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THE ACOUSTIC MODE IN NUMERICAL CALCULATIONS OF SUBSONIC COMBUSTION

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Resume - Cet article presente une revue des methodes pour le traitment des modes acoustiques dans les simulations numeriques de la combustion subsonique.

Abstract - A review is given of the methods for treating the acoustic mode in numerical calculations of subsonic combustion.

I. INTRODUCTION

In numerical calculations of subsonic combustion, treatment of the acoustic mode has been a problem for many researchers. It is widely believed that Mach number and acoustic wave effects are negligible in many subsonic combustion problems. Yet, the equations that are often solved contain the acoustic mode, and many numerical techniques for solving these equations are inefficient when the Mach number is much smaller than one.

This paper reviews two general approaches to ameliorating this problem. In the first approach, equations are solved that ignore acoustic waves and Mach number effects. Section II of this paper gives two such formulations which are called the Elliptic Primitive and the Stream and Potential Function formulations. We tell how these formulations are obtained and give some advantages and disadvantages of solving them numerically.

In the second approach to the problem of calculating subsonic combustion, the fully compressible equations are solved by numerical methods that are efficient, but treat the acoustic mode inaccurately, in low Mach number calculations. Section III of this paper introduces two of these numerical methods in the context of an analysis of their stability properties when applied to the acoustic wave equations. These are called the ICE[1] and acoustic subcycling[2] methods. It is shown that even though these methods are more efficient than traditional methods for solving subsonic combustion problems, they still can be inefficient when the Mach number is very small. Finally, a method called Pressure Gradient Scaling[3] is described that, when used in conjunction with either the ICE or acoustic subcycling methods, allows for very efficient numerical solution of subsonic combustion problems.

II. THE EQUATIONS OF SUBSONIC COMBUSTION

We first give the primitive equations of motion for a laminar flow of chemically reactive ideal gases.[4] The continuity equation of species k is

$$\frac{\partial \rho_k}{\partial t} + \underline{\nabla} \cdot \left[\rho_k (\underline{u} + \underline{V}_k) \right] = W_k \sum_{\ell} \dot{\omega}_\ell (\nu''_{k,\ell} - \nu'_{k,\ell}) \quad , \tag{1}$$

where ρ_k is the mass density of species k, $\underline{u}$ is the mixture mass-average velocity, $\underline{V}_k$ is the velocity of species k relative to $\underline{u}$, W_k is the molecular weight of species k, $\dot{\omega}_\ell$ is the reaction rate of reaction ℓ, and $\nu''_{k,\ell}$ and $\nu'_{k,\ell}$ are the backward and forward stoichiometric coefficients of species k in reaction ℓ. The specific forms of $\underline{V}_k$ and $\dot{\omega}_\ell$ will not concern us in this paper.

The mixture momentum equation is

$$\frac{\partial \rho \underline{u}}{\partial t} + \underline{\nabla}\cdot(\rho \underline{u}\underline{u}) + \underline{\nabla} p = \underline{\nabla}\cdot\underline{\underline{\sigma}} + \rho \underline{g} \quad . \tag{2}$$

The mixture density ρ is obtained from

$$\rho = \sum_k \rho_k \quad . \tag{3}$$

In Eq. (2) p is the static pressure, $\underline{\underline{\sigma}}$ is the viscous stress tensor, and $\underline{g}$ is the body acceleration on the fluid. The specific form of $\underline{\underline{\sigma}}$ will not concern us.

The mixture internal energy equation is

$$\frac{\partial \rho e}{\partial t} + \underline{\nabla}\cdot(\rho \underline{u} e) + p\underline{\nabla}\cdot\underline{u} = \underline{\underline{\sigma}}:\underline{\nabla}\underline{u} - \underline{\nabla}\cdot\underline{q} - \underline{\nabla}\cdot\left(\sum_k \rho_k \underline{V}_k h_k\right) \quad . \tag{4}$$

In Eq. (4), e is the internal energy (thermal plus chemical), $\underline{q}$ the heat flux vector (exclusive of enthalpy diffusion), and h_k is the enthalpy of species k.

The temperature T, pressure, and densities are related through the equations of state

$$p = \sum_k (\rho_k / W_k) R_o T \tag{5}$$

and

$$\rho e = \sum_k \rho_k \left[h_k(T) - R_o T / W_k\right] \quad , \tag{6}$$

where R_o is the universal gas constant.

The primitive Eqs. (1)-(6) apply to physical regimes that are not of interest in many combustion problems. They apply to flows of arbitrary Mach number, and their solutions have acoustic waves. In many combustion problems, the Mach numbers are small compared to unity, and it is widely believed that acoustic wave effects are negligible. The following question then arises: can we find a formulation of the equations that is specialized to low Mach number flows without acoustic waves and that is simpler and easier to solve numerically? This is really two questions. The answer to the first is that special formulations have been obtained for subsonic combustion problems. The answer to the second is that one can usually solve numerically the primitive equations as easily and inexpensively as any specialized formulation. The remainder of Section II will

give two subsonic formulations; in Section III we give reasons for our answer to the second question above.

A. The Elliptic Primitive Formulation

The first low Mach number formulation we call the Elliptic Primitive (EP) formulation. We first give the equations and then indicate how they are obtained. In this formulation, the momentum equation is slightly modified:

$$\frac{\partial \rho \underline{u}}{\partial t} + \underline{\nabla}\cdot(\rho \underline{u}\underline{u}) + \underline{\nabla} p' = \underline{\nabla}\cdot\underline{\underline{\sigma}} + \rho \underline{g} \quad . \tag{7}$$

The quantity p' is the pressure fluctuation about a mean value $\bar{p}$, which is spatially uniform. Solution for p' is an elliptic problem whose explicit form we will give later. An important feature of the EP formulation is that p' is uncoupled from the equation of state pressure:

$$\bar{p} = \sum_k (\rho_k / W_k) R_o T \quad . \tag{8}$$

Another important feature of the EP formulation is that an equation for the divergence of the velocity field is used.

$$\underline{\nabla}\cdot\underline{u} = -\frac{1}{\gamma \bar{p}} \frac{d\bar{p}}{dt} - \frac{\gamma - 1}{\gamma \bar{p}} \left[\underline{\nabla}\cdot\underline{q} + \sum_\ell \dot{\omega}_\ell \Delta h_\ell(T) + \sum_k \rho_k \underline{V}_k c_{p_k} \cdot \underline{\nabla} T \right]$$

$$+ \frac{\bar{W}}{\rho} \left[\sum_{k,\ell} \dot{\omega}_\ell (\nu''_{k,\ell} - \nu'_{k,\ell}) - \sum_k \underline{\nabla}\cdot(\rho_k \underline{V}_k / W_k)' \right] \quad , \tag{9}$$

where

$$\gamma = c_p / c_v = \frac{\sum_k Y_k c_{p_k}}{\sum_k Y_k (c_{p_k} - R_o / W_k)} \quad , \tag{10}$$

$$Y_k = \rho_k / \rho \quad , \tag{11}$$

$$c_{p_k} = \frac{dh_k}{dT} \quad , \tag{12}$$

$$\Delta h_\ell(T) = \sum_k h_k(T) W_k (\nu''_{k,\ell} - \nu'_{k,\ell}) \quad , \tag{13}$$

and

$$\bar{W} = 1 / \sum_k (Y_k / W_k) \quad . \tag{14}$$

From Eq. (9), the divergence $\underline{\nabla}\cdot\underline{u}$ can be non-zero because of changes in the mean pressure $\overline{p}$, because of local heat addition due to chemical reactions or heat and mass diffusion, or because of changes in the local mean molecular weight.

To determine how the mean pressure $\overline{p}$ changes, we must know the boundary conditions in our particular problem. In many cases combustion occurs in an open atmosphere, and we can assume

$$\overline{p} = \text{constant} \quad . \tag{15a}$$

When combustion occurs in an enclosure whose volume V is changing in time, then an equation for $\overline{p}$ is obtained by integrating Eq. (9) over the volume V:

$$\frac{1}{\overline{p}}\frac{d\overline{p}}{dt}\iiint_V \frac{1}{\gamma}\,d\underline{x} = -\frac{dV}{dt} + \iiint_V \left\{\frac{\overline{W}}{\rho}\left[\sum_{k,\ell}\dot{\omega}_\ell(\nu''_{k,\ell} - \nu_{k,\ell}) - \sum_k \underline{\nabla}\cdot(\rho_k\underline{V}_k/W_k)\right]\right.$$

$$\left. - \frac{\gamma-1}{\gamma\overline{p}}\left[\underline{\nabla}\cdot\underline{q} + \sum_\ell \dot{\omega}_\ell\Delta h_\ell(T) + \sum_k \rho_k\underline{V}_k c_{p_k}\cdot\underline{\nabla}T\right]\right\}d\underline{x} \quad . \tag{15b}$$

In the EP formulation, Eqs. (1), (7), (8), (9), and (15) are used.

To obtain the EP equations from the primitive equations, two assumptions are needed. First, we assume that the pressure solution p of the primitive equations can be decomposed into the sum of mean and fluctuating parts:

$$p = \overline{p}(t) + p''(\underline{x},t) \quad ,$$

where $|p''| \ll \overline{p}$. The fluctuation p'' differs from p' because acoustic pressure fluctuations are contained in it. Second, we assume that the solution changes negligibly when those terms in Eqs. (1)-(6) of relative order $|p''|/\overline{p}$ are neglected. These are the $p''\underline{\nabla}\cdot\underline{u}$ term in the energy equation (4) and the p'' term in Eq. (5). To obtain Eq. (9), one first derives the temperature equation from Eq. (4) using Eqs. (1) and (6), and then eliminates the substantial derivative of the temperature, DT/Dt, from this equation using Eq. (8). In this derivation, the viscous dissipation term $\underline{\underline{\sigma}}:\underline{\nabla}\underline{u}$ in Eq. (4) is neglected because it is negligibly small in subsonic combustion problems.

The assumption that $|p''| \ll \overline{p}$ is usually valid for subsonic combustion since we usually have

$$|p''|/\overline{p} = M^2$$

where M is the Mach number.[4] The validity of the second assumption, that we can neglect terms of relative order $|p''|/\overline{p}$, is problem-dependent. By neglecting these terms, we eliminate the acoustic mode from the equations. In many combustion problems, it is widely believed that acoustic waves are unimportant, but in some problems it is known that they are responsible for ignition or enhanced combustion rates.

An EP formulation was first used by Ramshaw and Trapp[5] in a two-phase flow application. An EP formulation for combustion was given, though not numerically solved, in Ref. 6. Paolucci and Chenoweth[7] have solved the EP equations numerically in two-dimensional combustion problems.

The biggest advantage to solving the EP equations occurs in one-dimensional problems. Here one usually knows the velocity at one or both boundaries, and the complete velocity field can be found from Eq. (9), which is easy to solve in one-dimension. Additional advantages of the EP formulation are that Eq. (6) need not be solved and that one need not account for the viscous dissipation terms.

It is sometimes fallaciously stated that the EP equations are to be preferred to the primitive equations for subsonic combustion problems, because numerical solutions of the primitive equations, in contrast to those for the EP equations, must satisfy the Courant sound speed restriction on the magnitude of the computational time step.[8] This restriction is that

$$\frac{c\delta t}{\delta x} \leq 1 \quad , \tag{16}$$

where c is the isentropic speed of sound and δt and δx are the computational time step and cell size. In subsonic combustion problems, Eq. (16) restricts δt to be intolerably small in comparison to problem times of interest. The fact is, however, that there are numerical methods for solving the primitive equations for which the restriction Eq. (16) is not necessary. This will be shown later.

In addition to the previously stated disadvantage that it ignores acoustic wave and compressibility effects, the EP formulation has two other disadvantages. The energy equation in the primitive equations can be formulated and finite-differenced in conservative form.[8] Because the EP formulation does not have an energy equation, this possibility is forsaken. Conserving energy in numerical calculations of combustion is important because it helps ensure that correct flame temperature, and hence accurate chemical reaction rates, are calculated. The second disadvantage is that solution for p' is an elliptic problem, and finite difference approximations to elliptic equations must usually be solved by time-consuming iterative procedures. As we shall see in Section III, the use of iterative procedures is also necessary for solving the difference approximations of one numerical method for the primitive equations.

B. Stream and Potential Function Formulation

In the second low Mach number formulation, the stream function and vorticity equations for constant density flows,[8] are generalized to apply to subsonic combustion. Since $\nabla \cdot \underline{u}$ is non-zero in combustion problems, there is not a stream function $\underline{\psi}$ such that $\nabla \times \underline{\psi} = \underline{u}$. The velocity $\underline{u}$ can nevertheless be expressed as the sum of a solenoidal part $\nabla \times \underline{\psi}$ and an irrotational part $\nabla\phi$, where $\underline{\psi}$ and ϕ are called stream and potential functions. Thus we call the second low Mach number formulation the stream and potential (SAP) function formulation.

In the SAP formulation, Eqs. (1), (8), (9), and (15) are retained, but the right-hand side of Eq. (9) is set equal to a scalar D. The velocity field is obtained from

$$\underline{u} = \nabla\phi + \nabla \times \underline{\psi} \quad , \tag{17}$$

where the potential function ϕ and stream function $\underline{\psi}$ are obtained by solving

$$\nabla^2\phi = D \tag{18}$$

and

$$\underline{\nabla} \times (\underline{\nabla} \times \underline{\psi}) = \underline{\omega} \quad , \tag{19}$$

where $\underline{\omega}$ is the vorticity. The vorticity equation is obtained by taking the vector curl of the equation for $\frac{\partial \underline{u}}{\partial t}$ derived from Eq. (7):

$$\frac{\partial \underline{\omega}}{\partial t} + \underline{\nabla}\cdot(\underline{u}\underline{\omega}) + \underline{\nabla} \times \left(\frac{1}{\rho}\,\underline{\nabla}p'\right) = \underline{\nabla}\cdot(\underline{\omega}\underline{u}) + \nabla \times \left(\frac{1}{\rho}\,\underline{\nabla}\cdot\underline{\underline{\sigma}}\right) \quad . \tag{20}$$

Finally, we must have an equation for p'. This is obtained by taking the divergence of the equation for $\frac{\partial \underline{u}}{\partial t}$:

$$\underline{\nabla}\cdot\left(\frac{1}{\rho}\,\underline{\nabla}p'\right) = -\frac{\partial D}{\partial t} - \underline{u}\cdot\underline{\nabla}D - \underline{\underline{\nabla u}}:\underline{\underline{\nabla u}}^{T} + \underline{\nabla}\cdot\left(\frac{1}{\rho}\,\underline{\nabla}\cdot\underline{\underline{\sigma}}\right) \quad , \tag{21}$$

where the superscript T denotes the transpose. Equation (21) is the elliptic equation for p' to which we have referred earlier.

The SAP equations have been used by Jones and Boris in their "slow flow" method.[9] It is the object of discrete vortex methods[10,11] to solve the SAP equations in the high Reynolds number limit, although these discrete methods are not yet usable for practical combustion problems because they ignore the term $\underline{\nabla} \times \left(\frac{1}{\rho}\,\underline{\nabla}p'\right)$ in the vorticity equation.

The advantage of the SAP formulation is that a vorticity equation is solved. In many problems, vorticity is confined to thin sheets or small subregions of the flow fields, and thus particle methods for solving Eq. (20) become very attractive because these have very little numerical diffusion and can provide high resolution where it is needed.[10,11] A disadvantage of the SAP equations is that in general three elliptic equations must be solved — Eqs. (18), (19), and (21).

III. NUMERICAL METHODS FOR THE PRIMITIVE EQUATIONS

This section is devoted to elaborating the statement of Section II that the primitive equations can usually be solved numerically as easily and inexpensively as the subsonic flow formulations. First, we perform a linear stability analysis of some common finite difference approximations to the acoustic wave equations. The analysis is done in order to introduce numerical methods for solving Eqs. (1)-(6) that allow one to circumvent the Courant sound speed restriction Eq. (16). We next show that these methods can become more inefficient as the Mach number is reduced, and we describe a method called Pressure Gradient Scaling (PGS) for improving the efficiency of low Mach number calculations. The main idea of the PGS method is that the Mach number can be increased in very low Mach number problems, improving computational efficiency without changing solu-

Eqs. (1)-(6) have the acoustic mode, is exploited in an efficient method that is not available for the EP or SAP formulations.

A. A Class of Numerical Methods for the Acoustic Equations

Consider a one-dimensional disturbance to an otherwise uniform fluid that is inviscid and non-reactive. Then Eqs. (1)-(6) have solutions that approximately satisfy the acoustic equations

$$\frac{\partial \rho'}{\partial t} + \rho_o \frac{\partial u}{\partial x} = 0$$

and (22)

$$\rho_o \frac{\partial u}{\partial t} + c_o^2 \frac{\partial \rho'}{\partial x} = 0 \quad ,$$

where $\rho = \rho_o + \rho'$ and $c_o^2 = \gamma \frac{R}{W} T_o$, ρ_o and T_o being the density and temperature of the undisturbed fluid. For the initial conditions

$$\rho'(x,o) = A\rho_o e^{ikx}$$

$$u(x,o) = Bc_o e^{ikx} \tag{23}$$

of a disturbance of wavelength $L = \frac{2\pi}{k}$, the solution to Eq. (22) is

$$\rho'(x,t) = \rho_o \left[\frac{A+B}{2} e^{ik(x-c_o t)} + \frac{A-B}{2} e^{ik(x+c_o t)} \right]$$

$$u(x,t) = c_o \left[\frac{A+B}{2} e^{ik(x-c_o t)} - \frac{A-B}{2} e^{ik(x+c_o t)} \right] \quad . \tag{24}$$

The general solution of the linear system Eqs. (22) is found by summing solutions of the form Eqs. (24) over all wavenumbers k. The solutions Eqs. (24) have the property that they have constant amplitudes and speeds c_o. In contrast, we shall see that in finite difference solutions to Eqs. (22), waves are both damped and travel with wavelength-dependent speeds (dispersion).

To implement numerical solution of Eqs. (22), we subdivide the computational region into a mesh of cells of uniform size δx. In the class of methods we consider, we employ a staggered mesh in which the densities and velocities are located a distance $\delta x/2$ apart. Thus we let $(\rho')_j^n$ and $u_{j+1/2}^n$ denote the computed approximations to $\rho'(j\delta x, n\delta t)$ and $u((j+1/2)\delta x, n\delta t)$, where δt is the computational time step. To calculate the values of $(\rho')_j^{n+1}$ and $u_{j+1/2}^{n+1}$ from known values at time $n\delta t$, we use the following finite difference approximations to Eq. (22):

$$\frac{(\rho')_j^{n+1} - (\rho')_j^n}{\delta t} + \rho_o \left[\theta \frac{u_{j+1/2}^{n+1} - u_{j-1/2}^{n+1}}{\delta x} + (1 - \theta) \frac{u_{j+1/2}^{n} - u_{j-1/2}^{n}}{\delta x} \right] = 0$$

$$\frac{u_{j+1/2}^{n+1} - u_{j+1/2}^{n}}{\delta t} + \frac{c_o^2}{\rho_o} \left[\phi \frac{(\rho')_{j+1}^{n+1} - (\rho')_j^{n+1}}{\delta x} + (1 - \phi) \frac{(\rho')_{j+1}^{n} - (\rho')_j^{n}}{\delta x} \right] = 0 \quad . \tag{25}$$

The parameters θ and ϕ, which can have values between 0 and 1, are used to vary the level of time-advancement of the finite difference approximations to the spatial derivatives. When θ and ϕ are both zero, the numerical scheme is purely explicit - that is, $(\rho')_j^{n+1}$ and $u_{j+1/2}^{n+1}$ are known explicitly in terms of calculated values of ρ' and u at time $n\delta t$. When θ and ϕ are both unity, the scheme is implicit, and $(\rho')_j^{n+1}$ and $u_{j+1/2}^{n+1}$ must be solved for implicitly from equations that couple their values at neighboring spatial points.

Numerical solutions of Eqs. (25) can again be found for the Fourier components. Substituting the values

$$(\rho')_j^n = A^n \rho_o \exp [ikj\delta x]$$

and

$$u_{j+1/2}^n = B^n c_o \exp [ik(j + 1/2)\delta x] \tag{26}$$

into Eqs. (25) and solving for A^{n+1} and B^{n+1} gives

$$\begin{pmatrix} A^{n+1} \\ B^{n+1} \end{pmatrix} = \begin{pmatrix} \frac{1 + a^2\theta(1 - \phi)}{1 - a^2\theta\phi} & \frac{a}{1 - a^2\theta\phi} \\ \frac{a}{1 - a^2\theta\phi} & \frac{1 + a^2\phi(1 - \theta)}{1 - a^2\theta\phi} \end{pmatrix} \begin{matrix} A^n \\ B^n \end{matrix} \tag{27}$$

where

$$a = -2iC \sin \psi/2 \quad ,$$

$$C = \frac{c_o \delta t}{\delta x}$$

is the Courant number, and

$\psi = k\delta x$

is the dimensionless wavenumber. The numerical solutions will be stable if and only if both eigenvalues of the above matrix have magnitudes less than or equal unity.

We examine the question of stability for three different cases. Case I is the fully-explicit scheme in which $\theta = \emptyset = 0$. For this case we find that both eigenvalues have magnitudes equal to $(1 + 4C^2 \sin^2 \psi/2)^{1/2}$, and thus all wavelengths are unstable. Case II is the fully-implicit scheme in which $\theta = \emptyset = 1$. Here we find that both eigenvalues have magnitudes $(1 + 4C^2 \sin^2 \psi/2)^{-1/2}$, and thus this scheme is unconditionally stable--that is, it is stable for all values of C. Case III is the numerical scheme with $\theta = 1$ and $\emptyset = 0$ (or $\theta = 0$ and $\emptyset = 1$). In this case we find that if $C \sin \psi/2 \leq 1$ then both eigenvalues have magnitudes equal to unity, but if $C > 1$ then the wavelength $L = 2\delta x$ is unstable. This is the shortest wavelength resolvable by the computational mesh. Thus in Case III we have an example of scheme for which the Courant condition must be satisfied for stability.

Case II corresponds to the ICE method.[1] In this method fully-implicit differencing is used for the pressure gradient term in Eq. (2) and the terms associated with dilatation of the velocity field in Eqs. (1) and (4). The result is a scheme for which the Courant condition [Eq. (16)] need not be observed. As can be seen from the magnitudes of the eigenvalues in Case II, acoustic waves are strongly damped, especially when C is large. This is not of concern to us in subsonic combustion problems, however, if the acoustic waves do not affect combustion. A disadvantage of the ICE method is that the implicit finite difference approximations must usually be solved by a time-consuming iterative procedure, and many commonly-used iterative procedures have the undesirable property that for the ICE equations they converge more slowly as the Mach number tends to zero. This will be shown subsequently.

The numerical scheme of Case III is used in the acoustic subcycling method of Haselman.[2] In this method the terms responsible for acoustic wave propagation are differenced using a subcycle time step δt_s that satisfies $\delta t_s \leq \delta t$ and $\frac{c\delta t_s}{\delta x} \leq 1$, and their calculation is repeated $\frac{\delta t}{\delta t_s}$ times (subcycles) each large time step δt. The remaining terms in the equations use the larger time step δt. Usually δt is governed by the constraint

$$\frac{u\delta t}{\delta x} = 1 \quad ,$$

and thus we have

$$\frac{\delta t_s}{\delta t} \leq M \quad . \tag{28}$$

Computational efficiency is gained in the acoustic subcycling method because only a small number of terms are differenced using the smaller time step δt_s and because $(\rho')_j^{n+1}$ and $u_{j+1/2}^{n+1}$ are explicitly calculable. This method is also neutrally stable and thus has less numerical damping than the ICE method, although this can be a disadvantage since we prefer a method that damps the short wavelength, unresolvable components of the numerical solution. The acoustic subcycling method also has the disadvantage that it becomes more inefficient as M

goes to zero since, according to Eq. (28), the number of subcycles is approximately 1/M.

B. Pressure Gradient Scaling and Some Point Relaxation Iteration Procedures

The Pressure Gradient Scaling (PGS) method[3] was developed to improve the efficiency at low M of the ICE and acoustic subcycling methods. The basic idea of the PGS method is to improve computational efficiency by increasing M while still keeping it small in an absolute sense (M << 1). Solution features of interest in many combustion problems are unaltered when M is varied below some small upper bound. This idea was first used in O'Rourke and Bracco.[6] The PGS method is implemented by solving a revised primitive equation system in which Eq. (2) is replaced by

$$\frac{\partial \rho \underline{u}}{\partial t} + \underline{\nabla}\cdot(\rho \underline{u}\underline{u}) + \frac{1}{\alpha^2}\underline{\nabla} p = \underline{\nabla}\cdot\underline{\underline{\sigma}} + \rho \underline{g} \quad , \tag{29}$$

where $\alpha > 1$. By an examination of the acoustic equations of this revised system, it is easily seen that the effect of the $1/\alpha^2$ factor before the pressure gradient term, is to lower the sound speed by a factor α and thus to increase M by the same factor. For details concerning the method, the reader is referred to Ref. 3.

It is obvious how the PGS method makes more efficient the acoustic subcycling method since the number of subcycles is approximately 1/M. We now show how the PGS method accelerates convergence of some iteration procedures that are often used in conjunction with the ICE method. Consider the fully-implicit approximation to the PGS acoustic equations:

$$\frac{(\rho')_j^{n+1} - (\rho')_j^n}{\delta t} + \rho_o \frac{u_{j+1/2}^{n+1} - u_{j-1/2}^{n+1}}{\delta x} = 0 \tag{30a}$$

$$\rho_o \frac{u_{j+1/2}^{n+1} - u_{j+1/2}^{n}}{\delta t} + \frac{c_o^2}{\alpha^2} \frac{(\rho')_{j+1}^{n+1} - (\rho')_j^{n+1}}{\delta x} = 0 \quad . \tag{30b}$$

By using Eq. (30b) to eliminate $u_{j+1/2}^{n+1}$ and $u_{j-1/2}^{n+1}$ from Eq. (30a), we find that we must solve the implicit system of equations

$$D_j = (\rho')_j^{n+1} - (\rho')_j^n - C_\alpha^2\left[(\rho')_{j+1}^{n+1} - 2(\rho')_j^{n+1} + (\rho')_{j-1}^{n+1}\right]$$

$$+ \frac{\rho_o \delta t}{\delta x}\left(u_{j+1/2}^n - u_{j-1/2}^n\right) = 0 \quad , \tag{31}$$

where $C_\alpha = \frac{c_o \delta t}{\alpha \delta x}$. The matrix associated with Eq. (31) is a tridiagonal matrix for which very efficient direct solution methods are available. For multidimensional problems, however, these direct solution methods are very inefficient. Thus we consider a class of methods, called point relaxation methods, for the

To define these point relaxation methods, we first introduce some notation. Let ρ_j^ν and D_j^ν be the approximate values of $(\rho')_j^{n+1}$ and D_j after ν iterations. The first point relaxation method is called Jacobi iteration. In this method we calculate $\rho_j^{\nu+1}$ from

$$\rho_j^{\nu+1} = \rho_j^\nu - \frac{D_j^\nu}{\left(\frac{\partial D_j}{\partial \rho_j}\right)} \quad , \tag{32}$$

where $\frac{\partial D_j}{\partial \rho_j} = \frac{\partial D_j}{\partial (\rho')_j^{n+1}}$.

Equation (32) would solve $D_j \equiv 0$ if D_j just depended on $(\rho')_j^{n+1}$ and not on $(\rho')_{j-1}^{n+1}$ and $(\rho')_{j+1}^{n+1}$. In Jacobi iteration, the D_j^ν in Eq. (32) are given by

$$D_j^\nu = D_j^{\nu-1} + \left(\frac{\partial D_j}{\partial \rho_{j-1}}\right)(\rho_{j-1}^\nu - \rho_{j-1}^{\nu-1}) + \left(\frac{\partial D_j}{\partial \rho_j}\right)(\rho_j^\nu - \rho_j^{\nu-1})$$

$$+ \left(\frac{\partial D_j}{\partial \rho_{j+1}}\right)(\rho_{j+1}^\nu - \rho_{j+1}^{\nu-1}) \quad . \tag{33}$$

This corresponds to calculating first all the D_j^ν in one pass through the computational mesh from Eq. (31) using the ρ_j^ν, and then calculating changes in density from Eq. (32) in a second pass. The D_j^ν we use in Eq. (32) do not depend on any densities for the next iterate level--that is, on the $\rho^{\nu+1}$. A second point relaxation procedure, called Gauss-Seidel iteration, differs from Jacobi iteration in that D_j^ν depends on the $\rho_{j-1}^{\nu+1}$:

$$D_j^\nu = D_j^{\nu-1} + \left(\frac{\partial D_j}{\partial \rho_{j-1}}\right)(\rho_{j-1}^{\nu+1} - \rho_{j-1}^\nu) + \left(\frac{\partial D_j}{\partial \rho_j}\right)(\rho_j^\nu - \rho_j^{\nu-1})$$

$$+ \left(\frac{\partial D_j}{\partial \rho_{j+1}}\right)(\rho_{j+1}^\nu - \rho_{j+1}^{\nu-1}) \quad . \tag{34}$$

This corresponds to calculating <u>both</u> D_j^ν and $\rho_j^{\nu+1} - \rho_j^\nu$ on the same pass through the computational mesh in order of ascending j, and adding the change in density to ρ_j^ν before going to the next computational cell. A third iterative procedure,

called Successive Over-relaxation (SOR) uses Eq. (34) for the D_j^ν but calculates changes in density from

$$\rho_j^{\nu+1} = \rho_j^\nu - \frac{\lambda D_j^\nu}{\left(\frac{\partial D_j}{\partial \rho_j}\right)} \quad , \tag{35}$$

where $1 < \lambda < 2$. In the past, Gauss-Seidel and SOR iteration have been more popular than Jacobi iteration because they converge in fewer arithmetic operations. Jacobi iteration is better suited to modern vector computers because the calculation of ρ_j or D_j need not be performed in sequence. In a code using Jacobi iteration on a vector computer, more operations are performed per unit of computer time.

All three methods become more inefficient when the Mach number is reduced. We now show this for Gauss-Seidel iteration. Using Eq. (32) to eliminate the density changes in Eq. (34), and then using Eq. (31) to evaluate $\frac{\partial D_j}{\partial \rho_j}$, $\frac{\partial D_j}{\partial \rho_{j-1}}$, and $\frac{\partial D_j}{\partial \rho_{j+1}}$, gives

$$D_j^\nu - \frac{C_\alpha^2}{1 + 2C_\alpha^2} D_{j-1}^\nu = \frac{C_\alpha^2}{1 + 2C_\alpha^2} D_{j+1}^{\nu-1} \quad . \tag{36}$$

Again we examine the behavior of the Fourier components of D_j^ν. Letting $D_j^\nu = A^\nu e^{ij\psi}$ where $\psi = k\delta x$ and substituting this into Eq. (36) gives

$$\frac{A^{\nu+1}}{A^\nu} = \frac{e^{i\psi}}{2 - e^{-i\psi} + 1/C_\alpha^2} \quad .$$

For small values of ψ (long wavelengths) and large values of C_α, we have

$$\left|\frac{A^{\nu+1}}{A^\nu}\right| = 1 - \psi^2 - 2/C_\alpha^2 + o\left(\psi^4, 1/C_\alpha^4, \frac{\psi^2}{C_\alpha^2}\right) \quad . \tag{37}$$

From Eq. (37) we can draw several conclusions. First we show the inefficiency of Gauss-Seidel iteration when M is reduced. If M is reduced for a fixed value of $\frac{u\delta t}{\delta x}$, then the Courant number $\frac{c\delta t}{\delta x}$ is increased. The quantity C_α is the Courant number when the PGS method is not in use. When C_α increases, the ratio in Eq. (37) increases, thus slowing the convergence rate since the errors D_j are then damped more slowly. This situation worsens when we refine the mesh and thereby introduce lower wavelength (smaller ψ) errors.

When the PGS method is used, however, and we lower the Mach number for a fixed value of $\frac{u\delta t}{\delta x}$, we can increase α to keep the value of C_α constant.[3] Thus the convergence rate is not worsened. Further the ratio in Eq. (37) does not increase above an upper bound as the mesh is refined.

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