1985

Complex Mach reflection in shock diffraction problems

Osamu Yamamoto

Iowa State University

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COMPLEX MACH REFLECTION IN SHOCK DIFFRACTION PROBLEMS

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Osamu Yamamoto

A Dissertation Submitted to the Graduate Faculty in Partial Fulfillment of the Requirements for the Degree of

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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>CHAPTER I. INTRODUCTION</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>CHAPTER II. SHOCK DIFFRACTION PROBLEMS</td>
<td>7</td>
</tr>
<tr>
<td>CHAPTER III. GOVERNING EQUATIONS AND TRANSFORMATIONS</td>
<td>13</td>
</tr>
<tr>
<td>Double Normalization</td>
<td>18</td>
</tr>
<tr>
<td>CHAPTER IV. FINITE-DIFFERENCE METHOD</td>
<td>21</td>
</tr>
<tr>
<td>Special Discretization Formula</td>
<td>22</td>
</tr>
<tr>
<td>CHAPTER V. INITIAL CONDITIONS</td>
<td>27</td>
</tr>
<tr>
<td>CHAPTER VI. BOUNDARY CONDITIONS</td>
<td>34</td>
</tr>
<tr>
<td>Wall Boundary</td>
<td>34</td>
</tr>
<tr>
<td>Ramp Boundary</td>
<td>35</td>
</tr>
<tr>
<td>Reflected Shock</td>
<td>36</td>
</tr>
<tr>
<td>Mach Stem</td>
<td>40</td>
</tr>
<tr>
<td>CHAPTER VII. CONTACT SURFACE CALCULATIONS</td>
<td>42</td>
</tr>
<tr>
<td>Coordinate System</td>
<td>42</td>
</tr>
<tr>
<td>Contact Surface Speed</td>
<td>48</td>
</tr>
<tr>
<td>CHAPTER VIII. NUMERICAL RESULTS</td>
<td>51</td>
</tr>
<tr>
<td>CHAPTER IX. CONCLUSIONS</td>
<td>68</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>69</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENT</td>
<td>72</td>
</tr>
<tr>
<td>APPENDIX A. METRICS OF DOUBLE NORMALIZATION</td>
<td>73</td>
</tr>
<tr>
<td>APPENDIX B. TRIPLE POINT SOLUTION</td>
<td>77</td>
</tr>
<tr>
<td>APPENDIX C. SPLIT COEFFICIENT MATRIX METHOD</td>
<td>84</td>
</tr>
<tr>
<td>APPENDIX D. JUMP CONDITION ACROSS THE DISCONTINUITY</td>
<td>92</td>
</tr>
</tbody>
</table>
LIST OF TABLES

TABLE 1. Metrics of contact surface normalizing transformation . . . 45
LIST OF FIGURES

FIGURE 1. Examples of shock diffraction ........................................... 2
FIGURE 2. Shock diffraction geometry .................................................. 3
FIGURE 3. Domains and boundaries of shock diffraction ............................. 4
FIGURE 4. Schematic diagram of RR and its shock polar .............................. 8
FIGURE 5. Schematic diagram of SMR and its shock polar ........................... 10
FIGURE 6. Schematic diagram of CMR and its shock polar .......................... 12
FIGURE 7. Typical complex Mach reflection ............................................. 14
FIGURE 8. Mesh system ........................................................................... 19
FIGURE 9. Reference mesh and floating grid points ................................... 24
FIGURE 10. Self-similar velocities across the reflected shock ....................... 31
FIGURE 11. Sublayer grid points at wall boundary .................................... 35
FIGURE 12. Isopycnics of complex Mach reflection ................................... 53
FIGURE 13. Comparison of wall density ................................................... 54
FIGURE 14. Numerical simulation of CMR, Isobars ................................... 56
FIGURE 15. Wall pressure and density ..................................................... 57
FIGURE 16. CMR ( $M_s = 1.89$, $\theta_r = 40^\circ$ ) ....................................... 60
FIGURE 17. Wall pressure and density ...................................................... 61
FIGURE 18. CMR ( $M_s = 2.20$, $\theta_r = 40^\circ$ ) ....................................... 62
FIGURE 19. Wall pressure and density ...................................................... 63
FIGURE 20. CMR ( $M_s = 2.50$, $\theta_r = 40^\circ$ ) ....................................... 64
FIGURE 21. Wall pressure and density ...................................................... 65
FIGURE 22. CMR ( $M_s = 2.70, \theta_r = 40^\circ$ ) ......... 66

FIGURE 23. CMR ( $M_s = 2.80, \theta_r = 40^\circ$ ) ......... 67

FIGURE 24. Schematic diagram of three shock confluence .... 80

FIGURE 25. Domain of dependence ......... 87

FIGURE 26. Discontinuity in an arbitrary domain ......... 92
CHAPTER I. INTRODUCTION

The study of shock diffraction is of considerable importance to fluid dynamics researchers in analyzing blast wave effect on ground structures and flight vehicles. Typical examples include reflection of a shock wave from the wing of a supersonic aircraft due to an external store and blast wave diffraction by a building (Figure 1).

The simplest laboratory experiment designed to study the shock diffraction problem consists of a two-dimensional ramp mounted on a shock tube wall. When a planar shock encounters a compression ramp, the ensuing shock diffraction pattern is determined by the Mach number of the incident shock, $M_s$, and the ramp angle $\theta_r$. The various combinations of $M_s$ and $\theta_r$ give rise to four different types of shock diffraction. These are regular reflection (RR), single Mach reflection (SMR), complex Mach reflection (CMR), and double Mach reflection (DMR). The various configurations are shown in Figure 2.

Although Ernst Mach (1) originally observed RR and SMR in 1878, little analytical or numerical work was done on shock diffraction until the 1940s when John von Neumann (2,3) rekindled interest in the problem. A few years later the CMR and DMR diffraction patterns were first identified by Smith (4) and White (5). The transitions among the various diffraction cases have received study both analytically and in the laboratory. Ben-Dor and Glass (6,7) have recently published data identifying the boundaries of the various diffraction regimes. These boundaries are shown in Figure 3.
FIGURE 1. Examples of shock diffraction
INCIDENT SHOCK

RAMP

VERTICAL SINGULARITY

REFLECTED SHOCK

VORTICAL SINGULARITY

INCIDENT SHOCK

SELF-SIMILAR STAGNATION POINTS

• NODAL + SADDLE

CONTACT SURFACE

自我相似超声速流动

REGULAR REFLECTION

TRIPLE POINT

MACH STEM

KINK

CONTACT SURFACE

SINGLE MACH REFLECTION

COMPLEX MACH REFLECTION

DOUBLE MACH REFLECTION

FIGURE 2. Shock diffraction geometry
Incident shock-wave Mach number, $M_s$

### Shock diffraction

<table>
<thead>
<tr>
<th>Region no.</th>
<th>Shock reflection</th>
<th>Flow deflection</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RR</td>
<td>Detached</td>
</tr>
<tr>
<td>2</td>
<td>SMR</td>
<td>Detached</td>
</tr>
<tr>
<td>3</td>
<td>SMR</td>
<td>Attached</td>
</tr>
<tr>
<td>4</td>
<td>CMR</td>
<td>Detached</td>
</tr>
<tr>
<td>5</td>
<td>CMR</td>
<td>Attached</td>
</tr>
<tr>
<td>6</td>
<td>DMR</td>
<td>Attached</td>
</tr>
<tr>
<td>7</td>
<td>DMR</td>
<td>Attached</td>
</tr>
</tbody>
</table>

**FIGURE 3.** Domains and boundaries of shock diffraction
In recent years, the numerical simulation of shock diffraction has shown potential for providing a vast amount of data which cannot be derived from shock tube experiments. Even so, very few numerical results are available today for the RR, SMR, and DMR cases.

One of the early numerical works using a finite-difference approach is that of Ludloff and Friedman (8). In their report, both elliptic and hyperbolic (time-asymptotic approach) formulations of the governing equations were used. The time-asymptotic approach was employed by Rusanov (9) and later by Schneyer (10) to solve for RR and SMR. However, their shock-captured results failed to correctly predict the actual physical flow across the shock wave. Kutler and Shankar (11) computed the solution for the RR case using a boundary shock-fitting approach. Their results show excellent agreement with the experimental data. In a continuation of that work, Shankar, Kutler, and Anderson (12) obtained numerical results for SMR using a boundary shock-fitting approach and treating the contact surface as a floating discontinuity. Their results predicted accurate shock shapes; however, the contact surface was not computed correctly. The most recent reported work on shock diffraction is that of Woodward and Colella (13). They have used a shock-capturing approach with an extremely fine mesh to compute the flowfield for the DMR case.

Unfortunately, earlier numerical results were obtained for isolated cases in RR, SMR, and DMR regimes, and no transition case from SMR to DMR has been computed. In the present study, solutions in the CMR
regime, starting from near SMR to just before the second triple-point forms, are computed in an attempt to study the evolution of the physical process governing the formation of a second triple point and a second Mach stem. To do this, the case with \( M_S = 1.89 \) and \( \Theta_r = 40^\circ \) (this case was computed as SMR earlier by Shankar, Kutler, and Anderson, and serves as the comparison of numerical results) is computed first with the initial conditions presented in Chapter V. Then the subsequent cases with increased \( M_S \) (\( \Theta_r \) is fixed) are computed using the previously computed results as the initial conditions. A comparison case with the experimental data (\( M_S = 2.67 \) and \( \Theta_r = 30^\circ \)) is computed by perturbing both \( M_S \) and \( \Theta_r \) from the earlier case. This also demonstrates the flexibility of the present numerical codes in computing various cases of shock diffraction.

A first-order accurate, explicit, split coefficient matrix (SCM) method is used to integrate the unsteady Euler equations. The boundary shock-fitting approach in conjunction with floating discontinuity-fitting is employed in order to show the sharp discontinuity across the contact surface and the details in the neighborhood of the vortical singularities.
CHAPTER II. SHOCK DIFFRACTION PROBLEMS

When a moving incident shock strikes a ramp with a large inclination angle \( (\theta_x > 50^\circ) \), regular reflection invariably occurs. The flow process through the incident shock and the reflected shock can be easily understood on the shock polar diagram. A typical RR case and its shock polar drawn relative to the incident shock are shown in Figure 4. The polar I corresponds to the incident shock and polar R corresponds to the reflected shock. The conditions indicated by 1 are in the undisturbed region ahead of the incident shock; 2 indicates conditions behind the incident shock; and 3 indicates conditions behind the reflected shock. When the ramp angle is given, the state 2 is determined by the shock angle \( \beta \) and the shock induced Mach number \( M_1 \). Upon passing through incident shock I, the flow is deflected by an angle \( \delta_1 \) from its original path. The boundary condition on the wall dictates that the flow must be deflected back to the original path through the reflected shock, i.e., the state 3 is found on the R polar where the net deflection angle \( \delta = \delta_1 + \delta_2 \) is zero.

The transition from regular to Mach reflection can be accomplished by decreasing the ramp angle \( \theta_x \). For a sufficiently weak incident shock, the transition results in a single Mach reflection. A typical SMR configuration and the associated shock polars are shown in Figure 5. Von Neumann (2) was the first to propose the detachment criterion for the transition from a regular to a Mach reflection. According to this criterion, the termination of regular reflection takes place when the
FIGURE 4. Schematic diagram of RR and its shock polar
detachment point of the reflected shock \( R' \) is tangent to the \( P/P_1 \) axis. Physically this condition means that the flow through the reflected shock turns just enough to become parallel with the ramp surface. There are two other criteria currently proposed; one is the mechanical equilibrium condition and the other is the sonic condition. The discussion of these criteria is presented in Refs. 14 and 15.

Further decrease in the ramp angle \( \theta_r \) from its critical value requires a three-shock confluence to satisfy the boundary conditions. Since the flow through the reflected shock cannot make a sufficiently large turn to become parallel with the ramp wall (see the \( R'' \) polar of Figure 5), the formation of the Mach stem and triple-point results. The flows behind the reflected shock and the Mach stem undergo different shock processes; therefore, two different thermodynamic states separated by a contact surface exist at the triple point. Physical conditions require that the pressures and the flow direction must be the same across the contact surface. These two states are indicated by 3 and 4 in Figure 5. It is important to note that in the SMR configuration, the flow behind the reflected shock is subsonic; therefore, downstream characteristics can reach to the reflection point.

When the incident shock strength increases, more gradual transition takes place from SMR to CMR. Typical CMR and its shock polar are shown in Figure 6. The transition from SMR to CMR is noted by a developing supersonic flow behind the reflected shock. Unlike the SMR case, downstream characteristics cannot reach to the reflection point; hence,
FIGURE 5. Schematic diagram of SMR and its shock polar
the reflected shock develops a slope inflection below the sonic point. In most CMR cases, an irregular shape develops on the reflected shock and on the contact surface. The details of these effects are discussed in Chapter VIII.
TRIPLE POINT TRAJECTORY

MACH STEM

CONTACT SURFACE

FIGURE 6. Schematic diagram of CMR and its shock polar
CHAPTER III. GOVERNING EQUATIONS AND TRANSFORMATIONS

A Cartesian coordinate system shown in Figure 7 is chosen to formulate the shock diffraction problem. The origin is located at the compression corner, and the x and y axes are oriented in the usual sense.

In an unsteady compressible flow in the (x,y)-plane, conservation of mass is expressed by

$$\rho_t + \rho(u_x + v_y) + \rho_x u + \rho_y v = 0$$  \hspace{1cm} (1)

and conservation of momentum of an inviscid fluid is given by

$$u_t + uu_x + vu_y + p_x/\rho = 0$$  \hspace{1cm} (2)
$$v_t + uv_x + vv_y + p_y/\rho = 0$$  \hspace{1cm} (3)

If heat transfer by friction, conduction and radiation is neglected, the conservation of energy is expressed by

$$S_t + uS_x + vS_y = 0$$  \hspace{1cm} (4)

where \(p\) and \(\rho\) denote the pressure and density respectively; \(u\) and \(v\) are the components of fluid velocity in the x and y directions; \(t\) denotes the time; and the entropy \(S\) is defined by

$$S = \ln p - \gamma \ln \rho$$  \hspace{1cm} (5)

As noted earlier, no characteristic length appears in this problem, and the shock pattern and the associated flowfield expands at a constant
FIGURE 7. Typical complex Mach reflection
rate. This type of flow is said to be self-similar in time, and solutions can be obtained by integrating the governing partial differential equations written in the self-similar coordinates. The self-similar transformation of the form

$$
\tau = \ln t \\
\xi = x/t \\
\eta = y/t
$$

was originally used by Jones et al. (16)

Application of the above coordinate transformation to the equations (1) to (4) results in

$$
(u-\xi)\rho_{\xi} + (v-\eta)\rho_{\eta} + \rho (u_{\xi} + v_{\eta}) = 0 \\
(u-\xi)u_{\xi} + (v-\eta)u_{\eta} + p\rho / \rho = 0 \\
(u-\xi)v_{\xi} + (v-\eta)v_{\eta} + p\rho / \rho = 0 \\
(u-\xi)S_{\xi} + (v-\eta)S_{\eta} = 0
$$

If we define the self-similar velocity components of the form

$$
U = u - \xi \\
V = v - \eta
$$

and eliminate \( \rho \) by the relation \( a^2 = \gamma \rho / \rho \), then the governing equations reduce to
where \( P \) in the above expressions is the logarithm of \( p \), \( a \) is the local speed of sound and \( \gamma \) is the ratio of specific heats.

It follows, since Equations (9) differ from those in the physical coordinates only by non-differential terms, that the system is elliptic, parabolic or hyperbolic according to

\[
U^2 + V^2 > a^2
\]  

In the CMR regime of shock diffraction, both subsonic and supersonic regions exist in the flowfield; hence, the system of equations (9) is a mixed set of elliptic and hyperbolic equations.

These equations can be made completely hyperbolic by reintroducing residual terms which will vanish as the time-asymptotic solution is computed. The hyperbolic system of equations is
The governing equations written in self-similar coordinates exhibit some unusual properties. The divergence form of the continuity equation may be written

\[ \rho \tau + (\rho U)_\xi + (\rho V)_\eta = -2\rho \]  

(12)

This shows that the continuity equation has a nonhomogeneous term corresponding to a sink distribution proportional to the local density. In addition, it can be shown that the energy equation may be written

\[ \frac{DH}{Dt} = - (U^2 + V^2) \]

(13)

where \( H \) is the total enthalpy. In this system, the total enthalpy is not constant along the streamlines and experiences changes proportional to the velocity squared.
Double Normalization

For the present study, a boundary shock-fitting approach is used to compute the reflected shock and the Mach stem. In the shock-fitting procedure these shocks are treated as computational boundaries, and the computational domain needs to be discretized uniformly between these boundaries and other boundaries formed by the wall and the ramp.

This is accomplished by a double normalization of the form

\[
X = \frac{\xi - \xi_r(Y,T)}{\xi_s(Y,T) - \xi_r(Y,T)}
\]

\[
Y = \frac{n}{n_m(X,T)}
\]

\[
T = \tau
\]

where \(\xi = \xi_r(Y,T)\) is the ramp boundary, \(\xi = \xi_s(Y,T)\) is the reflected shock and \(n = n_m(X,T)\) is the Mach stem equation.

The mesh system established by the double normalization is fixed and referred to as the reference mesh. It can be distinguished from the floating mesh on the contact surface which is free to move within the reference mesh. The distance between the ramp and the reflected shock is divided into \((j_{\text{max}} - 1)\) equal intervals with mesh spacing of \(\Delta X\), and the distance between the wall and the Mach stem is divided into \((i_{\text{max}} - 1)\) intervals with \(\Delta Y\) spacing. The mesh system generated by the double normalization is shown in Figure 8b.
REFLECTED
SHOCK

INCIDENT
SHOCK

CONTACT
SURFACE

TRIPLE
POINT

MACH
STEM

VORTICAL
SINGULARITY

REFLECTED
SHOCK

CONSTANT
X LINE

RAMP

WALL

STAGNATION
POINT

(a) Physical plane

(b) Computational plane

FIGURE 8. Mesh system
Application of the double normalization transformation to the self-similar Euler equations (11) yields

\[
\begin{align*}
\rho + \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} &= 0 \\
\mathbf{F} &= \rho \mathbf{U} + \rho \mathbf{a} \mathbf{U} - \rho \mathbf{a} \mathbf{a} \nabla \phi \\
\rho \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} &= 0
\end{align*}
\]

where \( \mathbf{U} \) and \( \mathbf{V} \) are contravariant velocity components of the form

\[
\begin{align*}
\mathbf{U} &= X_U + X_Y U + X_Y V \\
\mathbf{V} &= Y_U + Y_Y U + Y_Y V
\end{align*}
\]

Note that the entropy equation (11d) is uncoupled and already in a characteristic form; hence, it can be integrated independently from the rest of the equations. Necessary metrics of the transformation are derived in Appendix A.
CHAPTER IV. FINITE-DIFFERENCE METHOD

A first-order accurate, explicit, split coefficient matrix (SCM) method (17) is used to advance the flowfield in the time-asymptotic procedure. Details of the SCM method are presented in Appendix C. The SCM algorithm uses both forward and backward differences according to the characteristic direction of the governing hyperbolic system of equations. In the reference mesh interior where the computational grids are not crossed by a floating discontinuity, standard one-sided forward differences

\[
F_X^+ = \frac{F_{i+1,j} - F_{i,j}}{\Delta X} \\
F_Y^+ = \frac{F_{i+1,j} - F_{i,j}}{\Delta Y}
\] (17)

and one-sided backward differences

\[
F_X^- = \frac{F_{i,j} - F_{i,j-1}}{\Delta X} \\
F_Y^- = \frac{F_{i,j} - F_{i,1,j}}{\Delta Y}
\] (19)

are used.
Special Discretization Formula

The floating discontinuity-fitting technique introduces unequally spaced mesh intervals when a discontinuity is adjacent to a reference mesh point. Therefore the standard spatial differences (17 to 20) must be replaced by a special differencing approximation in order to maintain the stability and accuracy of the numerical scheme.

From the orientation of the contact surface with respect to the reference mesh (Figure 8b), it is natural to track the contact surface movement along the constant X lines, i.e., the contact surface position and its flow variables are computed on those points where the contact surface intersects with the constant X lines. On other floating grid points where the contact surface cuts the constant Y lines, the position and the flow variables are interpolated between neighboring floating grid points on the constant X lines.

Figure 9a shows the reference mesh in the vicinity of the contact discontinuity. The derivation of a special discretization formula is based upon weighting the contributions of neighboring mesh points (on the same side of the discontinuity) in such a way that the truncation error varies smoothly as the discontinuity cuts through the mesh.

Consider the approximation of derivatives at \((i,j)\). The ordinary Y backward difference (20) is replaced by

\[
F_Y^- = \frac{-1}{\Delta Y} \left[ \frac{2(2 - \varepsilon_Y)}{1 + \varepsilon_Y} F_s + (2 \varepsilon_Y - 3) F_{i,j} + \frac{(1 - \varepsilon_Y)(2 \varepsilon_Y - 1)}{1 + \varepsilon_Y} F_{i+1,j} \right]
\]

(21)
and the X forward difference (17) is replaced by

\[
F_X^+ = \frac{1}{\Delta X} \left[ \frac{2(2 - \varepsilon_X)}{1 + \varepsilon_X} F_{s',1} + (2\varepsilon_X - 3)F_{i,j} + \frac{(1 - \varepsilon_X)(2\varepsilon_X - 1)}{1 + \varepsilon_X} F_{i,j-1} \right]
\]

(22)

where

\[
\varepsilon_X = \frac{X_{s',1} - X_{i,j}}{\Delta X} \quad \text{and} \quad \varepsilon_Y = \frac{Y_{i,j} - Y_{s'}}{\Delta Y}
\]

The derivatives on the other side of the discontinuity are computed similarly. The truncation error for Equation (22) is given by

\[
(2\varepsilon_X^2 - 4\varepsilon_X + 1) \frac{\Delta X}{2} F_{XX}
\]

(23)

If point \((i,j-1)\) is not available when applying Equation (22), as is the case indicated in Figure 9b where two discontinuity points are close to each other, then \(F_X^+\) is approximated by

\[
F_X^+ = \frac{F_{s',1} - F_{s''}}{X_{s',1} - X_{s''}}
\]

(24)

If, however, the distance between the two discontinuity points is smaller than \(\Delta X\), the values at \((i,j)\) are interpolated between \(s'\) and \(s''\).

Point \((i,j-1)\) is not available when the discontinuity point is close to a boundary as shown in Figure 9c. In this case \(F_X^+\) is approximated by

\[
F_X^+ = \frac{F_{s} - F_{i,j-1}}{\varepsilon \Delta X}
\]

(25)
FLOATING DISCONTINUITY POINTS (Y-DIRECTION TRACKING)

INTERPOLATED DISCONTINUITY POINTS

FIGURE 9. Reference mesh and floating grid points
if \( \varepsilon \Delta X \) is greater than \( \varepsilon^* \Delta X \) which is the smallest spacing allowed in order to maintain the stability of the numerical scheme. The smallest spacing \( \varepsilon^* \Delta X \), for a given time step \( \Delta T \), is found by

\[
\varepsilon^* \Delta X = \Delta T \left| \frac{U}{a} \pm \sqrt{\frac{X_c^2 + X_h^2}{\gamma}} \right|_{\text{max}}
\] (26)

If, however, \( \varepsilon \Delta X \) is smaller than \( \varepsilon^* \Delta X \), then the derivatives are extrapolated along the boundary on the same side of the discontinuity.

So far, we have discussed the special discretization technique applied to the reference grid points. Next, the finite differences applied to the floating grid points are discussed.

In order to compute the contact surface properly, the floating discontinuity-fitting procedure requires the normalization of the distance between the contact surface and the Mach stem, and the distance between the contact surface and the wall boundary. Because of this normalization, X derivatives can be approximated from values on the floating grid points along the contact surface. However, approximation of Y derivatives still needs special discretization formulae because of unequally spaced mesh intervals adjacent to the contact surface.

Consider the approximation of Y derivatives at s in Figure 9a. Standard forward and backward differences may be replaced by

\[
F_{ys}^+ = \frac{-1}{\Delta Y} \left[ \frac{3}{1 + \varepsilon} F_s - 2F_{i,j} + \frac{2\varepsilon^* - 1}{1 + \varepsilon} F_{i,j+1} \right]
\] (27)

and
\[ F_{YS} = \frac{1}{\Delta Y} \left[ \frac{3}{1 + \varepsilon} F_s - 2F_{i,j-1} + \frac{2\varepsilon - 1}{1 + \varepsilon} F_{i,j-2} \right] \]  

(28)

where

\[ \varepsilon^+ = \frac{Y_{i,j} - Y_s}{\Delta Y} \]

\[ \varepsilon^- = \frac{Y_s - Y_{i-1,j}}{\Delta Y} \]

The truncation error for above formula is given by,

\[ (\varepsilon - 1) \frac{\Delta Y}{2} F_{YY} \]  

(29)

If \( F_{i+1,j} \) or \( F_{i-2,j} \) is not available, then a similar logic as before for the unequally spaced reference grid points may be used.
CHAPTER V. INITIAL CONDITIONS

For a given set of incident shock Mach number $M_s$ and ramp angle $\theta_r$, the flowfield must be initialized on all grid points in order to start the integration of the governing hyperbolic PDEs.

To initialize the flowfield at time $T = 1$, the pressure and the density are set equal to unity, and the velocity is set to be zero in the undisturbed region 1 (see Figure 7). The flow conditions in region 2, which are used as the upstream conditions for the reflected shock, are calculated from the following Rankine-Hugoniot relations:

\[
p_2 = p_1 \left[ 1 + \frac{2\gamma}{\gamma + 1} (M_s^2 - 1) \right]
\]

\[
\rho_2 = \rho_1 \frac{(\gamma + 1) M_s^2}{(\gamma - 1) M_s^2 + 2}
\]

\[
a_2 = \sqrt{\gamma \frac{p_2}{\rho_2}}
\]

\[
\bar{u}_1 = u_1 - q_s
\]

\[
\bar{u}_2 = \frac{\rho_1}{\rho_2} \bar{u}_1
\]

\[
u_2 = u_2 + q_s
\]

\[
v_2 = 0
\]
The triple point is located by first assuming its trajectory angle \( \chi \). Then, the triple point coordinates \((\xi, \eta)_{TP}\) are computed from

\[
\begin{align*}
\xi_{TP} &= M_s a_l = M_s \sqrt{T} \\
\eta_{TP} &= \xi_{TP} \tan(\chi + \theta_r).
\end{align*}
\] (37)

From the conditions in 1 and the triple point location, the solution of the three-shock confluence can be computed. This is discussed in Appendix B. The resulting information from the triple point calculations are the reflected shock slope \( \partial \xi_s / \partial \eta \), the contact surface slope \( \partial \eta_c / \partial \xi \), and the Mach stem slope \( \partial \eta_m / \partial \xi \), as well as the flow conditions on both sides of the contact surface.

A suitable standoff distance for the reflected shock is assumed so that a cubic polynomial can be used to approximate the initial shock shape between the triple point and the wall. The initial Mach stem shape between the triple point and the ramp surface is approximated in a similar manner. The contact surface is assumed to be a straight line from the triple point to the ramp with the slope \( \partial \eta_c / \partial \xi \) computed from the triple point solution.

The flow conditions behind the reflected shock are computed from the Rankine-Hugoniot relations (see Figure 10).

1. Unit normal and unit tangent vectors to the reflected shock;

\[
\begin{align*}
\hat{n} &= n_x \hat{i} + n_\eta \hat{j} = \frac{1}{\sqrt{1 + (\partial \xi_s / \partial \eta)^2}} \hat{i} - \frac{\partial \xi_s / \partial \eta}{\sqrt{1 + (\partial \xi_s / \partial \eta)^2}} \hat{j} \\
\hat{t} &= t_x \hat{i} + t_\eta \hat{j} = \frac{\partial \xi_s / \partial \eta}{\sqrt{1 + (\partial \xi_s / \partial \eta)^2}} \hat{i} + \frac{1}{\sqrt{1 + (\partial \xi_s / \partial \eta)^2}} \hat{j}
\end{align*}
\] (38) (39)
2. Self-similar velocity components in region 2;

\[ \vec{q}_2 = (u_2 - \xi_s) \hat{i} + (v_2 - \eta_s) \hat{j} \]  
(40)

\[ q_{2n} = \vec{q}_2 \cdot \hat{n} \]  
(41)

\[ q_{2t} = \vec{q}_2 \cdot \hat{t} \]  
(42)

where \((\xi_s, \eta_s)\) is a point on the reflected shock.

3. Relative velocity with respect to the moving shock;

\[ q_s = \frac{3\xi_s / \partial \tau}{n} \]  
(43) \hspace{1cm} (\partial \xi_s / \partial \tau \text{ is initially assumed zero.})

\[ \overline{q}_{2n} = q_{2n} - q_s \]  
(44)

\[ \overline{q}_{2n} = \frac{q_{2n}}{a_2} \]  
(45)

where \(q_s\) is the shock speed in its normal direction, and \(3\xi_s / \partial \tau\) is the component of shock speed with which the reflected shock is actually advanced.

4. Conditions behind the reflected shock;

\[ p_3 = p_2 \left[ 1 + \frac{2\gamma}{\gamma + 1} \left( \overline{M}_{2n}^2 - 1 \right) \right] \]  
(46)

\[ c_3 = c_2 \frac{(\gamma + 1) \overline{M}_{2n}^2}{\gamma (\gamma - 1) \overline{M}_{2n}^2 + 2} \]  
(47)
\[ \bar{q}_3 = \bar{q}_3 \frac{c}{c_1} \]  
\[ q_{3n} = \bar{q}_{3n} + q_s \]  
\[ q_{3t} = \bar{q}_{3t} \]  
\[ \bar{q}_3 = U \hat{i} + V \hat{j} = q_{3n} \hat{n} + q_{3t} \hat{t} \]  

The flow conditions behind the Mach stem can be computed in a similar fashion by replacing the upstream conditions.

The initial conditions along the wall boundary can be obtained by integrating the energy equation of the form

\[ U \frac{\partial}{\partial \xi} \left( \frac{a^2}{\gamma - 1} + \frac{U^2 + V^2}{2} \right) + V \frac{\partial}{\partial n} \left( \frac{a^2}{\gamma - 1} + \frac{U^2 + V^2}{2} \right) = -(U^2 + V^2) \]  

\[ \text{(52)} \]

At the wall, \( V \) is zero, and \( U \) is approximated by a linear variation,

\[ U = U_s \frac{\xi}{\xi_s}, \quad 0 \leq \xi \leq \xi_s \]  

\[ \text{(53)} \]

where \( U_s \) is the self-similar velocity at the shock, and \( \xi_s \) is the standoff distance. The integration of Equation (52) yields the local speed of sound as a function of position along the wall;

\[ \frac{a^2(\xi)}{a_s^2} = \frac{\gamma - 1}{2} U_s \left[ U_s \left( 1 - \frac{\xi^2}{\xi_s^2} \right) + \left( \xi_s - \frac{\xi^2}{\xi_s^2} \right) \right] \quad 0 \leq \xi \leq \xi_s \]  

\[ \text{(54)} \]
REFLECTED SHOCK

$\xi - \xi_s(x,t) = 0$

$\mathbf{q}_n = \mathbf{q}_s - \mathbf{q}_n$

FIGURE 10. Self-similar velocities across the reflected shock
where the subscript $s$ denotes values at the reflected shock. Using the entropy relation,

$$S = \ln p - \gamma \ln \rho = \gamma \ln \left( \frac{a^2}{\gamma} \right) - (\gamma - 1) \ln p$$ (55)

the pressure variation along the wall is found to be

$$\ln p(\xi) = \frac{\gamma \ln \left( \frac{a^2(\xi)}{\gamma} \right) - S}{\gamma - 1}$$ (56)

where the entropy $S$ is constant and the same as that behind the reflected shock.

The point where the contact surface meets the ramp is a vortical singularity. Since the self-similar velocity is zero, and the pressure achieves a local minimum at the vortical singularity, these variables along the ramp are approximated by a parabolic variation between the stagnation corner $O$ and the vortical singularity $VS$, and between $VS$ and the Mach foot $M$. The entropy between $O$ and $VS$ is constant and the same as that along the wall, and between $VS$ and $M$, it is constant and the same as that behind the Mach stem.

The velocity components along the contact surface are linearly interpolated between the triple point $TP$ and $VS$. Since the contact surface is a streamline, the entropy level on either side of the contact surface is constant and the same as that at the triple point.

Finally, the conditions on the interior grid points are initialized. Since the pressure is continuous across the contact
surface, the distribution on the interior grid points is approximated by a linear interpolation between the ramp and the reflected shock. The velocity components and the entropy are linearly interpolated between the ramp and the contact surface, and between the contact surface and the reflected shock.

The procedure described above is used to initialize the flowfield for the case of $M_s = 1.89$ and $\Theta_r = 40^\circ$ only, and the previously computed results are used as the initial conditions for other cases.

Starting with the initialized flowfield, the governing equations are integrated using an explicit, first-order SCM method.
CHAPTER VI. BOUNDARY CONDITIONS

The computational region is bounded by the wall, the ramp, the reflected shock, and the Mach stem. On these boundaries, only one-sided finite differences are available, and the SCM algorithm needs to be modified in order to account for the boundary conditions.

Wall Boundary

Since the shock diffraction pattern may be viewed as symmetric about the z-axis which coincides with the wall boundary, the method of reflection can be used to treat the wall boundary conditions. By providing an imaginary sublayer of grid points as illustrated in Figure 11, wall grid points are treated in the same way as any other interior grid points. In an actual computation, the following backward differences are substituted instead of increasing the number of grid points.

\[
P_{Y(1,j)}^- = \frac{P_{1,j} - P_{2,j}}{\Delta Y} = -P_{Y(1,j)}^+
\]

(57)

\[
U_{Y(1,j)}^- = \frac{U_{1,j} - U_{2,j}}{\Delta Y} = -U_{Y(1,j)}^+
\]

(58)

\[
V_{Y(1,j)}^- = \frac{0 - (-V_{2,j})}{\Delta Y} = V_{Y(1,j)}^+
\]

(59)

The entropy equation at the wall reduces to

\[
S_T + \bar{U}S_X = 0
\]

(60)
Since both velocity components vanish at the stagnation corner, the entropy value there needs to be artificially updated by assigning to it the entropy value of adjacent grid point.

Since the SCM method uses the characteristic information of the governing hyperbolic PDEs to advance the flowfield, Kentzer's characteristic approach (18) is most conveniently adapted to the SCM algorithm to treat the ramp boundary.
Normally, there are three compatibility equations available in the interior of the computational region. However, the compatibility equation associated with the characteristic pointing from the exterior of the domain toward the boundary cannot be used. Thus, there are only two equations available at the ramp boundary. The following two compatibility equations are derived in Appendix C.

\[
\begin{align*}
\rho_1 + \gamma_x \frac{\partial}{\partial x} + \frac{1}{2} \left[ 1 - \left( \frac{x^2 y^2 + x^2 y^2}{\gamma_x \gamma_y} \right) \right] \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left[ 1 + \left( \frac{x^2 y^2 + x^2 y^2}{\gamma_x \gamma_y} \right) \right] \frac{\partial^2}{\partial y^2} \\
- \frac{y}{a} \left( \frac{x^2 y^2 - x^2 y^2}{\gamma_x \gamma_y} \right) \frac{\partial^2}{\partial y^2} + 2y = 0
\end{align*}
\]

These equations are solved for the pressure and one of the velocity components. Then, the second velocity component can be computed from the flow tangency condition

\[
U = V \tan \theta
\]

Reflected Shock

At the reflected shock boundary, two characteristics; one stream line and one wave front characteristic, reaching from the upstream of the shock front must be eliminated. This results in the following compatibility equation available at the reflected shock.
Now $U_T$ and $V_T$ can be expressed in terms of $P_T$ using the Rankine-Hugoniot relations as follows. First, taking the time derivative of Equation (51),

$$\frac{\partial U_T}{\partial t} = \frac{\partial^n}{\partial \xi^2} n_\xi + q_{2n} \frac{\partial n_{\eta \xi}}{\partial t} - \frac{\partial q_{2n}}{\partial t} n_\eta - q_{2t} \frac{\partial n_\eta}{\partial t}$$

(65)

$$\frac{\partial V_T}{\partial t} = \frac{\partial^n}{\partial \eta^2} n_\eta + q_{3n} \frac{\partial n_{\xi \eta}}{\partial t} + \frac{\partial q_{2n}}{\partial t} n_\xi + q_{2t} \frac{\partial n_\xi}{\partial t}$$

(66)

where $\vec{n} = n_\xi \hat{i} + n_\eta \hat{j}$ is a unit normal vector to the shock, $q_{3n}$ is the normal component of the self-similar velocity behind the shock and $q_{2t}$ is the tangential component of the self-similar velocity ahead of the shock. The acceleration terms seen on the RHS of Equations (66) and (67) are obtained from Equations (41) to (51) as follows:

$$\frac{\partial q_{3n}}{\partial t} = \frac{\partial^2 U_T}{\partial t^2} - \frac{2 a}{\gamma + 1} \left( 1 + \frac{\bar{M}^2}{M^2} \right) \frac{\partial \bar{M}^2}{\partial t}$$

(67)

$$\frac{\partial q_{2n}}{\partial t} = \frac{\partial \xi_s}{\partial t} n_\xi + ( u_2 - \xi_s ) \frac{\partial n_\xi}{\partial t} - \frac{\partial n_\eta}{\partial t} n_\eta - \frac{\partial n_\eta}{\partial t}$$

(68)
\[ \frac{\partial q_{\xi}}{\partial t} = \frac{\partial q_s}{\partial t} \eta_t - (u_2 - \xi_s) \frac{\partial n}{\partial t} - \frac{\partial n_s}{\partial t} \eta_z - \eta_s \frac{\partial n_s}{\partial t} \]  
\hspace{0.5cm} (69)

where

\[ \frac{\partial n}{\partial t} = n_t \eta_t \frac{\partial q_s}{\partial \eta} \]  
\hspace{0.5cm} (70)

\[ \frac{\partial n_s}{\partial t} = -n_z \xi_t \frac{\partial q_s}{\partial \eta} \]  
\hspace{0.5cm} (71)

\( \frac{\partial q_s}{\partial \eta} \) is computed by a central difference of the shock speed \( \frac{\partial q_s}{\partial t} \), and \( \frac{\partial n_s}{\partial t} \) is set equal to zero since the reflected shock is tracked in the \( \xi \)-direction.

Now, from the pressure jump condition across the shock,

\[ P = \ln p_2 + \ln \left[ 1 + \frac{2}{\gamma + 1} \left( \frac{M^2}{2n} - 1 \right) \right] \]  
\hspace{0.5cm} (72)

we get

\[ \frac{\partial P}{\partial T} = \frac{4\gamma M^2}{2\gamma M^2 - (\gamma - 1) \frac{\partial T}{\partial T}} \frac{\partial M}{\partial T} \]  
\hspace{0.5cm} (73)

or

\[ \frac{\partial M}{\partial T} = \frac{M^2 - \frac{\gamma - 1}{2\gamma}}{2 \frac{M^2}{2n}} \frac{p}{T} \]  
\hspace{0.5cm} (74)
Substituting equation (74) into (67) and the acceleration terms into Equations (65) and (66) we have

\[
\left\{ 1 - \frac{\gamma}{a} \right\} \left[ \left( 1 + \frac{\bar{M}_2^2}{2n} \right) \left( \frac{\bar{M}_2^2}{2n} - \frac{\gamma - 1}{2\gamma} \right) \right] \left( X_\xi n_\xi + X_\eta n_\eta \right) P_T
\]

= R.H.S. of EQ. (64)

From the above expression, \( P_T \) is computed.

To update the shock position, we propose to compute the shock acceleration first. Rewriting Equation (43) we have,

\[
\frac{\partial \xi_s}{\partial \tau} = q_s n_\xi
\]

(76)

Taking the time derivative, and using Equation (70) we get the shock acceleration of the form

\[
\frac{\partial^2 \xi}{\partial \tau^2} = \frac{\partial q_s}{\partial \tau} n_\xi + n_\xi n_\eta \left( \frac{\partial \xi_s}{\partial \tau} \right) \left( \frac{\partial \xi_s}{\partial \eta} \right)
\]

(77)

where \( \partial q_s / \partial \tau \) is evaluated from Equation (44) as

\[
\frac{\partial q_s}{\partial \tau} = \frac{\partial q_{2n}}{\partial \tau} - a_2 \frac{\partial \bar{M}_{2n}}{\partial \tau}
\]

(78)

Substituting Equation (74) into the above expression,

\[
\frac{\partial q_s}{\partial \tau} = \frac{\partial q_{2n}}{\partial \tau} - a_2 \left[ \frac{\bar{M}_{2n}^2 - \gamma - 1}{2}\left( \frac{\bar{M}_{2n}^2}{2n} \right) \right] \frac{\partial P}{\partial \tau}
\]

(79)
New shock speed and shock position can be obtained by the simple integration,

\[
\frac{\partial \xi_s}{\partial t} \bigg|_{\text{new}} = \frac{\partial \xi_s}{\partial t} \bigg|_{\text{old}} + \frac{\partial^2 \xi_s}{\partial t^2} \Delta t \tag{80}
\]

and

\[
\xi_s \big|_{\text{new}} = \xi_s \big|_{\text{old}} + \frac{1}{2} \left( \frac{\partial \xi_s}{\partial t} \bigg|_{\text{new}} + \frac{\partial \xi_s}{\partial t} \bigg|_{\text{old}} \right) \Delta t \tag{81}
\]

The shock slope is computed by the central difference of the form

\[
\frac{\partial \xi_s}{\partial n} \bigg|_i = \frac{\xi_s \big|_{i+1} - \xi_s \big|_{i-1}}{2 \Delta n} \tag{82}
\]

With the new position, speed, and slope, the flow conditions behind the reflected shock are updated using Rankine-Hugoniot relations (46) to (51).

**Mach Stem**

For the Mach stem boundary, a compatibility equation similar to the one for the reflected shock is obtained. The derivation is shown in Appendix C, and only the result is presented here.
\[
P_T + \frac{X}{a} ( \eta \phi u_T + \eta \phi v_T ) = -\lambda^2 \frac{\partial^2}{\partial Y^2} \lambda
\]

\[
= -\frac{1}{2} \left[ 1 + \left( \frac{\eta \phi \psi + \eta \phi \psi^*}{\eta \phi \psi + \eta \phi \psi^*} \right) \right] \lambda^2 \frac{\partial^2}{\partial X^2} \lambda
\]

\[
= -\frac{1}{2} \left[ 1 - \left( \frac{\eta \phi \psi + \eta \phi \psi^*}{\eta \phi \psi + \eta \phi \psi^*} \right) \right] \lambda^3 \frac{\partial^3}{\partial X^3} \lambda
\]

\[
= -\frac{\lambda}{a} ( \eta \phi \psi - \eta \phi \psi^* ) \lambda^1 \frac{\partial^1}{\partial X^1} \lambda
\]

\[
= -\frac{\lambda}{a} ( \eta \phi \psi + \eta \phi \psi^* ) \frac{\partial^1}{\partial Y^1} \lambda
\]

\[
= -\frac{\lambda}{a} ( \eta \phi \psi + \eta \phi \psi^* ) \frac{\partial^1}{\partial \eta^1} \lambda
\]

A similar procedure, described for the reflected shock, can be followed in order to compute the flow conditions behind the Mach stem, provided appropriate changes in the upstream conditions are made.
CHAPTER VII. CONTACT SURFACE CALCULATIONS

During the early part of this study, the contact surface calculations were found to be extremely unstable. For example, if the initial conditions were not sufficiently close to the steady state solution while the reflected shock and the Mach stem were stable, the contact surface developed a highly irregular shape eventually causing the numerical calculations to diverge. Richtmeyer (19) reported similar difficulties in computing the contact surface and concluded that the instability is due to the physical structure of the contact surface. The unstable contact surface structure in shock diffraction has also been reported by USSR researchers (20). In Richtmeyer's progress report, he proposed to add artificial tension terms to make the contact surface calculations stable. The success of such an approach, however, has not been reported. In the present calculations, only correct mathematical formulae for the contact discontinuity, rather than introducing artificial terms, are used to compute the flow conditions and the position of the contact surface.

Coordinate System

While the boundary shock-fitting approach was used to treat the reflected shock and the Mach stem, the contact surface was computed by the floating discontinuity-fitting scheme (21). This approach of treating discontinuities in the computational domain has been successfully demonstrated in References (21), (22), and (23).
In order to compute the contact surface properly, the floating-fitting procedure requires derivatives along the contact surface as well as proper stretching factors for both sides of the contact surface. This is accomplished by writing the governing equations in the discontinuity oriented coordinate system, i.e., by normalizing the distance between the moving contact surface and the fixed boundaries in the direction of contact surface movement. From the expected topological changes in the contact surface, it seems natural to track the discontinuity points in the Y direction along constant X surfaces (see Figure 8). The required transformation is given by

\[
\begin{align*}
\bar{T} &= T \\
\bar{X} &= X \\
\bar{Y}_3 &= \frac{Y}{Y_c(X,T)} - 1 \quad \text{(reflected shock side)} \\
\bar{Y}_4 &= \frac{Y - Y_c(X,T)}{1 - Y_c(X,T)} \quad \text{(Mach stem side)}
\end{align*}
\]

where \( Y - Y_c(X,T) = 0 \) is the contact surface equation. Equation (84c) normalizes the distance between the contact surface and the wall, and Equation (84d) normalizes the distance between the contact surface and the Mach stem. Application of the normalizing transformation to the governing equations (15) results in

\[
Q_{\bar{T}} + [ \mathbf{A} ] Q_{\bar{X}} + [ \mathbf{B} ] Q_{\bar{Y}_k} + G = 0 \quad k = 3 \text{ or } 4
\]

where
\[
\begin{bmatrix} \tilde{E} \end{bmatrix} = \tilde{Y}_{kT} \begin{bmatrix} I \end{bmatrix} + \tilde{X}_{kX} \begin{bmatrix} A \end{bmatrix} + \tilde{Y}_{kY} \begin{bmatrix} B \end{bmatrix}
\] (86)

In the above expressions, \(Q,G,[A]\) and \([B]\) are the same as those of Equation (C2) in Appendix C, and \([I]\) is the identity matrix. Subscript \(k\) indicates the equations are either for the reflected shock side \((k=3)\) or for the Mach stem side \((k=4)\) of the contact surface. Necessary metrics of the transformation are tabulated in Table 1. \(\partial Y_c/\partial T\) is the contact surface speed and is computed from the jump conditions discussed later in this chapter. \(\partial Y_c/\partial X\) is the contact surface slope in the computational domain and can be computed by

\[
\frac{\partial Y_c}{\partial X} = \frac{Y_\zeta + Y_\eta \frac{\partial \eta_c}{\partial \zeta}}{X_\zeta + X_\eta \frac{\partial \eta_c}{\partial \zeta}}
\] (87)

where \(Y_\zeta, Y_\eta, X_\zeta\) and \(X_\eta\) are the metrics of reference mesh and those values on the contact surface may be obtained by a linear interpolation between the neighboring reference grid points. \(\partial \eta_c/\partial \zeta\) is the contact surface slope in the self-similar coordinate system.

The method of characteristics is employed to integrate the compatibility equations at the contact surface. In a discontinuity-fitting approach, differencing of flow variables across the discontinuity is not permitted. Therefore, the compatibility equations associated with the characteristics pointing from the other side of the contact surface cannot be used. Elimination of inappropriate
TABLE 1. Metrics of contact surface normalizing transformation

<table>
<thead>
<tr>
<th>Reflected shock side</th>
<th>Mach stem side</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \overline{V}_{3T} = -\frac{1}{Y_c(X,T)} \frac{\partial Y_c}{\partial T} )</td>
<td>( \overline{V}_{4T} = -\frac{1}{1 - Y_c(X,T)} \frac{\partial Y_c}{\partial T} )</td>
</tr>
<tr>
<td>( \overline{V}_{3X} = -\frac{1}{Y_c(X,T)} \frac{\partial Y_c}{\partial X} )</td>
<td>( \overline{V}_{4X} = -\frac{1}{1 - Y_c(X,T)} \frac{\partial Y_c}{\partial X} )</td>
</tr>
<tr>
<td>( \overline{V}_{3Y} = \frac{1}{Y_c(X,T)} )</td>
<td>( \overline{V}_{4Y} = \frac{1}{1 - Y_c(X,T)} )</td>
</tr>
</tbody>
</table>

characteristics results in two compatibility equations on each side of the contact surface. The procedure of obtaining these equations is similar to that of the SCM method described in Appendix C. The characteristics of \([A]\) are found in Appendix C. The characteristics of the \([B]\) matrix are found to be

\[
\lambda^1_{kY} = \hat{V}_k = \overline{V}_{kT} + \overline{V}_{kX} \overline{U}_k + \overline{V}_{kY} \overline{V}_k
\]

\[
\lambda^2_{kY} = \hat{V}_k + a_k \sqrt{\overline{Y}_k*}
\]

\[
\lambda^3_{kY} = \hat{V}_k - a_k \sqrt{\overline{Y}_k*}
\]

where
\[ \overline{V} = \sqrt{\overline{V}^{\kappa \xi} + \overline{V}^{\kappa \eta}} \]

and

\[ \overline{V}^{\kappa \xi} = \overline{V}_X \xi + \overline{V}_Y \xi \]
\[ \overline{V}^{\kappa \eta} = \overline{V}_X \eta + \overline{V}_Y \eta \]

In the above expressions, \( \overline{U} \) and \( \overline{V} \) are contravariant velocity components with respect to the \((X,Y,T)\) coordinate system. \( \overline{V} \) is the contravariant velocity component normal to the contact surface in \((X,Y,T)\) coordinate system and may be set equal to zero along the contact surface.

On the reflected shock side of the contact surface, we have two compatibility equations

\[ P = \frac{Y}{a} \left( \overline{V}^{\kappa \xi} U + \overline{V}^{\kappa \eta} V \right) = -\frac{1}{2} \left[ 1 + \frac{1}{2} \left( \overline{V}^{\kappa \xi} \eta + \overline{V}^{\kappa \eta} \xi \right) \right] \lambda \frac{3}{2} \frac{2}{X} \]
\[ - \frac{1}{2} \left[ 1 - \frac{1}{2} \left( \overline{V}^{\kappa \xi} \eta + \overline{V}^{\kappa \eta} \xi \right) \right] \lambda \frac{3}{2} \frac{2}{X} \]
\[ + \frac{Y}{a} \left( \overline{V}^{\kappa \xi} \xi - \overline{V}^{\kappa \eta} \eta \right) \lambda \frac{3}{2} \frac{2}{X} \]
\[ - \lambda \frac{3}{2} \frac{2}{Y} \]
\[ - \frac{Y}{a} \left( \overline{V}^{\kappa \xi} U + \overline{V}^{\kappa \eta} V \right) - 2Y \]
\[
\frac{\gamma}{a_3} \left( \frac{\overline{V}_3}{u_3} \overline{U}_3 \overline{T} - \frac{\overline{V}_3}{u_3} \overline{V}_3 \overline{T} \right) = - \frac{1}{2} \left( \frac{\overline{V}_3}{u_3} \frac{\overline{X}_3}{\overline{\eta}_3} = \frac{\overline{V}_3}{u_3} \frac{\overline{X}_3}{\overline{\eta}_3} \right) \left( \lambda_X^2 \chi^2 + \lambda_X^3 \chi^3 \right)
\]
\[
- \frac{\gamma}{a_3} \left( \frac{\overline{V}_3}{u_3} \frac{\overline{X}_3}{\overline{\eta}_3} + \frac{\overline{V}_3}{u_3} \frac{\overline{X}_3}{\overline{\eta}_3} \right) \lambda_X^1 \chi^1
\]
\[
- \frac{\gamma}{a_3} \left( \frac{\overline{V}_3}{u_3} \frac{\overline{U}_3}{u_3} \overline{V}_3 \overline{T} \right)
\]

(93)

where \(\lambda_X\) and \(\chi_X\) are the same as those found in Appendix C, and

\[
\frac{2 \gamma}{\eta} = \frac{P}{\eta} + \frac{\gamma}{a_3} \left( \frac{\overline{V}_3}{u_3} \frac{\overline{U}_3}{u_3} \overline{V}_3 \overline{T} \right)
\]

(94)

On the Mach stem side of the contact surface, we have

\[
P_T - \frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{U}_4}{u_4} \overline{T} + \frac{\overline{V}_4}{u_4} \frac{\overline{V}_4}{u_4} \overline{T} \right) = - \frac{1}{2} \left[ 1 - \left( \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} + \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} \right) \lambda_X^2 \chi^2 \right]
\]
\[
- \frac{1}{2} \left[ 1 + \left( \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} + \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} \right) \lambda_X^3 \chi^3 \right]
\]
\[
- \frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} - \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} \right) \lambda_X^1 \chi^1
\]
\[
- \lambda_X^2 \chi^2 \eta
\]
\[
+ \frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{U}_4}{u_4} + \frac{\overline{V}_4}{u_4} \frac{\overline{V}_4}{u_4} \overline{T} \right) = 2 \gamma
\]

(95)

\[
\frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{U}_4}{u_4} \overline{T} - \frac{\overline{V}_4}{u_4} \frac{\overline{V}_4}{u_4} \overline{T} \right) = - \frac{1}{2} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} - \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} \right) \left( \lambda_X^2 \chi^2 - \lambda_X^3 \chi^3 \right)
\]
\[
- \frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} + \frac{\overline{V}_4}{u_4} \frac{\overline{X}_4}{\overline{\eta}_4} \right) \lambda_X^2 \chi^2
\]
\[
- \frac{\gamma}{a_4} \left( \frac{\overline{V}_4}{u_4} \frac{\overline{U}_4}{u_4} - \frac{\overline{V}_4}{u_4} \frac{\overline{V}_4}{u_4} \overline{T} \right)
\]

(96)
where

$$\lambda^2_{\eta Y} = \lambda^2_{\eta Y} - \frac{\gamma}{a_0} \left( \frac{\bar{c}_{\eta \eta}}{a_0} U_{\eta Y} + \frac{\bar{c}_{\eta \gamma}}{a_0} V_{\eta Y} \right)$$  \hspace{1cm} (97)$$

An additional equation is supplied by the condition that no velocity flux is allowed across the contact surface. This is expressed by

$$\hat{n} \cdot (\hat{U}_3 \hat{i} + \hat{V}_3 \hat{j}) = \hat{n} \cdot (\hat{U}_4 \hat{i} + \hat{V}_4 \hat{j})$$  \hspace{1cm} (98)$$
or

$$n_\xi (U_3 - U_4) + n_\eta (V_3 - V_4) = 0$$  \hspace{1cm} (99)$$

where

$$\hat{n} = n_\xi \hat{i} + n_\eta \hat{j} = \frac{\partial n_\gamma}{\partial \xi} \hat{i} + \frac{-1}{1 + \left( \frac{\partial n_\gamma}{\partial \xi} \right)} \hat{j}$$  \hspace{1cm} (100)$$
is the unit normal vector to the contact surface.

Equations (92), (93), (95), (96) and (99) are solved simultaneously for five unknown variables, the pressure and the two velocity components on each side of the contact surface. The entropy levels are constant along the contact surface and the same as at the triple point.

Contact Surface Speed

In order to advance the contact surface position, its speed is computed first from the jump conditions which hold across the
discontinuity (24). Applying the jump condition derived in Appendix D to the present contact discontinuity, we have

$$- \frac{\partial Y}{\partial T} \left[ W \right] - \frac{\partial Y}{\partial X} \left[ X, W + X, E + X, F \right] + \left[ Y, W + Y, E + Y, F \right] = 0$$  \hspace{1cm} (101)$$

where the flux vectors are

$$W = \begin{bmatrix} \rho \\ \rho U \\ \rho V \end{bmatrix} \quad E = \begin{bmatrix} \rho U \\ P + \rho U^2 \\ \rho UV \end{bmatrix} \quad F = \begin{bmatrix} \rho V \\ P + \rho V^2 \end{bmatrix}$$  \hspace{1cm} (102)$$

and $[W]$ denotes the jump $W_3 - W_4$ in the quantity $W$. Suppose we choose to use the $X$-momentum equation (the same result will be obtained by the use of the continuity equation or the $Y$-momentum equation) in the jump condition (101). Then, the contact surface speed is

$$\frac{\partial Y}{\partial T} = \left( Y, - \frac{\partial Y}{\partial X} X, \right) \quad \frac{\partial Y}{\partial T} = \frac{\partial Y}{\partial \xi} \frac{\partial Y}{\partial \eta} \left( cU^2 \right) + \left( Y, - \frac{\partial Y}{\partial X} X, \right) \frac{\partial UV}{\partial T}$$  \hspace{1cm} (103)$$

and substituting Equation (87), we get

$$\frac{\partial Y}{\partial T} = \left( Y, - \frac{\partial Y}{\partial X} X, \right) \quad \frac{\partial Y}{\partial T} = \frac{\partial Y}{\partial \xi} \frac{\partial Y}{\partial \eta} \left( cU^2 \right) + \left( Y, - \frac{\partial Y}{\partial X} X, \right) \frac{\partial UV}{\partial T}$$  \hspace{1cm} (104)$$
The first term of Equation (104) is the grid speed and may be set equal to zero since the reference mesh is fixed by the double normalization (14). The condition (99) implies that

\[
\frac{\partial \eta_c}{\partial \xi} (U_3 - V_3) = \frac{\partial \eta_c}{\partial \xi} (U_4 - V_4) = q_c
\]  

(105)

where \(q_c\) is the contact surface speed in the physical space. Finally the contact surface speed in computational coordinates simplifies to

\[
\frac{\partial Y_c}{\partial \tau} = \frac{Y_c \frac{\partial X}{\partial \eta} - Y \frac{\partial X_c}{\partial \eta}}{X_c + X_h \frac{\partial \xi}{\partial \tau}} \left( \frac{\partial \eta_c}{\partial \xi} U - V \right)
\]  

(106)

The contact surface position is advanced by the simple integration

\[
Y_c(X,T)\big|_{new} = Y_c(X,T)\big|_{old} + \frac{\partial Y_c}{\partial \tau} \Delta T
\]  

(107)

After updating the new position, the slope can be computed by a curve fitting technique. In the present approach, a cubic spline is used to fit the contact surface. The spline fitting is progressed from the triple point down to the vortical singularity since the contact surface slope is known at the triple point from the solution of the three-shock confluence.
CHAPTER VIII. NUMERICAL RESULTS

The computational grid system for all cases presented in this chapter consists of 11 points in the X direction and 21 points in the Y direction. An average of 2000 time steps was taken to ensure the convergence of the solutions, which required approximately 16 minutes of computer time on a CDC CYBER 173.

Numerical results in the form of density contours are compared with Ben-Dor's experimental data (25) in Figure 12. The experimental conditions for the case were reported to be a Mach number of 3.74 and the ramp angle of 30 degrees. However, in order to achieve the same density ratio across the incident shock, the present numerical results were obtained for a Mach number of 3.67. The shock shape predicted by the numerical computation shows good agreement with the experimental data except at the bottom of the reflected shock, which is clearly due to the boundary layer along the wall and cannot be predicted by the present inviscid model. The trajectory angle of the present result is 8.74 degrees as compared to 8 degrees from experimental data. The end of contact surface is seen to form a vortex region in the shock tube experiment. This may be explained by the fact that the contact surface can be thought of as a vortex sheet, and the roll up at its end may be due to the viscous effect. In Figure 13, the density variations along the wall are compared. A similar tendency is observed along the ramp surface. Larger discrepancies are seen across the reflected shock and near the intersection of the slip surface and the ramp, which is referred to as the vortical singularity.
The present numerical results show that the vortical singularity is moved toward the Mach stem to develop the irregularly curved contact surface as depicted in Figure 12b. Examination of USSR reports (References 26 and 27) and the recent numerical work by Woodward and Collela (13) reveals a similar physical picture of this phenomena. The experimental data show the coalescing compression waves at the slope inflection on the reflected shock. This may be due to a supersonic turning of the flow behind the reflected shock. However, the present numerical results show a very weak compression wave emanating from immediately below the contact surface due to a subsonic flow deflection over the ramp. The supersonic flow seems to be directed in a straight path as can be seen from the straight contact surface and the straight reflected shock. However, the flow is gradually turned away from the ramp in the subsonic region below the sonic line because of the downstream characteristics reaching that region.

The numerical results are also compared with the earlier calculations of Shankar, Kutler, and Anderson (12) in Figures 14 and 15. A similar computational approach was used in this earlier study. The conditions for the comparative case were $M_s = 1.89$ and $\theta_r = 40^\circ$. The pressure contours show good agreement. The shape of the contact surface and the location of the vortical singularity show some differences. As noted earlier, these differences are probably due to difficulty in correctly treating the contact surface in Reference 12. Present results show a slightly curved contact surface reaching the ramp at a glancing
(a) Present numerical results, $M_s = 3.67$

(b) Experiment, Ben-Dor (Ref. 24)

$M_s = 3.74$

FIGURE 12. Isopycnics of complex Mach reflection ($\theta_r = 30^\circ$)
FIGURE 13. Comparison of wall density

- EXPERIMENT (24) DIATOMIC GAS N₂
- NUMERICAL PERFECT GAS
angle. The interferogram obtained by Law (28) shows a contact surface with a similar shape. The pressure variations along the wall are compared in Figure 15. The present results show more variation along the ramp surface, and the pressure reaches a lower minimum at the vortical singularity. This is because the flow along the contact surface is further expanded as it approaches the ramp surface tangentially.

A series of results are presented in Figures 16 to 23 in order to demonstrate the transition from single Mach reflection to double Mach reflection. These results were obtained by using the previously obtained results as an initial condition. The incident Mach number was gradually increased from 1.89 to 2.80, while the ramp angle was held constant at 40 degrees.

Figure 16 shows the pressure, the density, and the self-similar Mach number contours, and the self-similar velocity vector plot for $M_s = 1.89$. The Mach number $M_3$ behind the reflected shock at the triple point is computed to be 1.042. This case is in the CMR regime close to SMR. The reflected shock has monotonically increasing slope from the triple point to the wall where the shock terminates at a 90 degree angle. Isobars show that expansion takes place on both sides of the contact surface toward the vortical singularity. The stream lines may be visualized from the velocity vector plot and can be seen to converge at the vortical singularity.
FIGURE 14. Numerical simulation of CMR, Isobars ($M_s = 1.89, \phi_r = 40^\circ$)
FIGURE 15. Wall pressure and density
In Figure 17, the pressure along the wall is seen to reach a local minimum at that point. Ludloff and Friedman (8) predicted a similar result in their elliptic PDE formulation of the problem.

Figures 18 and 19 show the results for \( M_s = 2.20 \). Isobars and isopycnics show very little variation behind the Mach stem. Contrary to the previous case, a compression region is developed near the vortical singularity. Close examination of the self-similar velocity (Figure 18d) along the ramp reveals a stagnation point immediately below the vortical singularity and another vortical singularity further down the ramp where the majority of the stream lines converge. It can be seen from the Mach number contours (Figure 18c) that the development of the compression wave is due to the rapid deceleration of the flow in the vicinity of the new self-similar stagnation point. Despite the developing supersonic flow behind the reflected shock, no curvature inflection can be detected in the shock shape. This may be explained by the fact that the compression wave just developed near the ramp has not reached the reflected shock. Hence, the incoming flow through the shock is not affected. Another important observation throughout the present investigation is that the triple-point structure, i.e., the reflected shock, the contact surface, and the Mach stem, rotates counterclockwise (based on the figures depicted) as the incident Mach number is increased. Because of this, the flow bounded between the shock and the contact surface must deflect further as it approaches the ramp.

Therefore, the development of the compression wave is due to two
factors, larger flow deflection angle and flow with higher self-similar velocity approaching the ramp.

Figures 20 and 21 show the results for \( M_s = 2.50 \). The reflected shock develops a curvature inflection due to the compression wave reaching from the self-similar stagnation point immediately below the vortical singularity. The reflected shock and the contact surface are seen to be straight up to the sonic line. Higher stagnation pressure moves the end of the contact surface toward the Mach stem. The flow behind the Mach stem is continuously compressed toward the self-similar stagnation point (Figure 20a). The compression wave immediately below the contact surface has been reported in References 26 and 27.

The results for \( M_s = 2.70 \) are shown in Figure 22. The reflected shock can be seen to develop a kink, and the further development of the compression wave reaching the reflected shock is clear. The sonic line is just above the kink and a rapid compression takes place immediately below the kink in the shock wave.

The last case computed is for \( M_s = 2.80 \), and the results are shown in Figure 23. The sonic line is advanced to the kink, and hence, this case may be considered to be near the transition from CMR to DMR regime. The Mach number \( M_3 \) behind the reflected shock is computed to be 1.395. It is evident from these results that the incipient second Mach stem in DMR is formed from the coalescence of compression waves immediately behind the sonic line. A further increase in the upstream Mach number requires a strong shock instead of a finite compression wave in order to achieve the required pressure jump and a subsonic downstream flow.
FIGURE 16. CMR (M_s = 1.89, \theta_r = 40^\circ)
FIGURE 17. Wall pressure and density
FIGURE 18. CMR ( $M_s = 2.20, \theta_r = 40^\circ$ )
FIGURE 19. Wall pressure and density
FIGURE 20. CMR ( M_s = 2.50, \theta_r = 40^\circ )
FIGURE 21. Wall pressure and density
FIGURE 22. CMR ( $M_s = 2.70$, $\theta_r = 40^\circ$ )
FIGURE 23. CMR (M_s = 2.80, $\theta_r = 40^\circ$)
Numerical solutions of shock diffraction in the complex Mach reflection region have been obtained for the first time. A finite-difference scheme was used in conjunction with boundary shock and a floating discontinuity-fitting approach for the present study. The origination of a compression wave in CMR has been revealed, and its interactions with the reflected shock and the contact surface have been clearly demonstrated. It is evident from the results that an accurate computation of the contact surface, i.e., its position and shape, as well as its flow properties, is imperative for the accurate prediction of the developing compression wave. The supersonic flow region behind the reflected shock and the compression wave were found to be responsible for the formation of a smooth slope inflection (near SMR) and a kink (near DMR) on the reflected shock. It was observed during this investigation that the rotation of the triple-point structure is partly responsible for the development of compression waves with increasing incident Mach number. For the last case, the CMR flowfield immediately prior to the DMR regime has been computed, and the formation of the second triple point and the incipient second Mach stem is clearly seen. It requires further implementation of the present numerical code in order to actually compute a solution in the DMR regime. However, this study represents a significant step in the development of the numerical approach in analyzing shock diffraction problems.
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APPENDIX A. METRICS OF DOUBLE NORMALIZATION

The computational mesh system for the complex Mach reflection is established by a double normalization of the form:

\[ f(\xi, \eta, \tau; X, Y, T) = X - \frac{\xi - \xi_s(Y, T)}{\xi_s(Y, T) - \xi_f(Y, T)} = 0 \]

\[ g(\xi, \eta, \tau; X, Y, T) = Y - \frac{\eta}{\eta_m(X, T)} = 0 \]

\[ h(\xi, \eta, \tau; X, Y, T) = T - \tau = 0 \]

Note that \( \xi, \eta \) and \( \tau \) are the independent variables of the implicit functions \( f, g \) and \( h \).

The metrics of the transformation are found from vector calculus (29), and these are:

\[ X_\xi = - \frac{\partial (f, g, h)}{\partial (\xi, Y, T)} \]

\[ X_\eta = - \frac{\partial (f, g, h)}{\partial (\eta, Y, T)} \]

\[ X_\tau = - \frac{\partial (f, g, h)}{\partial (X, \tau, T)} \]

\[ Y_\xi = - \frac{\partial (f, g, h)}{\partial (X, \xi, T)} \]

\[ Y_\eta = - \frac{\partial (f, g, h)}{\partial (X, \eta, T)} \]

\[ Y_\tau = - \frac{\partial (f, g, h)}{\partial (X, \tau, T)} \]
\[
T_\tau = - \frac{\partial (f, g, h)}{\partial (X, Y, \tau)} \frac{1}{J}
\]
\[
T_\xi = - \frac{\partial (f, g, h)}{\partial (X, Y, \xi)} \frac{1}{J}
\]
\[
T_\eta = - \frac{\partial (f, g, h)}{\partial (X, Y, \eta)} \frac{1}{J}
\]

where

\[
J = \frac{\partial (f, g, h)}{\partial (X, Y, \tau)} = \begin{vmatrix} f_X & f_Y & f_T \\ g_X & g_Y & g_T \\ h_X & h_Y & h_T \end{vmatrix}
\]

is the Jacobian of \(f, g\) and \(h\) with respect to \(X, Y\) and \(Z\). After substituting the following identities;

\[
T_\tau = 1, \quad T_\xi = T_\eta = 0
\]
\[
f_X = g_T = h_T = 1
\]
\[
h_X = h_Y = 0
\]
\[
f_\tau = f_\xi = g_\tau = g_\xi = h_\tau = h_\xi = h_\eta = 0
\]

the metrics (A2) and the Jacobian (A3) are simplified to

\[
X_\tau = \frac{f_Y g_T - f_T}{J}, \quad X_\xi = \frac{f_\xi}{J}, \quad X_\eta = \frac{f_Y g_\eta}{J}
\]
\[
Y_\tau = \frac{f_\tau g_X - g_T}{J}, \quad Y_\xi = \frac{f_\xi g_X}{J}, \quad Y_\eta = \frac{g_\tau}{J}
\]

(A5)
\[ J = 1 - f_Y \frac{\partial Y}{\partial X} \]  

(A6)

The derivatives appear on the right hand side of (A5) are obtained as follows:

\[
\begin{align*}
    f_Y &= \frac{\partial \xi_s}{\partial Y} + X \left( \frac{\partial \xi_s}{\partial Y} - \frac{\partial \xi_s}{\partial Y} \right) \\
    f_T &= \frac{\partial \xi_s}{\partial T} + X \left( \frac{\partial \xi_s}{\partial T} - \frac{\partial \xi_s}{\partial T} \right) \\
    f_\xi &= -\frac{1}{\xi_s(Y, T) - \xi_r(Y, T)}
\end{align*}
\]

\[
\begin{align*}
    g_X &= \frac{Y}{\eta_m(X, T)} \frac{\partial \eta_m}{\partial X} \\
    g_T &= \frac{Y}{\eta_m(X, T)} \frac{\partial \eta_m}{\partial T} \\
    g_\eta &= -\frac{1}{\eta_m(X, T)}
\end{align*}
\]

(A7)

Finally, the geometric derivatives are obtained by

\[
\begin{align*}
    \frac{\partial \xi_s}{\partial Y} &= \frac{\partial}{\partial Y} \left( \eta \cot \theta_r \right) = \frac{\partial}{\partial Y} \left( \eta m(X=0) \cot \theta_r \right) = \xi_m(X=0) \\
    \frac{\partial \xi_s}{\partial \eta} &= \eta_m(X=1) \frac{\partial \xi_s}{\partial \eta} \\
    \frac{\partial \xi_s}{\partial T} &= Y \cot \theta_r \frac{\partial \eta_m}{\partial T} (X=U)
\end{align*}
\]

(A8)

where \( \frac{\partial \xi_s}{\partial \eta} \) is the slope of the reflected shock and numerically computed by a central difference; \( \frac{\partial \eta_m}{\partial \xi} \) is the Mach stem slope and computed in a similar manner; \( \frac{\partial \xi_s}{\partial T} \) and \( \frac{\partial \eta_m}{\partial T} \) are the reflected shock
speed and the Mach stem speed and computed by the shock-fitting procedure in Chapter VI.
APPENDIX B. TRIPLE POINT SOLUTION

In Chapter I, it was pointed out that various forms of shock diffraction depend on two parameters, the incident shock Mach number $M_s$ and the ramp angle $\theta_r$. In the following discussion, we assume $M_s$ and $\theta_r$ are given so that one of the Mach reflections (three-shock system) results.

Following the initialization of the flowfield discussed in Chapter V, the flow conditions in region 1 (see Figure 24a) are set equal to:

$$
\begin{align*}
p_1 &= 1 \\
p_1 &= 1 \\
u_1 &= 0 \\
v_1 &= 0 \\
a_1 &= \sqrt{\gamma \frac{p_1}{\rho_1}}
\end{align*}
$$

(B1)

In the physical plane, the triple point travels along a straight path denoted by the triple point trajectory angle $\chi$. To locate the coordinates of the triple point initially at $T = 1$, the trajectory angle must be assumed. In this study, an approximate $\chi$ was obtained either from experimental data (Reference 25) or from the previously computed results. Then, the triple point coordinates are

$$
\begin{align*}
\xi_{TP} &= M_s a_1 \\
\eta_{TP} &= \xi_{TP} \tan(\chi + \theta_r)
\end{align*}
$$

(B2)
The conditions in region 2 are easily obtained from the flow conditions in region 1 and the oblique shock relations. However, these relations are derived for a stationary shock; thus, the self-similar properties of the flowfield are utilized so that the shock structure can be viewed at rest. First, the self-similar velocity components are computed as

\[ U_1 = u_1 - \xi_{TP} = -\xi_{TP} \]  \hfill (B3)

\[ V_1 = v_1 - \eta_{TP} = -\eta_{TP} \]

Then, the conditions in region 2 are computed by

\[ M_{1n} = \frac{\sqrt{U^2 + V^2}}{a_1} \]

\[ \beta_1 = 90^\circ - (\chi + \theta_r) \]

\[ M_{1n} = M_1 \sin \beta_1 \]

\[ \delta_2 = \tan^{-1} \left[ \frac{2 \cot \beta_1 \left( \frac{M_{1n}^2 - 1}{(\gamma + 1) M_{1n}^2 - 2 M_{1n}^2 + 2} \right)}{1 + \frac{\gamma - 1}{\gamma + 1} \left( M_{1n}^2 - 1 \right)} \right] \]  \hfill (B4)

\[ M_2 \sin^2(\beta_1 - \delta_2) = \frac{1 + \frac{\gamma - 1}{\gamma + 1} \frac{M_2}{M_{1n}}}{\gamma M_{1n}^2 - \frac{\gamma - 1}{2}} \]

\[ p_2 = p_1 \left[ 1 + \frac{2}{\gamma + 1} \left( M_{1n}^2 - 1 \right) \right] \]

\[ c_2 = c_1 \frac{(\gamma + 1) M_{1n}^2}{(\gamma - 1) M_{1n}^2 + 2} \]
To compute the conditions in regions 3 and 4, an iterative procedure is developed to compute the solution of the three-shock confluence. The following procedure can be easily understood on the shock polar diagram shown in Figure 24b. First, the detachment point $D$ of the reflected shock is found from

$$\beta_{3\text{max}} = \sin^{-1}\sqrt{\frac{1}{\gamma M_2^2} \left[ \frac{\gamma + 1}{4} M_2^2 - 1 + \sqrt{\frac{(\gamma + 1) + \frac{\gamma^2 - 1}{2} M_2^2 + \frac{(\gamma + 1)^2}{16} M_2^4}{\gamma M_2^2}} \right]}$$

$$M_{2n} = M_2 \sin \beta_{3\text{max}}$$

$$\delta_{\text{max}} = \tan^{-1}\left[ \frac{2 \cot \beta_{3\text{max}} \left( M_{2n}^2 - 1 \right)}{(\gamma + 1) M_2^2 - 2 M_{2n}^2 + 2} \right]$$

$$\delta_{\text{min}} = \delta_2 - \delta_{\text{max}}$$

where $\delta_{\text{max}}$ is the maximum deflection angle achievable through the reflected shock. At this stage, the pressure difference across the contact surface may be computed. The pressure $p_{3D}$ on the reflected shock side is

$$p_{3D} = p_2 \left[ 1 + \frac{2\gamma}{\gamma + 1} (M_{2n}^2 - 1) \right]$$
FIGURE 24. Schematic diagram of three shock confluence
The shock angle $\beta_4$ corresponding to $\delta_4 = \delta_{3\text{min}}$ may be obtained from the solution of the following polynomial:

$$\sin^6 \beta_4 + \alpha_1 \sin^4 \beta_4 + \alpha_2 \sin^2 \beta_4 + \alpha_3 = 0 \quad \text{(B7)}$$

where

$$\alpha_1 = -\frac{M^2 + 2}{M^2} = -\gamma \sin^2 \delta_4$$

$$\alpha_2 = \frac{2 M^2 + 1}{M^2} + \left[ \frac{(\gamma + 1)^2}{\gamma M^2} + \frac{\gamma - 1}{M^2} \right] \sin^2 \delta_4$$

$$\alpha_3 = -\frac{\cos^2 \delta_4}{M^2}$$

The smallest of the three roots corresponds to a decrease in entropy and should be disregarded (Reference 30). The mid root corresponds to the weak shock solution, and the largest root corresponds to the strong shock solution which is required by the Mach stem. Then, the pressure $p_{4D}$ on the Mach stem side is

$$p_{4D} = p_1 \left[ 1 + \frac{2\gamma}{\gamma + 1} \left( M^2 \sin^2 \beta_4 - 1 \right) \right] \quad \text{(B8)}$$

If the pressure difference $p_{3D} - p_{4D}$ is zero, then the solution of three shock system would have been obtained. If, however, the two pressures are different, the following iterative procedure is used to compute the solution.
The idea of the iterative scheme is to adjust the net deflection angle $\delta_3$ in a systematic way until zero pressure difference (within a convergence tolerance) across the contact surface is achieved.

1. Compute $p_3$ and $p_4$ as described before, and define

$$ f^i = p_3 - p_4 \quad (B9) $$

If $|f^i| < \varepsilon$, then stop, where $\varepsilon$ is the preset convergence tolerance ($\varepsilon$ was set equal to $10^{-8}$).

2. Perturb $\delta_3$ by a small fixed amount $\Delta \delta_3$ ($\Delta \delta_3$ was set to 0.01°).

$$ \delta_3^* = \delta_3 + \Delta \delta_3 \quad (B10) $$

3. Compute $\beta_3$ from the polynomial (B7) using $\delta = \delta_2 - \delta_3^*$. If $p_{3D} > p_{4D}$ then $\beta_3 = \text{mid root}$, if not, $\beta_3 = \text{largest root}$.

4. Compute $\beta_4$ from (B7) using $\delta = \delta_3^*$.

5. Compute $p_3$ and $p_4$ from Equations (B6) and (B8), and set

$$ f^* = p_3 - p_4 \quad (B11) $$

6. Approximate the derivative of $f^i$ by

$$ \frac{df}{d\delta_3} = \frac{f^* - f^i}{\Delta \delta_3} \quad (B12) $$

7. Update the deflection angle by
\[
\delta_{3}^{i+1} = \delta_{3}^{i} - \frac{f_{i}}{d \delta_{3}} \tag{B13}
\]

and repeat from step 2 with \(i = i + 1\).

After the convergence criterion is satisfied, the following information can be obtained. The reflected shock slope at the triple point is

\[
\frac{\partial \xi_{S}}{\partial \eta} = \tan (\beta_{1} + \beta_{3} + \delta_{2}) \tag{B14}
\]

the slope of the Mach stem is

\[
\frac{\partial \eta_{M}}{\partial \xi} = \tan (\beta_{4} + \chi + \theta_{r}) \tag{B15}
\]

and the contact surface slope is

\[
\frac{\partial \eta_{C}}{\partial \xi} = \tan (\delta_{3} + \chi + \theta_{r}) = \tan (\delta_{4} + \chi + \theta_{r}) \tag{B16}
\]

Finally, the rest of the flow conditions on each side of the contact surface can be computed from the oblique shock relations (46) to (51) in Chapter V.
APPENDIX C. SPLIT COEFFICIENT MATRIX METHOD

In the present work, the governing gas dynamic equations presented in Chapter III are integrated by a first-order accurate, explicit finite difference method, the split coefficient matrix (SCM) method. The SCM method uses the information propagated along the characteristics of the hyperbolic system of equations to advance the dependent variables in the time-like direction. In this appendix, the governing equations written in the self-similar coordinate system are further developed into a split coefficient matrix form.

The nonconservative form of the gas dynamic equations (15) in Chapter III may be written in a vector form

\[ \dot{Q} + [A] Q_x + [B] Q_y + G = 0 \]  

(C1)

where

\[ Q = \begin{bmatrix} P \\ U \\ V \end{bmatrix} \quad G = \begin{bmatrix} 2Y \\ U \\ V \end{bmatrix} \]  

\[ [A] = \begin{bmatrix} \bar{U} & \gamma X_{\xi} & \gamma X_{\eta} \\ \frac{a^2}{Y} X_{\xi} & \bar{U} & 0 \\ \frac{a^2}{Y} X_{\eta} & 0 & \bar{U} \end{bmatrix} \quad [B] = \begin{bmatrix} \bar{V} & \gamma Y_{\xi} & \gamma Y_{\eta} \\ \frac{a^2}{Y} Y_{\xi} & \bar{V} & 0 \\ \frac{a^2}{Y} Y_{\eta} & 0 & \bar{V} \end{bmatrix} \]
Here, the entropy equation is omitted since it is already in a characteristic form and can be integrated separately from the rest of the equations.

If we write the coefficient matrices \([A]\) and \([B]\) in a characteristic form, Equation (C1) is equivalent to

\[
Q_T + T_A \Lambda_A T_A^{-1} Q_X + T_B \Lambda_B T_B^{-1} Q_Y + G = 0
\]

where \(\Lambda_A\) is the characteristic matrix whose diagonal elements are the eigenvalues of the coefficient matrix \([A]\), and \(T_A\) is the similarity transformation matrix whose rows are the left eigenvectors associated with the diagonal elements of \(\Lambda_A\). The elements of these matrices are:

\[
\Lambda_A = \begin{bmatrix}
\bar{U} & 0 & 0 \\
0 & \bar{U} + a \sqrt{X^2} & 0 \\
0 & 0 & \bar{U} - a \sqrt{X^2}
\end{bmatrix}
\]

\[
T_A^{-1} = \begin{bmatrix}
0 & \bar{X}_\eta & -\bar{X}_\xi \\
\frac{a}{\sqrt{X^2}} & \bar{X}_\xi & \bar{X}_\eta \\
-\frac{a}{\sqrt{X^2}} & \bar{X}_\xi & \bar{X}_\eta
\end{bmatrix}
\]
where

\[ T_A = \frac{1}{2 \sqrt{X^*}} \begin{bmatrix} 0 & \frac{Y}{a} & -\frac{Y}{a} \\ 2 X^*_\phi & X^*_\phi & X^*_\phi \\ -2 X^*_\eta & X^*_\eta & X^*_\eta \end{bmatrix} \]

The transformation matrices corresponding to the \([B]\) matrix have the same form except \(X\) and \(U\) are replaced by \(Y\) and \(V\), respectively. Then, the split coefficient matrix form is defined by

\[ Q_T + T_A \Lambda^+ A_T^{-1} Q_X + T_A \Lambda^- A_T^{-1} Q_X^+ + T_B \Lambda^+ B_T^{-1} Q_Y + T_B \Lambda^- B_T^{-1} Q_Y^+ + G = 0 \] (C4)

where \(\Lambda_A\) is split into two diagonal matrices \(\Lambda^+_A\) whose diagonal contains only positive eigenvalues and \(\Lambda^-_A\) whose diagonal elements are all negative. \(\Lambda_B\) is separated likewise.
Now, in order for the characteristic information to be correctly propagated, the space derivatives must be differenced according to the characteristic directions. For example, the derivative \( Q_x \) must be approximated by a backward difference since it is associated with the positive characteristics. This reasoning is clearly understood from the domain of dependence illustrated in Figure 25. A forward difference is indicated by the + sign over the space derivatives, and a backward difference is indicated by the - sign.

![Figure 25. Domain of dependence](image-url)
Expanding Equation (C4), we have the following compatibility equations applicable to the interior of the computational domain

\[
P_\tau + \frac{1}{2} \lambda^2_X \lambda^2_X + \frac{1}{2} \lambda^3_X \lambda^3_X + \frac{1}{2} \lambda^2_Y \lambda^2_Y + \frac{1}{2} \lambda^3_Y \lambda^3_Y + 2\gamma = 0
\]

\[
U_\tau + \frac{1}{2} \frac{a}{\gamma} \frac{X}{\xi} \left( \lambda^2_X \lambda^2_X - \lambda^3_X \lambda^3_X \right) + \frac{1}{2} \frac{a}{\gamma} \frac{Y}{\xi} \left( \lambda^2_Y \lambda^2_Y - \lambda^3_Y \lambda^3_Y \right) + \frac{X}{\eta} \frac{\lambda^1_X \lambda^1_X}{X} + \frac{Y}{\eta} \frac{\lambda^1_Y \lambda^1_Y}{Y} + U = 0
\]

\[
V_\tau + \frac{1}{2} \frac{a}{\gamma} \frac{X}{\eta} \left( \lambda^2_X \lambda^2_X - \lambda^3_X \lambda^3_X \right) + \frac{1}{2} \frac{a}{\gamma} \frac{Y}{\eta} \left( \lambda^2_Y \lambda^2_Y - \lambda^3_Y \lambda^3_Y \right) - \frac{X}{\xi} \frac{\lambda^1_X \lambda^1_X}{X} - \frac{Y}{\xi} \frac{\lambda^1_Y \lambda^1_Y}{Y} + V = 0
\]

where

\[
\lambda^1_X = \bar{U} \quad \lambda^1_Y = \bar{V}
\]

\[
\lambda^2_X = \bar{U} + a \sqrt{X} \quad \lambda^2_Y = \bar{V} + a \sqrt{Y}
\]

\[
\lambda^3_X = \bar{U} - a \sqrt{X} \quad \lambda^3_Y = \bar{V} - a \sqrt{Y}
\]

\[
\xi^1_X = \frac{X}{\eta} \frac{U_X}{U} - \frac{X}{\xi} \frac{V_X}{V}
\]

\[
\xi^2_X = \frac{P_X}{a} \left( \frac{X}{\xi} \frac{U_X}{U} + \frac{X}{\eta} \frac{V_X}{V} \right)
\]

\[
\xi^3_X = \frac{P_X}{a} \left( \frac{X}{\xi} \frac{U_X}{U} + \frac{X}{\eta} \frac{V_X}{V} \right)
\]

\[
\xi^1_Y = \frac{Y}{\eta} \frac{U_Y}{U} - \frac{Y}{\xi} \frac{V_Y}{V}
\]

\[
\xi^2_Y = \frac{P_Y}{a} \left( \frac{Y}{\xi} \frac{U_Y}{U} + \frac{Y}{\eta} \frac{V_Y}{V} \right)
\]
\[ \lambda^3_Y = P_Y - \frac{Y}{a} \left( Y^\rho U_Y + Y^\eta V_Y \right) \]

All spatial derivatives are differenced according to the sign of the eigenvalues multiplying them.

At the computational boundaries, only one-sided differences (either in the X or Y direction depending on the boundary) are available. Therefore, special compatibility equations must be developed for such places. At the ramp boundary, the characteristic \( \lambda_X^2 \) is positive and is directed toward the boundary from the exterior of the domain. Therefore, the compatibility equation associated with the \( \lambda_X^2 \) characteristic must be discarded and replaced by an auxiliary equation applicable to the boundary. This is done by first premultiplying Equation (C3) by \( T_A^{-1} \) to obtain

\[ T_A^{-1} Q_T + \Lambda_A T_A^{-1} Q_X + T_A^{-1} T_B \Lambda_B T_B^{-1} Q_Y + T_A^{-1} G = 0 \]  \hspace{1cm} (C6)

Then, the second row of the above equation is discarded. The resulting compatibility equations are: These equations are:

\[ P_T + \lambda^1_X \lambda^2_X + \frac{1}{2} \left[ 1 - ( \frac{X^\rho Y^\rho + X^\eta Y^\eta}{\zeta^\rho \zeta^\rho + \eta^\rho \eta^\rho} ) \right] \lambda^2_Y \lambda^2_Y \]

\[ + \frac{1}{2} \left[ 1 + ( \frac{X^\rho Y^\rho + X^\eta Y^\eta}{\zeta^\rho \zeta^\rho + \eta^\rho \eta^\rho} ) \right] \lambda^3_Y \lambda^3_Y \]

\[ - \frac{Y}{a} \left( \frac{X^\rho Y^\rho - X^\eta Y^\eta}{\zeta^\rho \eta^\rho} \right) \lambda^1_Y \lambda^1_Y + 2Y = 0 \]  \hspace{1cm} (C7)
\[ V_T + \frac{1}{2} a \frac{\partial}{\partial \eta} \left( \frac{\partial x^*_v}{\partial \eta} - \frac{\partial x^*_v}{\partial \eta} \right) \left[ \lambda_1^2 \lambda_2^2 - \lambda_3 \lambda_3^3 \right] \]
\[ - \frac{\partial x^*}{\partial \eta} \left( \frac{\partial x^*_v}{\partial \eta} + \frac{\partial x^*_v}{\partial \eta} \right) \lambda_1^2 \lambda_2^2 + V = 0 \]

The auxiliary equation at the ramp boundary may be the flow tangency condition

\[ U = V \cot \theta \]

At the reflected shock boundary, the characteristics \( \lambda_X^1 \) and \( \lambda_X^3 \) must be eliminated. The resulting compatibility equation is

\[ P_T + \frac{\lambda}{\eta} \left( \frac{\partial x^*_v}{\partial \eta} U + \frac{\partial x^*_v}{\partial \eta} V \right) + \lambda_1^2 \lambda_2^2 \]
\[ + \frac{1}{2} \left[ 1 + \left( \frac{\partial x^*_v}{\partial \eta} \frac{\partial x^*_v}{\partial \eta} \right) \lambda_2^2 \lambda_3^2 \right] \]
\[ + \frac{1}{2} \left[ 1 - \left( \frac{\partial x^*_v}{\partial \eta} \frac{\partial x^*_v}{\partial \eta} \right) \lambda_2^3 \lambda_3^3 \right] \]
\[ + \frac{\lambda}{\eta} \left( \frac{\partial x^*_v}{\partial \eta} - \frac{\partial x^*_v}{\partial \eta} \right) \lambda_1 \lambda_2^1 \]
\[ + \frac{\lambda}{\eta} \left( \frac{\partial x^*_v}{\partial \eta} U + \frac{\partial x^*_v}{\partial \eta} V \right) + 2\gamma = 0 \]

The Rankine-Hugoniot relations applicable to the shock front are used to replace the missing equations at the reflected shock boundary. At the Mach stem boundary, a similar procedure is followed to eliminate the characteristics \( \lambda_Y^1 \) and \( \lambda_Y^3 \). The resulting compatibility equation at the Mach stem is
\[ P + \frac{Y}{a} ( Y U + Y V ) + \frac{\lambda^2}{Y} \frac{\partial^2}{\partial Y^2} \]

\[ + \frac{1}{2} \left[ 1 + \left( \frac{a Y}{a Y} + \frac{a Y}{a Y} \right) \right] \frac{\lambda^2}{\frac{\partial}{\partial X}} \frac{\partial^2}{\partial X^2} \]  

\[ + \frac{1}{2} \left[ 1 - \left( \frac{a Y}{a Y} + \frac{a Y}{a Y} \right) \right] \frac{\lambda^3}{\frac{\partial}{\partial X}} \frac{\partial^3}{\partial X^3} \]

\[ + \frac{Y}{a} \left( \frac{a Y}{a Y} - \frac{a Y}{a Y} \right) \frac{\lambda^1}{\frac{\partial}{\partial X}} \frac{\partial^1}{\partial X^1} \]

\[ + \frac{Y}{a} ( Y U + V ) + 2Y = 0 \]  

Missing equations are replaced by the shock relations similar to those used at the reflected shock.
APPENDIX D. JUMP CONDITION ACROSS THE DISCONTINUITY

Consider a hyperbolic system of gas dynamic equations written in the conservation law form

\[ W_T + E_X + F_Y + B = 0 \]  \hspace{1cm} \text{(D1)}

in a domain \( D \) of the \((X,Y,T)\) space. The domain \( D \) is divided into \( R_1 \) and \( R_2 \) by the surface \( C(X,Y,T) = 0 \) (Figure 26).

FIGURE 26. Discontinuity in an arbitrary domain
W, E and F are continuous in $R_1$ and $R_2$, but have discontinuity across the surface $C(X,Y,T) = 0$. Then, $W$ is said to be a weak solution in $D$ if it satisfies the equation

$$\int_D (W \phi_T + E \phi_X + F \phi_Y + B \phi) \, dX \, dY \, dT = 0 \quad (D2)$$

where $\phi(X,Y,T)$ is an arbitrary test function which is continuous and has continuous derivatives in $D$, and vanishes on the boundary and the exterior of $D$. Integrating $(D2)$ by parts, we get

$$\int_{R_1} (W_T + E_X + F_Y + B ) \phi \, dX \, dY \, dT + \int_{R_2} (W_T + E_X + F_Y + B ) \phi \, dX \, dY \, dT$$

$$\quad + \int_C \left( \begin{bmatrix} E \\ F \\ W \end{bmatrix} \cdot \mathbf{n}_1 + \begin{bmatrix} E \\ F \\ W \end{bmatrix} \cdot \mathbf{n}_2 \right) \phi \, ds = 0 \quad (D3)$$

where $\mathbf{n}_1$ is the unit normal to the $R_1$ side of the discontinuity surface, and $\mathbf{n}_2$ is the unit normal to the $R_2$ side of $C$.

The first two integrals are zero from the conservation equations $(D1)$. Observing $\mathbf{n}_1 = -\mathbf{n}_2$, we can write the last integral as

$$\int_C \left( \begin{bmatrix} E \\ F \\ W \end{bmatrix}_1 - \begin{bmatrix} E \\ F \\ W \end{bmatrix}_2 \right) \cdot \mathbf{n}_1 \phi \, ds = 0 \quad (D4)$$
Since the integral (D3) vanishes for all test functions, we arrive at the jump condition

\[ n_t [W] + n_x [E] + n_y [F] = 0 \]  

which holds across the surface \( C(X,Y,T) \), where \([W]\) represents the jump in the quantity \( W \), and the normal vector is given by

\[ \hat{n} = n_x \hat{i} + n_y \hat{j} + n_t \hat{k} = \frac{\nabla C(X,Y,T)}{|\nabla C(X,Y,T)|} \]