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NUMERICAL METHODS FOR

LARGE-SCALE, TIME-DEPENDENT

PARTIAL DIFFERENTIAL EQUATIONS

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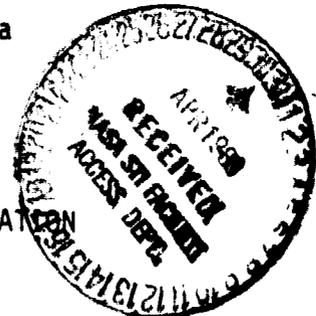
LARGE-SCALE, TIME-DEPENDENT

PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

A survey of numerical methods for time dependent partial differential equations is presented. The emphasis is on practical applications to large scale problems. A discussion of new developments in high order methods and moving grids is given. The importance of boundary conditions is stressed for both internal and external flows. A description of implicit methods is presented including generalizations to multidimensions. Shocks, aerodynamics, meteorology, plasma physics and combustion applications are also briefly described.

TABLE OF CONTENTS

1. Introduction

In the construction of numerical solutions to large scale problems one wishes to have a code with many different characteristics. Examples of these properties include efficiency both in terms of computer time and computer storage and also ease of use. Frequently a code is constructed to be used by other people who do not have a detailed knowledge of the algorithm. Hence, one does not want a program which requires the specification of many nonphysical parameters or one that requires intervention on the part of the user. Lagrangian codes are frequently complex and may require operator intervention for rezoning. Hence, we shall concentrate on Eulerian methods.

In contrast to ordinary differential equations it does not seem advisable to introduce general packages for time dependent partial differential equations. In one space dimensions a number of packages exist usually based on an ODE solver. These packages are useful when one wants a quick answer to a simple problem. However, the programs are far from optimal both in terms of computer time and computer storage [115]. Hence, for realistic physical models with many complicated equations which are to be solved many times it is necessary to develop a code for each problem. This is especially true for multidimensional problems. The range of solutions including both smooth and discontinuous flows demands that the algorithm be carefully matched with the physics. Depending on many

factors one may need either an explicit or implicit scheme. Accuracy and geometrical considerations will determine whether high or low accuracy methods (in both space and time) are more appropriate.

In the following sections we will discuss in more detail many of the factors that influence the choice of a scheme. Special attention will be paid to the treatment of boundaries. After a general discussion of standard boundary treatments attention will be focused on moving boundaries. Artificial boundaries to simulate an infinite domain create other difficulties which will be analyzed. In all these cases the interplay between the physics and the numerics will be stressed. Implicit methods and applications to specific problems are discussed with special emphasis on shocks and on steady state solutions.

2. Boundary Treatment

Since much of this study deals with nonstandard boundary problems we shall first review the basic theory. For a numerical method to be useful we require that it be stable and also converge. Hence, small perturbations in the problem should give rise to small perturbations in the solution. We first consider the model equation

$$(2.1) \qquad u_t + Au_x = 0$$

with A a constant n×n matrix and $0 \leq x \leq 1$. Let A be symmetric and have k positive eigenvalues, n-k negative eigenvalues. It is then straightforward to show that (2.1) is well posed only if k linearly independent conditions are imposed at $x = 0$ and n-k conditions at $x = 1$. This number of conditions is also sufficient for well posedness as long as no variables corresponding to characteristic variables coming into the boundary, from inside the region, are specified.

For a numerical method it is necessary to specify the correct number of boundary conditions as given by the differential equation. In general one requires some method to numerically determine the boundary values for the other, nonspecified variables. If the boundary treatment is not done correctly then errors are generated at the boundary which propagate into the domain of integration and create instabilities. Especially for nonlinear problems these instabilities frequently do not manifest themselves at the

boundaries but rather along sonic lines or stagnation
points. It is a nontrivial task to trace the source of
the difficulty to a mistreatment of the boundary [137].

For simplicity we shall assume that the numerical
scheme uses information only at the point of interest and
at its immediate two neighbors at various time levels. Then
Kreiss has shown [81], [110] that the stability for a
scalar equation can be analyzed by assuming a solution of
the form

$$u_j^n = U \kappa^j z^n$$

and only considering the semi-infinite domain $0 \leq x < \infty$.
If there are solutions to the interior and boundary differ-
ence schemes with $|\kappa| < 1$ and $|z| > 1$ then the initial-
boundary scheme is unstable. If there are no nontrivial
solutions with $|\kappa| < 1$ and $|z| > 1$ then the scheme is
stable. If there are solutions with $|\kappa| = 1$, $|z| = 1$
more care is required. For additional details see the survey
by Morton [140].

For systems of equations or schemes that require more
than three mesh points at a time level the theory is more
complicated. For systems, the algebra of solving the equa-
tions for complex κ and z is large and needs to be done
for each system of equations. Gottlieb, Gunzburger and
Turkel [72] have shown how the scalar results can be extended
to systems of equations if one takes into account the
characteristic variables (see also [28]). If this is not

done examples are given to show that troubles can occur.
Several examples are presented in later chapters. Engquist
and Smedsaas [55] have a method of lines code that automa-
tically accounts for the characteristic variables.

For several of the standard schemes, boundary condi-
tions have been analyzed by several authors. We shall
present a brief outline of the results.

1.   Leapfrog method:

    a. Extrapolation in space is unstable.

    b. Extrapolation in space-time is stable.

    c. A one-sided Euler method is stable.

We again emphasize that these results are true only for a
scalar equation. As mentioned above the scalar results can
be extended to systems if the numerical boundary treatment
is done on the correct characteristic variables rather than
on the natural variables. The given boundary conditions
can consist of any combination of variables that yields a
well posed differential problem.

2.   Lax-Wendroff method:

This is usually implemented by a two step Richtmyer
or a two step MacCormack method. The MacCormack method
is easier to implement as no half points are required and
boundary conditions can be imposed after the first step.
The treatment   of parabolic terms is also easier using
the MacCormack scheme.

    a. Space extrapolation at the conclusion of the two
        steps is stable.

    b. A one-sided Euler method at the conclusion of the
        two steps is stable.

    c.   Extrapolation at the intermediate step of the
        Richtmyer method is unstable.

    d.   Extrapolation or one-sided differences at the
        intermediate step or final step of the MacCormack
        method is stable.

These boundary treatments are discussed in detail in [71].
Method d is particularly easy to implement and will be
discussed in more detail in the next section where it is
extended to higher order methods. In many cases one sided
differences are equivalent to extrapolation of fluxes to
artificial points exterior to the region. The choice
between these options is based on programming ease.

3.   Implicit methods:

    a.   Space extrapolation is stable.

    b.   The box scheme is stable and very accurate.

    c.   Explicit one sided differences can lead to
        stability limits on Δt ([172]).

Many numerical tests have confirmed the analysis of
Kreiss for both simple test cases and complicated problems.
At present one difficulty is to extend these results, in a
useful manner, to multidimensional problems. Abarbanel and
Gottlieb [3] have considered the leapfrog scheme while
Bayliss (private communication) has analyzed methods based
on splitting techniques. In practice most of the one

dimensional results generalize to the multidimensional situation. In the coming chapters we shall consider practical generalizations to higher order methods, moving boundaries and radiation boundaries.

The numerical treatment of boundaries for parabolic equations is usually simpler than that described above since all the variables are prescribed. Some difficulties may arise when derivative boundary conditions are given, this is especially true for nonrectangular regions [195].

More serious difficulties occur when the highest space derivatives are multiplied by a small (but fixed) parameter, e.g. high Reynolds number flow. Most schemes contain some numerical viscosity and so one must ensure that the numerical viscosity does not overwhelm the physical viscosity. In general this is only true in boundary layers where the large gradients enhance the physical viscosity. Therefore, when the computations do not resolve the boundary layer it is not reasonable to impose parabolic-type boundary conditions. When one uses a coarse mesh near the boundary one is effectively ignoring the viscous effects and only considering the inviscid equations. So, with coarse grids near the boundary one should use hyperbolic-like boundary conditions. Failure to do this leads to cell Reynolds number restrictions [158].

To clarify this point we consider a model problem; the steady state linearized Burgers equation

$$(2.2a) \qquad u_{xx} = Ru_x , \qquad R > 0 , \qquad 0 \leq x \leq 1$$

with boundary conditions

(2.2b) $u(0) = 1$ $u(1) = 0$.

The solution is given by

(2.3) $u(x) = (e^R - e^{Rx})/(e^R - 1)$.

For R large the solution is approximately equal to 1 everywhere except for a boundary layer near $x = 1$. Solving (2.2) by central differences we have

(2.4a) $v_{j+1} - 2v_j + v_{j-1} = R_\Delta (v_{j+1} - v_{j-1})$ with

(2.4b) $R_\Delta = R\Delta x$, $v_0 = 1$, $v_N = 0$

This has the solution

(2.5) $v_j = \dfrac{Q^j - Q^N}{1 - Q^N}$, $Q = \dfrac{2 - R_\Delta}{2 + R_\Delta}$.

R_Δ is generally called the cell Reynolds number or the Peclet number. For R_Δ larger than 2 , Q is negative and so v_j is oscillatory. As R_Δ increases ,   Q approaches -1 and v_j acquires a large $2\Delta x$ oscillation which has nothing in common with the analytic solution (see also [158]).

One way to avoid this situation is to construct schemes, at least near boundaries, which do not have any cell Reynolds number restriction [6], [36], [41]. Alternatively one can match the interior scheme with an asymptotic expansion for the boundary layer [82]. Where feasible stretched grids should be used to resolve the boundary layers. When the

position of the boundary layer is not known in advance or is nonuniform along the boundary this is a difficult process.

The important point is that this oscillation is entirely due to faulty boundary treatment, i.e., nonresolution of the boundary layers. For example, specifying $u_x = 0$ at $x = 1$ rather than $u = 0$ eliminates these oscillations. This is a practical method for outflow boundary conditions [84]. Alternatively, one can specify combinations of u and higher order derivatives at the boundary. As Δx goes to zero this combination should reduce to $u(1) = 0$ and so the scheme converges for fixed R. As R_Δ increases the boundary condition should approximate some extrapolation formula which is stable for the hyperbolic difference approximation. For example, we can replace (2.4b) by

$$(2.4c) \qquad v_N + R_\Delta(v_N - v_{N-1}) = 0$$

The solution to (2.4) is then given by

$$(2.6) \qquad v_j = AQ^j + 1 - A \; ; \quad A = (1 - Q^N + R_\Delta Q^{N-1}(1-Q))^{-1}$$

By inspection v_j converges to $u(x_j)$ as Δx goes to zero. As R_Δ increases beyond 2, Q becomes negative and oscillations appear. However, the factor A in front of the oscillatory part becomes small and so the oscillations do not disturb the solution. In more practical situations the first difference $v_N - v_{N-1}$ can be replaced by higher differences for greater accuracy. Similarly, more complicated weights than simply R can be constructed. For

multidimensional problems R_Δ varies locally in both
space and time. The downstream boundary conditions can
also create oscillations when the mesh does not resolve
the boundary layers. Correct treatment of the downstream
boundaries eliminates this difficulty [95].

This provides an additional example of the ill effects
of improper boundary treatment. As before the effects
propagate into the interior and cannot always be easily
traced back to its proper source.

3. HIGHER ORDER METHODS — FORMULATION

As computer hardware improved, the need for more sophisticated numerical algorithms became obvious. In the early stages of software development a standard technique was a first order method while a high order method signified a second order method. Computers were not sufficiently fast to consider two dimensional problems with fine meshes and so only low accuracy results were obtained. With the advent of faster and more structured computers it is now reasonable to achieve one percent accuracy for many two dimensional time dependent problems. Three dimensional problems are being solved with coarse meshes. With this situation it is necessary to analyze higher order methods. When one wishes accuracies of the order of one to five percent the higher order methods allow for a coarser grid than first or second order methods with no loss in accuracy. This coarser grid means that both computer storage and computer running time can be decreased without any deterioration in the solution. When even more accurate solutions are needed the advantages of the higher order methods are more pronounced. The results of [188] show that even with low accuracy requirements the fourth order method was more efficient.

Higher order methods may not always be advantageous or feasible. Higher order methods usually require more computer time per time step than lower order methods. Hence, efficiency is increased only if a coarser mesh can be used. There are various circumstances where the mesh is

constrained by considerations other than accuracy and hence
little is achieved by higher order methods. One case is
when the geometry of the problem demands a large number of
points. For example, if one wishes to describe the many
perturbations on a real wing then one needs many more
points than are needed for reasonable accuracy with a
second order method. Another example occurs in meteorolog-
ical flows over the globe. The accuracy of any algorithm
is limited by uncertainties in the physics of the model and
in observational data. However, one cannot choose too
coarse a grid or the topography of the earth is distorted.
Similar situations occur in other fields where the basic
equations being integrated have only limited validity.
However, for the majority of cases where the mesh is
constructed mainly on accuracy considerations the use of
higher order methods can lead to large savings in time and
storage. Furthermore, the implementation of these methods
frequently does not require large modifications to existing
codes.

The construction of higher order methods has proceeded
along one of three lines. Either extensions of existing
finite difference methods, or finite element methods or
spectral methods. Multidimensional finite element methods
have not proven very successful for hyperbolic problems.
There are problems with the inversion of a large
unstructured but sparse matrix and have thus far not
competed successfully with standard alternating direction

techniques or explicit methods. Furthermore, finite element methods do not automatically yield stable boundary treatment (see e.g. [72] and [80]) and so much of their justification for elliptic problems does not generalize. In this section we shall discuss finite difference methods and spectral methods.

High order finite difference methods have the advantage that they are similar to lower order methods. Hence, their implementation is easier and usually does not require major modifications to existing programs. Spectral methods are even higher order and frequently are "infinite" order methods. They have limited applicability to problems with complex boundaries (see however [151]) and their suitability for shock problems needs further investigation. It is possible to construct unconditionally stable spectral methods; also boundary conditions are more straightforward with spectral methods. We shall concentrate on the so called pseudospectral or collocation methods as they have wide range of applicability. Galerkin spectral methods are more costly because of the need to calculate convolution sums. Hence, they are limited to equations with a quadratic nonlinearity in which case fast methods are available to calculate the convolution sums [149]. Even in this case they are two to three times slower than a pseudospectral method.

We first consider the one-dimensional equation

$$(3.1) \qquad u_t + f_x = 0$$

and some extensions of standard second order methods.

The leapfrog approximation to (3.1) is given by

$$(3.2) \qquad u_j^{n+1} = u_j^{n-1} - \lambda(f_{j+1}^n - f_{j-1}^n)$$

with $\lambda = \Delta t/\Delta x$. A fourth order extension suggested by Kreiss and Oliger [111] is

$$(3.3) \quad u_j^{n+1} = u_j^{n-1} - \frac{\lambda}{6}[8(f_{j+1}^n - f_{j-1}^n) - (f_{j+2}^n - f_{j-2}^n)]$$

At the boundaries (3.3) can be supplemented by (see [64] and [143]

$$u_0^{n+1} = u_0^{n-1} - \frac{\lambda}{3}(-11f_0^n + 18f_1^n - 9f_2^n + 2f_3^n)$$
$$+ \frac{11\lambda\rho}{6}(u_0^{n+1} - 2u_0^n + u_0^{n-1})$$

(3.4) and

$$u_1^{n+1} = u_1^{n-1} - \frac{\lambda}{3}(-2f_0^n - 3f_1^n + 6f_2^n - f_3^n)$$
$$+ \frac{\lambda\rho}{2}(u_1^{n+1} - 2u_1^n + u_1^{n-1})$$

with $\rho \geq$ spectral radius of $A = \partial f/\partial u$.
These equations can be trivially solved for u_0^{n+1} and u_1^{n+1}.
Similar expressions can be derived for u_N^{n+1} and u_{N-1}^{n+1}.
To these conditions must be appended the appropriate
boundary conditions. This scheme is stable if $\lambda \frac{\partial f}{\partial u} \leq .72$.

Another standard scheme is the Lax-Wendroff method.
A two step version proposed by MacCormack [124] is

$$(3.5) \qquad \begin{aligned} u_j^{(1)} &= u_j^n - \lambda(f_{j+1}^n - f_j^n) \\ u_j^{n+1} &= \frac{1}{2}[u_j^n + u_j^{(1)} - \lambda(f_j^{(1)} - f_{j-1}^{(1)}] \ . \end{aligned}$$

Another variant uses backward differences for the predictor and forward differences for the corrector. A fourth order extension is given by Gottlieb and Turkel [69], [188].

$$u_j^{(1)} = u_j^n + \frac{\lambda}{6} (7f_j^n - 8f_{j+1}^n + f_{j+2}^n)$$

(3.6)

$$u_j^{n+1} = \frac{1}{2} [u_j^n + u_j^{(1)} - \frac{\lambda}{6} (7f_j^{(1)} - 8f_{j-1}^{(1)} + f_{j-2}^{(1)})] .$$

The boundary treatment for the predictor is

$$u_{N-1}^{(1)} = u_{N-1}^{(1)} - \frac{\lambda}{6} (4f_N^n - f_{N-1}^n - 4f_{N-2}^n + f_{N-3}^n)$$

(3.7a)

$$u_N^{(1)} = u_N^n - \frac{\lambda}{6} (15f_N^n - 28f_{N-1}^n + 17f_{N-2}^n - 4f_{N-3}^n)$$

and for the corrector

$$u_0^{n+1} = \frac{1}{2} [u_0^n + u_0^{(1)} - \frac{\lambda}{6} (4f_3^{(1)} - 17f_2^{(1)} + 28f_1^{(1)} - 15f_0^{(1)})]$$

(3.7b)

$$u_1^{n+1} = \frac{1}{2} [u_1^n + u_1^{(1)} - \frac{\lambda}{6} (-f_3^{(1)} + 4f_2^{(1)} + f_1^{(1)} - 4f_0^{(1)})] .$$

The boundary conditions (3.7) are identical to using cubic extrapolation to calculate the fluxes exterior to the domain and then using (3.6). There exists another variant with backward differences in the predictor and forward differences for the corrector. For fourth order accuracy, in space, one must alternate the two variants. This scheme is stable if $\lambda \frac{\partial f}{\partial u} \leq 2/3$.

16

The schemes that have been presented are second order
in time. It is possible to develop four step methods that
are fourth order in both space and time. One such method
is

$$u_{j+\frac{1}{2}}^{(1)} = \frac{1}{2}(u_{j+1}^{n} + u_{j}^{n}) - \frac{\lambda}{2}(f_{j+1}^{n} - f_{j}^{n})$$

$$u_{j}^{(2)} = \frac{-u_{j+1}^{n} + 10u_{j}^{n} - u_{j-1}^{n}}{8} - \frac{\lambda}{2}(f_{j+\frac{1}{2}}^{(1)} - f_{j-\frac{1}{2}}^{(1)})$$

(3.8)

$$u_{j+\frac{1}{2}}^{(3)} = \frac{-(u_{j+2}^{n} + u_{j-1}^{n}) + 9(u_{j+1}^{n} + u_{j}^{n})}{8}$$

$$+ \lambda [f_{j+1}^{(2)} - f_{j}^{(2)} + \frac{1}{8}(-f_{j+2}^{n} + 3f_{j+1}^{n} - 3f_{j}^{n} + f_{j-1}^{n})]$$

$$u_{j}^{n+1} = u_{j}^{n} + \frac{\lambda}{6} [f_{j+\frac{1}{2}}^{(3)} - f_{j-\frac{1}{2}}^{(3)} + f_{j+1}^{(2)} - f_{j-1}^{(2)}$$

$$+ \frac{1}{2}(-f_{j+\frac{3}{2}}^{(1)} + 7f_{1+\frac{1}{2}}^{(1)} - 7f_{j-\frac{1}{2}}^{(1)} + f_{j-\frac{3}{2}}^{(1)})$$

$$+ \frac{1}{16}(-f_{j+2}^{n} + 10f_{j+1}^{n} - 10f_{j-1}^{n} + f_{j-2}^{n})] \; .$$

This scheme is stable if $\lambda \frac{\partial f}{\partial u} \leq 1$.

Other variants are given in [1] and extensions to
multidimensions are described in [186]. Third order methods
in time are given by Burstein and Mirin [30] and Rusanov [164],
[165]. Steppeler developed third order methods in space
and time based on an explicit evaluation of the Taylor
Series combined with a third order finite element approxi-
mation [175], [176].

An alternative approach is to use Richardson extrapolation at each time step to increase the local accuracy in time. For the leapfrog method, which is symmetric about $t + \Delta t/2$, this is straightforward while for the multistep methods it is more complicated. This approach increases the domain of dependence and also decreases the time step allowed by stability. It has the advantage of simplicity and of generalizing to multidimensions ([187]).

The schemes considered until now have been explicit methods that are fourth order in space. We now present higher order implicit methods. Comparisons between explicit and implicit schemes are presented in Section 5. We consider the compact implicit scheme [149], [202].

$$(3.9) \quad (\frac{1-\alpha}{2}) \Delta u_{j-1}^n + \alpha \Delta u_j^n + (\frac{1-\alpha}{2}) \Delta u_{j+1}^n$$

$$= - \frac{\lambda}{2} [\xi (f_{j+1}^{n+1} - f_{j-1}^{n+1}) + (1-\xi)(f_{j+1}^n - f_{j-1}^n)]$$

with $\Delta u_j^n = u_j^{n+1} - u_j^n$.

If $\alpha = 1$ we have the standard implicit schemes. These are second order in time when $\xi = 1/2$ and unconditionally stable for $\xi \geq 1/2$. If $\alpha = 2/3$ the schemes are fourth order in space. To solve (3.8) requires an iteration procedure. An alternative is to expand f^{n+1}. Let $A = \frac{\partial f}{\partial u}$, then a substitute for (3.9) is

$$(3.10) \quad (\frac{1-\alpha}{2} - \lambda \xi A^n) \Delta u_{j-1}^n + \alpha \angle u_j^n + (\frac{1-\alpha}{2} + \lambda \xi A^n) \Delta u_{j+1}^n$$

$$= - \frac{\lambda}{2} (f_{j+1}^n - f_{j-1}^n)$$

This scheme has the same formal order of accuracy in space and time as (3.9). Experience has shown that if one is approaching a steady state or else if the time evolution is slow then (3.10) is accurate even with large time steps (see [14]). However, for some problems the iteration procedure may be necessary. For sufficiently large time steps approaching a steady state and $\xi = 1$ it can be shown that (3.10) is approximately Newton's method for solving nonlinear equations [105].

Using a trapezoidal rule with end corrections it is possible to construct a fourth order in space and time formula that requires only three mesh points in the x direction. Let A be the Jacobian of f with respect to u. Then (3.9) can be replaced by

(3.11)
$$\frac{1}{6}(-4\Delta u^n_{j-1} + \Delta u^n_j - 4\Delta u^n_{j+1})$$

$$= -\frac{\lambda}{4} [f^{n+1}_{j+1} - f^{n+1}_{j-1} + f^n_{j+1} - f^n_{j-1}]$$

$$-\frac{\lambda^2}{12} [A^{n+1}_{j+\frac{1}{2}}(f^{n+1}_{j+1} - f^{n+1}_j) - A^{n+1}_{j-\frac{1}{2}}(f^{n+1}_j - f^{n+1}_{j-1})$$

$$+ A^n_{j+\frac{1}{2}}(f^n_{j+1} - f^n_j) - A^n_{j-\frac{1}{2}}(f^n_j - f^n_{j-1})]$$

If one wishes to linearize this scheme with fourth order accuracy in time, one must first calculate a second order accurate predictor. Hence, the generalization of (3.10) requires a predictor and corrector step. An additional difficulty with (3.11) is that the matrix

inversion is stable only when $A\frac{\Delta t}{\Delta x} \leq 1$. Hence, even though the scheme is unconditionally stable one must restrict the time step in order to get a well conditioned matrix problem. Furthermore, it is difficult to generalize (3.11) to multi-dimensional problems since an alternating direction method will reduce the time accuracy of the algorithm. This scheme as well as some noncompact higher order implicit methods are described in [92]. Fourth order, in space, methods for equations with both hyperbolic and parabolic terms are considered in [41] and [161]. Some comparisons for the boundary layer equations are presented in [205]. It is also possible to construct higher order methods for these problems by combining high order Dufort-Frankel and leapfrog methods [68], [111].

Since these schemes are compact, special schemes are only required at the boundary. The author has found that the box scheme is especially accurate even though it reduces the order of accuracy. Hence, a boundary treatment for (3.10) would be

$$(3.12) \qquad (\frac{1 - \lambda A^n}{2}) \Delta u_0^n + (\frac{1 + \lambda A^n}{2}) \Delta u_1^n = -\lambda (f_1^n - f_0^n) \quad .$$

Further discussion of implicit methods is presented in section 5.

All the above methods are extensions of standard finite difference formulas. Hence, they have the advantage that it would not involve much programming effort to change an existing code. However, although they are of higher order

they are still only fourth order accurate in space. An alternative is to use a pseudo-spectral scheme. For sufficiently smooth solutions these methods converge faster than any power of the mesh size (see [70]).

For periodic boundary conditions the most appropriate expansion series is the Fourier series. To solve (3.1) with a leapfrog-like method in time one algorithm is

$$(3.13) \qquad u_j^{n+1} = u_j^{n-1} - 2(\Delta t f_x)_j^n$$

where

$$(3.14) \qquad (\Delta t f_x)_j^n = \sum_{k=-N}^{N} i \, \hat{f}_k \, G(k \, \Delta t) \, e^{\pi i j k/N}$$

where $G(k \, \Delta t) = k \, \Delta t + O\big((k \, \Delta t)^3\big)$. Given f this requires two fast Fourier transforms. A good choice for G is

$$(3.15) \quad G(k \Delta t) = (8 \sin (k\sigma \, \Delta t) - \sin(2k\sigma\Delta t)/6\sigma$$

with $c \geq 1.4 \cdot$ (spectral radius of $\frac{\partial f}{\partial u}$). This scheme is unconditionally stable.

For problems requiring some dissipation one can replace the leapfrog method by a Runge-Kutta method. If one wishes to use a splitting method for multi-dimensional cases then in practice one is limited to second order in time methods. Unfortunately, the second order Runge-Kutta method is unconditionally unstable for the Fourier method. Hence, we consider a modified method similar to (3.13 - 3.14). The modified Euler scheme is given by

$$\bar{u} = u^n - \Delta t f_x^{(n)}$$

(3.16)

$$u^{n+1} = \tfrac{1}{2}(\bar{u} + u^n - \Delta t \bar{f}_x)$$

with

$$(\Delta t f_x)_j^n = \sum_{k=-N}^{N} \hat{f}_k G_1(k\Delta t) e^{\pi i j k/N}$$

(3.17)

$$(\Delta t \bar{f}_x)_j = \sum_{k=-N}^{N} \hat{\bar{f}}_k G_2(k\Delta t) e^{\pi i j k/N}$$

with $G_1(k\Delta t) \simeq k\Delta t$, $G_2(k\Delta t) \simeq k\Delta t$ for small $k\Delta t$. Choosing $G_1(k\Delta t) = G_2(k\Delta t) = k\Delta t$ the stability condition is $AN^2\Delta t \leq 8$ with $A = \partial f/\partial u$ [70]. Since this is very restrictive we substitute this with

$$G_1(k\Delta t) = (-e^{2z} + 8e^z - 7)/6\sigma$$

(3.18)

$$G_2(k\Delta t) = (7 - 8e^{-z} + e^{-2z})/6\sigma$$

where $z = ik\sigma\Delta t$ and $\sigma > 1.4\sigma(A)$. As before the scheme is unconditionally stable with these parameters.

If we consider the simplified equation

(3.19)
$$u_t + a(x)u_x = 0 \quad ,$$

the standard stability proof for the Fourier method is valid only if $a(x)$ doesn't change sign (see [57]). The correct analysis of (3.19) when $a(x_0) = 0$ depends on

distinguishing between mesh-stability and time-stability. The Fourier method for (3.19) is stable for $0 < t < T$ as the number of modes increases. Hence, by the Lax-Equivalence theorem the approximation converges to the analytic solution. However, for a fixed number of modes the error may increase exponentially as time increases (when $a(x_0) = 0$). Hence, the Fourier method in its original form may not be useful when $a(x)$ changes sign [74]. To overcome this difficulty we replace $G_1(k\Delta t)$ by $G_1(k\Delta t)\rho(k)$ and similarly for G_2 in (3.21). We choose the cutoff $\rho(k)$ so that it is one for small k and goes to zero for the highest modes. Majda et al. [131] and Kreiss and Oliger [113] have shown that this modification to the Fourier method is stable. In fact, using these cutoffs with a Chebyshev method (to be described) one can solve the Riemann problem of fluid dynamics and resolve the shock and contact discontinuity within one mesh width (D. Gottlieb, private communication).

For bounded domains, an expansion in Chebyshev polynomials is more appropriate. Since the eigenvalues of the operator have a negative real part, we consider a two step scheme rather than a leapfrog method. Hence, we have

$$u^{n+\frac{1}{2}} = u^n - \frac{1}{2}(\Delta t f_x)_j^n$$

(3.20)

$$u^{n+1} = u_j^n - (\Delta t f_x)_j^{n+\frac{1}{2}} \quad .$$

Let $x_j = \cos \pi j/N$, one can then expand

(3.21) $\qquad f_j = \sum\limits_{k=0}^{N} a_k T_k(x_j) \qquad j=0,\ldots,N$

where [70]

(3.22) $\quad a_k = \dfrac{1}{c_k} \sum\limits_{j=0}^{N} \dfrac{1}{c_j} f_j \cos \dfrac{\pi j k}{N} . \qquad c_0 = c_N = 2$

$$c_\ell = 1 \qquad \ell = 1,\ldots N-1 .$$

Equation (3.22) is solved using the FFT. We then have

(3.23) $\qquad (\Delta t f_x)_j = \sum\limits_{k=0}^{N} b_k T_k(x_j)$

with

(3.24) $\qquad b_k = \dfrac{2}{c_k} \sum\limits_{\substack{\ell=k+1 \\ \ell+k \text{ odd}}}^{N} a_\ell G(\ell \Delta t)$

and $G(\ell \Delta t) = \ell \Delta t + O((\Delta t)^3)$. In this case a reasonable choice is (see [73]), $z = e^{-\alpha \ell \Delta t}$, and

(3.25) $\qquad G(\ell \Delta t) = (11 - 18z + 9z^2 - 2z^3)/6\alpha$,

with α approximately equal to the spectral radius of $\dfrac{\partial f}{\partial u}$.

The extension to multidimensional problems in rectangular domains is straightforward. The leapfrog

methods generalize in the obvious manner. For the Runge-
Kutta methods splitting techniques are avai'able for multi-
dimensions while for the implicit methods alternating
direction techniques are the most appropriate.

We have stressed methods that are second order in time.
There are several reasons why higher order methods in time
are less appropriate. First, the extension to several
dimensions is complicated as splitting and alternating
direction methods are second order in time unless complicated
algorithms are constructed. The necessity for a full multi-
dimensional scheme usually results in a method which requires
many operations per time step. For problems where the time
dependent equations are being used as a relaxation scheme
to a steady state there is no obvious advantage to a higher
order method in time. Even for time dependent problems the
important physical phenomena frequently move at speeds
considerably slower than the fastest signal speed allowed by
the equations. Hence, these motions are usually easy to resolve
and only the variation in space is rapid requiring higher order
techniques. The other major argument for second order schemes
in time is that one can always increase the time accuracy by
taking smaller time steps. The computer work involved varies
linearly with the time step and so this may be more efficient
than a costly high order method. Furthermore, choosing
smaller time steps does not increase the storage. However,

for explicit methods doubling the mesh points increases the work by 2^{d+1} in d dimensions and the storage requirements increase by 2^d. Hence, the use of high order methods in space to limit the number of mesh points can be very advantageous. Furthermore, one can increase the accuracy in time by locally using Richardson extrapolation [187]. In general it is not known when higher order methods in space or time are more efficient than lower order methods. One case where the author has found higher order methods, in time, useful is instability studies. Time inaccuracies can introduce errors which cause artificial instabilities. As more experience is gained better guidelines should be available.

4. HIGH ORDER METHODS -- RESULTS

In [150] and [186] a range of problems are considered to demonstrate the advantage of high order methods. Here we consider two of these cases which illustrate many of the phenomena of more complex situations.

The first problem is flow in a nozzle. The equations are one dimensional but many two dimensional effects are included by specifying $A(x)$ the area of the nozzle at position x. The equations of motion are

$$(A\rho)_t + (\rho A u)_x = 0$$

$$(4.1) \qquad (A\rho u)_t + [A(\rho u^2 + p)]_x = A_x p$$

$$(AE)_t + [Au(E + p)]_x = 0$$

with $\qquad p = (\gamma-1)(E - \frac{1}{2}\rho u^2)$ and $\gamma = 1.4$.

The solution to the steady state equations is known for both smooth and shocked profiles [43]. Hence, we march the equations toward a steady state and we can then compute the errors between the computational solution and the known analytical solution.

We linearize (4.1) about a constant state (ρ_0, u_0, E_0) and drop lower order terms. One then finds that the characteristic values λ and eigenfunctions v are given by

$$(4.2a) \qquad \lambda_1 = u_0 \qquad v_1 = \left(\frac{u_0^2}{2} - \frac{c_0^2}{\gamma-1}\right)\rho - u_0 \rho u + E$$

$$(4.2b) \quad \lambda_2 = u_0 + c_0 \quad v_2 = u_0 \left[\frac{u_0}{2} - \frac{c_0}{\gamma-1} \right] \rho - \left[u_0 - \frac{c_0}{\gamma-1} \right] \rho u + E$$

$$(4.2c) \quad \lambda_3 = u_0 - c_0 \quad v_3 = u_0 \left[\frac{u_0}{2} + \frac{c_0}{\gamma-1} \right] \rho - \left[u_0 + \frac{c_0}{\gamma-1} \right] u + E$$

$$\text{with} \quad c_0^2 = \gamma(\gamma-1) \left[\frac{E_0}{\rho_0} - \tfrac{1}{2} u_0^2 \right] .$$

At the inlet the flow is subsonic and we specify ρ and E equal to the known steady solution. This is supplemented by a difference equation for the characteristic variable v_3 which is coming into the boundary. Given ρ, E and v_3 one can trivially solve for ρu. With the explicit method it was not found very important to solve for v_3 rather than ρu. However, with the implicit method and large time steps the use of (4.2c) was crucial. As pointed out before the use of noncharacteristic boundary treatment frequently manifested itself as a negative pressure at the sonic point. The only way of identifying it as a boundary difficulty was to observe that the difficulty disappeared when one solved for v_3 rather than ρu by the boundary difference scheme.

For smooth solutions no boundary conditions are specified at the exit. Hence, the special boundary treatment is used for all three variables. For a shocked profile the pressure is specified at the exit. Again, with the explicit schemes it was not found necessary to use characteristic variables. Instead we calculated ρ and ρu by finite

difference approximations to (4.1). E was then calculated knowing ρ, ρu and p. With the implicit methods one must first linearize the given boundary condition so that iteration is not required. This is similar to the manner in which (3.10) was derived. Then $p^{n+1} = p_{exit}$ is replaced by

$$(4.3) \qquad \frac{u_0^2}{2} \Delta \rho - u_0 \Delta m + \Delta E = \frac{p_{exit} - p^n}{\gamma - 1} ; \quad \Delta \rho = \rho^{n+1} - \rho^n$$

By inspection one verifies that in the steady state $p = p_{exit}$. (4.3) is supplemented by two equations based on the box scheme (3.13) for the characteristic variables v_1 and v_2. For the higher order methods $A'(x)$ must be also calculated to the same order. Hence, for all problems both $A(x)$ and $A'(x)$ were given analytically. For the examples considered $A(x)$ was chosen as a hyperbolic cosine.

For smooth profiles, it was found that the major difficulty occurred at the throat where the flow is sonic. When an artificial viscosity is not used many of the methods gave rise to an expansion shock. For most of the problems the solution is considered at steady state if p changed by less than $\varepsilon = 10^{-5}$ in one time step. For some of the runs with high resolution a smaller ε was chosen.

In Table 4.1 we present the results for a smooth profile. The explicit MacCormack methods did not require an artificial viscosity while the implicit method did. When needed the artificial viscosity is added explicitly

at time t even for the implicit methods. We see from the table that the fourth order explicit method is more than twice as efficient as the corresponding second order method. It also requires less than half the storage to achieve three digit accuracy in the steady state. For four digit accuracy the efficiency factor increases to 16.

For implicit methods the accuracy and stability depends very much on the boundary treatment. In [72] it is proved that one does not need to include the given boundary conditions in the implicit method. Instead, after each time step one can correct for the boundary conditions. For equations (4.1) it was found that this worked only for time steps less than three times the Courant limit, otherwise nonlinear instabilities arose. For larger time steps it was necessary to incorporate the given boundary conditions in the matrix to be inverted. With time steps of about 15 times the Courant limit steady state was reached very rapidly. In this case the higher order method was only about thirty percent more efficient. We speculate that in going to a steady state the use of the lower order box scheme at the boundary deteriorates the accuracy. For a wave equation the fourth order implicit method was 3-4 times more efficient than the second order implicit method (see also [63]). For both these cases there is no improvement in either accuracy or in the rate of convergence when a second order in time method is used rather than a first order in time method.

This problem, (4.1), was also solved with the Chebyshev collocation method (3.16) - (3.17) with $G_1(k\Delta t) = G_2(k\Delta t) = k\Delta t$. This is stable with time steps about .1 times the Courant limit. The error at the steady state is concentrated at the sonic point. A simple automatic postprocessor at the conclusion of the code removes this error. The result is an error level 20 times smaller than with the fourth order method, as seen in table 4.1b.

We next consider (4.1) with a shocked profile. The solution to most of the methods is not a monotone function of the mesh. Hence, instead of comparing schemes for a given error tolerance we find the asymptotic rate of accuracy. This is found by a least square estimate based on about 50 runs with different meshes. If one includes the shock area in the error analysis then all the methods converge like $(\Delta x)^{1/2}$ in the L_2 norm and as Δx in the L_1 norm. When we exclude a fixed physical distance about the shock the scheme behaves statistically according to the formal accuracy of the method. With the implicit methods instabilities appeared when time steps larger than five times the Courant limit were used.

As the second example we consider a two dimensional problem in dynamic acoustics. The equations are given by (7.1) where the radiation boundary treatment for this problem is discussed. The numerical algorithm used to solve this problem is the second and fourth order two step schemes (3.5) and (3.6) together with a splitting of

the two dimensional problem into a series of one dimensional problems. This code was run on the CDC-STAR at NASA Langley. More details of the algorithm are found in [10].

Two cases are considered here. In the first case the mean flow is zero and the forcing function is a delta function in space and harmonic in time; for this case the analytic solution is known. The fourth order method is more accurate than a second order method with twice as many mesh points. The efficiency gain is about 400 percent at large error tolerances and increases at lower error tolerances.

In the second case we use a realistic mean flow modeled after experiments and a harmonic source located two jet diameters downstream of the jet exit. Varying the mesh and boundaries demonstrates that the fourth order method with 12000 points yields essentially the analytic result. We then measure the peak acoustic pressure as a function of the angle. The fourth order method with 8800 points gives much better accuracy than the second order method with 16000 mesh points. The fourth order method is now being routinely used to solve problems with a variety of sources including pulses, convecting sources and quadrapoles. Second order methods would not be feasible for these problems because of storage and cost limitations.

In general we have found the fourth order methods to be three to five times faster while still giving accuracy

comparable with the second order method. The savings in storage is a factor of two per space dimensions. For error levels less than one percent the efficiency of the higher order methods increase. Similar conclusions were reached in [150]. Coding changes for the finite difference methods are minimal given a second order program with either an explicit or implicit scheme.

On some simple problems spectral methods behave even more efficiently than the fourth order schemes. However, they require coding a new program with careful attention being paid to the implementation. At present there has been little experience with these methods for large scale hyperbolic problems especially in complex geometries or with nonsmooth profiles.

TABLE 4.1a

Smooth Solution to System (4.1) with errors $\approx 10^{-3}$.

Method	Order	N	CFL	Viscosity Factor	L^2 Error Steady State
MacCormack (3.5)	2	41	0.90	0.0	1.93×10^{-3}
Two Step (3.6)	4	21	0.60	0.0	8.15×10^{-3}
Fully Implicit (3.9, $\xi = 1$, $\alpha = 1$)	2	37	1.00	0.40	1.05×10^{-3}
Fully Implicit	2	37	10.0	0.40	9.97×10^{-4}
Crank-Nicolson (3.9, $\xi = \frac{1}{2}$, $\alpha = 1$)	2	35	1.0	0.40	1.11×10^{-3}
Crank-Nicolson	2	35	10.0	0.40	1.11×10^{-3}
Fully Implicit (3.9, $\xi = 1$, $\alpha = 2/3$)	4	23	1.0	0.40	1.22×10^{-3}
Fully Implicit	4	29	10.0	0.30	1.26×10^{-3}

TABLE 4.1b

Smooth Solution to System (4.1) with errors $\approx 10^{-4}$

Method	Order	N	CFL	Viscosity Factor	L^2 Error Steady State
MacCormack (3.5)	2	171	0.90	0.0	1.01×10^{-4}
Two Step (3.6)	4	39	0.60	0.0	1.09×10^{-4}
Fully Implicit	2	111	10.0	0.4	1.07×10^{-4}
Fully Implicit	4	51	10.0	0.4	1.20×10^{-4}
Chebyshev	∞	33	0.10	0.0	1.16×10^{-5}

5. IMPLICIT METHODS

The use of implicit methods to solve hyperbolic equations has been increasing in recent years (see e.g. [20], [87]). The rationale behind this is that implicit methods are frequently unconditionally stable. Choosing large time steps can then more than compensate for the extra work per time step.

Even though there are no stability restrictions on the time step nevertheless the time step is still restricted by accuracy requirements. We consider the simplest equation

$$(5.1) \qquad u_t - u_x = 0 \qquad \qquad 0 \le x \le 2\pi$$

which we approximate by the Crank-Nicolson scheme

$$(5.2) \qquad v_j^{n+1} - v_j^n = \frac{\Delta t}{4\Delta x}\left(v_{j+1}^{n+1} - v_{j-1}^{n+1} + v_{j+1}^n - v_{j-1}^n\right) \quad .$$

Assume $v_j^n = \sin(jk\Delta x)$. Since the Crank-Nicolson formula (5.2) is nondissipative the only errors are phase errors, so that $v_j^{n+1} = \sin(jk\Delta x + \alpha)$. For the differential equations $\alpha_A = k\Delta t$. The numerical phase for (5.2) is given by

$$(5.3) \qquad \alpha_N = \sin^{-1}\left[\frac{\frac{\Delta t}{\Delta x}\sin(k\Delta x)}{1 + (\Delta t)^2 \sin^2(k\Delta x)/4(\Delta x)^2}\right]$$

In Table 5.1 we present the phase errors α_N/α_A for $k\Delta x = \frac{\pi}{20}, \frac{\pi}{10}$, and $\frac{\pi}{4}$. We note that the phase errors increase dramatically as we choose $\Delta t/\Delta x$ much larger than one.

This is because the Courant condition $\Delta t/\Delta x \leq 1$ has physical significance beyond a formal stability condition. With larger time steps we are not following the wave correctly.

The justification for implicit methods arises only by considering equations more complicated than a wave equation. A simple model is provided by

$$(5.4) \qquad u_t + u_x = A(1-p)\cos(x-pt) \quad .$$

A solution to (5.4) is

$$(5.5) \qquad u(x,t) = A\cos(x-pt) + B\cos(x-t) \quad .$$

If $p \ll 1$ and $B \ll 1$ then accuracy requirements only demand

$$(5.6) \qquad \frac{p\Delta t}{\Delta x} \approx 1$$

which is much weaker than the stability criterion for explicit schemes $\Delta t/\Delta x \leq 1$.

Another example is provided by systems of equations with widely separated eigenvalues. For simplicity we consider the uncoupled system

$$(5.7) \qquad \begin{aligned} u_t + au_x &= 0 \\ v_t + bv_x &= 0 \end{aligned}$$

with $u = A \sin(x-at)$, $v = B \sin(x-bt)$ and $A << B$, $a >> b$. As before explicit schemes require $a\Delta t/\Delta x \leq 1$. However, since $A << B$ accurate solutions only require $b\Delta t/\Delta x \leq 1$.

Both of these examples demonstrate the phenomena of different time scales. For these problems the time step of an explicit method would be limited by the speed of the fastest possible mode. For implicit methods the time step is chosen to resolve the slower modes which carry most of the energy. Both these simple illustrations have many practical applications. For example a slowly oscillating wing or rotor will induce wave motion with much slower speeds than that of free motion. In meteorology or plasma physics the usual speeds of propagation are much smaller than the fastest signal speed. These will be discussed further in chapter 8. The possible extensions of explicit methods for these problems will also be discussed.

A similar justification for implicit method occurs when the time step for an explicit method would vary dramatically between different regions. An extreme example occurs in laser fusion where the diffusitivity can change by many orders of magnitude across the domain. In magnetic fusion the existence of near vacuum regions create areas of very high speeds compared with the center of the plasma. In other problems similar effects occur due to different mesh sizes in different regions. For problems

in meterology the time step for an explicit scheme is
determined by the small mesh volumes near the pole due
to converging latitude lines. In Navier-Stokes problems
with boundary layers extremely small mesh sizes occur
near the body in order to resolve the boundary layer.
In all these problems the time step of an explicit scheme
is governed by a small region which may not be the area
requiring the greatest resolution in time.

A second type of problem suitable for implicit
method are those cases for whicn only the steady-state
solution is desired. The time dependent equations are
used merely as a device for obtaining iterative solutions
to the steady state equations. In this case there is no
need for the numerical method to accurately follow the
transient. Indeed, one way to accelerate the iteration
process is to make the scheme inconsistent with the transi-
ent solution. We only need guarantee that the numerical
steady state achieved is independent of the iteration
procedure. Consider the general equation

$$(5.8) \qquad u_t = L\, u \ .$$

A simple way to ensure the correct steady state is to
solve for $u^n = u^{n+1} - u^n$ at each time step. The algorithm
then has the form

$$(5.9) \qquad Q^n \Lambda u^n = L\, u^n \ .$$

The steady state is defined by $\Delta u^n = 0$ and so we have $L u^n = 0$. Since the time accuracy is not important we do not wish to iterate at each time step. In the interest of efficiency Q^n should not depend on the unknown variable u^{n+1}. In many cases this can be achieved without loss of accuracy by a linearization procedure such as introduced in [14], [23], and [122]. Higher order (in space) of these schemes were defined by (3.10) and (3.11).

If we use the backward Euler formula for (5.8) we have

$$(5.10) \qquad \Delta u^{n+1} = \Delta t \, L \, u^{n+1} \quad .$$

Linearizing, this equation we have that

$$(5.11) \qquad \frac{1}{\Delta t}(I - \Delta t J^n) \Delta u^n = L u^n \quad ,$$

J is the Jacobian of L with respect to u. As Δt increases this scheme approaches the Newton-Raphson iteration

$$(5.12) \qquad -J^n \Delta u^n = L u^n \quad .$$

This is a property only of the backward Euler formula and is not true for other selections of parameters in (3.9).

In general it is not necessary that Q^n be a function of the exact Jacobian of L since we are only interested in the steady state. This freedom can be utilized in several different ways. One possibility is to change Q^n in such a

way as to simplify the solution of the linear set of equations (5.11). In most cases Q^n involves block tridiagonal matrices. If these matrices can be inverted by Gaussian eliminations without pivoting then the inversions can be accomplished by the Thomas algorithm in $O(m^3 N)$ operations where m is the block size and N is the number of mesh points (see [103]). Hence, for general block tridiagonal matrices and m larger than 3 or 4, most of the work is in inverting the full blocks. When the fluid dynamic equations are written in velocity form these blocks can be decomposed as a direct sum of smaller blocks and so the process can be speeded up [23]. When the momentum form of the fluid equations are used full blocks occur. However, by using the freedom in Q^n one can simplify these blocks at the expense of making the numerical scheme inconsistent with the time dependent equations [174]. In fact even when solving the steady equations directly using Newton's method [17] J need not be the Jacobian of L. This generalization leads to the use of quasi-Newton methods (for a survey see [46]).

Alternatively one can choose Q^n in such a manner as to speed up the convergence. McDonald and Briley [128] consider methods with different Δt at different mesh points. This can be viewed as a matrix conditioning of the linear equations. This is especially promising for parabolic equations in two space dimensions where the theory of parameter selection for A.D.I. methods is well developed.

Implicit methods have the disadvantage that they require
the solution of a large number of coupled equations at each
time step. Therefore, the reduction in the number of time
steps compared with explicit methods must be weighed by
the increase in the number of arithmetic operations
required for each step. To simplify the inversion process
in several dimensions alternating direction methods are
generally used. In this case one needs to invert a block
tridiagonal matrix for each direction. As mentioned pre-
viously this is very expensive when the block sizes get
large. For example, in the magnetohydrodynamic case the
blocks are 8×8 matrixes. In combustion problems there
is at least one partial differential equation per species.
Hence, for complicated chemical processes very large blocks
can be generated. These situations render standard implicit
methods impractical as the work increases with the cube of
the block size. In some cases one can use knowledge of the
block structure to reduce this work [23]. However, when
shocks appear and the conservative forms of the equations
must be used, full matrices are unavoidable.

Furthermore, the Thomas algorithm is an inherently
serial algorithm and so inefficient for many vector pro-
cessors. In three space dimensions one can perform many
tridiagonal inversion simultaneously to partially vectorize
the procedure. However, this demands large storage require-
ments. The use of a cyclic reduction method is more efficient
for a vector machine but is still very far from optimal for
these pipeline machines. Hence, many of the advantages of
A.D.I. are negated on machines as the STAR-100.

An additional difficulty with alternating direction methods is that they introduce $O((\Delta t)^2)$ perturbations into the matrix Q^n of (5.10). In this case the scheme no longer approximates the Newton method for large Δt and consequently there is a reduction in the rate of convergence to a steady state. Marching to a steady state using large time steps one wants to use the delta form (5.10) so as to ensure that the steady state is independent of Δt. In two space dimensions the alternating direction methods which solve for u^{n+1} and Δu^n are equivalent, but in three dimensions they are not. The three dimensional algorithm is unconditionally stable in the linear case if one solves for u^{n+1} but the steady state depends on Δt. On the other hand if one solves for Δu^n to produce a steady solution independent of Δt, the algorithm is unconditionally unstable for scalar problems. As the entropy equation is essentially a scalar equation this method has difficulties for many systems. Only the addition of viscous terms can stabilize the procedure.

Several alternatives have recently been advanced as substitutes to alternating direction methods. Steger and Warming [176] have suggested splitting the flux vector into two parts corresponding to the positive and negative eigenvalues. Each part is then solved using the one sided differences appropriate for the corresponding eigenvalue. Jameson and Turkel [105] have proposed a method based on a LU decomposition. In this method the lower and upper factors

are chosen for computational ease. The resulting scheme
can be chosen to be second order accurate in space. It is
demonstrated that the crucial ingredient is that each of
the L and U factors be diagonally dominant. The dia-
gonal dominance of the final scheme is irrelevant. This
scheme is stable for one, two and three dimensions. A
common feature of both these schemes is that only two factors
appear independent of the number of space dimensions. For
one dimension this is a disadvantage since it introduces
perturbations of order $(\Delta t)^2$ and so slows down the con-
vergence rate. However, for three space dimensions the
A.D.I. schemes have changes of order $(\Delta t)^3$ from the back-
ward Euler method and so converge to a steady state even
slower than these methods for large Δt. The requirement
of three sweeps through the mesh for a three dimensional
A.D.I. method is also a disadvantage when not all the infor-
mation can be stored in core.

Since the backward Euler method is a good approximation
to Newton's method it may be advantageous to use this method
even for multidimensional problems. The resulting matrix
is no longer tridiagonal and hence it is necessary to find
some efficient method to invert the matrix. Band Gaussian
elimination solvers require excessive core especially since
pivoting must be used. For parabolic problems that arise
in laser fusion Kershaw [108] has used a conjugate gradient
method for inverting the matrix. Similarly Orszag [151] has
advocated the use of conjugate gradient to invert the full

matrices that arise from spectral methods. Brackbill [20] has used a SOR method in conjunction with his implicit method for the nonlinear MHD equations.

Until now we have concentrated on the rate of convergence to a steady state. An equally important topic is the accuracy in the steady state. We wish to stop the iteration process in such a manner so that the error in the iteration process is below the truncation error of the steady state scheme. In using (5.10) we have assumed that in the steady state $\Delta u^n = 0$. In many codes, one iterates until Δu^n is below some given error tolerance, ε. We then have that $Lu^n = Q^n \varepsilon$ so that the error in Lu is effected by the operator, Q. Therefore, it is better to use the residual Lu^n as a measure of the steady state rather than Δu^n. Since, L is in general not an elliptic operator it is difficult to measure the deviation of u^n from the steady state, even given that $Lu^n = \varepsilon$. It is also important to choose initial conditions that are a reasonable guess to the steady state solution.

In summary, implicit methods have been successful when one is careful to match the physics with the method. These methods are less appropriate for wave-like equations where one wishes to follow all the possible modes of propagation.

Attention to boundary treatment is even more important for implicit methods than for explicit methods. This is mainly because one wishes to use the implicit methods with

large time steps.   In many calculations one could use any
one sided difference to some equation to supplement the given
boundary conditions as long as small time steps were used.
However, for large time steps it was essential, for
nonlinear stability, that the characteristics variables,
e.g. (4.2), be used.   Sköllermo [172] gives examples where
the use of an explicit boundary method can force a stabi-
lity condition for the entire method.

For complicated flows the choice of a poor boundary
treatment may be difficult to judge.   For example, in-
correct treatment of outflow boundaries will severly slow
the rate of convergence to a steady state.   Rudy and
Strikwerda [162],[163] and Thomas [182] demonstrate
that overspecification can be particularly inefficient.
However, if one judges the results by comparison with
experiment one would never sense the incorrect boundary
treatment.   Gustaffson and Kreiss [85] show that for this
case the steady state may depend on the initial conditions.
In any case it would not be obvious that the slow rate of
convergence is due to the boundary treatment.   Thomas [182]
describes boundary treatments for other types of boundaries
that occur in Navier-Stokes flow (see also [4]).

Due to the unconditional stability of implicit
schemes it is not clear how to choose the time step.   One
simple procedure is

$$\frac{(\Delta t)^{n+1}}{(\Delta t)^{n}} = \frac{\dfrac{\| \Delta u^{n} \|}{\| u^{n} \|}}{\dfrac{\| \Delta u^{n-1} \|}{\| u^{n-1} \|}} \quad ; \quad \Delta u^{n} = u^{n} - u^{n-1}$$

for some choice of norm. This has been used successfully in plasma diffusion problems (D. Nelson, private communication). A more sophisticated choice is to compare two iterates for time t as is done in o.d.e. solvers. When going to a steady state Δt can be viewed as an interation parameter, as discussed previously.

TABLE 5.1

Phase errors for the Crank-Nicolson method as a function of the time step.

$\Delta t/\Delta x$ \ $k\Delta x$	$\dfrac{\pi}{20}$	$\dfrac{\pi}{10}$	$\dfrac{\pi}{4}$
.1	.995	.983	.900
1.	.993	.976	.865
2.	.987	.954	.783
3.	.978	.921	.641
5.	.949	.837	.262
10.	.845	.365	.070
50.	.063	.016	.003

46

6. MOVING BOUNDARIES AND ADAPTIVE GRIDS

In the usual fluid dynamical situation boundaries are considered as fixed in time. In many situations, especially for analytical results, the fluid is considered as being confined to a rectangular or circular region. However, in many circumstances one must include the motion of the boundary as an important element of the problem. The movement of the boundary arises from many different factors which require different methods.

The simplest situation arises when the boundary moves in response to an external force. This may represent a moving piston, a diaphragm or similar devices. The next situation occurs when the boundary represents a free surface. In this case the boundary represents the separation between the domain of interest and some other region, for instance a vacuum or the general atmosphere. The outer region presents no resistance and the boundary moves in accordance with the forces exerted on it by the interior material. This occurs when metals are subject to a high temperature or pressure and begin to flow. Other examples occur when liquids are not in a container, as in water over a dam or water waves or raindrops. The most difficult problem arises when the moving boundary represents an interface between different materials. In many cases these are materials subject to the same differential equations. The two materials differ only in their density or other material properties. The simplest such case is a

contact discontinuity in fluid mechanics where both sides
are the same material but jumps occur across the moving
surface. In other situations the media on the two sides of
the moving boundary are represented by different
differential equations. Such conditions arise when an
explosive gas impinges on a solid material. Another
example is the interface between a plasma and a vacuum.
In the latter case hyperbolic time dependent equations
describe the motion of the plasma while the magnetic field
in the vacuum is given by a time independent Poisson equa-
tion. In these cases the boundary moves as a result of
imbalance of forces from the two sides.

The standard techniques to solve such problems are
Lagrangian methods (see e.g. [19], [20], [96], [197]).
With such schemes the boundaries are coordinate lines;
this simplifies the algorithm. However, Lagrangian methods
have several drawbacks. They are usually low order methods
especially in regions where the mesh is nonuniform. When the
motions are large the grid undergoes severe distortions which
require rezoning the mesh. This rezoning is quite difficult
in three dimensions. The rezoning usually results in a loss
of mass and so should not be done too frequently. In
addition, the rezoning formulas are usually not automated
and require intervention by the user. The main drawback of
Lagrangian methods is that they are very complicated and
not user oriented. One method of simplifying the rezoning

difficulty is to use triangular meshes. At each time
step reconnections are made when appropriate. This
method developed by Fritts and Boris [60] has been
applied to problems involving high shear. As a dual
to this method is a scheme devised by Peskin [153] which
is a grid free Lagrangian method. This latter scheme
has been applied to the incompressible Navier-Stokes
equations. A difficulty with both these methods are
that they are difficult to couple with implicit time
algorithms and also the extension to three dimensions
is computationally complicated due to the many possible
configurations.

At the opposite end one can use a strictly Eulerian
approach and integrate across the boundary. To prevent
smearing of the interface one adds some artificial compres-
sion after each time step [91]. The location of each
material is identified by a color function which is 1 in
one region and 0 in the other region. This color function
satisfies a convection equation which itself must be
solved numerically without smearing. This method has not
been used extensively on large scale problems and its
applicability for multidimensional problems is question-
able. It would be difficult to implement at interfaces
where jump conditions need to be satisfied. These jump
conditions depend on the physics of the situation and
cannot be derived just from properties of the differential
equation.

One alternative is to map each region onto a rectangle.
If this mapping is done at each time step then one must
interpolate between the grids at successive time steps.
Instead, one can initially find a grid by any package,
e.g. [184]. This gives new coordinates $\xi = \xi(x,y)$,
$\eta = \eta(x,y)$. We now allow the new coordinates to vary
with time, so that $\xi = \xi(x,y,t)$ and η $\eta(x,y,t)$. Given
the differential equation

(6.1)
$$w_t + f_x + g_y = 0 \quad .$$

This gets transformed into (see [154], [193])

(6.2)
$$q_\tau + F_\xi + G_\eta = 0$$

with

$$q = I\,W$$

(6.3a)
$$F = I(\xi_t w + \xi_x f + \xi_y g)$$

$$G = I(\eta_t w + \eta_x f + \eta_y g)$$

and

$$\xi_t = -x_t \xi_x - y_t \xi_y$$

(6.3b)
$$\quad .$$

$$\eta_t = -x_t \eta_x - y_t \eta_y$$

$$I = x_\xi y_\eta - x_\eta y_\xi$$

(6.3c)

$$J = \xi_x \eta_y - \xi_y \eta_x = 1/I$$

In order to determine all these quantities we require
the grid point speeds (x_t, y_t). One method is to construct
a new grid at the advanced time. This can be done either as
a function of gradients in the problem [50] or by solving an
elliptic equation. Given (x, y) at t and $t + \Delta t$ (x_t, y_t)
can be calculated. An iterative procedure would be more
costly but also more stable. Hindeman et al.[98] prefer
differentiating the elliptic equation for (x, y) with
respect to t. This yields a linear elliptic equation for
(x_t, y_t). Given (x_t, y_t) on the boundary this equation is
solved at each time level. It is also important to solve
for the gird in a manner which is consistent with the
numerical solution of the differential equations [183].

These procedures require the solution of an elliptic
equation at each time step. It is not clear that the over-
head required by the mapping justifies its use. In addition,
we would like to use information about the gradients of
the solution to construct the grid at the new time level.
At this time it is not known what are reasonable ways of
accomplishing this especially for multidimensions. For
example, it is well known that we can not allow the image
of a square in (ξ, η) to become too distorted or else in-
accuracies and instabilities may occur. Also, if the grid
changes too rapidly in time one would expect difficulties.
An experimental program for a parabolic problem is presented
in [50] while one for hyperbolic systems is presented in [98].
Oliger [146] and Yanenko [207] also investigate adaptive
grids from a more theoretical viewpoint.

The differential equations are solved on the fixed Eulerian mesh. At mesh points far from the boundary the standard Eulerian scheme is used. At grid points near the boundary one sided differences are used. Alternatively the fluxes can be extrapolated to the outside of each domain and then the standard scheme is used. The boundary itself is identified by a series of Lagrangian tracer particles which are allowed to move through the fixed Eulerian mesh. This boundary is used only to keep the regions separate and prevent diffusion of one material into another region. The only communication between different regions is via jump conditions across an interface. No differential equations are integrated across a boundary.

As an example of the difficulties encountered with moving surfaces we discuss the impact of materials at high speeds. Metals impacted by gases or by other metals are subjected to high pressures which will deform the metal. The metals display elastic-plastic deformations. The differential system for these situations is given by the Prandtl-Reuss equations [97]. As usual, p, u, v, e represent the density, velocities and internal energy respectively. The total stress are given by $\tau_{ij} = S_{ij} - p\delta_{ij}$ S_{ij} are stress deviatories and p is the thermodynamic pressure. When the deviatories are less than the stress limit, i.e. $\int S_{ij}^2 \leq \kappa^2$ the flow is elastic. For $\int S_{i,j}^2 = \kappa^2$ the flow is plastic. κ^2 is constant in the simplest of models but is a function of various dependent

variables when work hardening is included. We shall consider these equations with cylindrical symmetry.

Let $\dfrac{d}{dt} = \dfrac{\partial}{\partial t} + u \dfrac{\partial}{\partial z} + v \dfrac{\partial}{\partial r}$. Then the equations in the generalized elastic regime are given by

$$\frac{d\rho}{dt} + \rho\left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) = - \frac{\rho v}{r}$$

$$\rho \frac{du}{dt} + \frac{\partial p}{\partial z} - \frac{\partial S_{11}}{\partial z} - \frac{\partial S_{12}}{\partial r} = \frac{S_{12}}{r}$$

$$\rho \frac{dv}{dt} + \frac{\partial p}{\partial r} - \frac{\partial S_{12}}{\partial z} - \frac{\partial S_{22}}{\partial r} = \frac{\partial S_{22} + S_{11}}{r}$$

$$\rho \frac{de}{dt} - (S_{11}-p) \frac{\partial u}{\partial z} - (S_{22}-p) \frac{\partial v}{\partial r} - S_{12}\left(\frac{\partial v}{\partial z} + \frac{\partial u}{\partial r}\right)$$

(6.4)
$$= - \frac{v(S_{11} + S_{22} + p)}{r}$$

$$\frac{dS_{11}}{dt} = 2 \mu \, \epsilon_{11}$$

$$\frac{dS_{12}}{dt} = 2 \mu \, \epsilon_{12}$$

$$\frac{dS_{22}}{dt} = 2 \mu \, \epsilon_{22}$$

with the strain rates ϵ_{ij} given by

$$\epsilon_{11} = \frac{1}{3}\left(2\,\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} - \frac{v}{r}\right)$$

$$(6.5) \qquad \epsilon_{12} = \frac{1}{2}\left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial z}\right)$$

$$\epsilon_{22} = \frac{1}{3}\left(2\,\frac{\partial v}{\partial r} - \frac{\partial u}{\partial z} - \frac{v}{r}\right)\ .$$

To this we append an equation of state

$$(6.6) \qquad p = p(\rho,\epsilon)\ .$$

Since these equations are hyperbolic we can construct characteristic equations for which differentiations in only two space-time directions occur. In contrast to the fluid dynamic equation there are two speeds of propagation. The first is the shear or transverse speed given by

$$(6.7a) \qquad c_s^2 = \mu/\rho\ .$$

There is also the compressive or longitudinal speed

$$(6.7b) \qquad c_d^2 = c^2 + 4\mu/3\rho$$

where

54

(6.7c)
$$c^2 = \frac{\partial p}{\partial \rho}$$

is the fluid dynamic sound speed. In addition to these
two conoids there are three quantities that propagate
along stream lines. Hence, in total there are seven
sets of bicharacteristics.

In the interior we solve (6.4) by any dissipative
conservative scheme. We do not follow the shocks explicit-
ly but instead capture them. The elimination of shock
fitting eliminates many of the complexities of the problem
and allows us to concentrate on fitting the interfaces.
Since shocks are compressive it is possible to follow them
without shock fitting. However, contact discontinuities
will be unacceptably smeared unless some special procedure
is followed. Hence, all free surfaces or interfaces are
followed explicitly to prevent their diffusion.

Due to the complications of the boundary we have
chosen a simple scheme for the Eulerian mesh. All the
results were obtained using a two step scheme devised by
Burstein [29] This scheme uses data at a nine point
rectangular lattice at the time level t to advance to $t+\Delta t$.
At points far from the boundary the computation is straight-
forward. At mesh points near the boundary the fluxes at arti-
ficial points outside the domain are found by extrapolation.
Quadratic extrapolation including the values at the
boundary is used because of the complexities that arise

with an arbitrarily shaped boundary. After the flux
extrapolation the nine point scheme can be used without
any complications. Each side of an interface is updated
independently. In no case are values on one side of the
boundary used to update variables on the other side. In
many cases different grids are used in different regions
so that it would be difficult to integrate across an
interface even for quantities that are continuous across
the interface.

All boundaries, which move through the fixed Eulerian
mesh, are marked by Lagrangian tracer particles with
position (z,r) and velocity (u_B, v_B). For interfaces between
two regions there are marker particles on both sides of the
moving boundary. The motion of these particles is governed
by the equations

$$\frac{dz}{dt} = u_B(z,r,t)$$

(6.8)

$$\frac{dr}{dt} = v_B(z,r,t) \ .$$

The velocity (u_B, v_B) is the local fluid velocity and is
found by extrapolation from the interior. Across an inter-
face only the normal velocity is continuous. Hence, there
will be a tangential slippage of the position of the tracer
particles on one side of the interface with respect to the
other side. The system of equations (6.8) are solved for
the new positions $z(t + \Delta t)$, $r(t + \Delta t)$ at each boundary
point by a first order method.

56

Since each tracer particle is moved independently the distance between these particles will vary. In many cases the particles will bunch up in some regions with very few boundary particles in other sections. To prevent this the particles are rezoned if the distance between two particles differs by more than 25 percent from the average distance between particles. This rezoning consists of creating a new set of tracer particles which are equally spaced. Any information needed at the tracer particles are found by interpolation. All distances and interpolation formulas are calculated in terms of arc length along the boundary. This is a one dimensional operation and so much simpler than a full Lagrangian rezone of the entire two dimensional grid. Furthermore, since the interior values are unaffected by this transformation, the rezoning procedure cannot affect the conservation of mass, momentum or energy.

In order to advance the solution we need the dependent variables at the boundary itself. It is here that the jump conditions affect the solution. We first describe the boundary conditions at an interface separating two contiguous elastic domains. The physical laws that apply at material interface boundaries are (1) continuity of the normal velocity, u_n , (2) continuity of the normal stress, τ_{nn} , and (3, 4) the specification of the shear stress, τ_{ng} , on each side of the interface as a given function of

the normal stress.   Here we only consider the condition
that τ_{ng} = 0 on each side of the interface, which is the
free slip condition.   One could also consider welded sur-
faces where laws (3, 4) are replaced by the condition that
the entire stress matrix be continuous across the inter-
face.

It may be verified that, for the elastic equations,
there are four characteristic waves emanating from the mov-
ing interface, i.e., from each side of the interface two
waves propagate away from the boundary. Hence, at the
interface boundary, a total of four conditions need to be
specified, so that by satisfying the above physical laws at
the interface boundary, the boundary motion can be determined.

To implement the boundary conditions we consider a
coordinate system with coordinates, n the normal and s
the tangent to the boundary at each marker point along the
boundary. Let S(z,r) be the deviatoric stress tensor as
a function of (z,r). Let R be the rotation matrix

$$(6.9a) \qquad R = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} ,$$

with θ the angle measured clockwise from the Z axis
to the normal. Then

$$(6.9b) \qquad S(n,s) = R\,S\,(z,r)\,R^{t}$$

58

is the rotated deviatoric tensor. In this reference
frame, the stress tensor T with components τ_{ij} can
be computed. The velocity vector is given by

$$(6.9c) \qquad \begin{pmatrix} u_n \\ u_s \end{pmatrix} = R \begin{pmatrix} u \\ v \end{pmatrix} .$$

To find the boundary values at the new time step we
must calculate fourteen quantities corresponding to the
seven dependent variables on each side of the interface.
Since we are given four conditions we must supplement this
by ten additional pieces of information. As discussed
before we shall use the characteristic variables to ob-
tain this information. We consider the interface as in-
creasing in the counterclockwise direction. We denote
by superscript 1 the region to the left and superscript
2 the region to the right of the interface. The normal
direction is taken as going from region one to region and
the tangential direction counterclockwise. As stated
before the signals c_d, c_s propagating to the right bring
two pieces of information to the boundary from the interior
of region one. Similarly for region two we consider the
signals $-c_d$, $-c_s$ travelling from right to left. In
addition, we have three pieces of information on each side
that travels along stream lines. Using the
characteristic variables (see [33]) we find that

(6.10a)
$$u_n^{(1)} - u_n^{(2)} = 0$$

(6.10b)
$$p^{(1)} - S_{nn}^{(1)} - \left[p^{(2)} - S_{nn}^{(2)} \right] = 0$$

(6.10c)
$$S_{ns}^{(1)} = 0$$

(6.10d)
$$S_{ns}^{(2)} = 0$$

(6.10e)
$$\rho^{(1)} c^{(1)^2} - p^{(1)} = \bar{\rho}^{(1)} c^{(1)^2} - \bar{p}^{(1)}$$

(6.10f)
$$\rho^{(2)} c^{(2)^2} - p^{(2)} = \bar{\rho}^{(2)} c^{(2)^2} - \bar{p}^{(2)}$$

(6.10g)
$$\frac{4\mu^{(1)}}{3\rho_0^{(1)}} p^{(1)} + c^{(1)^2} S_{nn}^{(1)} = \frac{4\mu^{(1)}}{3\rho_0^{(1)}} \bar{p}^{(1)} + c^{(1)^2} \bar{S}_{nn}^{(1)}$$

(6.10h)
$$\frac{4\mu^{(2)}}{3\rho_0^{(2)}} p^{(2)} + c^{(2)^2} S_{nn}^{(2)} = \frac{4\mu^{(2)}}{3\rho_0^{(2)}} \bar{p}^{(2)} + c^{(2)^2} \bar{S}_{nn}^{(2)}$$

(6.10i)
$$\frac{2\mu^{(1)}}{3\rho_0^{(1)}} \left[p^{(1)} - S_{nn}^{(1)} \right] - c_d^{(1)^2} S_{nn}^{(1)}$$

$$= \frac{2\mu^{(1)}}{3\rho_0^{(1)}} \left[\bar{p}^{(1)} - \bar{S}^{(1)} \right] - c_d^{(1)^2} \bar{S}_{nn}^{(1)}$$

(6.10j)
$$\frac{2\mu^{(2)}}{3\rho_0^{(2)}} \left[p^{(2)} - S^{(2)} \right] - c_d^{(2)^2} S_{nn}^{(2)}$$

$$= \frac{2\mu^{(2)}}{3\rho_0^{(2)}} \left[\bar{p}^{(2)} - \bar{S}_{nn}^{(2)} \right] - c_d^{(2)^2} \bar{S}_{nn}^{(2)}$$

$$(6.10k) \qquad u_s^{(1)} - \frac{1}{\rho_0^{(1)} c_d^{(1)}} \, S_{ns}^{(1)} = \bar{u}_s^{(1)} - \frac{1}{\rho_0^{(1)} c_d^{(1)}} \, \bar{S}_{ns}^{(1)}$$

$$(6.10\ell) \qquad u_n^{(1)} + \frac{p^{(1)} - S_{nn}^{(1)}}{\rho_0^{(1)} c_d^{(1)}} = \bar{u}_n^{(1)} - \frac{\bar{p}^{(1)} - \bar{S}_{nn}^{(1)}}{\rho_0^{(1)} c_d^{(1)}}$$

$$(6.10m) \qquad u_s^{(2)} + \frac{1}{\rho_0^{(2)} c_d^{(2)}} \, S_{ns}^{(2)} = \bar{u}_s^{(2)} + \frac{1}{\rho_0^{(2)} c_s^{(2)}} \, \bar{S}_{ns}^{(2)}$$

$$(6.10n) \qquad u^{(2)} - \frac{p^{(2)} - S_{nn}^{(2)}}{\rho_0^{(2)} c_d^{(2)}} = \bar{u}_n^{(2)} - \frac{\bar{p}^{(2)} - \bar{S}_{nn}^{(2)}}{\rho_0^{(2)} c_d^{(2)}}$$

In these equations the bar on the right hand side indicates
quantities that already have been computed. In all the
examples presented they were computed using nearest
point extrapolation from the interior of the appropriate
domain (see also [40]). The subscripts n and s refer
to the normal and tangential directions as given by (6.9).
The sound speeds c_s, c_d, c were defined in (6.7), while
ρ_0 denotes a reference density usually taken as the density
of the marker particle at the previous time step. Note, all
material properties differ between the two sides of the
interface.

Solving the system of equations (6.10) we find that

$$(6.11a) \qquad u_n^{(1)} = u_n^{(2)} = \frac{\bar{u}_n^{(2)} + r\bar{u}^{(1)}}{r + 1} - \frac{\kappa}{r + 1} \frac{1}{\rho_0^{(1)} c_d^{(1)}} \left[\bar{\tau}_{nn}^{(2)} - \bar{\tau}_{nn}^{(1)} \right]$$

with

$$(6.11b) \qquad \kappa = \rho_0^{(1)} c_d^{(1)} / \rho_0^{(2)} c_d^{(2)} \; .$$

Thus, the normal velocity is a weighted average of the extrapolated normal velocities from the two sides, the weight being the ratio of the acoustic impedances. In addition there is a correction term dependent on the difference in the extrapolated normal stresses. As usual $\tau_{nn} = p - S_{nn}$. In a similar manner we have

$$(6.11c) \qquad \tau_{nn}^{(1)} = \tau_{nn}^{(2)} = \frac{\tau_{11}^{(1)} + \kappa \bar{\tau}_{11}^{(2)}}{\kappa + 1} + \frac{\rho_0^{(1)} c_d^{(1)}}{\kappa + 1} \left(\bar{u}_n^{(1)} - \bar{u}_n^{(2)} \right) \; .$$

and

$$(6.11d) \qquad p^{(1)} = \bar{p}^{(1)} + \frac{c^{(1)^2}}{c_d^{(1)^2}} \left(\tau_{nn}^{(1)} - \bar{\tau}_{nn}^{(1)} \right) \qquad ;$$

$$S_{nn}^{(1)} = p^{(1)} - \tau_{nn}^{(1)}$$

$$(6.11e) \qquad p^{(2)} = p^{(2)} + \frac{c^{(2)^2}}{c_d^{(2)^2}} \left(\tau_{nn}^{(2)} - {}^{-(2)}_{nn} \right) \qquad ;$$

$$S_{nn}^{(2)} = p^{(2)} - \tau_{nn}^{(2)} \; .$$

Similarly we can solve for u_s and S_{ss} on each side. The complete recipe for dertermining the values assigned to dependent variables on each side of the interface is given by the following algorithm.

(i)   Extrapolate, from the interior to the boundary, the deviatoric stresses S, pressure p, internal energy e, and velocity components u, v on each side of the interface.

(ii)   Transform the stress and velocity components from the z,r-coordinate system, to the n,s-coordinate system.

(iiia)   Use (6.11c) to calculate τ_{nn} , then

(iiib)   Calculate pressure on each side using
$$p^{(i)} = S_{nn}^{(i)} - \tau_{nn} , \quad i = 1,2.$$

(iv)   Apply the slip free condition: $\tau_{ns}^{(i)} = S_{ns}^{(i)} = 0$, $i = 1,2.$

(v)   Transform the deviatoric stresses back to the z,r-coordinate system using (iv) and the extra-extrapolated values $\tau_{nn}^{(i)}$, $\tau_{ss}^{(i)}$, $i = 1,2.$

(vi)   Calculate u_n using (6.11a); then

(vii)   Convert the velocity components to the z,r-coordinate system using (vi) and the extrapolated values $u_s^{(i)}$, $i = 1,2.$

(viii)   Calculate densities from the equation of state $\rho^{(i)} = F_i(p^{(i)}, e^{(i)})$ using (iiib) and the extrapolated values $e^{(i)}$, $i = 1,2.$

We note that the continuity of normal stress is not used to calculate the deviatorics but instead is used to compute p. This algorithm has been chosen so that the formulas are valid even if one or both materials are purely inviscid. In the limiting case of infinite density ratio

across the interface, i.e., $\rho^{(1)}/\rho^{(2)} \to 0$, the above algorithm coincides with the common driver-driven model where $\tau_{nn} = \bar{\tau}_{nn}^{(1)}$ and $u_n = \bar{u}_n^{(2)}$.

The method described above applies equally well to free surfaces if we interpret one of the domains to exhibit material properties such that all dependent variables are zero. For definiteness denote the vacuum side by super-script (2); then

$$(6.10b') \qquad \tau_{nn} = \tau_{nn}^{(2)} = 0 ,$$

and the slip free condition is

$$(6.10c') \qquad \tau_{ns} = 0 .$$

In many problems there exist regions with large gradients. These gradients need to be resolved in order to have an accurate solution. To prevent an excess of grids a stretching is introduced which is a function of only one coordinate transform. We denote the transformed variables by (α, β). By use of the implicit function theorem it is possible to transform divergence free quations from the physical space (z,r) to the computational space (α, β) in such a manner that the new equations are still in diver-gence free form. A consequence of this is that shocks will be computed with the correct jump conditions in the computational plane.

In most problems in ballistics the large gradients occur near the axis of symmetry. For these cases we used a transformation (see [160]).

64

$$(6.12a) \quad \beta = 1 - \log \left(\frac{b+a-r}{b-a+r}\right) / \log \left(\frac{b+a}{b-a}\right)$$

with $b = 1/(1 - d/a)$. This maps the interval $(0,a)$ into $(0,1)$ and d is the boundary layer thickness. For the acoustic problem discussed in the next section an alternate stretching was used.

$$(6.12b) \quad r = \beta \left[1 - ae^{-b\beta^2}\right].$$

This is inverted numerically to find $\beta = \beta(r)$. For the acoustics problem the transform was used in both the z and r directions. In both cases one of the free parameters controls the size of the gradients while the other controls the size of the boundary layer effect induced by the transform.

Another alternative is to choose new coordinate points, β_i, in some a priori manner. Cubic splines can then be used to construct the derivatives at β_i. The coordinate transformation generated in this manner need not be monotone. To enforce monotonicity one may need to alter slightly the β_i so that no abrupt jumps occur. Even though this procedure is not automatic it allows the construction of flexible coordinate systems. Since the mesh generation is done only for each geometry the inconvenience is not great. The author has used this method to construct a mesh system for a generalization of (4.1) that is being used for optimization studies for the national transonic tunnel at NASA Langley Research Center.

Due to the complicated geometry of the tunnel it was necessary to refine the mesh in several different sections of the domain; this made it difficult to use analytic transformations. The disadvantage of this method is more pronounced when one wishes to frequently change the mesh or change the geometry of the configuration.

In other problems, as the shaped charge, transformations are needed because of the shape of the domain. Even if a domain is rectangular if it is not properly aligned with the coordinate axes a large waste of grids will occur. In the shaped charge the initial shape of the liner is a rectangle rotated about 30° with respect to the axis of symmetry. The length of the liner is about 100 times larger than the width. For this case it was necessary to introduce the computational coordinates (α, β) via a full two dimensional transform. Even though this complicates the equations it presents an enormous savings in both computer time and storage. Due to the moving boundary it is sometimes necessary to introduce time dependent transformations. In all these cases the coordinate transform is given analytically. Hence, it does not map the physical region into a perfect rectangle but rather into a computational region which is in some sense reasonable.

The code described above, SMITE, has been applied to
numerous problems in elasticity and plasticity. These
include application to bars impacting on other bars or into
plates as well as problems with shaped charges and explo-
sives. All these applications involve highly distorted
boundaries together with the interaction of many shocks.

To illustrate this method and its range of applicabi-
lity we present two examples. In the first case we consider
an aluminum sphere impacting on a tungsten disc. The initial
configuration is shown in figure 6.1a The configuration
after 25 microseconds is shown in figure 6.1b. The sphere
has flattened out and is extended normal to the axis of
symmetry. The disc has also been indented. Obviously,
large distortions have occurred in both materials. These
graphs were obtaining the system (6.4) - (6.6) with the
inclusion of plasticity.

The first example illustrated the interaction of two
metals. In the second example we consider a gas-metal
interface. The initial configuration is shown in figure
6.2a. The larger region is a gas with ignition occuring
at the origin. A blast wave propagates through the gas and
impinges on the metal. The solution after 35 micro-
seconds is shown in figure 6.2b. The gas has expanded
outward while the metal has split into two sections.
The larger section is a slug which contains most of the
mass. In addition, there is a jet region which moves
rapidly to the right. Additional examples are given in
[31] and [33].
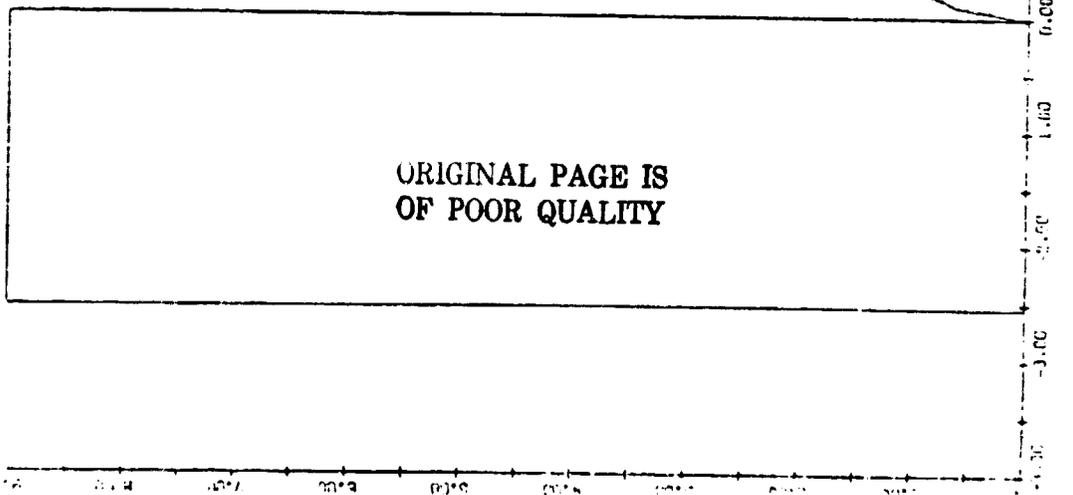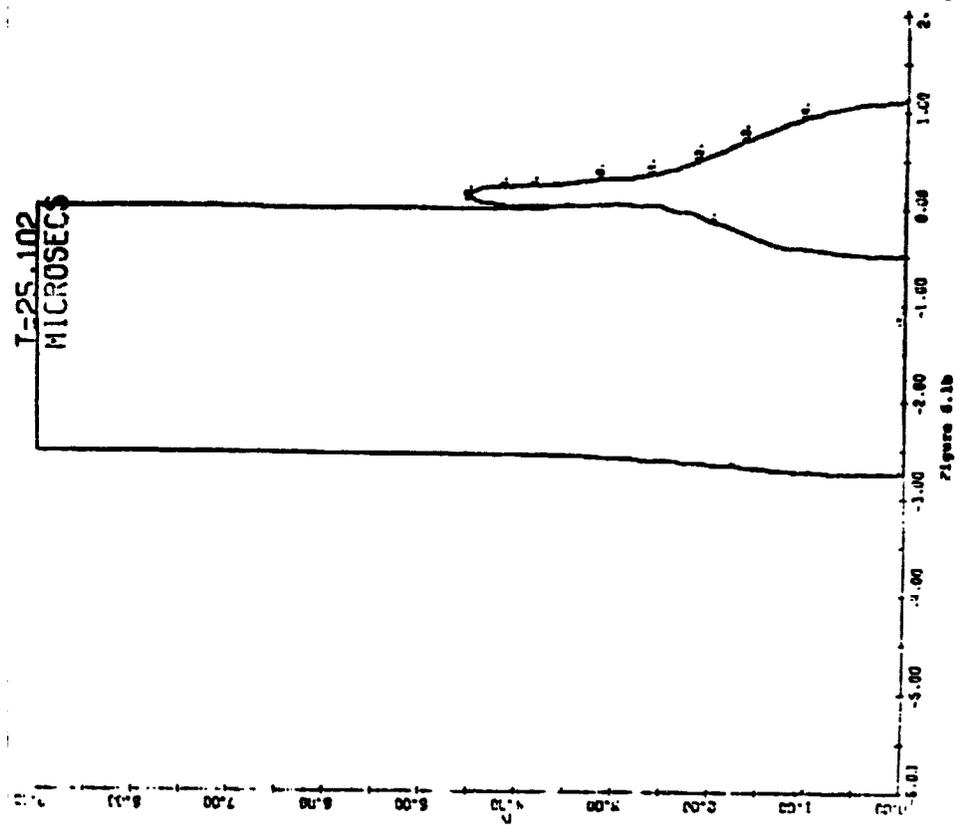
T-25.102
MICROSECS

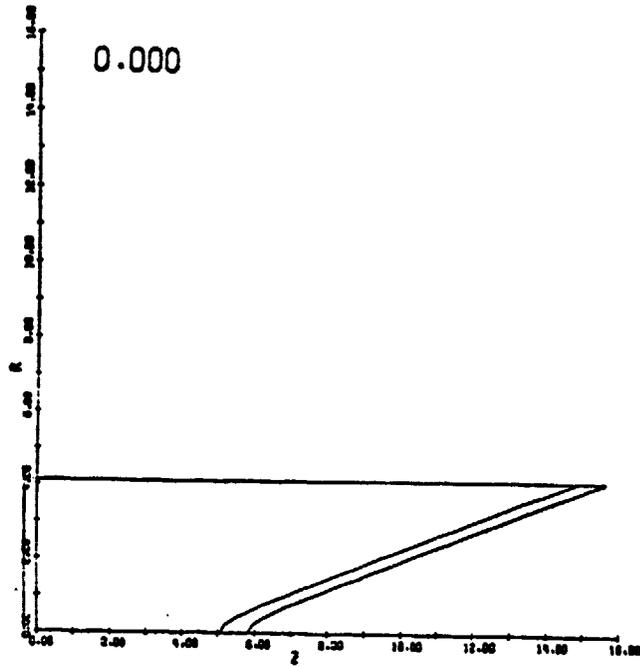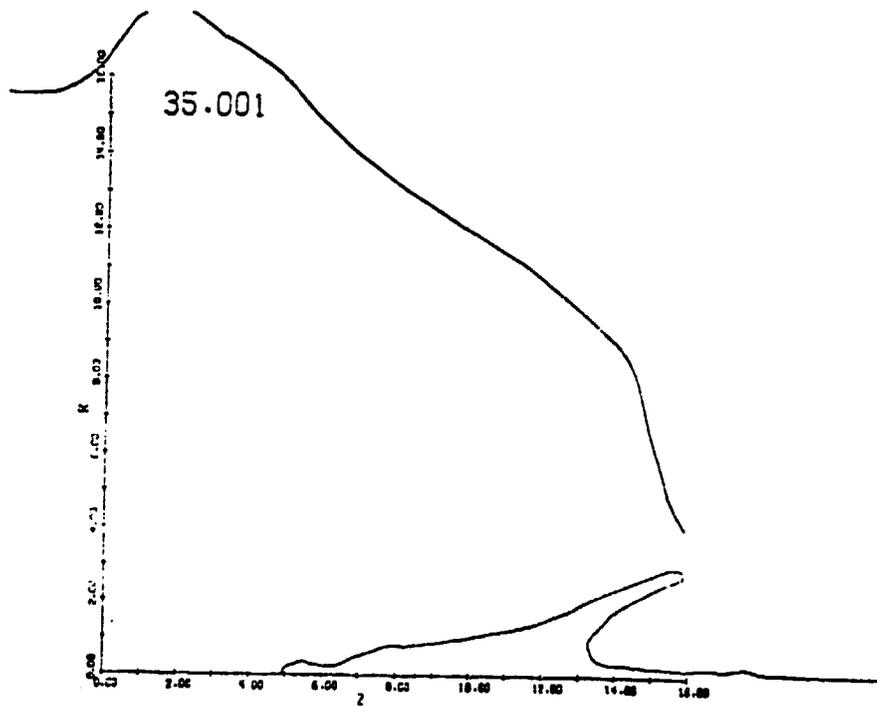Figure 6.1b

T=0.000
MICROSECS

Figure 6.1a

Figure 6.2a

Figure 6.2b

7. RADIATION BOUNDARY CONDITIONS

In many problems of interest one is interested in solving the equations in an infinite domain. For computational expediency one needs to compute in a bounded domain. One possibility is to map the infinite domain onto a bounded one. However, in many circumstances this mapping can aggravate the situation especially if the solution is oscillatory at infinity or the mapping has a singularity (see [79]). An alternative possibility is to insert an artificial boundary and then impose boundary conditions on this surface to simulate an infinite domain, i.e. there should be no reflections from the boundary back into the domain. Unless certain restrictions are met this will in general not be possible [85].

In general one cannot construct boundary conditions that give no reflections. Instead one wishes to consider conditions which are in some sense better. The notion of better can be defined in many ways. Some of them are

(1) the reflections decrease rapidly as the position of the boundary goes to infinity

(2) the reflections decrease for longer wave lengths

(3) the reflections decrease as the incident wave approaches in a direction more normal to the boundary

(4) the reflections are decreased so that the approach to a steady state is accelerated.

One approach to decreasing reflections is to introduce a viscosity near the boundary or to introduce a sponge

layer [148]. With this approach it is not clear what effect the boundary treatment has on the interior dynamics. In addition it is difficult to improve these methods if one wishes to further decrease the reflections. Conditions 2 and 3 were used by Engquist and Majda [53], [54] to construct an asymptotic set of nonreflecting conditions based on pseudodifferential operators. The higher order methods require Padé approximations for stability. Rudy and Strikwerda [162] have constructed, by heuristic arguments, a radiation boundary condition based on (4).

Gustaffson and Kreiss [85] have shown that in general one can not construct nonreflecting boundary conditions unless the behavior of the solution is known in the neighborhood of infinity. We adopt their procedure and construct boundary conditions which are based on an asymptotic expansion of the solution valid for large distances. As with all asymptotic expansions we expect reasonable results even when the artificial boundary is brought in quite close to the region of interest. Extensive numerical tests indeed confirm that the domain of integration can be very constricted when one uses the higher order boundary operators.

Specifically, we consider the linearized Euler equations in cylindrical coordinates.

$$\rho_t + (\rho u_0 + u)_z + (\rho v_0 + v)_r + \frac{\rho v_0 + v}{r} = F_1$$

$$(7.1) \qquad u_t + (u u_0 + \rho)_z + (u v_0)_r = u v_{0,r} - v u_{0,r} + F_2$$

$$v_t + (v u_0)_z + (v v_0 + \rho)_r = v v_{0,z} - u v_{0,z} + F_3$$

where $(u_0(z,r), \ v_0(z,r))$ represents the mean flow. The mean density is assumed constant and is scaled so that $\rho_0 = 1, \ c_0 = 1$.

In order for it to be feasible to integrate (6.1) in a bounded domain it is necessary to assume that the mean flow and the forcing terms decay as r or z go to infinity (see e.g. [85]). Hence for sufficiently large d (where $d^2 = r^2 + z^2$) (7.1) can be approximated by the wave system

$$
\begin{aligned}
\rho_t + u_z + v_r + \frac{v}{r} &= 0 \\
u_t + \rho_z \qquad\quad &= 0 \\
v_t + \rho_r \qquad\quad &= 0
\end{aligned}
$$

(7.2)

or since p is linearly related to ρ

(7.3) $$ p_{tt} - \nabla^2 p = 0 $$

where ∇^2 is the Laplacian in cylindrical coordinates.

To find radiation conditions we first consider (7.3) in spherical coordinates and let d represent the spherical radius. It is known [11] and [59] that p has a formal expansion in terms of travelling waves

(7.4) $$ p = \sum_{j=1}^{\infty} \frac{f_j(t-d,\theta)}{d^j} $$

where θ represents the angular dependence of p. One can then verify that

(7.5) $$ \frac{\partial p}{\partial t} + \frac{\partial p}{\partial d} = O\left(\frac{1}{d^2}\right) $$

$$(7.6) \qquad \frac{\partial p}{\partial t} + \frac{\partial p}{\partial d} + \frac{p}{d} = O(\frac{1}{d^3})$$

We note that the approximation to (7.5) $\frac{\partial p}{\partial t} + \frac{\partial p}{\partial d} = 0$ is just what one would obtain from a one dimensional characteristic theory. More generally, let

$$L = \frac{\partial}{\partial t} + \frac{\partial}{\partial d}$$

$$(7.7)$$

$$B_m = \prod_{j=1}^{m} (L + \frac{2j-1}{d}) = (L + \frac{2m-1}{d}) B_{m-1} \quad .$$

It follows from (7.4) that

$$(7.8) \qquad B_m p = O\left(\frac{1}{d^{2m+1}}\right)$$

It is shown in [11] that boundary conditions $B_m p = 0$ all lead to well posed problems in the sense of Kreiss [81]. Furthermore, one can show that errors in the solution decrease as d goes to infinity. In particular for the first order approximation (7.6) we can show that the error $\tilde{p}$ between the solutions in the bounded and infinite domains satisfies

$$(7.9) \qquad \iint (\tilde{p}_t^2 + \tilde{p}_x^2) \, dV \leq \int g^2 \, dS$$

where $g = O(1/d^3)$. In general for the mth order approximation (7.8) we can show that

$$(7.10) \qquad \| \tilde{p} \|^2 \leq K \| | g | \|$$

where $g = O(1/d^{m+1})$ and $||\cdot||$, $|||\cdot|||$, are appropriate norms.

The extension to cylindrical coordinates is straight-forward since

(7.11) $\qquad r = d \cos \theta$, $\qquad d^2 = r^2 + z^2$

$\qquad\qquad\qquad z = d \sin \theta$, $\qquad \tan \theta = \dfrac{z}{r}$

Hence, all derivatives with respect to d can be expressed as derivatives with respect to z and r. In fact one can show by induction that only derivatives tangential to the boundary need appear.

The lowest order approximations in spherical coordinates are given by

(7.12a) $\qquad\qquad B_1 p = \dfrac{\partial p}{\partial t} - \dfrac{\partial p}{\partial d} + \dfrac{p}{d} = 0$

(7.12b) $\qquad B_2 p = \dfrac{\partial^2 p}{\partial t^2} + 2 \dfrac{\partial^2 p}{\partial t \partial d} + \dfrac{\partial^2 p}{\partial d^2} + \dfrac{4}{d} \dfrac{\partial p}{\partial t} + \dfrac{4}{d} \dfrac{\partial p}{\partial d} - \dfrac{2p}{d^2} = 0$

For cylindrical symmetry we have by (7.11) that

(7.13) $\qquad \dfrac{\partial p}{\partial d} = \dfrac{\partial p}{\partial r} \cos \theta + \dfrac{\partial p}{\partial z} \sin \theta = -\left[\dfrac{\partial v}{\partial t} \cos \theta + \dfrac{\partial u}{\partial t} \sin \theta \right]$

Hence, we can replace (7.12) by

(7.14a) $\qquad B_1 p = \dfrac{\partial}{\partial t} [p - u \sin \theta - v \cos \theta] + \dfrac{p}{d} = 0$

$$B_2 p = (1 + \cos^2 \theta) \frac{\partial^2 p}{\partial t^2} - 2 \left[\cos \theta \frac{\partial^2 u}{\partial t^2} + \sin \theta \frac{\partial^2 v}{\partial t^2} \right]$$

$$(7.14b) \qquad - \cos 2\theta \frac{\partial^2 v}{\partial r \partial t} - \sin 2\theta \frac{\partial^2 u}{\partial r \partial t} + \frac{\cos^2 \theta}{r} \frac{\partial v}{\partial t}$$

$$+ \frac{4}{d} \left[\frac{\partial p}{\partial t} - \cos \theta \frac{\partial u}{\partial t} - \sin \theta \frac{\partial v}{\partial t} \right] + \frac{2p}{d^2} = 0$$

In order to illustrate the advantage of even the first order boundary condition we present one example. (7.1) was integrated using a mean flow obtained from experimental data. The source was taken as a single monopole along the axis of symmetry. In figure (7.1) we plot the pressure as a function of time for a fixed axial point. In figure (7.1a) the characteristic (or Sommerfeld) condition

$$(7.15) \qquad \frac{\partial p}{\partial t} + \frac{\partial p}{\partial r} = 0$$

was used. The spurious reflections from the boundary are evident. In figure (7.1b) we present the solution using the first order boundary condition, $B_1 p = 0$. This solution no longer has any spurious reflections. These comparisons were made with the boundary at fixed distance. Varying the position of the artificial boundary it was found that, using the first order boundary condition, one could bring the boundary quite close to the sources without loss of accuracy. For distributed sources, moving

sources or a quadrapole it became necessary to use higher order boundary conditions. Further comparisons are presented in [10] and [11].

The problems in dynamic jet acoustics present severe difficulties for any numerical scheme. One wishes to find the acoustic pressure in the far field which necessitates many grid points. However, the grid must be constructed so that there is high resolution near the origin to resolve the sources and the mean flow. In addition one wishes to verify long term patterns of the pressure. This requires accuracy over many time steps. To have any chance of solving this problem requires attention to the methods described in the past few sections. The use of high order methods is required to limit the number of mesh points. In addition the artificial boundaries must be brought in as far as possible to further limit the number of mesh points. This requires boundary conditions that severely restrict the reflection of waves from the artificial boundary. Careful attention to the stretching of the grid is also necessary. With all the above considerations a realistic two dimensional problem still requires about 35,000 mesh points for reasonable accuracy. This required the use of explicit methods that could be executed very efficiently on a pipeline computer. This problem shows that a successful code for a large scale problem requires an efficient algorithm and boundary conditions; a careful attention to the physics as well as to computer architecture.

For many applications one is interested in the fluid
dynamic equations linearized about a mean state a uniform
state which is nonzero at infinity. Let p_∞, ρ_∞, u_∞
represent the mean state in the far field and define
$c_\infty^2 = \gamma p_\infty / \rho_\infty$. We assume that v_∞ is zero. The two
dimensional analog of (7.2) is

$$u_t + u_\infty u_x + \frac{1}{\rho_\infty} p_x = 0$$

(7.16)
$$v_t + u_\infty v_x + \frac{1}{\rho_\infty} p_y = 0$$

$$p_t + u\, p_x + \gamma p_\infty (u_x + v_y) = 0 \ .$$

This is equivalent to the convective wave equation

$$(7.17) \qquad p_{tt} + 2u_\infty p_{xt} + u_\infty^2 p_{xx} - c_\infty^2 (p_{xx} + p_{yy}) = 0 \ .$$

By a change of variables this can be transformed to the
wave equation. We then transform the boundary conditions
$B_m p = 0$ to this coordinate system. When all is finished
we transform back to the (x,y) system. The first order
boundary condition for (7.16) then becomes, [13]

$$(7.18) \qquad \frac{r}{d} \frac{1}{\sqrt{c_\infty^2 - u_\infty^2}} \frac{\partial p}{\partial t} - \frac{\rho_\infty c_\infty^2}{c_\infty^2 - u_\infty^2} \frac{x}{d}\left(\frac{\partial u}{\partial t} + u_\infty \frac{\partial v}{\partial y}\right)$$

$$- \rho_\infty \frac{y}{d}\left(\frac{\partial v}{\partial t} + u_\infty \frac{\partial v}{\partial x}\right) + \frac{p - p_\infty}{2d} = 0$$

where $d^2 = x^2 + y^2$ and $r^2 = \left[\dfrac{c_\infty^2}{c_\infty^2 - u_\infty^2}\right] x^2 + y^2$. When $u_\infty = 0$ this reduces to the previous boundary condition. When u_∞ is larger than c_∞ the outflow is supersonic and no boundary conditions can be specified at the artificial boundary. The boundary condition (7.18) has been used for the Navier-Stokes equations with a subsonic outflow. The use of (7.17) substantially increased the rate of convergence to a steady state solution. The unknown linearized state (ρ_∞, u_∞, c_∞) was taken from the previous time step. A generalization of (7.15) for nonlinear problems is considered by Hedstrom [94].

It is also possible to generalize this theory to the three dimensional Helmholtz equation

$$(7.18) \qquad \Delta p + k^2 p = 0 .$$

The analog of (7.4) is

$$(7.19) \qquad p = e^{-ikr} \sum_{j=1}^{\infty} \frac{f_j(\theta,\phi)}{r^2} .$$

The radiation boundary conditions are then given by $B_m p = 0$ with

$$(7.20) \qquad B_m = \prod_{j=1}^{m} \left(-ik + \frac{\partial}{\partial r} + \frac{2j-1}{r}\right) .$$

This procedure is ordered by first operating with $j = 1$ and continuing until $j = m$. In [12] energy estimates are obtained for the error using (7.20). Numerical computations

presented in [12] demonstrate that for many cases one need only take ten mesh points normal to the boundary, independent of k, in solving (7.18). The boundary conditions apply to the Laplace equation when $k = 0$ in (7.18) and (7.20). Extensions to two dimensions are also considered in [13].
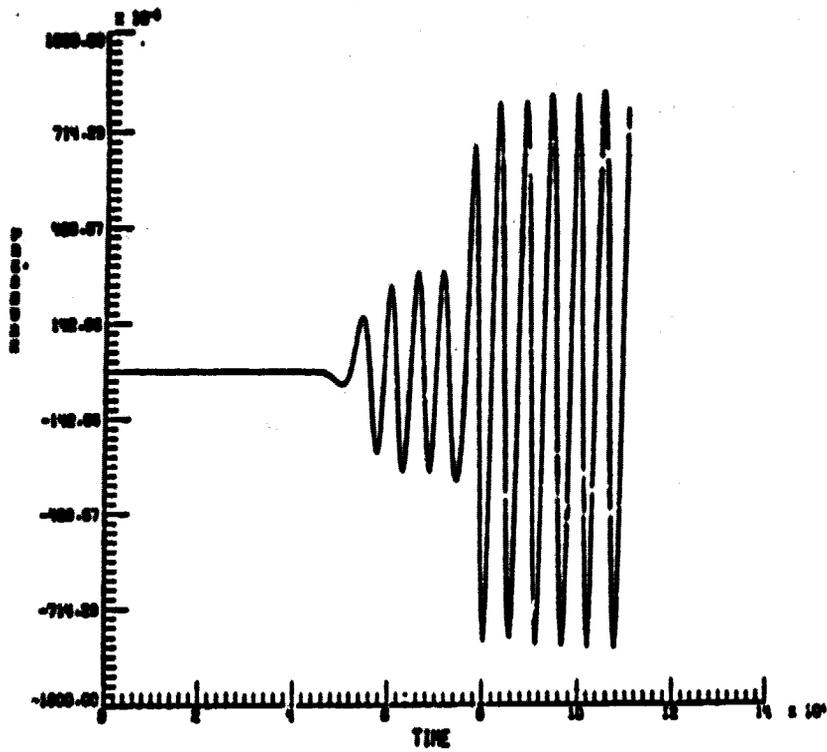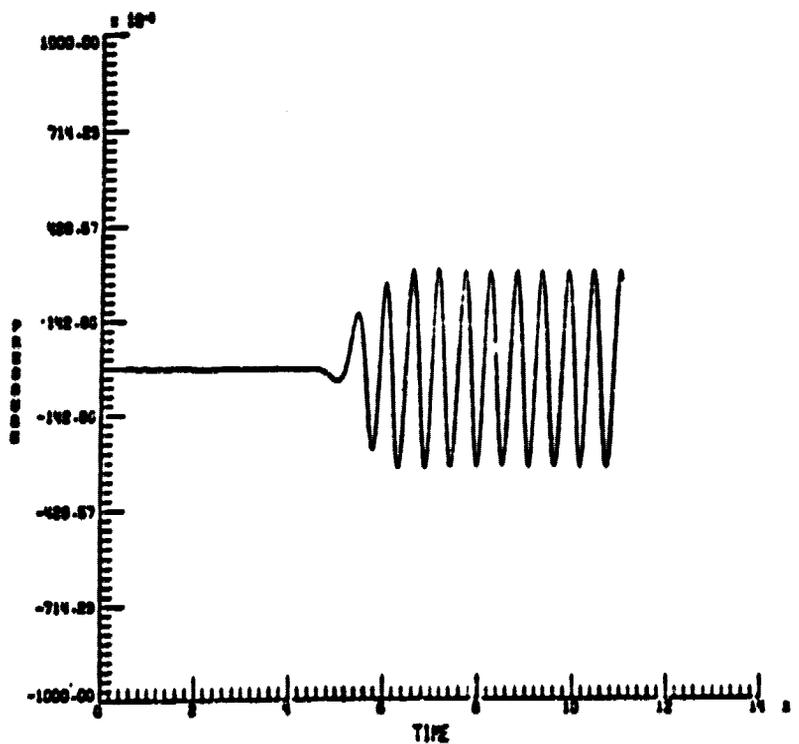
Figure 7.1a. Sommerfeld Condition

Figure 7.1b. Improved Radiation Condition, $B_{1p} = 0$.

8. APPLICATIONS

In the previous sections we have tried to stress the
interplay between the numerical scheme and the physics of
the problem. In particular we strongly feel that there is
no such thing as a universal or ultimate scheme. The
variety of phenomena described by time dependent partial
differential equations demands a variety of numerical
methods. In this section we shall describe some difficulties
that arise in particular situations. Due to a shortage of
space we can only sketch these difficulties with a brief
description of possible remedies. References to the litera-
ture will be given for a more extensive discussion of indi-
vidual situations.

A. Shocks

When dealing with nonlinear systems the solution
does not always remain smooth even when the initial data is
smooth. Instead surfaces of discontinuities, called shocks
arise. The solution is smooth on either side of the shock
and across the shock the solution is governed by jump condi-
tions. These shocks are an inherently nonlinear phenomena.
Linear discontinuities such as contact discontinuities can
also occur. For a survey of the analytical theory of shocks
see [118].

The standard convergence theorems for numerical
schemes are based on the assumption that the solution is
smooth (see [156]). When shocks occur it is well known that
one can construct reasonable schemes that converge to a

solution with the wrong shock location (e.g. [116], [209]).
One alternative is to use the differential equations only
in smooth regions. The shock itself is followed explicitly
using the Rankine-Hugoniot relations supplemented by char-
acteristic data (see [140], [152], [166]). For complex
flows with several intersecting shocks this is difficult.
Furthermore, there is the additional difficulty of predicting
the generation of shocks that do not exist initially. The
introduction of viscous terms further complicates the
method.

An alternative to fitting the shock is the so-called
shock capturing method. Lax and Wendroff [116] showed that
if the equations are written in divergence-free form

$$(8.1) \qquad\qquad u_t + \operatorname{div} f = 0$$

and if the numerical method also has this property then
when the scheme converges it will give the correct shock
speeds. Because of the ease of use, this method has dominated
the computation of shocked flows. We note that the use of
divergence-free form is not necessary. Instead one can integrate
(8.1) as a quasi-linear system and compensate for this by
the addition of terms that depend on the mesh (see [209]).
It is also well known that the use of the divergence free
form is not sufficient to give the correct shock speed.
Once one generalizes the definition of a solution to allow
discontinuous solutions then the solution to (8.1) is no
longer unique. One must demand additional constraints, e.g.
that entropy increase across the shock, in order to have a

unique solution (see [118] for additional information). For
first order systems necessary and sufficient conditions which
guarantee entropy satisfying discrete shock profiles are
given by Majda and Ralston [132].

The use of the difference scheme across the shock has
several disadvantages. In some cases it has been found that
non-physical rarefaction shocks can appear ([90], [125]) i.e.,
the entropy condition is violated. This generally happens
at a sonic line or a stagnation point where an eigenvalue of
the system becomes zero. All the known examples for model
equations exhibit troubles only when the coefficient in the
equation passes through zero. The usual second order schemes,
Lax-Wendroff or MacCormack, have a dissipative mechanism
which vanishes when an eigenvalue of $\frac{\partial f}{\partial x}$ in (8.1) is zero.
Hence, in these circumstances the scheme is effectively non-
dissipative and so it is no surprise that difficulties can
occur. Another difficulty of higher order method is that
overshoots can occur in the neighborhood of shocks even when
the shock speeds are calculated correctly.

The standard cure to these difficulties is to add an
artificial viscosity term to the scheme. This viscosity
should be constructed so that it does not affect the accuracy
of the scheme in the smooth portion of flow. It also should
not vanish at the sonic lines or the stagnation points. In
practical computations several viscosities have been suggested
which work reasonably well [29], [49]. Majda and Osher
[130], [133] have suggested some viscosities for which
they can prove the convergence of the scheme to the correct

solution. Lerat and Peyret [120] have shown that one can
lessen the impact of the oscillations by choosing the
correct variant of MacCormack's method (3.5). This becomes
difficult for complicated flow patterns. Lerat [121]
discusses the addition of nonlinear correction terms to
reduce the oscillations. These latter studies are based
on the modified equation approach [100], [171], [194].
These corrections have been of a very specialized and
problem dependent nature.

It is known that monotone schemes have the property
that overshoots do not occur and that they give the correct
shock locations [90]. Unfortunately, linear monotone schemes
are only first order accurate. Crandall and Majda [44]
have considered generalizations of monotone schemes as well
as extensions to several dimensions by using splitting methods.
They demonstrate that splitting the equations into one
dimensional portions can have strange effects on the
shocked solution. The definition of monotonicity for
systems of equations is not clear.

An alternative to using monotone first order methods
everywhere is to use these methods only near the shock
and to use a higher order method in the smooth portion
of the flow [88]. Rather than using different schemes
in different regions it is easier to automatically com-
bine these schemes using hybrid techniques [89]. The
monotone methods produce excessive smoothing of the shock
profile. Several nonlinear corrections have been suggested
[18], [91], [191], [208] to prevent this smearing.

A simpler technique is to use the scheme without the addition of any artificial viscosity. At the completion of each step one filters the solution to remove any oscillations. The simplest way to accomplish this is with a Shuman filter [88]. Let $\bar{u}$ represent the solution to any finite difference scheme at time t. We then define the corrected solution to be

$$(8.2a) \qquad u_j^n = \bar{u}_j + \theta_{j+\frac{1}{2}}(\bar{u}_{j+1} - \bar{u}_j) - \theta_{j-\frac{1}{2}}(\bar{u}_j - \bar{u}_{j-1}) \ .$$

with

$$(8.2b) \qquad\qquad 0 < \theta_j < \tfrac{1}{2} \ .$$

For (8.2) to be second order accurate, in space, we require that $\theta_j = 0(\Delta x)$ in the smooth regions of the flow. (8.2) can be viewed as the second step of a splitting process which adds the viscous terms $(\theta u_x)_x$. Hence, stability is ensured whenever the basic numerical algorithm is absolutely stable. A reasonable choice for θ is [92]

$$(8.2c) \quad \theta_{j+\frac{1}{2}} = \alpha \left[\frac{\sigma_{j+2} - \sigma_{j+1} - 2(\sigma_{j+1} - \sigma_j) + (\sigma_j - \sigma_{j-1})}{|\sigma_{j+2} - \sigma_{j+1}| + 2|\sigma_{j+1} - \sigma_j)| + |\sigma_j - \sigma_{j-2}|} \right]$$

where $0 < \alpha < \tfrac{1}{2}$ and σ is a function of $\bar{u}$. For the fluid dynamic equations one frequently chooses σ as the density.

The various techniques discussed all reduce oscillations in the neighborhood of a shock. It is not clear

whether one needs to remove these oscillations except
for aesthetic reasons. This seems to be problem dependent.
For problems with combustion, it is imperative to prevent
oscillations which may falsely trigger the combustion
process. For steady state calculations with separate
shocks the oscillations probably do little harm to the
total solution. For dynamic situations with interacting
shocks the situation is less clear.

Shocks are inherently stable and compressive phenomena.
Hence, even without shock fitting the shock is smeared over
only a few mesh points even for long periods of time.
However, contact discontinuities continue to spread in
time. Hence, in multidimensions where coarse grids are
necessary one cannot resolve contact discontinuities over
long periods of time. One can try to convert these dis-
continuities into pseudo-shocks [91]. Alternatively one
can use fitting techniques only for contact discontinuities.
One such technique was described in section 6 for the inter-
face between different materials.

Numerical evidence indicates that if higher order
methods are used in smooth parts of the flow then errors
in the shock area do not propagate into the smooth region
[188]. Since contact discontinuities are a linear phenomena
it seems that errors in the discontinuity region may
contaminate the entire domain of integration. For
linear problems with discontinuities a straightforward
method will yield only second order accuracy even in

smooth regions [129]. The accuracy of the method can be
recovered by pre- and post-processing [138]. For non-
linear problems preprocessing and postprocessing will not
work. On the other hand there are indications that there
is no need for any adjustments for shocks ([119], [188]).
In fact preliminary computations demonstrate that one can
achieve one point shocks and contact discontinuities
using Chebyshev spectral methods (3.16 - 3.18). Small
oscillations appear which can be removed by a postprocessor
(D. Gottlieb, private communication).

When using implicit methods to compute the solution
to shocked flows, computational experience indicates that
one can not use time steps more than about three or four
times the local Courant limit, even for stationary shocks
(e.g. [93]). In many practical situations this is not a
serious limitation as the time step for an explicit scheme
would be goverened by regions other than the shock region.
For example, in a shock-boundary layer interaction the time
step is goverened by the boundary layer mesh and not the
shock. Hence, an implicit method can still use time steps
about fifty times larger than those used by an explicit
method.

B. Multidimensional Problems

In several of the previous chapters we have dis-
cussed methods for one dimensional problems. For practical
applications one needs multidimensional codes. For some

methods as leapfrog it is straightforward to construct a stable multidimensional scheme. Even in this case the most straightforward version can lead to restrictive time steps. Consider the equation

$$(8.3) \qquad u_t + A u_x + B u_y = 0 \ .$$

The straightforward leapfrog method for this equation is

$$(8.4) \qquad u_{i,j}^{n+1} = u_{i,j}^{n-1} - \frac{\Delta t}{\Delta x} A_{i,j}^n \left(u_{i+1,j}^n - u_{i-1,j}^n \right)$$

$$- \frac{\Delta t}{\Delta y} B_{i,j}^n \left(u_{i,j+1}^n - u_{i,j-1}^n \right) \ .$$

This is stable if

$$(8.5a) \qquad A \sin \xi + B \sin \eta \leq 1$$

for all ξ and η. In the worst case this can demand $\|A\| \leq \frac{1}{2}$, $\|B\| \leq \frac{1}{2}$. For the fluid dynamic equations (8.4) is stable when

$$(8.5b) \qquad \Delta t \left[\sqrt{\left(\frac{u}{\Delta x}\right)^2 + \left(\frac{v}{\Delta y}\right)^2} + \sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2} \ c \right] \leq 1 \ .$$

Abarbanel and Gottlieb [2] have pointed out that one can improve this stable condition by averaging the derivatives. In particular we can replace (8.4) by

(8.6) $\quad u_{i,j}^{n+1} = u_{i,j}^{n-1} - \frac{\Delta t}{2\Delta x} A_{i,j}^n$

$$\cdot \left[\left(u_{i+1,j+1}^n + u_{i+1,j-1}^n - u_{i-1,j+1}^n - u_{i-1,j-1}^n \right) \right]$$

$$- \frac{\Delta t}{2\Delta y} B_{i,j}^n$$

$$\cdot \left[\left(u_{i+1,j+1}^n + u_{i-1,j+1}^n - u_{i+1,j-1}^n - u_{i-1,j-1}^n \right) \right] \cdot$$

This is now stable when

(8.7) $\qquad \frac{\Delta t}{\Delta x} A \leq 1 \quad , \quad \frac{\Delta t}{\Delta y} B \leq 1$

which is optimal. Similar extension to three dimensions
exist except that the averaged scheme is no longer optimal
but still better than the standard leapfrog method. Exten-
sions to arbitrary dimensions are considered in [201].
A similar gain is achieved for the fourth order leap-
frog method (S. Abarbanel and D. Gottlieb, private commu-
nication).

For implicit methods the extension to multidimensions
is less straightforward. The obvious generalization of one
dimensional schemes leads to the necessity of inverting
large sparse matrices which are no longer tridiagonal.
To avoid this problem one usually employs an alternating
direction method to reduce the problem to a sequence of one
dimensional problems. McDonald and Briley [128] have stressed
the importance of doing this in such a manner that each
portion of the split is consistent with the original equations.
In chapter 5 we have indicated some of the disadvantages of

A.D.I. These include a reduction in the rate of convergence to a steady state and also instability for some important three dimensional versions.

For the usual multistep explicit methods one can construct full two dimensional versions. This has been done by Richtmyer [156], Burstein [29], MacCormack [124], Turkel, Abarbanel and Gottlieb [186] among others. These schemes usually have a restricted stability criterion. More important, it is difficult to treat different directions in a different manner in order to take advantage of the physics of the situation. Strang [179], Yanenko [206], and Marchuk [134] have introduced the concept of splitting the equation into several components. We consider the general equation

$$(8.8) \qquad u_t = M_x u + M_y u + M_z u = M u \ .$$

Here, we have arbitrarily split the right hand side into three portions. Frequently these splits are identified with separate dimensions. However, in other applications other splits are indicated by the physics (see e.g. [135] and section D). We now consider the subsystems

$$(8.9) \qquad v_t = M_x v \quad ; \quad v_t = M_y v \quad ; \quad v_t = M_z v$$

and we denote the numerical solution to these subsystems by

$$(8.10) \quad v^{n+1} = L_x v^n \quad ; \quad v^{n+1} = L_y v^n \quad ; \quad v^{n+1} = L_z v^n$$

respectively. We can reconstruct the solution to (8.8) by

(8.11a)
$$u^{n+1} = L_x L_y L_z u^n .$$

This is a first order, in time, approximation to (8.8).
In order to make the approximation second order in time we
follow (8.11a) by

(8.11b)
$$u^{n+2} = L_x L_y L_z u^{n+1} .$$

This is stable if each of the one dimensional operators
are strongly stable. Gourlay and Morris [75], [76] have
considered the implementation using multistep methods.
Gottlieb [67] has shown that this 2-cycle of permutations
is second order even for nonlinear equations. This splitting
in two or three space dimensions coupled with some multi-
step scheme has been very successful for many applications.
One can show that one achieves the optimal time steps. One
can also treat different directions in different manners.
For example, MacCormack [125] uses the operator in the y
direction more often, with smaller time steps, than the
operator in the x direction. This compensates for the
finer mesh in the y direction. Alternatively, one could
couple Fourier methods in periodic directions with finite
difference or Chebyshev methods in directions with boundaries.
For a further description of details see [77].

As with all methods splitting techniques have their drawbacks. One immediate difficulty is that the intermediate steps have no physical interpretations. Hence, if the coefficients of the equations or the boundary conditions depend explicitly on time it is not clear which time to use for the middle steps. This is compounded if multi-step methods are used for the one-dimensional operator. Additional difficulties are encountered when the solution has a shock inclined to one of the coordinate directions. Crandall and Majda [45] have shown that unusual occurences happen in this case. The efficiency of the random choice method also deteriorates in the presence of oblique shocks when splitting is used (Chorin, personal communication).

Another difficulty occurs when some subsidiary constraints are intrinsic to the solution. For example, for the Maxwell equations the condition $\text{div} \, B = 0$ can be viewed as an initial condition. For problems with variable coefficients (8.10) is not symmetric in x and y even though the operators appear in a symmetric fashion. Hence, numerically $\frac{\partial}{\partial t} \, \text{div} \, B$ is nonzero. This introduces a non-physical Lorenz force which can cause numerical instabilities. The author has done extensive calculations with the nonlinear ideal MHD equations. When dimensional splitting was used nonphysical instabilities always occurred. This also occurs when Lagrangian schemes are used in MHD (Brackbill and Barnes [21]). A similar situation occurs in the

incompressible Navier-Stokes equations where $\text{div}\,u = 0$
must be satisfied. In this case the situation is improved
by explicitly adding terms involving $\frac{\partial}{\partial t}\,\text{div}\,u$ to the
equations. This does not affect the analytic solution
since $\text{div}\,u = 0$. However, the numerical solution can be
stabilized by such a procedure (see [86], [99]).

C. Aerodynamics

Aerodynamics is frequently divided into internal
and external flows. Internal aerodynamics describes flows
in nozzles, ducts and turbomachinery. These flows usually
involve complex flow patterns and frequently require the
addition of chemistry models to study the propagation of
flames. Boundary conditions are extremely important for
internal flows. These flows are usually subsonic or
transonic with maximum Mach numbers of about 1.3. Hence,
one is frequently not interested in shocks and can frequently
dispense with the conservation forms of the difference
equations. This is especially important for implicit methods.
The block structure of the matrices to be inverted are much
more complicated when the divergence form of the equations
must be used. The velocity form of the equations frequently
allows the decoupling of the blocks into a direct sum of
smaller blocks (see [23]). It is much faster to invert
three scalar tridiagonal matrices than to invert one block
tridiagonal matrix with 3×3 blocks. Hence, it is computa-
tionally important to utilize the proper form of the equations.

For large systems arising from chemical models this is even
more important. An extensive discussion of implicit methods
for internal flows is given by McDonald and Briley [128].

For both internal and external flows one must use a mesh
that resolves the boundary layers. This can be done by
a mesh stretching or a finite volume technique. In many
situations one is only interested in the steady state solution.
For this case implicit methods are becoming popular. As
mentioned in section 5 the implicit methods become more
inefficient as the complexity of the equations increase.
This complexity can be created by the existence of many
equations or the existence of cross derivatives. For many
aerodynamic flows one simplifies the full Navier-Stokes
equations to the so called "thin layer" approximations [175]
so that the flow is essentially unidirectional [51]. This
is useful only when the boundary layer has some simple
structure parallel to the body. An alternative is the
rapid solver proposed by MacCormack [126]. Details of these
approaches are given in the article by Hollanders and
Viviand [101]. An alternative to using the time dependent
equations is trying to solve the steady state equations
directly. Iterative methods have not proved to date, to
be very promising. One possibility is to use Newton's
method for linearizing the problem coupled with Gaussian
elimination. This has been carried out by Blomster and
Sköllermo [17] and Rizzi []57]. The major difficulty
with this approach is that the bandwidth of the matrix

increases rapidly as finer meshes are needed for more
realistic situations. This is especially severe in three
space dimensions. Alternate linerizations, such as
Schubert's methods, may alleviate the difficulty since one
can account for the sparsity of the matrix to be inverted
(see e.g. [136], [167]).

An important problem in using the time dependent
equations to achieve a steady state is finding ways to
accelerate the convergence to the steady state. One such
method is to use different time steps at different mesh
points. For explicit methods the time steps could be
chosen so as to satisfy the local stability limit (Burstein,
personal communication). For implicit methods large time
steps can be viewed as an iteration parameter. Some ideas
for optimizing this parameter were discussed in chapter 5.

Even more important is the proper implementation of
initial and boundary conditions. Rudy and Strikwerda [163]
have considered the effect of various boundary treatments
on the acceleration to steady state. Over-specification at
inflow can accelerate the convergence but frequently leads
to oscillations in the steady state. Under-specification
at outflow can prevent the achievement of the steady state.
The use of a radiation boundary condition can dramatically
decrease the number of steps required to achieve the
steady state. An analytic treatment of several boundary
treatments is provided in [147].

The correct choice of initial data is also important
in achieving a rapid steady state. When the initial data
does not satisfy the boundary conditions waves can arise
which take a long time to dissipate. One procedure is
to use a primitive form of the multi-grid method [22].
In this case we solve the equations on a coarse grid.
This can be done rapidly and so the initial guess is not
important. The converged solution is then used as an
initial guess for the next finer grid. A pyramid of
grids can be used until the finest grid is reached. Most
of the work is done on the finest grid and so the
coarser girds do not increase the work by very much. By
providing an excellent initial guess this process can sub-
stantially accelerate the process of reaching a steady
state.

For complex three dimensional flows it is likely that
all the processes described above and in chapter 5 will
be necessary to achieve a steady state within a reasonable
number of iterations. For surveys of methods for the
Navier-Stokes equations see [7], [35], [137], [154].
In addition there will be, in the future, more of a
need for internal accuracy checks, e.g. changing the
mesh size. This is crucial for investigating the effect
of various acceleration techniques on the accuracy of
the steady state solution. In most studies the only
accuracy checks are comparisons of averaged quantitities

with experimental data, e.g. skin friction, drag, etc.
These comparisons ignore any oscillations or other diffi-
culties that may occur locally in sections of the flow.

d. Meterorology

The problems that occur in computational meteorology
are very different from those in aerodynamics. First,
in meteorology one is interested in the dynamic behavior
of the model. Even in climatology one wishes to find
statistical averages rather than a steady state solution.
Furthermore, the equations of motion are a classical
example of a system with different time scales. Allowable
speeds in the atmosphere range from sound waves down to
Rossby waves. The physically dominating Rossby waves
are about 20-30 times slower than the speed of sound.
Nevertheless, if one uses an explicit scheme the time
steps is restricted by the fastest possible modes of
propagation. A further restriction on numerical methods
is that one wishes to limit the amount of dissipation
introduced by the scheme. The long term weather patterns
are governed by a delicate balance between heating due
to solar radiation and dissipation due to friction and
interactions with the oceans. For long term weather pre-
diction it is essential that the numerical method does
not interfere with this balance.

As a simplified set of equations we analyze the
shallow water equations in cartesian coordinates.

(8.12a)
$$u_t + uu_x + vu_y = -gh_x + fv$$

(8.12b)
$$v_t + uv_x + vv_y = -gh_y - fu$$

(8.12c)
$$h_t + uh_x + vh_y = -h(u_x + v_y).$$

(u,v) are the velocity components and h is the equivalent height of the atmosphere. g and f are taken to be constants. The phase speeds of the system are

(8.13)
$$\omega_1 = u \sin \theta + v \cos \theta$$
$$\omega_{2,3} = \omega_1 \pm \sqrt{gh + f^2}$$

In this simple system ω_1 represents the important Rossby wave while $\omega_{2,3}$ are the relatively less important gravity waves. The flow is called geostrophic if the right hand side of (8.12a) and (8.12b) are zero. The flow is incompressible if the right hand side of (8.12c) is zero. The real atmosphere is quasi-geostrophic and almost incompressible. This is the cause of the small amount of energy in the gravity waves.

One way to overcome the difficulty with the different time scales is to use a semi-implicit method. In this method the right hand side of (8.12) is treated implicitly while the convective terms are treated explicitly. The resulting stability condition then depends only on the

velocities and not on the sound speed, $\sqrt{gh}$. A further
analysis of this is presented in Elvius and Sundstrom [52].
Navon [144] has combined a semi-implicit method together
with the linearization technique described in section 5.
He found that it was necessary to iterate the procedure
once in order to maintain the accuracy. Isaacson,
Marchesin and Zwas [104] have used a fully implicit compact
fourth order method coupled with linearization algorithm.
The scheme (3.9) was generalized to two dimensions by using
an alternating direction method. They found that the
correct treatment of the singularity at the pole was
necessary to maintain stability. The order of the factors
in the A.D.I. method was also crucial for stability.
Williamson [200] has compared the effectiveness of high
order schemes for the primitive equations. He found that
the horizontal diffusion term had a greater effect than
the order of the scheme. The introduction of topography
further complicates the comparison since for realistic
grids large mountain chains are described by relativity
few grid points leading to large gradients in the vertical
variable.

Gadd [62] has suggested splitting the system into fast
and slow components and treating each separately with a
Lax-Wendroff method. This has the disadvantage of using a
dissipative method. It is possible to use a similar idea
with the leapfrog method by using two grids. The convective

terms are differenced on the fine grid while the right
hand side of (8.12) is differenced on a coarse grid but
with a compact fourth order method. The resulting
approximation to (8.12) is given by

$$
u_{i,j}^{n+1} = u_{i,j}^{n-1} - \lambda \left[u_{i,j}^{n} \left(u_{i+1,j}^{n} - u_{i-1,j}^{n} \right) \right.
$$

$$
\left. + v_{i,j}^{n} \left(v_{i,j+1}^{n} - v_{i,j-1}^{n} \right) \right]
$$

$$
- \frac{\lambda g}{p} \left(h_{i+p,j} - h_{i-p,j} \right)
$$

$$
+ \frac{\Delta t f}{3} \left(4 v_{i,j}^{n} + v_{i+p,j}^{n} + v_{i-p,j}^{n} \right) \quad ,
$$

$$
(8.14) \qquad v_{i,j}^{n+1} = v_{i,j}^{n-1} - \lambda \left[u_{i,j}^{n} \left(v_{i+1,j}^{n} - v_{i-1,j}^{n} \right) \right.
$$

$$
\left. + v_{i,j}^{n} \left(v_{i,j+1}^{n} - v_{i,j-1}^{n} \right) \right]
$$

$$
- \frac{\lambda g}{p} \left(h_{i,j+p} - h_{i,j-p} \right)
$$

$$
- \frac{\Delta t f}{3} \left(4 u_{i,j}^{n} + u_{i,j+p}^{n} + u_{i,j-p}^{n} \right) \quad ,
$$

$$h_{i,j}^{n+1} = h_{i,j}^{n-1} - \lambda \left[u_{i,j}^{n} \left(h_{i+1,j}^{n} - h_{i-1,j}^{n} \right) \right.$$

$$+ v_{i,j}^{n} \left(h_{i,j+1}^{n} - h_{i,j-1}^{n} \right) \Bigg]$$

$$- \frac{\lambda h_{i,j}^{n}}{p} \left[4 \left(u_{i+p,j}^{n} - u_{i-p,j}^{n} + v_{i,j+p}^{n} - v_{i,j-p}^{n} \right) \right.$$

$$+ u_{i+p,j+p}^{n} - u_{i-p,j+p}^{n} + u_{i+p,j-p}^{n} - u_{i-p,j-p}^{n}$$

$$\left. + v_{i+p,j+p} - v_{i+p,j-p} + v_{i-p,j+p} - v_{i-p,j-p} \right]$$

with $\lambda = \dfrac{\Delta t}{\Delta x} = \dfrac{\Delta t}{\Delta y}$.

An additional difficulty that occurs in meterology is due to the spherical coordinate system used for the globe. The coordinate singularity at the pole together with the convergence of the latitude lines at the poles forces an unrealistically small time step for explicit schemes. Many attempts at using other coordinate systems or patching several coordinate systems have not been very successful. To enable the use of larger time steps some smoothing algorithm is used near the poles to eliminate the higher frequencies. In figure (6.1) we display a contour map of h for the solution to the shallow water equations in spherical coordinates. This solution used 3 minute time steps and includes Fourier filtering near the poles (see [190], [199]). In figure (6.2) is shown a second graph using the scheme (8.14) together with

Fourier filtering. This allowed 7½ minute time steps.
A leap frog method without any filtering could use only
½ minute time steps with the grid used.

More realistic models are based on the primitive
equations and also contained many levels in the vertical
direction. Usually a pressure-like coordinate is used
in the vertical direction. Even though many calculations
have been performed with the primitive equations
Oliger and Sundström [147] have shown that the system is
not well-posed. Browning [26] has proposed a substitute
which is a proper limit of hyperbolic equations.

In volume 17 of *Methods of Computational Physics* a
variety of methods are presented for solving these equations.
Spectral, pseudospectral and finite element methods all
present advantages and disadvantages for large scale
problems. To date there has been little comparison of
these numerical techniques under real-life situations.

   e. Combustion

       The replacement of an ideal gas by a real gas
and the inclusion of chemical processes introduces
several new difficulties into the computation. Because
of the exponential dependence of the ignition on the
termperature it is critical that there be no overshoots
in the computation of shocks. False overshoots can ig-
nite the chemistry at entirely incorrect places and times
and completely invalidate the computation. As previously

mentioned one alternative is to introduce severe dissipa-
tion.   Anti-diffusion is later added to sharpen the
shock profile (see [18], [91], [191]). An additional
difficulty is the introduction of many new equations
when many chemical species are present. This is a parti-
cular difficulty for implicit methods as the work increases
with m^3 where m is the number of equations. In certain
cases Briley and McDonald [24] have shown that these
matrices can be simplified.

Since the flame occupies only a small region of the
computational domain it is necessary to introduce a fine
mesh which moves adaptively in time. Efficient ways of
changing the grid, especially for several space dimensions
are unknown. One way of moving the mesh for one space
dimension is given in [50]. An additional difficulty with
combustion problems is the stiffness of the ordinary
differential equations which describe the chemistry. This
necessitates much smaller time steps for the chemistry than
for the fluid dynamics. This can be partially alleviated
by using splitting techniques (section b) to split the
chemical and fluid dynamical portions of the calculation.

A different approach to these problems was introduced
by Chorin [38]. He extended a probabilistic method due
to Glimm [65] into a practical method. The random choice
method is based on _ne solution to many Riemann problems.
In each interval the solution is considered to consist of
two constant states with a discontinuity between them. The

solution is advanced to the next time level by analytically
solving this local Riemann problem and then choosing the
new constant state to be the solution evaluated at a random-
ly chosen point within the mesh. This method has the pro-
perty that the discontinuity is sharp (in a probabilistic
sense) without overshoots. Hence, there is no need for
artificial dissipation or a moving grid. A drawback of the
method is that it is at best first order accurate in the
smooth regions of the flow. Since convergence is guaranteed
only in a probabilistic sense accuracy for any given compu-
tation may be poor. This depends crucially on the choice
of sampling. It is expensive to calculate exactly the solu-
tion to a Riemann problem at every mesh point and each time
level. An alternative is to solve the Riemann problem with
a finite difference method [93]. This also has the advantage
that it easily generalizes to complex systems of equations.
The present extension to several dimensions is based on
splitting techniques. As this reduces the effectiveness of
the method other approaches are being investigated [66].
Sod [173] has compared this method with some finite difference
schemes for simple shock problems.

104

f. Plasma Physics

The simplest set of equations that describe a plasma are the ideal MHD equations developed by Lunquist [123]. These form a set of eight nonlinear symmetric hyperbolic equations. Grad [78] has shown that the full equations include all of standard fluid dynamics within a small range of parameter space in the MHD equations. Hence, all the difficulties discussed in the previous sections automatically occur in MHD. In order to make the problems manageable one can only treat simpler problems than those solved for the Navier-Stokes equations. This is even more true when more relevant equations, as the Vlasov or Fokker-Planck equations are considered. For these equations only one dimensional or simple geometries can be considered.

As a simple illustration we consider the steady state equations. For the Navier-Stokes equations we can solve the full system with the time derivatives set equal to zero. Some of these methods were described in section c and others are described in more detail by Hollanders and Viviand [101]. For ideal MHD even the case with no flow, i.e., $u = 0$, is nontrivial. In this case the equations become

$$\nabla p = \nabla \times \nabla \times B$$

(8.15)

$$\operatorname{div} B = 0 \qquad .$$

This system of four equations for p, B_x, B_y, B_z has two real and two imaginary characteristics. Hence, this is a mixed hyperbolic-elliptic system. For three dimensional systems in a torus it is not even clear that the differential system is well posed. By imposing additional constraints Betancourt and Garabedian [16], [9] have obtained solutions to (8.15) for three dimensional configurations. Brackbill [20] has obtained solutions by using the full time dependent MHD equations and marching to a steady state while removing kinetic energy so that $u = 0$ in the limit. It is obviously much more difficult to do the type of steady state calculations that are commonplace in aerodynamic flows.

In addition to the steady state, or equilibrium problems, one is also interested in the stability of the equilibrium. When one wishes to study nonlinear stability the main technique is to integrate the time dependent equations. As mentioned in section b one difficulty is introduced by the constraint $\text{div}\,B = 0$. If $\frac{\partial}{\partial t}\,\text{div}\,B$ is nonzero numerically it can introduce false sources of instability. Hence, stable equilibria can appear as unstable equilibria (see also [21], [142]).

For the time dependent equations there are three sound speeds known as the fast (or magneto-acoustic) speed, the Alfven speed and the slow speed (see e.g. [39]). Many of the instabilities in a torus occur at the Alfven speed which can be much smaller than the fast speed. Hence, we again face the

phenomena of different time scales. We wish to use time
steps based on the Alfven speed without sacrificing stability.
One approach is to use an implicit, alternating direction
method (see [122]). However, this requires the inversion of
block 8×8 tridiagonal matrices which is time consuming.
Plasma flow has the property that most of the change occurs
along magnetic flux surfaces and not across them. By using
flux surfaces on a coordinate system one can separate out
the fast and slower motions. Since the Alfven wave is
incompressible this can be used to set up a scheme which
uses time steps based on the Alfven speed (see [106]). The
main disadvantage is that the method fails when the flux
lines no longer provide a reasonable coordinate system.
Another approach is to use a semi-implicit method (Brackbill,
private communication) similar to that in section d. One
can now use a standard Eulerian or Lagrangian grid. The
size of the matrices to be inverted are severely reduced
while the time step is governed by the Alfven time step.

When considering non-ideal effects the major effect
is resistivity rather than viscosity. While this still
introduces parabolic terms nevertheless the physical
effects are quite different. It is well known that
resistivity can frequently cause instabilities that did
not exist in the ideal case [48]. As with the Navier-Stokes
it is necessary to resolve boundary layers where the
resistive effects are dominant. An additional difficulty
with plasma physics is the existence of a vacuum outside

the plasma. The magnetic field in the vacuum is governed
by an elliptic equation which must be couped with the time
dependent MHD equations across a moving interface. When
solving the plasma-vacuum problem Lagrangian type methods
or flux surface methods have been used. The Eulerian
methods usually represent the plasma as a low density plasma.

We have concentrated on the application of MHD to
magnetic controlled thermonuclear reactions. Another
application is to astrophysics. For these problems
radiation boundary conditions as described in chapter
7 are important. Another important area is laser fusion.
In this area the introduction of artificial boundaries
is also important. In addition, these problems frequently
have regions with extremely different properties as the
pellet is compressed. Hence, the methods must be capable
of handling changes in coefficients in the range of 15
orders of magnitude. Further discussion of methods for
plasma physics are given in [155] and also volume 16 of
Methods of Computational Physics.

g. Other Applications

In this brief survey we have shown some of the
difficulties that occur in specific applications.
Naturally this survey cannot cover all topics. One major
field which has not been discussed is two phase flow.
Aspects of that field are discussed by H. Wirz [203].

Another field which was touched on briefly in chapter 8
is acoustics. This includes such diverse fields as
seismology, underwater acoustics and jet acoustics. Each
of these present their own difficulties. In seismology
in particular one tends to use second order equations
rather than first order systems. The occurrence of
layered media introduces other difficulties. Both interior
and exterior ballistics provide problems with extreme dis-
tortion of materials. Due to the high pressures and tem-
peratures even metals deform. Hence, one cannot
integrate in a region with fixed boundaries. Instead,
the motion of the free surfaces and interfaces must be
calculated. An additional difficulty is the existence
of a plastic regime. For this regime the deviatoric
stresses remain on the yield surface, i.e.,
$\sum s_{i,j}^2 = K$. It is a nontrivial problem to enforce this
constraint numerically. A survey of numerical methods
in elastodynamics is given in [5].

One major field which has not been discussed is that
of incompressible flow. Discussion of finite difference
methods is given in a companion article by Krause [109]
(see also [61] and [185]). There has also been much work
in the application of finite element approaches to solving
the time dependent incompressible Navier-Stokes equations
(see e.g. [58], [25], [102]. Of particular note is the
recent use of grid-free methods. Chorin [37] used a method
based on the interaction of a finite number of vortices.

Combination grid-vortex methods have considered in [27], [127], and [167]. Peskin [153] has advocated the use of a Lagrangian grid free method. These codes have been used for many aeronautical purposes. The use of these codes for biological studies is complicated by the fact the boundaries which represent tissue material, are permeable [151]. The spectral methods can also be viewed as grid-free methods. Applications of spectral methods to incompressible flows are surveyed in [150]

Boundary layer computations have been dominated by the use of fourth order finite difference and finite element algorithms (e.g. [41], [107], [161], [196], [205]). A major difficulty in the practical use of these codes is the lack of sufficiently accurate turbulence models. Extensions of the mathematical models to detached and reverse flow is also being investigated [34]. The boundary layer equations are a parabolic system. Other parabolic problems include heat flow and diffusion problems. Diffusion problems are of major importance for such diverse fields as oil studies, plasma diffusion and biological processes.

Transonic flow calculations have been mainly based on the potential equation. Recent progress in the field has been presented in [204] and in the Proceedings of the Fourth AIAA Computational Fluid Dynamics Conference.

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