## Effective Treatment of the Singular Line Boundary Problem for Three-Dimensional Grids

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## **Abstract**

 $\mathbf{T}$  HREE-DIMENSIONAL grids of rotation contain a singular line where the radial grid planes meet. When the flow equations are transformed into generalized coordinates, a mathematical singularity is introduced into the governing equations. Specifically, the grid Jacobian J becomes infinite along the singular line. This can introduce nonphysical perturbations in the flow solution, particularly if a finite-difference solution algorithm is used. A number of recent publications <sup>1-5</sup> have discussed problems associated with the singular line.

This paper presents a method for eliminating the axis singularity. The governing equations are reformulated using a redefined grid Jacobian that can be evaluated at the singular line. This allows a finite-difference algorithm to compute a smooth, continuous solution in the region of the singular line.

## **Contents**

A typical grid over a three-dimensional blunt body is shown in Fig. 1. It consists of a series of radial grid planes that meet along a common or singular line usually emanating from the nose of the body. In the following discussions the singular line is assumed to lie on the x axis.

The solution procedure normally employed by CFD algorithms is to transform the governing equations and grid coordinates from a Cartesian (x, y, z) coordinate system to a generalized  $(\xi, \eta, \zeta)$  coordinate system. The Navier-Stokes equations expressed in vector form in generalized coordinates are

$$\frac{\partial \hat{Q}}{\partial t} + \frac{\partial \hat{E}}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} + \frac{\partial \hat{G}}{\partial \zeta} = \frac{\partial \hat{R}}{\partial \xi} + \frac{\partial \hat{S}}{\partial \eta} + \frac{\partial \hat{T}}{\partial \zeta}$$
(1)

with

$$\hat{Q} = J^{-1}Q \qquad \hat{E} = J^{-1}[\xi_x E + \xi_y F + \xi_z G]$$

$$\hat{F} = J^{-1}[\eta_x E + \eta_y F + \eta_z G] \qquad \hat{G} = J^{-1}[\zeta_x E + \zeta_y F + \zeta_z G]$$
(2)

where E, F, and G are the inviscid Cartesian flux vectors. The grid Jacobian J used in the preceding expressions and to compute the metric terms,  $\xi_x$ ,  $\xi_y$ ,  $\xi_z$ ,  $\eta_x$ , etc., is defined as

$$J = \left[ x_{\xi} (y_{\eta} z_{\xi} - y_{\xi} z_{\eta}) - x_{\eta} (y_{\xi} z_{\xi} - y_{\xi} z_{\xi}) + x_{\xi} (y_{\xi} z_{\eta} - y_{\eta} z_{\xi}) \right]^{-1}$$
 (3)

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Along the singular line, the spatial derivatives in the circumferential direction,  $x_{\eta}$ ,  $y_{\eta}$ , and  $z_{\eta}$ , are all zero, making the grid Jacobian defined by Eq. (3) infinite. The metric terms are either infinite or indeterminate. No information is allowed to pass from the singular line boundary to the interior causing spurious perturbations in the computed flow solution.

A finite value for the singular line Jacobian can be obtained by extrapolation from interior grid points or by setting  $y_{\eta}$  and  $z_{\eta}$ , or  $x_{\eta}$  and  $y_{\eta}$  depending on the axis orientation to small finite values. However, these approximate methods yield unsatisfactory results when used with a finite-difference flow solver.

It is possible to redefine the grid Jacobian such that it is no longer infinite on the singular line. The grid Jacobian is written as the product of two quantities

$$J = (1/r)\,\overline{J}\tag{4}$$

where r is the radial distance from the singular line  $(y^2 + z^2)^{\frac{1}{2}}$ . The modified Jacobian  $\overline{J}$  is finite throughout the entire computational domain. It is equivalent to the grid Jacobian obtained if the Navier-Stokes equations were originally expressed in cylindrical,  $(x, r, \theta)$ , coordinates and can be computed from the expression

$$\overline{J} = \left[ x_{\xi} (r_{\eta} \theta_{\zeta} - r_{\zeta} \theta_{\eta}) - x_{\eta} (r_{\xi} \theta_{\zeta} - r_{\zeta} \theta_{\xi}) + x_{\zeta} (r_{\xi} \theta_{\eta} - r_{\eta} \theta_{\xi}) \right]^{-1}$$
 (5)

If Eq. (4) is inserted in Eq. (1) and the chain rule used to remove the r term from the partial differential equations, the governing equations become

$$\frac{\partial \overline{Q}}{\partial t} + \frac{\partial \overline{E}}{\partial \xi} + \frac{\partial \overline{F}}{\partial \eta} + \frac{\partial \overline{G}}{\partial \zeta} + \frac{\overline{H}}{r} = \frac{\partial \overline{R}}{\partial \xi} + \frac{\partial \overline{S}}{\partial \eta} + \frac{\partial \overline{T}}{\partial \zeta} + \frac{\overline{W}}{r}$$
 (6)

The vector quantities are now scaled by the modified, or cylindrical, grid Jacobian.

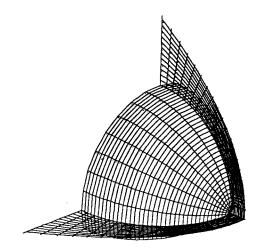


Fig. 1 Generic blunt body grid with axis singular line.

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$$\begin{split} \overline{Q} &= \overline{J}^{-1}Q & \overline{E} &= \overline{J}^{-1}[\xi_x E + \xi_y F + \xi_z G] \\ \overline{F} &= \overline{J}^{-1}[\eta_x E + \eta_y F + \eta_z G] & \overline{G} &= \overline{J}^{-1}[\zeta_x E + \zeta_y F + \zeta_z G] \end{split}$$

The viscous vectors are similarly scaled. The metric quantities,  $\xi_x$ ,  $\xi_y$ ,  $\xi_z$ ,  $\eta_x$ , etc., are first computed using cylindrical coordinates and then converted to Cartesian. Equation (6) is identical to that obtained if the cylindrical Navier-Stokes equations are transformed to generalized coordinates. The additional source-like vectors  $\overline{H}$  and  $\overline{W}$ , are defined as

$$\overline{H} = [r_{\xi}\overline{E} + r_{\eta}\overline{F} + r_{\zeta}\overline{G}] \qquad \overline{W} = [r_{\xi}\overline{R} + r_{\eta}\overline{S} + r_{\zeta}\overline{T}] \qquad (7)$$

The singularity has, in effect, been transferred to these two source-like vectors. Since the source vectors are not evaluated along the singular line where r=0, the source vectors are never singular. For grids over bodies of rotation where  $x_{\eta}=r_{\eta}=0$ , the source vector  $\overline{H}$  is given by

$$\overline{H} = \overline{J}^{-1} \begin{bmatrix} \rho v_r \\ \rho u v_r \\ \rho v v_r + p \cos \theta \\ \rho w v_r + p \sin \theta \\ (e + p) v_r \end{bmatrix}$$
(8)

$$v_r = v \cos \theta + w \sin \theta$$
  $\theta = \tan^{-1}(z/y)$ 

Mach 20, inviscid, perfect gas flow was computed over a sphere at zero angle of attack using the Cartesian grid Jacobian and cylindrical grid Jacobian formulations. A zeroth-order extrapolation boundary condition at the singular line was used for both algorithms. The velocity components v and w are set to zero along the singular line, which is also the stagnation line for this case. The inviscid fluxes were differenced using Van Leer flux vector splitting.<sup>6</sup>

To give the grid Jacobian some noninfinite value for the Cartesian grid Jacobian case, the points on the singular line were given finite values of y and z corresponding to the points being distributed on a circle of radius  $1.0 \times 10^{-7}$  normalized with respect to the sphere radius centered on the x axis. Thus, the only difference between the two solutions is the use of the Cartesian or cylindrical grid Jacobian formulation.

Solutions computed using both methods are compared against data produced by Lyubimov and Rusanov.<sup>7</sup> They utilized a shock-fitting iterative difference scheme, referred to as a constant direction scheme, to compute inviscid flow over simple bodies of revolution at various Mach numbers. This

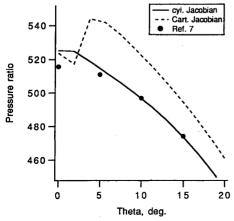


Fig. 2 Surface pressure ratio.

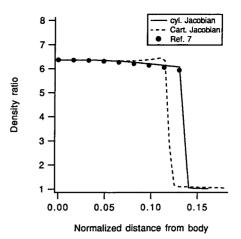


Fig. 3 Density ratio along stagnation line.

allows a comparison between an independent calculation and the results computed in this study.

Figure 2 shows normalized pressure along the body surface in the region of the singular line. The stagnation point and singular line are at  $\theta=0$ . The Cartesian grid Jacobian pressure profile exhibits a sawtooth pattern near the singular line. The computed radial velocity is not zero along the stagnation line as it should be. The three-dimensional cylindrical grid Jacobian solution shows none of these problems and computed pressure values compare closely with Ref. 7. Away from the singular line, the Cartesian grid Jacobian solution gradually approaches that of the other solutions.

Figure 3 shows the stagnation line normalized density profile of the three solutions. The cylindrical grid Jacobian density values and shock standoff distance compare closely with the results obtained in Ref. 7. The Cartesian grid Jacobian solution, however, significantly underpredicts shock standoff distance

When the cylindrical grid Jacobian technique was applied to compute flow over a body at a nonzero angle of attack it did not perform as well. The effect of the two source vectors,  $\vec{H}$  and  $\vec{W}$ , is to force the radial velocity to zero when r approaches zero. This is the proper effect if the singular line coincides with the stagnation line but not if the body is at an angle of attack with respect to the flow. Future research will be directed to extending the technique to nonzero angle-of-attack cases.

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