A new finite-difference scheme for singular differential equations in cylindrical or spherical coordinates

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It is well known that the standard finite-difference scheme for approximating the radial derivative in polar coordinates (*r*-derivative) in Laplace's Equation has difficulty capturing the singular (logarithmic) behavior of the solution near the origin. By choosing a non-standard finite difference scheme ("logarithmic differencing") the singular behavior can be captured with a significantly smaller local truncation error. In the almost-trivial 1-dimensional case, the singular behavior is captured *exactly*. A number of numerical examples are given which illustrate the utility of the new scheme.

1 Introduction

This paper discusses a method for computing numerical solutions to partial differential equations and ordinary differential equations written in spherical or cylindrical coordinates. It involves a new way to discretize the operator $\mathcal{R} \equiv r^p \frac{d}{dr}$, where p = 1is the cylindrical coordinates case and p = 2 is the spherical coordinates case.

The scheme introduced in this paper was first presented in Buckmire's 1994 thesis [1], in which particular slender bodies of revolution were found to possess shock-free flows. The problem is formulated using transonic small disturbance theory found in [2], [3] and [4], among other sources. Cole & Schwendeman announced the first computation of a fore-aft symmetric shock-free transonic slender body in [6]. Computationally, the problem involves numerically solving a boundary value problem with an elliptic-hyperbolic partial differential equation (the Kármán-Guderley equation) in cylindrical coordinates, with a singular inner Neumann boundary condition at r = 0 and a non-singular outer Dirichlet boundary condition

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far away from r = 0. Namely,

$$(K - (\gamma + 1)\phi_x)\phi_{xx} + \phi_{\tilde{r}\tilde{r}} + \frac{1}{\tilde{r}}\phi_{\tilde{r}} = 0.$$
(1)

$$\phi(x,\tilde{r}) \to S(x)\log\tilde{r} + G(x), \quad \text{as } \tilde{r} \to 0, \ |x| \le 1$$
(2)

$$\phi(x, \tilde{r})$$
 bounded, for $\tilde{r} = 0, |x| > 1.$

$$\phi(x,\tilde{r}) \to \frac{\mathcal{D}}{4\pi} \frac{x}{(x^2 + K\tilde{r}^2)^{3/2}}, \qquad \text{as } (x^2 + \tilde{r}^2)^{1/2} \to \infty.$$
 (3)

In (1), (2) and (3) the variable \tilde{r} is a scaled cylindrical coordinate, K is the transonic similarity parameter, \mathcal{D} is the dipole strength and $\phi(x, \tilde{r})$ is a velocity disturbance potential. Both S(x) and G(x) are bounded functions. The main point of sketching the boundary value problem here is to emphasize that the function G(x) which occurs in (2) needs to be computed very accurately, because the pressure coefficient on the body depends directly on G'(x). Computing it is complicated by the fact that $\phi(x, \tilde{r})$ and $S(x)\log\tilde{r}$ are becoming singular as $\tilde{r} \to 0$, which is where the boundary condition must be evaluated. Thus a numerical scheme was needed to compute the solution accurately as $\tilde{r} \to 0$. This was the motivation for the scheme introduced in this paper.

In 1971, Murman and Cole [5] introduced a numerical scheme which was the first of its kind to be able to handle mixed-type elliptic-hyperbolic partial differential equations like the Kármán-Guderley equation. The method is now known as "Murman-Cole switching" and is a particular scheme to discretize the x-derivatives in the partial differential equation. It is fitting that the new scheme which deals with the discretization of the r-derivatives in the same PDE is presented at a gathering honoring the contributions of Julian Cole.

2 Discretizing the operator $\mathcal{R} \equiv r^p \frac{d}{dr}$

This section shall explain the discretization of \mathcal{R} , limited to the p = 1 case; the p = 2 discretization is derived in a similar manner. Consider the quantity B(r) which is defined as

$$B(r) = \mathcal{R}u = \frac{r^p du}{dr},$$

where u = u(r) is an unknown function (the solution) the operator \mathcal{R} acts on.

The first step in the discretization of the operator is to choose a grid $\{r_j\}_{j=0}^N$ on the interval $0 \le r \le 1$ where

$$0 \leftarrow r_0 < r_1 < r_2 < \ldots < r_j < \ldots < r_N = 1.$$
(4)

On the grid defined in (4) one has discrete forms of the quantities of interest, such as $u(r_j) = u_j$ and $B_{j+1/2} = \left. r^p \frac{d}{dr} \right|_{r=r_{j+1/2}}$ where $r_{j+1/2} = \frac{r_j + r_{j+1}}{2}$.

There are two choices of discretizing B(r), the standard forward-difference approximation method and the new scheme, which shall be compared with each other.

$$B_{j+1/2}^{(1)} = r_{j+12/\frac{u_{j+1} - u_j}{r_{j+1} - r_j}}$$
(5)

$$B_{j+1/2}^{(2)} = \frac{u_{j+1} - u_j}{\log(r_{j+1}) - \log(r_j)} = \frac{u_{j+1} - u_j}{\log(r_{j+1}/r_j)}$$
(6)

The standard scheme in (5) shall be referred to as Scheme⁽¹⁾ and the new scheme in (6) shall be referred to as Scheme⁽²⁾. Scheme⁽²⁾ can be obtained by assuming that B(r) should be constant on each subinterval (r_j, r_{j+1}) of the grid. If one relates B(r) back to the physical fluid mechanics problem we want to solve, it corresponds to a mass flux. The relationship between $B_{j+1/2}$ and u_j and u_{j+1} solves the simple boundary value problem

$$ru' = B_{j+1/2} = \text{constant} \tag{7}$$

$$u(r_j) = u_j \tag{8}$$

$$u(r_{j+1}) = u_{j+1}.$$
(9)

The solution to this is $u(r) = B_{j+1/2} \log r + C$, which, when one applies the boundary conditions (8) and (9) leads to the formula

$$B_{j+1/2} = \frac{u_{j+1} - u_j}{\log(r_{j+1}/r_j)}.$$

3 Applying the method

The question to be asked now is, how well does the new scheme given in (6) work? This question will be answered by giving an example of the new scheme being applied to a simple differential equation. The Kármán-Guderley equation (1) and the associated boundary conditions of (2) and (3) can be related to the simpler boundary value problem given below

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) + qu = 0, \qquad q \text{ constant} \qquad (10)$$

$$\left. r \frac{du}{dr} \right|_{r=0} = S, \tag{11}$$

$$u(1) = G. \tag{12}$$

If one linearizes and substitutes $\phi(x,r) = u(r)e^{ikx}$ into (1) one will obtain the above boundary value problem. This simple boundary value problem is used as the test problem to benchmark the new finite-difference scheme instead of the transonic smalldistrurbance equation (1) one is really interested in solving, because the simpler problem has a known exact solution involving logarithms and Bessel functions, depending on the value of $q = k^2$. The exact solution can be written as

$$q > 0, \qquad u(r) = \frac{\pi}{2} SY_0(r\sqrt{q}) + (G - S\frac{\pi}{2}Y_0(\sqrt{q}))\frac{J_0(r\sqrt{q})}{J_0(\sqrt{q})}$$
(13)

$$q = 0, \qquad u(r) = S \log r + G \tag{14}$$

$$q < 0, \qquad u(r) = \frac{-\pi}{2} SK_0(r\sqrt{-q}) + (G + S\frac{\pi}{2}K_0(\sqrt{-q}))\frac{I_0(r\sqrt{-q})}{I_0(\sqrt{-q})}.$$
 (15)

First consider the q = 0 model problem. The differential equation in this case is simply

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) = B'(r) = 0.$$

This has the simple solution B(r) = constant. Using the boundary condition at $r = 0, B(0) = S \Rightarrow B(r) = S$. Thus the discrete version of the model equation which is being solved is

$$B_{j+1/2} = S. (16)$$

Using scheme⁽¹⁾ (the standard forward-difference approximation)

$$B_{j+1/2} = r_{j+1/2} \frac{u_{j+1} - u_j}{r_{j+1} - r_j} = S$$

$$\Rightarrow u_j = u_{j+1} - 2S \frac{r_{j+1} - r_j}{r_{j+1} + r_j} \quad \text{with } u_N = G.$$

This is a simple marching scheme which allows one to compute all the u_j , $j = 0, \ldots, N$ starting from $u_N = G$ and "marching" down to u_0 .

Using scheme $^{(2)}$ (the new scheme) the discrete equation to be solved is

$$B_{j+1/2} = \frac{u_{j+1} - u_j}{\log(r_{j+1}/r_j)} = S$$
$$\Rightarrow u_j = u_{j+1} - S\log(\frac{r_{j+1}}{r_j}), \quad \text{with } u_N = G$$

Scheme⁽²⁾ also leads to a marching scheme which solves the model equation exactly by definition. This happens because the scheme was derived assuming that B(r) would be constant on each subinterval. For this model equation B(r) = S, so it is the same constant, namely S on each subinterval. So scheme⁽²⁾ is exact for this model equation where q = 0. A similar idea of deriving a finite-difference scheme by using a discretization which solves a simple version of the differential equation one is actually interested in solving is given in Scharfetter & Gummel [8].

Compare the two schemes by looking at the difference between the numerical solution each generates, at each grid point.

$$e_j = u_j^{(1)} - u_j^{(2)} \tag{17}$$

where $u_j^{(1)}$ is the solution to the equation obtained using scheme⁽¹⁾ and $u_j^{(2)}$ is the solution to the equation obtained using scheme⁽²⁾.

$$e_{j} = u_{j+1}^{(1)} - 2S \frac{r_{j+1} - r_{j}}{r_{j+1} + r_{j}} - u_{j}^{(2)} + S\log(\frac{r_{j+1}}{r_{j}})$$

$$= e_{j+1} - 2S\delta_{j} + S\log\left(\frac{1 + \delta_{j}}{1 - \delta_{j}}\right)$$
(18)

where $\delta_j = \frac{r_{j+1} - r_j}{r_{j+1} + r_j}$. The symbol δ_j is a characteristic of the grid disretization somewhat akin to grid separation.

If $\delta_j \ll 1$, then using a simple Taylor series expansion

$$\frac{e_j - e_{j+1}}{S} = \frac{2}{3}\delta_j^3 + \frac{2}{5}\delta_j^5 + \dots$$
(19)

Thus the local discretization error made by the typical difference scheme is $O(\delta_j^3)$, which implies that the global error is $O(\delta_j^2)$. However, suppose that δ_j is not small for all j. Remember that δ_j depends on the choice of $\{r_j\}_{j=0}^N$. It is a characteristic of the grid discretization. For example, suppose that the choice is to use a uniform grid. In that case,

$$r_j = jh,$$
 $h = \frac{1}{N}, \quad j = 0, ..., N.$

In this case $\delta_j = \frac{r_{j+1} - r_j}{r_{j+1} + r_j} = \frac{h}{jh + (j+1)h} = \frac{1}{2j+1}$. Clearly, $\frac{1}{2N+1} \leq \delta_j \leq \frac{1}{3}$. So the parameter δ_j varies depending on what grid point it is evaluated at, but at j = 1, δ_1 is a constant which does not depend on N or h which means that as $h \to 0$ (or $N \to \infty$) the local discretization error, which is $O(\delta_j^3)$ does not get smaller and go to zero, but in fact the error at j = 1 is O(1)!

A uniform grid is a bad choice to pick when discretizing the domain if one is solving a differential equation with a $r^p \frac{d}{dr}$ operator and the domain includes the singular point r = 0, i.e. singular differential equations. A better grid choice is to ensure that the grid has the property that δ_j is small for all j. The easiest way to do that is to pick one value of δ for all j. The value can be chosen by looking at the definition of δ_j and re-arranging it to give a marching scheme which chooses the appropriate grid discretization $\{r_j\}_{j=0}^N$.

$$\delta_j = \frac{r_{j+1} - r_j}{r_{j+1} + r_j} \Rightarrow r_j = \left(\frac{1 - \delta_j}{1 + \delta_j}\right) r_{j+1}, \quad \text{with } r_N = 1$$

For example, if one lets $\delta_j = 1/N$,

$$r_j = \left(\frac{1-1/N}{1+1/N}\right)r_{j+1} = \frac{N-1}{N+1}r_{j+1}$$

which implies that $r_j = \alpha^{N-j}r_N$, where $\alpha = \frac{1-\delta}{1+\delta} = \frac{N-1}{N+1} < 1$. This grid choice corresponds to an approximately exponentially stretched grid, with many points clustered near r = 0. This analysis supports the grid choice used by Krupp & Murman [7] to solve the Kármán-Guderley equation back in 1972.

The standard forward-difference scheme can be used to solve singular differential equations, but the grid must be chosen intelligently. Using the new scheme there is flexibility about what kind of grid to use.



FIG. 2. Error Due to $scheme^{(2)}$

4 Numerical Results

Consider how the competing schemes fare when used to solve the $q \neq 0$ model problems. Exact solutions are known, so one can compare the absolute error scheme⁽¹⁾ makes in solving the problem to the absolute error scheme⁽²⁾ makes to solve the identical problem. The numerical results are given in Figures 1 and 2. In all cases, the new scheme is more accurate than the standard scheme. Even when scheme⁽²⁾ is used on a uniform grid but scheme⁽¹⁾ is used on an exponentially-stretched grid the new scheme fares better. Both schemes get worse errors as the point at which the inner boundary condition is evaluated approaches zero. For the numerical results given in Figures 1 and 2, a grid was chosen consisting of N = 50 points and then a series of computations performed solving the model problem (15) using a value of $q = \pm 1$. By choosing steadily decreasing values for α the degree to which the grid was exponentially stretched was increased, culminating in the final run with $r_0 = 10^{-9}$.

5 Conclusions

A new finite-difference scheme has been introduced to deal with differential equations in cylindrical or spherical co-ordinates. It appears to tackle singular problems more accurately and efficiently than other standard schemes. The author urges others to use this new scheme and look forward to hearing how it fares when used to solve other differential equations numerically. Future research will involve using the ideas in this paper to attempt to derive other similar finite-difference schemes.

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