

Alternate treatments of jacobian singularities in polar coordinates within finite-difference schemes*

Alexys Bruno-Alfonso^{1†}, Luben Cabezas-Gómez², Helio Aparecido Navarro³

¹ Departamento de Matemática, Faculdade de Ciências de Bauru, UNESP-Universidade Estadual Paulista, Bauru 17033-360, Brazil

² Departamento de Engenharia Mecânica, Pontifícia Universidade Católica de Minas Gerais, Coração Eucarístico, Belo Horizonte, MG, 30535-901, Brazil

³ Departamento de Engenharia Mecânica, Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos 13566-590, Brazil

(Received January 5 2011, Accepted February 22 2012)

Abstract. Jacobian singularities of differential operators in curvilinear coordinates occur when the Jacobian determinant of the curvilinear-to-Cartesian mapping vanishes, thus leading to unbounded coefficients in partial differential equations. Within a finite-difference scheme, we treat the singularity at the pole of polar coordinates by setting up complementary equations. Such equations are obtained by either integral or smoothness conditions. They are assessed by application to analytically solvable steady-state heat-conduction problems.

Keywords: finite difference, polar coordinates, Jacobian determinant

1 Introduction

Partial differential equations (PDEs) serve as mathematical models for physical phenomena such as diffusion and heat transfer, wave propagation and stationary fields. Of course, besides the differential equation, one should take into account boundary conditions and, when applicable, initial conditions as well. Thus, depending on the geometry of the spatial domain, the problem may be simplified when written in terms of curvilinear coordinates. Moreover, the PDE usually contains differential operators like gradient, divergence, Laplacian, and curl. While these operator take simple forms in Cartesian coordinates (x, y), their curvilinear versions may be rather cumbersome. To fix ideas, we consider a right-handed system of orthogonal coordinates (p, q), i.e., such that $x_p x_q + y_p y_q = 0$ and $x_p y_q - x_q y_p > 0$. In two dimensions, the gradient, divergence, Laplacian, and curl, may be written as^[10]

$$\vec{\nabla}u = \frac{1}{h_p} \frac{\partial u}{\partial p} \hat{e}_p + \frac{1}{h_q} \frac{\partial u}{\partial q} \hat{e}_q,\tag{1}$$

$$\vec{\nabla} \cdot \vec{U} = \frac{1}{J} \left[\frac{\partial}{\partial p} \left(h_q \, U_p \right) + \frac{\partial}{\partial q} \left(h_p \, U_q \right) \right] \tag{2}$$

$$\nabla^2 u = \frac{1}{J} \left[\frac{\partial}{\partial p} \left(\frac{h_q}{h_p} \frac{\partial u}{\partial p} \right) + \frac{\partial}{\partial q} \left(\frac{h_p}{h_q} \frac{\partial u}{\partial q} \right) \right],\tag{3}$$

$$\vec{\nabla} \times \vec{U} = \frac{1}{J} \left[\frac{\partial}{\partial p} \left(h_q \, U_q \right) - \frac{\partial}{\partial q} \left(h_p \, U_p \right) \right],\tag{4}$$

^{*} The authors thank the Brazilian research funding agencies CNPq, FAPESP and FAPEMIG for financial support. A. B.-A. is grateful to G. V. B. de Souza for useful discussions.

[†] Corresponding author. Tel.: +55-14-3103 6086. Fax: +55-14-3103 6096. *E-mail address*: alexys@fc.unesp.br.

respectively, where $h_p = \sqrt{x_p^2 + y_p^2}$ and $h_q = \sqrt{x_q^2 + y_q^2}$ are the scale factors, $J = h_p h_q$ is the Jacobian determinant, $\hat{e}_p = (x_p, y_p) / h_p$ and $\hat{e}_q = (x_q, y_q) / h_q$ are the unit vectors of the curvilinear coordinates, $U_p = \vec{U} \cdot \hat{e}_p$ and $U_q = \vec{U} \cdot \hat{e}_q$. In this way, one may clearly see that differential operators in Eqs. (1) ~ (4) have singularities at zeros of J. For short, these are called as Jacobian singularities.

When (p,q) are the usual polar coordinates (ρ,θ) satisfying $x = \rho \cos(\theta)$, $y = \rho \sin(\theta)$, the scale factors are $h_{\rho} = 1$ and $h_{\theta} = |\rho|$, the Jacobian determinant is $J = |\rho|$, and the unit vectors are $\hat{e}_{\rho} = (\cos(\theta), \sin(\theta))$ and $\hat{e}_{\theta} = (-\sin(\theta), \cos(\theta))$. Therefore, the only Jacobian singularity occurs at $\rho = 0$. In this sense, one should carefully treat differential equations containing the above mentioned operators, whenever the spatial domain contains the pole $\rho = 0$.

In the available literature, several approaches have been developed to obtain numerical solutions of PDEs in curvilinear coordinates where Jacobian singularities occur. Some authors exclude the corresponding points of the finite-difference mesh^[1, 4, 7]. In particular, Mohseni and Colonius [4] have used a computational domain where r takes either positive or negative values, while $0 \le \theta \le \pi$. In other approaches, a derivation of a limiting PDE has been proposed^[6, 9]. Contantinescu and Lele [2, 3] have developed a numerical method where governing equations for the flow at the polar axis are derived by series expansions. Moreover, Fukagata and Kasagi [5] introduced a single-valued representation of the velocity components at r = 0, based on the series expansion of Constantinescu and Lele [2, 3] and considering an energy-conservative numerical scheme. However, according to Morinishi et al [8], those authors did not consider the momentum conservation at the pole in order compute the velocity components at pole. In this sense, Morinishi et al [8] have introduced a novel treatment of the pole, using a discrete radial momentum equation with a fully conservative convection scheme at the pole. In other words, they obtained the radial velocity at the pole based on the radial momentum equation with a fully energy-conservative convection scheme.

In this paper, a finite-difference scheme in polar coordinates is set up to solve PDE problems. As usual, we consider $\rho \ge 0$ and $0 \le \theta \le 2\pi$. Moreover, the pole $\rho = 0$ belongs to the discretization mesh and the corresponding equation is derived. This is done by following two methods: (i) integration of both sides of the PDE over an infinitesimal region containing the pole and (ii) applying differentiability conditions at the pole. To assess these approaches, we solve problems which model heat-transfer processes. The cases where the unknown function is either a scalar or a vector field are addressed. A central-difference discretization of second order is used, including Dirichlet boundary conditions at the physical boundaries. Excellent agreement between numerical and analytical solutions is obtained in all cases. The extension of the present method to cylindrical and spherical coordinates is straightforward. In this way, the present ideas should find further application in modelling physical systems and processes like laminar and turbulent isothermal fluid flow, convection heat-transfer phenomena, mechanical waves, electromagnetic fields and quantum states.

2 Derivation of complementary conditions

2.1 A scalar function in polar coordinates

Let us consider a physical problem modelled by a PDE in a domain D with boundary C in Cartesian coordinates. The origin O(0,0) is assumed to be an inner point of D, as shown in Figure 1. When the boundary C is given by simple formulas in polar coordinates (ρ, θ) , with $\rho \ge 0$ and $0 \le \theta \le 2\pi$, it may be advantageous to set up the mathematical problem in the variables ρ and θ .

To be concrete, we deal with a stationary heat-transfer process in a thin homogeneous circular plate where thermal energy may be transferred from/to the environment either across the plane circular faces or the thin cylindrical surface at the plate edge. More specifically, we assume that energy interchange across the plane faces is given by the source function s(x, y), bounded and integrable over D. Moreover, the two-dimensional energy-flux density is denoted by the vector field $\vec{U}(x, y) = -k \nabla u(x, y)$, where k is the two-dimensional thermal conductivity. Then, because of the energy conservation, we have:

$$\vec{\nabla} \cdot \vec{U}(x,y) = s(x,y). \tag{5}$$

Consequently, the temperature distribution satisfies the Poisson equation:

World Journal of Modelling and Simulation, Vol. 8 (2012) No. 3, pp. 163-171

$$\nabla^2 u(x,y) = -\frac{s(x,y)}{k}.$$
(6)

165

Furthermore, the polar version of this equation is:

$$\frac{\partial^2 u}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial u}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} = -\frac{s}{k},\tag{7}$$

and the Jacobian singularity at $\rho = 0$ is apparent in the second and third terms in the left-hand side of this equation.



Fig. 1. Schematic representation of the physical domain Fig. 2. Computational domain and finite-difference D, its boundary C and the pole (0,0) mesh in polar coordinates

Because of the Jacobian singularity under investigation, the polar-to-Cartesian mapping may lack inverse. In fact, all points $(0, \theta)$ map into the origin of the Cartesian coordinates, i.e., the pole. Therefore, there is a certain value u_0 such that:

$$u(0,\theta) = u_0,\tag{8}$$

for all $0 \le \theta \le 2\pi$. Moreover, both sides of Eq. (5) may be integrated over a small disk of radius ε centered at the pole. This leads to:

$$\int_{0}^{2\pi} \frac{\partial u}{\partial \rho}(\varepsilon, \theta) \ d\theta = -\frac{\pi \, \varepsilon^2 \, \bar{s} \, (\varepsilon)}{k},\tag{9}$$

where $\bar{s}(\varepsilon)$ is the mean value of s(x, y) over the small disk. Since this source function is bounded, so it is $\bar{s}(\varepsilon)$, and the right-hand side of Eq. (9) tends to zero as $\varepsilon \to 0^+$. Hence, in this limit we obtain:

$$\int_{0}^{2\pi} \frac{\partial u}{\partial \rho} (0^+, \theta) \, d\theta = 0.$$
⁽¹⁰⁾

In some cases, boundary conditions are such that temperature depends on ρ alone, i.e., $u(\rho, \theta) = u(\rho)$. Therefore, according to Eq. (10), the condition at the pole reads:

$$u'(0^+) = 0. (11)$$

In the finite-difference calculations presented below, we may use discretized versions of Eq. (6) for inner mesh points with $\rho \neq 0$, and Eqs. (8) and (10) for mesh points with $\rho = 0$. Things may become simpler when the unknown function is smooth, i.e., when u(x, y) is known to be differentiable. For instance, this will be the case when u varies smoothly over a smooth boundary C and the source tem is also smooth. Under these conditions, U should be smooth along any straight line passing along the pole. By taking the a vector of the line as $\hat{e}_{\rho} = (\cos(\theta), \sin(\theta))$, the lateral derivatives at the pole are: A. Bruno-Alfonso & L. Cabezas-Gómez & H. Navarro: Alternate treatments of jacobian singularities

$$\lim_{\rho \to 0^-} \frac{u(\rho, \theta) - u(0, \theta)}{\rho} = \lim_{\rho \to 0^+} \frac{u(-\rho, \theta) - u(0, \theta)}{-\rho} = -\lim_{\rho \to 0^+} \frac{u(\rho, \theta \pm \pi) - u(0, \theta \pm \pi)}{-\rho}$$
$$= -\frac{\partial u}{\partial \rho} (0^+, \theta \pm \pi), \quad \lim_{\rho \to 0^+} \frac{u(\rho, \theta) - u(0, \theta)}{\rho} = \frac{\partial u}{\partial \rho} (0^+, \theta).$$

Here we have taken into account Eq. (8) and identity $u(-\rho, \theta) = u(\rho, \theta \pm \pi)$. Hence, differentiability of u leads to:

$$\frac{\partial u}{\partial \rho}(0^+,\theta) = -\frac{\partial u}{\partial \rho}(0^+,\theta \pm \pi),\tag{12}$$

for all values of θ . We also note that, to determine the value of u_0 , one further condition at the pole is needed. Since an arbitrary value of θ may be chosen for the finite-difference scheme, we take $\theta = 0$ and obtain condition:

$$\frac{\partial u}{\partial \rho}(0^+, 0) = -\frac{\partial u}{\partial \rho}(0^+, \pi).$$
(13)

This equation may be used for smooth solutions instead of Eq. (10).

For the sake of completeness, we note that for axially symmetric solutions, i.e., when $u(\rho, \theta) = u(\rho)$, Eq. (12) leads to Eq. (11). Moreover, in other cases, by integrating both sides of Eq. (12) from $\theta = 0$ to $\theta = \pi$, one obtains Eq. (10).

2.2 A vector function in polar coordinates

We now consider a vector function $\vec{U}(x,y) = (X(x,y), Y(x,y))$ satisfying a PDE problem in a spatial domain D containing the pole, as shown in Fig. 1. For simplicity, we restrict ourselves to problems where the solution is known to vary smoothly. In other words, we assume both X(x,y) and Y(x,y) to be differentiable scalar functions. Therefore, we may apply the ideas developed for u(x,y) in the previous section. However, we deal with their dependence on the polar coordinates, i.e., $X(\rho, \theta)$ and $Y(\rho, \theta)$.

On the one hand, from Eq. (8), there should be constants X_0 and Y_0 such that:

$$X(0,\theta) = X_0, \quad Y(0,\theta) = Y_0,$$

for all values of θ . On the other hand, from Eq. (12), we get:

$$\frac{\partial X}{\partial \rho}(0^+,\theta) = -\frac{\partial X}{\partial \rho}(0^+,\theta+\pi), \quad \frac{\partial Y}{\partial \rho}(0^+,\theta) = -\frac{\partial Y}{\partial \rho}(0^+,\theta+\pi).$$
(14)

Now we denote the radial and azimuthal components of the vector field \vec{U} as $v(\rho, \theta)$ and $w(\rho, \theta)$. Hence,

$$v(\rho,\theta) = \vec{U} \cdot \hat{e}_{\rho} = (X(\rho,\theta), Y(\rho,\theta)) \cdot (\cos(\theta), \sin(\theta)) = X(\rho,\theta) \cos(\theta) + Y(\rho,\theta) \sin(\theta),$$

$$w(\rho,\theta) = \vec{U} \cdot \hat{e}_{\theta} = (X(\rho,\theta), Y(\rho,\theta)) \cdot (-\sin(\theta), \cos(\theta)) = -X(\rho,\theta) \sin(\theta) + Y(\rho,\theta) \cos(\theta)$$

Their values at the pole satisfy:

$$v(0,\theta) = X(0,\theta) \cos(\theta) + Y(0,\theta) \sin(\theta) = X_0 \cos(\theta) + Y_0 \sin(\theta),$$
(15)

$$w(0,\theta) = -X(0,\theta) \sin(\theta) + Y(0,\theta) \cos(\theta) = -X_0 \sin(\theta) + Y_0 \cos(\theta).$$
(16)

Moreover, from these equations we obtain the radial derivatives at the pole, namely:

$$\frac{\partial v}{\partial \rho} \left(0^+, \theta \right) = \frac{\partial X}{\partial \rho} \left(0^+, \theta \right) \, \cos(\theta) + \frac{\partial Y}{\partial \rho} \left(0^+, \theta \right) \, \sin(\theta), \tag{17}$$

$$\frac{\partial w}{\partial \rho} \left(0^+, \theta \right) = -\frac{\partial X}{\partial \rho} \left(0^+, \theta \right) \sin(\theta) + \frac{\partial Y}{\partial \rho} \left(0^+, \theta \right) \cos(\theta), \tag{18}$$

WJMS email for contribution: submit@wjms.org.uk

166

respectively. Therefore, by combining Eqs. (14), (17) and (18), we get:

$$\begin{aligned} \frac{\partial v}{\partial \rho} \left(0^+, \theta + \pi \right) &= \frac{\partial X}{\partial \rho} \left(0^+, \theta \right) \ \cos(\theta) + \frac{\partial Y}{\partial \rho} \left(0^+, \theta \right) \ \sin(\theta), \\ \frac{\partial w}{\partial \rho} \left(0^+, \theta + \pi \right) &= -\frac{\partial X}{\partial \rho} \left(0^+, \theta \right) \ \sin(\theta) + \frac{\partial Y}{\partial \rho} \left(0^+, \theta \right) \ \cos(\theta). \end{aligned}$$

This means that polar components of \vec{U} satisfy:

$$\begin{cases} \frac{\partial v}{\partial \rho}(0^+,\theta) = \frac{\partial v}{\partial \rho}(0^+,\theta+\pi) \\ \frac{\partial w}{\partial \rho}(0^+,\theta) = \frac{\partial w}{\partial \rho}(0^+,\theta+\pi) \end{cases}$$
(19)

for all values of ϑ . Again, to determine the values X_0 and Y_0 , we only need to apply Eq. (19) to a single arbitrary value of θ . For simplicity, we take: $\theta = 0$ to obtain

$$\begin{cases} \frac{\partial v}{\partial \rho}(0^+,0) = \frac{\partial v}{\partial \rho}(0^+,\pi) \\ \frac{\partial w}{\partial \rho}(0^+,0) = \frac{\partial w}{\partial \rho}(0^+,\pi) \end{cases}$$
(20)

Hence, complementary conditions for a vector function at $\rho = 0$ are Eqs. (15), (16) and (20). Those conditions are used in the finite-difference scheme below.

3 Finite-differences and complementary conditions

We consider the computational domain to be a circular disk of radius R centered at the pole. Hence, polar coordinates take values in the ranges $0 \le \theta \le 2\pi$ and $0 \le \rho \le R$. We uniformly divide these intervals into N and M parts, respectively. The resulting mesh is given by $\theta_n = (n-1) \ \Delta \theta$ and $\rho_m = m \ \Delta \rho$, with $\Delta \theta = 2\pi/N, \ \Delta \rho = R/(M+1), n = 1, 2, ..., N$ and m = 0, 1, ..., M + 1. Conveniently, N is taken as an even number. In this way, $\theta_{1+N/2} = \pi$, i.e., π is among the azimuthal nodes (see Fig. 2). The temperature distribution in a circular plate occupying the region R is supposed to be described by the function $u(\rho, \theta)$ and its node values are denoted by $u_{m,n} = u(\rho_m, \theta_n)$.

3.1 Scalar unknown

To assess the complementary equations derived in subsection 2.1, we calculate the temperature distribution obeying Eq. (7), with source function $s(\rho, \theta) = s_0 \left[33 (\rho/R)^{3/2} - 9 (\rho/R)^{1/2} \right] \cos(2\theta)$ and boundary condition $u(R, \theta) = T_0 \sin^3(\theta - \pi/3)$.

The nodes with $2 \le n \le N - 1$ and $1 \le m \le M$ are inner points of the mesh in Fig. 2. At those points, the finite-difference version of Eq. (7) is written by using central differences as:

$$\frac{u_{m-1,n} - 2u_{m,n} + u_{m+1,n}}{(\Delta\rho)^2} + \frac{u_{m+1,n} - u_{m-1,n}}{2\rho_m \,\Delta\rho} + \frac{u_{m,n-1} - 2u_{m,n} + u_{m,n+1}}{\rho_m^2 \,(\Delta\theta)^2} = -\frac{s_{m,n}}{k},\tag{21}$$

with $s_{m,n} = s(\rho_m, \theta_n)$. It is worthy to notice that all points with $1 \le m \le M$ and either n = 1 or n = N lay at the boundary of the mesh in Fig. 2, but they correspond to inner points of the circular domain D. Hence, we may extend the validity of Eq. (21) by making the replacements $u_{m,0} \to u_{m,N}$ and $u_{m,N+1} \to u_{m,1}$. Moreover, for m = 1, we follow Eq. (8) and make:

$$u_{0,n} = u_0$$

for all $1 \le n \le N$ and, for m = M, we take into account the discretized boundary condition, i.e.,

$$u_{M+1,n} = T_0 \sin^3(\theta_n - \pi/3).$$
 (22)

In this way, we have got a system of N M linear equations for u_0 and the N M unknowns $u_{m,n}$ with $1 \le n \le N$ and $1 \le m \le M$.

The remaining equation follows from Eq. (10) and has the form:

$$\sum_{n=1}^{N} \frac{\partial u}{\partial \rho} (0^+, \theta_n) = 0.$$
(23)

Since the radial derivative in this sum may be estimated in terms of three points, namely:

$$\frac{\partial u}{\partial \rho}(0^+, \theta_n) = \frac{4u_{1,n} - 3u_0 - u_{2,n}}{2\,\Delta\rho},\tag{24}$$

Eq. (23) gives an equation for u_0 , i.e.,

$$u_0 = \frac{1}{3N} \sum_{n=1}^{N} \left(4 \, u_{1,n} - u_{2,n} \right) \,. \tag{25}$$

Consequently, Eqs. (21), (22) and (25) form a system of 1 + N M equations for u_0 and $u_{m,n}$ with $1 \le n \le N$ and $1 \le m \le M$.

We also note that for a smooth solution we may use Eq. (13) instead of Eq. (10). Hence, from Eq. (24) we obtain:

$$u_0 = \frac{2}{3}(u_{1,1} + u_{1,1+N/2}) - \frac{1}{6}(u_{2,1} + u_{2,1+N/2}),$$
(26)

which may be used instead of Eq. (25).

For the sake of comparison, it is useful to bear in mind that the present problem has a rather simple analytical solution, namely:

$$\frac{u(\rho,\theta)}{T_0} = \frac{1}{4} \left[\frac{3\rho}{R} \sin(\theta - \pi/3) + \frac{\rho^3}{R^3} \sin(3\theta) \right] + 4\sigma \left[\left(\frac{\rho}{R}\right)^{5/2} - \left(\frac{\rho}{R}\right)^{7/2} \right] \cos\left(2\theta\right),$$

with $\sigma = R^2 s_0/(kT_0)$ being a dimensionless parameter which characterizes the intensity of the heating source. Moreover, the two-dimensional energy-flux density is given by:

$$\vec{U}\left(\rho,\theta\right) = -k\,\vec{\nabla}u = -\frac{\partial u}{\partial\rho}\,\hat{e}_{
ho} - \frac{1}{
ho}\,\frac{\partial u}{\partial\theta}\,\hat{e}_{
ho}.$$

Therefore, its polar components $v(\rho, \theta)$ and $w(\rho, \theta)$ satisfy:

$$\frac{Rv(\rho,\theta)}{kT_0} = -\frac{3}{4} \left[\sin(\theta - \pi/3) + \frac{\rho^2}{R^2} \sin(3\theta) \right] - 2\sigma \left[5\left(\frac{\rho}{R}\right)^{3/2} - 7\left(\frac{\rho}{R}\right)^{5/2} \right] \cos(2\theta)$$
$$\frac{Rw(\rho,\theta)}{kT_0} = -\frac{3}{4} \left[\cos(\theta - \pi/3) + \frac{\rho^2}{R^2} \cos(3\theta) \right] + 8\sigma \left[\left(\frac{\rho}{R}\right)^{3/2} - \left(\frac{\rho}{R}\right)^{5/2} \right] \sin(2\theta).$$

Figs. 3 and 4 display the contour plot of u(x, y) and the stream lines of $\vec{U}(x, y)$, respectively. Vector $\vec{U}(x, y)$ is perpendicular to contour lines and points toward the low-temperature side of the line.

3.2 Vector unknown

From the analytical solution presented in the previous section, it is straightforward to show that the polar components of the energy-flux density satisfy the following Dirichlet boundary conditions:

$$\frac{Rv(R,\theta)}{kT_0} = -\frac{3}{4} \left[\sin(\theta - \pi/3) + \sin(3\theta) \right] + 4\sigma \cos(2\theta) \,. \tag{27}$$

$$\frac{Rw(R,\theta)}{kT_0} = -\frac{3}{4} \left[\cos(\theta - \pi/3) + \cos(3\theta) \right].$$
(28)



Fig. 3. Contour plots of the steady-state tempera- Fig. 4. Solid oriented curves are stream lines of the ture distribution, in units of T_0 , for a uniform cir- heat current corresponding to temperature distribution cular plate of radius R with the Dirichlet condition and conditions in Fig. 3. Dotted lines are contour lines $T(R, \theta) = T_0 \sin^3(\theta - \pi/3) \text{ and heating function in Fig. 3}$ $s(\rho, \theta) = s_0 \left[33 (\rho/R)^{3/2} - 9 (\rho/R)^{1/2} \right] \cos(2\theta), \text{ with}$ $R^2 s_0 = k T_0$

Then, in order to assess the complementary equations derived in subsection 2.2, we may try to calculate the vector field $\vec{U}(\rho,\theta)$. Of course, we should set up differential equations for $v(\rho,\theta)$ and $w(\rho,\theta)$. On the one hand, since $\vec{U}(\rho, \theta)$ is a gradient, its curl must vanish. Following Eq. (4), this leads to:

$$\frac{\partial w}{\partial \rho} + \frac{w}{\rho} - \frac{1}{\rho} \frac{\partial v}{\partial \theta} = 0.$$
⁽²⁹⁾

On the other hand, by using Eq. (2), we rewrite Eq. (6) as:

$$\frac{\partial v}{\partial \rho} + \frac{v}{\rho} + \frac{1}{\rho} \frac{\partial w}{\partial \theta} = s.$$
(30)

To set up the finite-difference scheme, we use the same mesh as in the previous section, denoting $v_{m,n} =$ $v(\rho_m, \theta_n)$ and $w_{m,n} = w(\rho_m, \theta_n)$. By using the same discretization procedure, Eqs. (29) and ((30) lead to:

$$\frac{w_{m+1,n} - w_{m-1,n}}{2\,\Delta\rho} + \frac{w_{m,n}}{\rho_m} - \frac{v_{m,n+1} - v_{m,n-1}}{2\,\rho_m\,\Delta\theta} = 0,$$
$$\frac{v_{m+1,n} - v_{m-1,n}}{2\,\Delta\rho} + \frac{v_{m,n}}{\rho_m} + \frac{w_{m,n+1} - w_{m,n-1}}{2\,\rho_m\,\Delta\theta} = s_{m,n}$$

These later equations are valid for $1 \le n \le N$ and $1 \le m \le M$, provided replacements $v_{m,0} \to v_{m,N}$, $w_{m,0} \rightarrow w_{m,N}$, $v_{m,N+1} \rightarrow v_{m,1}$, and $w_{m,N+1} \rightarrow w_{m,1}$ are made when needed. Moreover, when m = 1, we make use of Eqs. (15) and (16) to write:

$$v_{0,n} = X_0 \, \cos(\theta_n) + Y_0 \, \sin(\theta_n),\tag{31}$$

$$w_{0,n} = -X_0 \sin(\theta_n) + Y_0 \cos(\theta_n).$$
 (32)

The boundary Eqs. (27) and (28) are written as:

$$\frac{R v_{M+1,n}}{k T_0} = -\frac{3}{4} \left[\sin(\theta_n - \pi/3) + \sin(3\theta_n) \right] + 4\sigma \, \cos(2\theta_n) \,,$$
$$\frac{R w_{M+1,n}}{k T_0} = -\frac{3}{4} \left[\cos(\theta_n - \pi/3) + \cos(3\theta_n) \right] \,.$$

Furthermore, Eqs. (20), (24), (31) and (32) lead to the complementary conditions:

A. Bruno-Alfonso & L. Cabezas-Gómez & H. Navarro: Alternate treatments of jacobian singularities

$$X_0 = \frac{2}{3}(v_{1,1} - v_{1,1+N/2}) - \frac{1}{6}(v_{2,1} - v_{2,1+N/2}), \quad Y_0 = \frac{2}{3}(w_{1,1} - w_{1,1+N/2}) - \frac{1}{6}(w_{2,1} - w_{2,1+N/2})$$

This leaves us with 2 + 2M N equations for X_0 , Y_0 and the unknowns $v_{m,n}$ and $w_{m,n}$, with $1 \le n \le N$ and $1 \le m \le M$.

4 Convergence of numerical results

The finite-difference schemes described above lead to linear systems which may be solved by using a computational algebraic system such as Mathematica^[11]. For simplicity, we take M = N, thus we are able to investigate the convergence of results as a function of N. For the case of scalar unknown, we define:

 $\varepsilon_N = \max\left\{ \left| u_{m,n} - u(\rho_m, \theta_n) \right| : \ 0 \le m \le M, \ 1 \le n \le N \right\},\$

as the maximum error of the finite-difference calculation. By using $N = 20, 22, \ldots, 60$, the finite-difference



Fig. 5. The maximum error of the finite-difference scheme for scalar unknown as a function of , with being the number of angular divisions. Panel (a) (b) comes from the use of Eq. (25) and (26) as the complementary condition at the pole



Fig. 6. The maximum error of the finite-difference scheme for vector unknown as a function of 1/N, where N is the number of angular divisions

results for the temperature distribution essentially reproduce the exact solution displayed in Fig. 3, where $\sigma = 1$. This is apparent in Fig. 5, where the maximum error ε_N is shown as a function of 1/N. Panels (a) and (b) correspond to Eq. (25) and (26), respectively. We note that in both cases the error converges to zero as N grows. In fact, the error is essentially proportional to $1/N^2$.

The analysis of convergence for the case of vector unknown follows the same idea. Namely, we define:

$$\varepsilon_N = \max\left\{ \left\| \vec{U}_{m,n} - \vec{U}(\rho_m, \theta_n) \right\| : \ 0 \le m \le M, \ 1 \le n \le N \right\},\tag{33}$$

as the maximum error of the finite-difference calculation. Figure 6 displays the maximum error ε_N as a function of 1/N. This error converges to zero as N grows, being roughly proportional to $1/N^2$.

170

5 Conclusions

We have derived complementary conditions at geometrical singularities of PDEs in polar coordinates both for scalar and vector unknowns. Their finite-difference versions were applied to solve heat-transfer problems in a circular disk. A very good agreement between numerical and analytical solutions was obtained. As the number of mesh points increases, error decreases roughly as the inverse of the square of such number, showing that the employed discretization scheme have a second order accuracy.

Present approach is promising for application in the solution of other physical problems of interest, like laminar and turbulent isothermal fluid flow, convection heat-transfer phenomena, mechanical waves, electromagnetic fields and quantum states in curvilinear coordinates. The present approach is quite general for smooth solutions and does not avoid the pole. This idea may be extended to spherical and other curvilinear coordinates.

Of course, further numerical tests in time-dependent and non-linear problems, like those involving Navier-Stokes equations, should be performed in order to establish the overall applicability of the proposed methodology.

References

- [1] V. Arpaci. Conduction Heat Transfer. Addison-Wesley Publishing Company, New York, 1966.
- [2] G. Constantinescu, S. Lele. A new method for accurate treatment of flow equations in cylindrical coordinates using series expansions. in: *CTR Annual Research Briefs 2000, Center for Turbulence Research*, NASA Ames and Stanford University Press, Stanford, CA, 2001, 199–210.
- [3] G. Constantinescu, S. Lele. A highly accurate technique for the treatment of flow equations at the polar axis in cylindrical coordinates using series expansions. *Journal of Computational Physics*, 2003, **183**: 165–186.
- [4] G. Davies. A note on a mesh for use with polar coordinates. Numerical Heat Transfer, 1979, 2: 261–266.
- [5] K. Fukagata, N. Kasagi. Highly energy-conservative finite difference method for the cylindrical coordinate system. *Journal of Computational Physics*, 2002, **181**: 478–498.
- [6] M. Griffin, E. Jones, et al. A computational fluid dynamic technique valid at the centerline for non-axisymmetric problems in cylindrical coordinates. *Journal of Computational Physics*, 1979, **30**: 352–360.
- [7] K. Mohseni, T. Colonius. Numerical treatment of polar coordinate singularities. *Journal of Computational Physics*, 2000, 157: 787–795.
- [8] Y. Morinishi, O. Vasilyev, T. Ogi. Fully conservative finite difference scheme in cylindrical coordinates for incompressible flow simulations. *Journal of Computational Physics*, 2004, 197: 686–710.
- [9] N. Ozisik. Boundary Value Problems of Heat Conduction. Dover Publications Incorporated, New York, 1989.
- [10] K. Riley, M. Hobson. Essential Mathematical Methods for Physical Sciences. Cambridge University Press, Cambridge, 2011.
- [11] S. Wolfram. *The Mathematica Book*, 2, Cambridge University Press, 1996.