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COMPUTATIONAL ASPECTS OF GLIMM'S METHOD

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ABSTRACT

The application of Glimm's method to the equations of gas dynamics is considered. In particular, its advantages are discussed for situations in which chemical reactions occur in the gas.

Computational Aspects of Glimm's Method

by

Alexandre Joel Chorin

1. Introduction and general considerations.

In [9] Glimm introduced an approximate method for constructing solutions of systems of nonlinear hyperbolic conservation laws. This construction is the basis for his beautiful existence theorem in the large (with restrictions on the type of systems allowed and on the size and variation of the data). Some interesting generalizations of Glimm's proof have become available (see e.g. [7], [8], [11, [13]). Since 1965 there have been a number of attempts to use Glimm's construction as an computational tool, but they have not been brought to completion (or to publication), because it is quite clear that in most problems Glimm's construction is less accurate and more expensive than alternative methods. It has, however, turned out in the last few years that there are problems in which Glimm's construction is in fact very useful as a practical tool. These problems involve flow with multiple phases and/or chemical reactions, and the reasons for the usefulness of Glimm's method will become apparent in the course of the discussion. It also turns out that the method is being used under conditions where the assumptions in the available proofs are not satisfied, and a host of interesting open questions are in need of answers.

We begin by describing the method briefly. Consider the hyperbolic system of equations

$$\underline{v}_t = (\underline{f}(\underline{v}))_x, \quad \underline{v}(x,0) \quad \text{given}, \tag{1}$$

where $\underline{v}$ is the solution vector, and subscripts denote dif-

ferentiation. The time t is divided into intervals of length k. Let h be a spatial increment. The solution is to be evaluated at the points (ih,nk) and $((i+\frac{1}{2})h, (n+\frac{1}{2})k)$, $i = 0, \pm 1, \pm 2, \ldots$, $n = 1,2,\ldots$. Let $\underline{u}_i^n$ approximate $\underline{v}(ih,nk)$, and $\underline{u}_{i+1/2}^{n+1/2}$ approximate $\underline{v}((i+\frac{1}{2})h,(n+\frac{1}{2})k)$. The algorithm is defined if $\underline{u}_{i+1/2}^{n+1/2}$ can be found when $\underline{u}_i^n$, $\underline{u}_{i+1}^n$ are known. Consider the following Riemann problem:

$$\underline{v}_t = (f(\underline{v}))_x \ , \ t > 0, \quad -\infty < x < +\infty,$$

$$\underline{v}(x,0) = \begin{cases} \underline{u}_{i+1}^n & \text{for} \quad x \geqslant 0, \\ \underline{u}_i^n & \text{for} \quad x < 0. \end{cases}$$

Let $\underline{x}(x,t)$ denote the solution of this problem. Let θ_i be a value of a variable θ, $-\frac{1}{2} \leqslant \theta \leqslant \frac{1}{2}$. Let P_i be the point $(\theta_i h, \frac{k}{2})$, and let

$$\tilde{\underline{w}} = \underline{w}(P_i) = \underline{w}(\theta_i h, \tfrac{k}{2})$$

be the value of the solution $\underline{w}$ of the Riemann problem at P_i. We set

$$\underline{u}_{i+1/2}^{n+1/2} = \tilde{w}.$$

In other words, at each time step, the solution is first approximated by a piecewise constant function; it is then advanced in time exactly, and new values on the mesh are obtained by sampling.

It is clear that the applicability of the method depends on one's ability to find appropriate allowable solutions of the Riemann problem. The systems under consideration in practice are simplified versions of very complex systems; the omitted equations or terms survive in the form of algebraic constraints on the allowable waves. These constraints define what is allowable. It is one of the major attractions of Glimm's method that it allows one to impose the appropriate constraints with elegant ease.

The rate of convergence of the method (i.e. the error as a function of k and h) depends on how judiciously the θ's are chosen. The θ's must tend to equipartition on $[-1/2, 1/2]$. Various strategies for choosing the θ's are described in [2]; they lead to a method which is almost of first order accuracy. It is clear that the method cannot be more accurate than first order, since, depending on the choice of θ, a value of the solution may become attached to either one of two neighboring points. A more important quantity is the resolution of the method, i.e. its ability to conserve information above waves and their interactions without smoothing. It is shown in [2] that the method has high resolution under conditions where its natural competitors are fitting methods, i.e. methods which treat discontinuities as if they were internal boundaries.

2. Glimm's method in gas dynamics.

I intend to explain in some detail how Glimm's method is used in the analysis of reacting gas flow in one dimension. As a first step, we discuss the flow of chemically inert polytropic gas. The equations of motion are

$$\rho_t + (\rho v)_x = 0 \tag{2a}$$

$$(\rho v)_t + (\rho v^2 + p)_x = 0 \tag{2b}$$

$$e_t + ((e + p)v)_x = 0 \tag{2c}$$

where ρ is the density of the gas, v is its velocity, p is the pressure and e is the energy per unit volume; we have

$$e = \rho\varepsilon + \tfrac{1}{2}\rho v^2 \tag{2d}$$

where ε, the internal energy per unit mass, is given by

$$\varepsilon = \frac{1}{\gamma-1}\frac{p}{\rho} \tag{2e}$$

where $\gamma > 1$ is a constant. Glimm's method rests on the solution of the Riemann problem for these equations. Its convergence has been studied in [12] under the assumption

that the data have small variation.

Given a right state $S_r(\rho_r, p_r, v_r, e_r)$ and a left state $S_\ell(\rho_\ell, p_\ell, v_\ell, e_\ell)$, the solution of the Riemann problem consists of, from right to left: The right state S_r, a right wave which either a shock or a rarefaction, a middle right state S_{*r}, a slip line across which p and v (but not necessarily ρ or e) are continuous, a middle left state $S_{*\ell}$, a left wave which is either a shock or a rarefaction, and the left state S_ℓ. Let p_{*r} (resp. $p_{*\ell}$) be the pressure in S_{*r} (resp. $S_{*\ell}$). If $p_{*r} \leq p_r$ the right wave is a rarefaction, and if p_{*r} is known, S_{*r} can be determined from S_r, p_{*r}, the constancy of the appropriate Riemann invariant, and the isentropic equation of state. If $p_{*r} > p_r$ the right wave is a shock. The well-known fact that a shock is supersonic with respect to gas in front of it and subsonic with respect to the gas behind it is in fact the condition which ensures that S_{*r} behind a shock can be uniquely determined if S_r and p_{*r} are known. This can be readily seen by drawing and counting the characteristics entering the shock, see e.g. [6]. Similar considerations apply to the determination of $S_{*\ell}$ when $p_{*\ell}$ and S_ℓ are given. The condition $p_{*r} = p_{*\ell}$ ensures that the number of equations equals the number of unknowns. The resulting system of equations has a unique real solution, and can be solved e.g. by Godunov's iteration ([10], see also [14], [1], [2]).

Boundary conditions in a mixed initial value boundary value problem are readily imposed once it is noticed that the slip line separates the fluid initially to its right from the fluid initially to its left. One then designs Riemann problems at the walls in which the slip line has the appropriate velocity (see e.g. [3]). These considerations completely define Glimm's method for a one dimensional inert gas.

3. Glimm's method and the Riemann solution for nonconducting rapidly reacting gas.

We now consider the flow of a gas in which chemical reactions are taking place very rapidly and the heat con-

duction and viscosity are zero. The equations of motion are

$$\rho_t + (\rho v)_x = 0 \tag{3a}$$

$$(\rho v)_t + (\rho v^2 + p)_x = 0 \tag{3b}$$

$$e_t + ((e + p)v)_x = 0 \tag{3c}$$

$$e = \rho\varepsilon + \tfrac{1}{2}\rho v^2 \tag{3d}$$

as in (2), but now

$$\varepsilon = \varepsilon_i + q \tag{3e}$$

where ε_i is the interval energy per unit mass,

$$\varepsilon_i = \frac{1}{\gamma_0 - 1}\frac{p}{\rho} \quad \text{for unburned gas,} \tag{3f}$$

$$\varepsilon_i = \frac{1}{\gamma_1 - 1}\frac{p}{\rho} \quad \text{for burned gas,} \tag{3g}$$

and q is the energy of formation which can be released through chemical reaction, $q = q_0$ for unburned gas, $q = q_1$ for burned gas. If the chemical reaction is exothermic (i.e. gives out heat) and $\gamma_1 = \gamma_0$, then $\Delta = q_1 - q_0 < 0$. We shall assume that $\gamma_1 = \gamma_0 = \gamma$ to reduce the amount of writing.

The chemical reaction is assumed to occur very fast, and the reaction zone is idealized a s a discontinuity. The jump condition across a discontinuity can be readily derived (see e.g. [6]), and some manipulation leads to the following identities:

$$-M = \rho_1(v_1 - U) = \rho_0(v_0 - U), \tag{4a}$$

$$M^2 = -\frac{p_0 - p_1}{\tau_0 - \tau_1}, \tag{4b}$$

and

$$2\mu^2 H = p_0(\tau_0 - \mu^2\tau_1) - p_1(\tau_1 - \mu^2\tau_0) - 2\mu^2\Delta, \tag{4c}$$

where $\tau \equiv 1/\rho$, the index 0 refers to unburned gas, the index 1 refers to burned gas, $\mu^2 = \frac{\gamma-1}{\gamma+1}$, and U is the velocity of the discontinuity. Equation (4c) describes the locus of states (τ_1,p_1) which can be connected to (τ_0,p_0) by an infinitely thin reaction zone with energy release Δ. (See Fig. 1). The curve $H = 0$ is called the Hugoniot curve. The lines through (τ_0,p_0) tangent to $H = 0$ are called the Rayleigh lines and the points of tangency S_1 and S_2 are called the Chapman-Jouguet (CJ) points.

One portion of the Hugoniot curve is omitted because it would yield complex values of M (equation (4b))-clearly an impossibility. The upper branch of the curve is called the detonation branch; the part above S_1 the strong detonation branch, the part below S_1 the weak detonation branch. The lower part of the curve is the deflagration (or flame) branch. The gas burns if the temperature $T = p/\rho$ reaches a value above a critical temperature ("ignition temperature") T_c. This burning is irreversible and occurs at most once for each fluid particle.

Consider a right state $S_r(\rho_r,p_r,v_r,e_r)$ in which the gas is not burned, i.e. $q = q_0$, and consider the states S to which it can be connected by a shock, a rarefaction, or a reaction zone. If $T = p/\rho$ in S is such that no burning occurs, then we are back in the situation of the preceding section, and a knowledge of the pressure p in S will determine S. Suppose T in S is such that burning does occur. If p in S is given and is above the pressure in the Chapman-Jouguet state S_1, one can show that the geometry of the characteristics is such that p in S and S_r will determine S, as would have been the case with a shock. However, if p in S is below p in S_1 the situation is more complex. Weak detonations more more rapidly then the sound speed behind them (see [6]) and the state behind them is undetermined. Fortunately, one can show that weak detonations do not occur if the energy release is due to a chemical reaction in which the proportion of fuel burned remains between 0 and 100%. What can occur is a CJ detonation. The velocity of CJ detonation S_1 equals the speed of sound behind it, and it can thus be

followed by a rarefaction. S_1 is entirely determined by S_r, and if p in S is given, it determines S by connecting it to S_1 by a rarefaction ([6], [2]).

One can further show that in the absence of heat conduction the only deflagration which can occur is one across which p is constant and there is no mass flow -- i.e., such a deflagration is indistinguishable from a slip line (see e.g. [2]). Thus, the Riemann problem for equations (3) can be reduced to the Riemann problem for an inert gas, as long as one allows the right and left waves to be not only rarefactions or shocks, but also strong detonations or CJ detonations followed by rarefactions. A shock is the special case of a strong detonation with $\Delta = 0$, and a CJ detonation followed by a rarefaction is merely a rarefaction connected to a state S_1 entirely determined by either S_r on the right or S_ℓ on the left. Godunov's algebraic iteration procedure for solving the Riemann problem easily generalizes to the reacting case ([2]).

It is interesting to note that the elimination of parts of the Hugoniot curve by physical constraints, which makes the Riemann problem determinate, has a strong qualitative resemblance to the procedures used to define an appropriate Riemann solution for problems of the form $u_t + f_x$, where f is a non-convex function of u (see e.g. [7]), or to gas flow problems where the gas has a nonconvex equation of state ([16]).

Furthermore, the discussion just given should put in evidence some of the practical advantages of Glimm's method. Consider a problem whose solution consists of a CJ detonation followed by a rarefaction moving down a tube. The velocity and pressure profiles in such a wave are not monotonic, and may contain a very sharp spike at the detonation. Such a wave is very difficult to describe by a finite difference method, but will be described nearly perfectly by Glimm's method.

4. Reacting gas flow with heat conduction and finite rate chemistry.

We now consider how the method just described can be generalized to the case of flow with realistic chemistry and

finite heat conduction. Finite heat conduction is important since one of the main mechanisms of flame (deflagration) propagation is the conduction of heat which ignites new fluid (the other major mechanism is the diffusion of chemical species which can be treated by similar methods but which we shall not consider here). The full equations which describe the flow are enormously complex (see e.g. [17]) and must be simplified before they can be used or else the calculation becomes prohibitively expensive and the results impossible to interpret. An appropriate simplified model is:

$$\rho_t + (\rho v)_x = 0 \tag{5a}$$

$$(\rho v)_t + (\rho v^2 + p)_x = 0 \tag{5b}$$

((5a,b) are identical to (3a,b)),

$$e_t + ((e + p)v)_x - \lambda T_{xx}, \quad T = p/\rho \ , \tag{5c}$$

$$e = \rho\varepsilon + \tfrac{1}{2}\rho v^2, \tag{5d}$$

$$\varepsilon = \frac{1}{\gamma-1}\frac{p}{\rho} + Zq, \quad 0 \leqslant Z \leqslant 1, \tag{5e}$$

$$Z = Z(\underline{s}), \ \gamma = \gamma(\underline{s}), \ \underline{s} = (s_1,\ldots,s_n), \tag{5f}$$

$$\frac{d\underline{s}}{dt} = G(T,\underline{s}) \tag{5g}$$

where λ is the heat conduction, q is the total available chemical energy, Z is the fraction of energy still not released, and equation (4f) and (5g) express the fact that Z is a function of the progress of a chemical reaction which is described by a suitable kinetic scheme. A simple model of (5f), (5g) is the set of equations

$$\frac{dZ}{dt} = -KZ, \qquad \gamma = \text{constant},$$

where $K = 0$ if $T = p/\rho \leqslant T_0$, $K = K_0 = \text{constant} > 0$ if $T > T_0$. K_0 is the reaction rate and T_0 is the ignition temperature. If λ is not very small and K_0 is not very

large, the added equations can be handled by a standard fractional step procedure and taken outside the Riemann problem. However, if λ is very small and K_0 is large one has to find a suitable approximate Riemann solution which takes their effects into account.

The remarkable fact is that this can be done; it can be done most economically by making the following approximations: in the case of a detonation of finite structure, the state behind the detonation is the CJ state. In a case of a deflagration, there is no change of pressure across the deflagration. These approximations are in fact in very good agreement with experimental fact and with the relevant theory, and allow one to use the construction of the preceding section almost without change. For details, see e.g. [4], [15]. As a result, Glimm's method is capable of handling flows which contain hydrodynamic effects and chemical effects of widely different time scales.

For another type of application of Glimm's method, see [5].

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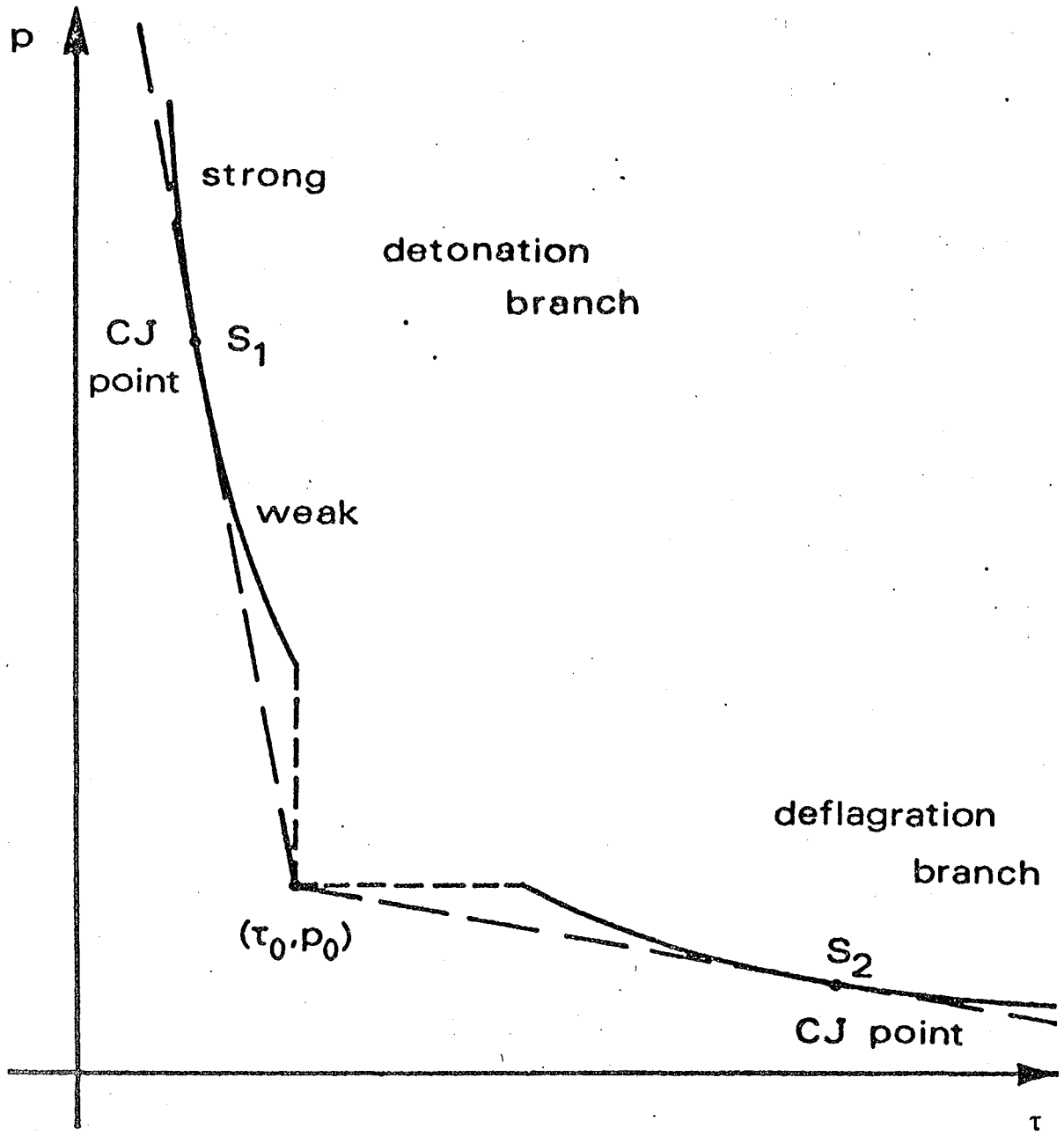

Fig. 1

The Hugoniot Curve

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