SHOCK CAPTURING USING FLUX-CORRECTED TRANSPORT ALGORITHMS WITH ETC (U)

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A numerical technique has been developed for capturing complex, nonsteady shock structures in multidimensions. The technique relies on moving the computational mesh with the shock wave so that the features of principal interest appear approximately stationary. The method has been implemented using coordinate-split Flux-Corrected Transport (FCT) algorithms which allow the mesh to evolve arbitrarily with respect to the fluid in each coordinate. The grid may thus be optimized in response to the needs of a
given problem. Synchronizing the grid and fluid motions permits significant reduction of numerical transients and eliminates numerical diffusion. Shocks develop naturally, with no fitting. The method is illustrated by calculating complex, two-dimensional Mach reflection phenomena associated with airblasts and shock diffraction on wedges. The numerical results are in good agreement with available experimental data.
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A numerical technique has been developed for capturing complex, nonsteady shock structures in multidimensions. The technique relies on moving the computational mesh with the shock wave so that the features of principal interest appear approximately stationary. The method has been implemented using coordinate-split Flux-Corrected Transport (FCT) algorithms which allow the mesh to evolve arbitrarily with respect to the fluid in each coordinate. The grid may thus be optimized in response to the needs of a given problem. Synchronizing the grid and fluid motions permits significant reduction of numerical transients and eliminates numerical diffusion. Shocks develop naturally, with no fitting. The method is illustrated by calculating complex, two-dimensional Mach reflection phenomena associated with airblasts and shock diffraction on wedges. The numerical results are in good agreement with available experimental data.

INTRODUCTION

Numerical solution of transient multidimensional gas dynamics problems is always nontrivial. When, in addition, the problem involves reflecting supersonic flows, large variations in length scales in both space and time, or phenomena for which neither analytic solutions nor detailed experimental observations are at hand, the state of the computational art is challenged. Such a problem arises in calculating the oblique reflection of shocks from solid surfaces in planar geometries (e.g. shock tube experiments) or axisymmetric geometries (e.g. airblasts). The complications arise mainly from the presence of Mach reflections which occur when a shock front impinges on a reflecting surface at angles of incidence sufficiently far from normal. The formation of a Mach stem and, consequently, of a slip surface intersecting the triple point (the confluence of the incident, Mach, and reflected waves) results from the requirement that the flow behind the reflected shock be parallel to the reflecting surface, which cannot be achieved through regular reflection.

Attempts to calculate the properties of the flow in Mach reflections date back at least to von Neumann and the research which grew out of the wartime explosive studies. For the simplest problem, that of a planar shock.
reflecting from a plane surface, Jones, Martin, and Thornhill\textsuperscript{5} noted that it
is possible to reduce the number of independent variables to two by transform-
ing to the similarity variables $x/t$, $y/t$, a device that was also used by
Kutler, et al\textsuperscript{6}. Ben-Dor\textsuperscript{7} developed a theory which used shock polars to explain
some of the features of this problem, and solved the system of algebraic equations
obtained by combining the jump conditions across the various disconti-
nuities (Courant and Friedrichs)\textsuperscript{8} to describe the flow in the neighborhood of
the triple point. To date, no satisfactory treatment of the complete flow
field has been published, although some features (like the shape of various
waveforms) are quite easy to model.

In connection with studies of both chemical and nuclear explosions there
have been many attempts to model a spherical blast wave reflecting from the
ground, the so-called height-of-burst (HOB) problem. The hydrodynamic pheno-
mena in the two cases are identical, although nonideal effects (primarily ex-
plusive afterburn in the first instance and radiation preheating in the second)
are different. Previous attempts to model two-dimensional complex shock re-
fection have suffered from restriction to describing part of the system, the
use of a special assumption like that of self-similarity, or less than satis-
factory agreement with experimental data.\textsuperscript{9}

The calculations discussed here represent a step forward in overcoming
these difficulties. They differ from previous numerical work in incorporating
two important computational developments: Flux-Corrected Transport (FCT)\textsuperscript{10} and
an adaptive regridding procedure, called "sliding rezone",\textsuperscript{11} which optimizes
the mesh point distribution and hence the resolution of surfaces of disconti-
nuity.

FCT is a finite-difference technique for solving the fluid equations in
problems where sharp discontinuities arise (e.g. shocks, slip surfaces and
contact surfaces). It modifies the linear properties of a second- (or higher)
order algorithm by adding a diffusion term during convective transport, and
then subtracting it out "almost everywhere" in the antidiffusion phase of each
time step. The residual diffusion is just large enough to prevent dispersive
ripples from arising at the discontinuity, thus ensuring that all conserved
quantities remain positive. FCT captures shocks accurately over a wide range
of parameters. No information about the number or nature of the surfaces of
discontinuity need be provided prior to initiating the calculation.

The FCT routine used in the present calculations, called JPBFCT (an ad-
vanced version of ETBFCT)\textsuperscript{12}, consists of a flexible, general transport module
which solves 1-D fluid equations in Cartesian, cylindrical, or spherical geo-
metry. It provides a finite difference approximation to the conservation laws
of the general form:

$$\frac{\partial}{\partial t} \int \phi dV = -\int \phi \left( u - \bar{u} \right) \cdot dA + \int T dA$$  \hspace{1cm} (1)

where $\phi$ represents the mass, momentum, energy or mass species in cell $\Omega(t)$,
$u$ and $\bar{u}$ represent the fluid and grid velocities, respectively, and $T$ repres-
sents the pressure/work terms. This formulation allows the grid to slide with
respect to the fluid without introducing any additional numerical diffusion.
Thus, knowing where the features of greatest interest are located, one can
concentrate fine zones where they will resolve these features most effectively
as the system evolves (Fig. 1).

In the next section we describe the computational techniques used to solve
the wedge problem and present the results of four simulations carried out to
reproduce experimental results of Ben-Dor and Glass.\textsuperscript{13} In Section III we pre-
sent a parallel discussion for a HOB calculation. Finally, in Section IV we
summarize our conclusions.
Fig. 1. Adaptive grids for a) planar shocks on wedge (double Mach shock features are indicated); b) and c) HOB problem initially and at transition point (grid lines in fine-zone region are indistinguishable).

SHOCK-ON-WEDGE CALCULATIONS

The JPBFCT algorithm was used in a 2-D Cartesian version of the FAST2D code to model the reflections of planar shocks from wedges of 20° to 60° and varying shock strengths. Four general classes which include regular, single, complex and double Mach reflection were calculated (referred to as cases a,b,c,d respectively). The bottom of the mesh, treated as a reflecting boundary, modeled the surface of the wedge. Quantities on the right hand boundary and on the top were set equal to the ambient values. The remaining boundaries were treated as permeable. In the single, complex, and double Mach reflection cases, the mesh was anchored on the left, essentially at the wedge tip where the incident shock first strikes, while the zones were stretched by a scaling factor proportional to \( t \) as soon as the reflection region filled a substantial portion of the grid. In case (d), the double Mach reflection case, the opening angle is so small that the incident shock has to traverse many zones before the mach stem has grown large enough to be well resolved. For this reason, the problem was solved on a uniform mesh in the frame of reference fixed.
to the reflection point, with stretching being initiated after the first Mach stem reached \( \approx 20 \) cells in length. The timestep was recalculated at every cycle with a Courant number of 0.5.

Figure 2 shows the pressure and density contours and the velocity field for cases a, b, c, d. The pertinent shock phenomena can be easily identified: incident shock, contact surface, first and second Mach stems. As shown in Fig. 1, the zoning is particularly sparse except for the region of interest. Adequate resolution of the key surfaces (contact and second Mach stem) is obtained with 5 zones in each direction. The accuracy can be evaluated by comparing the experimental density distributions along the wall (Fig. 3).

Fig. 2 - Pressure and density contours and flow velocity vectors (in frame of reflection point) for planar waves with Mach number \( M \) reflecting from wedges with angle \( \theta \) for (a) \( M=2.03, \theta=60^\circ \); (b) \( M=2.82, \theta=20^\circ \); (c) \( M=5.29, \theta=30^\circ \); (d) \( M=7.03, \theta=50^\circ \).
Fig. 3. Comparison of density (in units of ambient density $\rho_0$) for cases (a), (b), (c), (d) of Fig. 2 vs. distance from corner. Points are measured values reported in Ref. 13.

HEIGHT OF BURST CALCULATIONS

Next, we performed a numerical simulation of a 1KT nuclear detonation at 31.7 m HOB, a case which could be readily compared with high explosive data. A constant ambient atmosphere was used with a density of $1.22 \times 10^{-3}$ g/cm$^3$ and pressure $1.01 \times 10^6$ dynes/cm$^2$. To relate the energy and density to the pressure, a real-air equation of state (EOS) was used. This table-lookup EOS was derived from theoretical calculations by Gilmore$^{14,15}$ for equilibrium properties of air and has been vectorized for the Advanced Scientific Computer.$^{16}$ The internal energy density used in the call to the EOS is found by subtracting kinetic energy from total energy; this can be negative due to truncation (phase) errors. When this occurred, the value of the pressure was reset to zero.

The transition from regular reflection to double Mach reflection occurs at a ground range approximately equal to the HOB. The size of the mesh should
therefore be roughly twice the HOB in both directions. The upper boundary should be far enough away from the blast front to be non-interfering. We chose boundaries of 55 m for the radial direction and 103.5 m for the axial direction. The fine grid in the radial direction contained 140 out of 200 total zones, each 5 cm in length. The rightmost zones were 80 cm in length, and a smoothing involving 40 zones was performed between the regions to guarantee that the zone sizes varied slowly. In the axial direction the fine grid contained 75 out of 150 total zones, each 5 cm in length. Beyond that region the zones were geometrically increased by a factor of 1.112.

Placement of the fine grid at the origin of the mesh (ground zero, the point at which reflection first occurs) was determined to be optimum for capturing peak pressure in the airblast wavefront. Thus, as the expanding wave moves along the ground surface, the fine grid is always locked to it and each point along the blast front encounters the same spatial gridding as it approaches the ground. By treating each point of the incident front in the same manner, we insure that the calculation is internally consistent and that the computed transition point is accurate to within the limits of the resolution.

The initialization provides a strong shock with approximate Mach number $M=12$. This speed and the need for restart capability led to the choice of 200 timesteps as an interval for the spatial display (snapshots). The dump interval that resulted was $\Delta t \approx 0.3$ milliseconds (ms). These dumps were stored on magnetic tape and post-processed.

A fit to the 1-D nuclear blast flow field (Ref. 17) was used to initialize the energy and mass density and velocity field at 3.76 ms. The corresponding peak overpressure was 113 bars. After the 1 KT flow field was laid down inside a radius of 31.6 m, the fine-zone grid was activated to follow the peak pressure as it moved along the ground surface, modelled as a perfectly reflecting boundary. This region comprised 140 zones, and a switch was set to keep 40 of these zones ahead of the reflection point. Permeable boundary conditions are used on the top and right edges of the mesh, i.e., density, pressure and velocity are set equal to ambient preshock conditions. Reflecting conditions were applied to the left and bottom. The total elapsed physical time in the 2-D calculation, 7.6 ms, required 5600 cycles. Times are referred to $t=0$ at the start of the calculation.

The numerical simulation begins just before the shock first reflects from the ground. Fig. 4a indicates the pressure and density contours and velocity vectors at time 3.18 ms. In Fig. 4b the reflected shock is shown moving upward, the outward flow begins to stagnate at the ground (transition). Fig. 4c, $t=5.99$ ms, shows an enlargement of the shockfront, and the development of the Mach stem, slip surface and second Mach stem. The angle of the shock front with respect to the ground is increasing with time so that the effective wedge angle is decreasing. From Ben-Dor and Glass one expects a transition to double Mach stem to occur at approximately 45°. The angle in Fig. 4b is about 45° and the shock front has entered the transition phase. Figure 4d shows the fully developed shock structure at 7.79 ms. Clearly visible is the second Mach stem and a vortex region behind the first Mach stem. Toeing out of the first Mach stem can be also seen in the contours of Fig. 4d and occurs as the fluid rolls forward where the slip line would otherwise intersect the ground. The velocity field in Fig. 4d also shows this detail.

One should also note the reflected shock properties. The reflected shock propagates rapidly through the high temperature fireball, due to the high local sound speed. The shape of this reflected wave is a primary difference between the ROB case and the wedge case. The other major difference, of course, is the spherically expanding blast wave which decreases in strength approximately proportional to $r^{-2}$. 

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Finally we consider the pressure/distance relation for the HOB case. In Fig. 5 we compare the results of the numerical simulation with the data of Carpenter and with empirical analysis. Carpenter's data are based upon careful HOB experiments with 8 lb PBX9404 spheres. The empirical analysis was based on a 1 KT nuclear free air curve and HOB construction factors. The calculated values in the regular reflection regime are 20% low and may be attributed to a combination of FCT clipping, the resolution of the grid, and inaccuracies in the initialization of the flow field. During and after Mach reflection, the peaks remain low until the Mach stem structure has grown large enough to be resolved on the mesh. By the time it occupies a region of 15 cells high and 35 cells wide, the peak pressures are in good agreement with the HE data and the empirical analysis.
SUMMARY AND CONCLUSION

The complex 2-D Mach reflection phenomena associated with shock diffraction on wedges and height-of-burst explosions have been modeled with the FAST2D computer code. Four wedge cases—regular, single, complex and double Mach reflection—have been calculated and the results compared to experiments. A nuclear detonation (1 KT at 31.7m HOB) was also simulated. The results give insight into the formation and subsequent evolution of the Mach stem, the triple point and the contact discontinuity. The transition from regular reflection to double Mach reflection is predicted. Excellent agreement with Ben-Dor's data is obtained. We suggest that the first signal for transition is the appearance of a second peak behind the shock front due to stagnation in the flow. Calculated first and second pressure peaks versus distance in the HOB case agree both with the HE data and analysis to within 20%.

The use of the adaptive regridding procedure, called "sliding rezone", along with the FCT algorithm allows one to accurately predict the nonsteady shock structures in two dimensions for diffractions on wedges and HOB cases. Comparison with data for both wedges and HOB yields the best results obtained to date.

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