicted by theory and the results \( \tau = -1/h \) and \( \tau = -1/h^2 \) are displayed in Table 3. The results supports the theoretical derivations.

### 3.3. Model problem 3

The polar singularity was modelled by, \( u_i + \frac{1}{y} u_x = 0, \ 0 \leq x, y \leq 1 \). This equation is discretized as outlined in (2.2). We choose \( A = \text{diag}(a(y_0), ..., a(y_M)) \), where \( a(y_0) = 1/y_0 \) and \( a(y_i) = 1/y_i, \ i = 1..M \). That is, we commit a first-order error along the line \( y = 0 \). We need boundary conditions at \( x = 0 \) and choose \( \tau_1 = -a(y_i) \) at \( y_i \) in (2.2). Further, \( \tau_2 = 0 \) in (2.2). We use the exact solution \( u = \sin(yx - t) \) to provide boundary and initial data. We do not need to redo a similar analysis but only interpret this case from the results of the constant coefficient. For each \( y \neq 0 \) the equation is approximated to design order. If we assume that the 4-2 is employed, we have third-order global convergence. In other words, for \( N \times M - 1 \) points the error is \( O(h^3) \). For \( y = 0 \) we approximate \( 1/y \) by \( 1/y_1 = 1/h_y \) and we commit a first-order error on \( N \) points. We assume that \( h_x \sim h_y \sim h \). Then the overall \( l_2\)-error, \( e_{l_2} \), is computed as,

\[
e_{l_2}^2 = h^2 \sum_{i=1}^{N} \sum_{j=1}^{M} e_j^2 \sim h^2 \left( N(M - 1)(h^3)^2 + N(h^2)^2 \right) \sim h^2(h^4 + h) \sim h^{3.5}
\]

or, \( e_{l_2} \sim h^{1.5} \). The computational results are displayed in Table 4 and the convergence rate is 1.5 as predicted. As mentioned above, we need not supply any boundary condition at \( y = 0 \). However, at any boundary we may enforce the exact solution, if known, as a
Table 4. Errors and convergence rates at $t = 0$ for the 4-2 scheme with $a = 1/y$ and first-order approximation of $1/y$ at $y = 0$.

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<tr>
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Table 5. Errors and convergence rates at $t = 0$ for the 4-2 method with $a = 1/y$ and first-order approximation of $1/y$ at $y = 0$. A penalty term enforce the exact solution along the slip boundary $y = 0$.

<table>
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boundary condition. In this case we know the exact solution and we choose $\tau_2 = -a(y_0)$. As the previous analysis suggests, we should gain one order of accuracy at $y = 0$ (and globally.) We note that Table 5 supports that conclusion.

3.4. Advection equation on the circle segment

We will compute the solution to the advection equation with the 4-2 method on the circle segment shown in Figure 1. The grid spacing is equidistant meaning $\Delta r = \text{constant}$ and $\Delta \phi = \text{constant}$ with $N + 1$ points in both directions, implying that $h_\xi = h_\eta = 1/N$. (The general coordinate $\xi$ corresponds to $r$ and $\eta$ to $\theta$.) We use the scheme (2.2) for the equation (2.6) with $a = 0.9$ and $b = -\sqrt{1 - a^2}$ and compute two different cases:

(a) $(\tau_1)_j = -\hat{a}(x_0, x_j)$ and $(\tau_2)_i = \hat{b}(x_i, y_N)$. (A local penalty parameter is computed at each gridpoint.)

(b) $(\tau_1)_j = -\hat{a}(x_0, x_j)/h_\xi$ and $(\tau_2)_i = \hat{b}(x_i, y_N)$.

In the first case, we commit an $O(h)$ error along the line $\xi = 0$. The penalty strength at $\xi = 0$ is the marginal scaling for stability. Hence, this case corresponds to Model Problem 3 without the extra penalty term at $y = 0$. We would expect the $l_2$ convergence rate to be 1.5 and the $l_\infty$ convergence rate to be 1, which is the case in Table 6.

The second case corresponds to Model Problem 3 with the additional penalty at $y = 0$ in the sense that the penalty is unnecessary strong for pure stability purposes. However, the effect is an increased convergence rate by one order in both $l_2$ and $l_\infty$, which is observed in Table 7.

3.5. Grid singularity at outflow boundary.

So far, we have only considered the case of a grid with boundary condition at the singularity. To study the case of a grid singularity at an outflow we consider Model Problem
Stable and high-order accurate finite difference schemes on singular grids

<table>
<thead>
<tr>
<th>N</th>
<th>$l_2$-error</th>
<th>$q_2$</th>
<th>$l_{\infty}$-error</th>
<th>$q_{\infty}$</th>
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</thead>
<tbody>
<tr>
<td>10</td>
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<td>-</td>
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<td>0.9798</td>
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</table>

Table 6. Errors and convergence rates on the circle segment grid at $t = 0$ for the 4-2 method with $(\tau_1)_j = -\tilde{a}(x_0, x_j)$.

<table>
<thead>
<tr>
<th>N</th>
<th>$l_2$-error</th>
<th>$q_2$</th>
<th>$l_{\infty}$-error</th>
<th>$q_{\infty}$</th>
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</thead>
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<td>1.8902</td>
</tr>
</tbody>
</table>

Table 7. Errors and convergence rates on the circle segment grid at $t = 0$ for the 4-2 method with $(\tau_1)_j = -\tilde{a}(x_0, x_j)/h_\xi$.

2, modified to a left-going wave problem.

$$u_t - a(x)u_x = 0, \quad a(x) = \frac{1}{x}, \quad u(1, t) = g(t), \quad 0 \leq x \leq 1$$

(3.15)

The idea is to try to increase the accuracy of the approximated metric coefficient at the left boundary. The naive approach is to extrapolate to higher order using the ansatz, $a(x_0) \approx \alpha a(x_1) + \beta a(x_2)$, and Taylor expand.

$$a(x_0) \approx \alpha(a(x_0) + a'(x_0)(x_1 - x_0) + a''(x_0)\frac{(x_1 - x_0)^2}{2})$$

$$+ \beta(a(x_0) + a'(x_0)(x_2 - x_0) + a''(x_0)\frac{(x_2 - x_0)^2}{2}).$$

(3.16)

We have to interpret the derivatives as limits as $x_0 \to 0$. Then we obtain the conditions,

$$\alpha + \beta = 1, \quad \alpha h + 2h\beta = 0, \quad \alpha = 2, \beta = -1.$$  

(3.17)

This is the same solution we would obtain if we had fit a linear polynomial between $x_1$ and $x_2$ and extrapolated to $x_0$. The Taylor expansions, however, gives insight in the errors committed. The convergence rates obtained using this kind of extrapolation is shown in Table 8. $p$ is the order of the extrapolation polynomial, i.e. $p = 0$ is the previously used simple extrapolation from a close neighbor. $p = 1$ the linear extrapolation derived above, and $p = 2$ a second-order polynomial. As is clearly seen, trying to extrapolate to higher order does not raise the accuracy. To explain these results, we consider the first error term of (3.16).

$$e = \alpha a''(x_0)\frac{(x_1 - x_0)^2}{2} + \beta a''(x_0)\frac{(x_2 - x_0)^2}{2}.$$  

(3.18)

Let $x_0$ approach 0 and compute the limit, $e = \alpha \frac{1}{h} + \beta \frac{1}{h^2}$. We conclude that the error at $x_0$ is a term $a(x_0 + h)$, i.e. a first order error, which explains the results in Table 8. Of
### Table 8

<table>
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<tr>
<th>$p$</th>
<th>$l_2$-error</th>
<th>$q$</th>
<th>$l_2$-error</th>
<th>$q$</th>
<th>$l_2$-error</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
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<td>-</td>
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<td>2.0267</td>
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</table>

Eq (3.15) approximated with the 4-2 scheme. Extrapolation of $-1/x$ to $x = 0$ with polynomial order $p$.

### Table 9

<table>
<thead>
<tr>
<th>$N$</th>
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<tr>
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<td>4.4241e-07</td>
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</tbody>
</table>

Table 9. Eq (3.15) approximated with the 4-2 scheme. $-1/h^2$ approximating $-1/x$ at $x = 0$.

### Table 10

<table>
<thead>
<tr>
<th>$\sqrt{N}$</th>
<th>$l_2$-error</th>
<th>$q_2$</th>
<th>$l_{\infty}$-error</th>
<th>$q_\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
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<td>0.0136</td>
<td>-</td>
</tr>
<tr>
<td>21</td>
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<td>1.5097</td>
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<td>1.0128</td>
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</tbody>
</table>

Table 10. Circle segment with outflow at singular point ($a = -1, b = 0$). Zeroth-order interpolation of $y_0, x_0$ to $x = 0.5, y = 0$.

course, extrapolation only gives smaller leading error term with higher polynomial order if the extrapolated function is sufficiently smooth, which was not the case above. This leads us to extrapolate the smooth inverse of $1/x$.

That is, we approximate $x_0 = 0$ to second order accuracy, i.e. $x_0 = x' = h^2$, such that $1/x_0$ is approximated by $1/x' = 1/h^2$ which is a second-order approximation and the entire scheme should recover third-order accuracy. Indeed, this is confirmed in Table 9. Again, the numerical scheme becomes more stiff. Applying the same idea to the circle segment suggest that $y_0$ and $x_0$ should be extrapolated to second-order accuracy. In our example the functions are linear and we use a linear extrapolation to a point $O(\Delta r^2)$ away from the singularity. The results are displayed in Table 10 and 11. As is seen we get the predicted convergence rate 2 in $l_\infty$. We have confirmed that the maximum errors occur at the singular point and get an approximate convergence rate of 2.5 in $l_2$. 
3.6. Time step limits

Both the proposed remedies for the grid singularity introduces a stiness to the problem, if
compared to the same problem on a non-singular grid. However, if we accept the choice
of a singular grid transformation and still want to compute a solution, the time step
restriction is unavoidable. Consider,

\[ u_t + a(x)u_x = 0 \]  \hspace{1cm} (3.19)

Then the CFL constraint is \( \Delta t < c \cdot a(x)/h \) where \( c \) is a constant depending on the choice
of numerical scheme. As an example, we use model problem 1 where \( a(x) = 1/x \). The
more accurate we want to approximate \( a(0) \), the more stiff the problem becomes.

4. The Euler equations

We will demonstrate the robustness of the proposed techniques using the Euler equa-
tions of gas dynamics. We will consider an analytical vortex solution that enables us to
measure the error. Since the flows will be subsonic there will be boundary conditions
both at inflows and at outflows but not on all variables. Hence, we will use the technique
where the metric coefficients are approximated (and not the remedy utilizing stronger
penalties). The computations will be carried out with the multi-block SBP-SAT finite
difference code SUMb. The Euler equations are stated on conservative form and since the
previous analysis was carried out on primitive form, we will briefly discuss the differences
with respect to the metric approximations. The Euler equations in a Cartesian system
can be stated as,

\[ u_t + F_x + G_y = 0 \] \hspace{1cm} (4.1)

where \( u \) are the conservative variables and \( F, G \) are the fluxes. Applying a coordinate
transformation results in,

\[ (Ju)_t + (J\xi_x F + J\xi_y G)_\xi + (J\eta_x F + J\eta_y G)_\eta = 0. \] \hspace{1cm} (4.2)

We note that \( J\xi_x = y_\eta, J\xi_y = -x_\eta, J\eta_x = -y_\xi, J\eta_y = x_\xi \) are not singular but well-defined
on the grids we have considered. Hence, it is only \( J \) appearing in the time derivative
that is troublesome. To compute \( J \), we use the approximations of the metric coefficients
discussed at length above. We use the analytical solution as initial and boundary data.
The Mach number is 0.5 and the solution is computed with the 4-2 scheme marched with
a 3rd-order explicit Runge-Kutta scheme on 4 different meshes. The domain is seen in
Figure 2 and the grid sizes are: 33 \times 17 points (grid 1); 65 \times 33 points (grid2); 129 \times 65 points
(grid 3); 257 \times 129 points (grid 4). At \( T = 0.6 \) the \( l_2 \)-errors, \( l_\infty \)-errors and convergence

<table>
<thead>
<tr>
<th>( \sqrt{N} )</th>
<th>( l_2 )-error</th>
<th>( q_2 )</th>
<th>( l_\infty )-error</th>
<th>( q_\infty )</th>
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</thead>
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</tr>
<tr>
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</tr>
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</table>

Table 11. Circle segment with outflow at singular point \((a = -1, b = 0)\). Linear interpolation
of \( y_\eta, x_\eta \) to a point \( h^2 \) away from \( x = 0.5, y = 0 \).
rates are displayed in Table 12. We note that the computational convergence rates, are close to the theoretical 1.5 in $l_2$ and 1 in $l_\infty$. Also, the computations are perfectly stable on all grids and we note that the 4-2 method is quite accurate although the formal order is degraded due to the singularity. In Figure 2 the density is shown at $T = 0.6$ for two different grids: the coarsest (grid 1) and the second finest (grid 2). We observe that on grid 3 an almost perfect solution is obtained but even the solution on the coarsest mesh is good.

5. Conclusions

We have considered fictitious singularities introduced by the mapping of a non-square computational grid to a square that results in singular metric coefficients. We approach this problem by studying one-dimensional model problems and present two ways of handling the singularity, while keeping design order of the scheme.

The first remedy is applicable to SBP-SAT schemes and requires only a crude and simple approximation of the metric coefficients (one can even choose them to be an arbitrary constant). The accuracy is recovered through a stronger enforcement of the penalty boundary conditions.

The second technique, is a sufficiently accurate extrapolation of the metric coefficients to a point that approaches the singularity sufficiently fast. This solution is generally applicable to any stable finite difference scheme. However, care has to be taken when the metric coefficients are extrapolated and naive extrapolations do not improve the accuracy. Numerical examples supports the linear analysis for both remedies.

Both methods yield a more stiff set of ordinary differential equations to solve, compared to the same problem on a non-singular grid. The additional stiffness is proportional to the strength of the singularity. We show that this is a natural CFL constraint.

Finally, we show how to interpret the results for a system of equations in conservative form. We demonstrate that the non-linear two-dimensional Euler equations computed with the 4-2 scheme is robust with the second technique and obey the same accuracy properties as the linear counterpart.

REFERENCES


Stable and high-order accurate finite difference schemes on singular grids

Figure 2. The density of the Euler vortex solution at $T = 0.6$. The top figure computed with the 4-2 method on Grid 3 and the bottom figure on Grid 1.


