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NOTE

Convergence Acceleration for Steady Flame Computations

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1. INTRODUCTION

Different techniques have been developed to compute compressible low-Mach number flows. Reviews can be found in [1, 2]. To overcome the stiffness of the equations that appears for small Mach numbers, one can use preconditionning, implicit or semi-implicit methods, flux-vector splittings, or multigrid methods. False-transient methods, based on the artificial compressibility technique [3] and originally developed for incompressible flows [4], have also been extended to compressible flows using a low-Mach formulation of the equations [5]. However, these techniques have been rarely applied to combustion simulations where high density and temperature variations, a stiff energy source term, and real gas properties make the coupling between the energy, momentum, and continuity equations complex and difficult to capture. The application of compressible low-Mach number techniques to combustion problems is therefore not straightforward, and specific scaling methods have been developed [6, 7]. However, these methods also imply a modification of the conservation equations, which may raise some difficulties in complex configurations.

We propose here a simple method to efficiently accelerate convergence of flame computations, *without changing the nature of the full compressible conservation equations and their coupling*. Following the same idea as preconditioning and pressure scaling methods, the acoustic characteristic time is artificially reduced to become of the order of the convective time, but *no simplification of the equations is made*. The originality of this method is that it modifies the characteristic time of the the unsteady coupling between the flame and the flow but does not affect the nature of the coupling and leaves the steady solution unchanged.

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2. METHODOLOGY

The idea of the proposed method is to decelerate acoustic waves while keeping the time evolution of the flame unchanged. This is simply done by running the calculation at an artificially reduced pressure $P^* = P/\alpha^2$, where α is the acceleration factor, without modifying the temperature or the density (so that the equation of state now reads $P^* = \rho r T/\alpha^2$). The corresponding sound speed $c^* = \sqrt{\gamma P^*/\rho} = c/\alpha$ is therefore reduced, leading to a greater CFL-based time step $dt^* = \alpha dt$. This is quite different from false-transient methods where the pressure scaling appears only in the artificial pressure time-derivative term, added to the energy equation [5] (or the continuity equation in incompressible flows [3]), in order to allow the use of time-marching algorithms. The present scaling technique is closer to the method of [7], with the difference that we do not use the low-Mach number approximation.

Introducing P^* into the Navier–Stokes equations does not modify the continuity and mass fractions equations. On the other hand the momentum and pressure (or internal energy) equations take the form

$$\frac{\partial U_i}{\partial t} = -U_j \frac{\partial U_i}{\partial x_j} - \frac{\alpha^2}{\rho}\frac{\partial P^*}{\partial x_i} + \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j}$$

$$\alpha^2 \frac{\partial P^*}{\partial t} = -\gamma \alpha^2 P^* \frac{\partial U_j}{\partial x_j} - U_j \alpha^2 \frac{\partial P^*}{\partial x_j} + (\gamma - 1)\left[\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + \Phi_v + \dot{Q}\right],$$

where τ_{ij} is the stress tensor, Φ_v the viscous dissipation function, and $\dot{Q}$ any other source term (chemical heat release in combustion). It appears in these equations that simply replacing P by P^* leads to a modified steady solution because of the scaling by α^2 of some but not all terms of the right hand side (RHS). To avoid this we modify the RHS and solve for the following reduced equations (combined with the non-modified continuity and mass fractions equations),

$$\left(\frac{\partial U_i}{\partial t}\right)^* = -\frac{1}{\alpha^2} U_j \frac{\partial U_i}{\partial x_j} - \frac{1}{\rho}\frac{\partial P^*}{\partial x_i} + \frac{1}{\alpha^2}\frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial P^*}{\partial t} = -\gamma P^* \frac{\partial U_j}{\partial x_j} - U_j \frac{\partial P^*}{\partial x_j} + \frac{\gamma - 1}{\alpha^2}\left[\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + \Phi_v + \dot{Q}\right]$$

so that

$$\left(\frac{\partial U}{\partial t}\right)^* = \frac{1}{\alpha^2}\frac{\partial U}{\partial t}, \qquad \frac{\partial P^*}{\partial t} = \frac{1}{\alpha^2}\frac{\partial P}{\partial t}.$$

Integrating this reduced system in time gives

$$d\rho^* = \frac{\partial \rho}{\partial t} dt^* = \alpha d\rho, \qquad dU^* = \left(\frac{\partial U}{\partial t}\right)^* dt^* = dU/\alpha$$

$$dP^* = \frac{\partial P^*}{\partial t} dt^* = dP/\alpha, \qquad dY^* = \frac{\partial Y}{\partial t} dt^* = \alpha dY$$

$$dT^* = \alpha^2 dP^*/\rho r - \alpha^2 d\rho^* P^*/\rho^2 r = \alpha dT.$$

The density, temperature, and mass fractions are advanced in time with an acceleration factor α, while the dynamics variables U and P are advanced in time with a deceleration factor α.

The steady state solution obtained with this reduced system is unchanged compared to the original system as only time derivatives have been modified (only the LHS terms for the reduced momentum and pressure equations are scaled by $1/\alpha^2$ as compared to the original terms). Finally, the modifications of the conservation equations to yield the reduced system are the following:

- Continuity, no modification
- Velocity, divide the convective term and the viscosity by α^2
- Pressure, divide the viscosity, thermal conductivity, and source term by α^2
- Mass fraction, no modification.

Note that the equation of state must be modified too.

The maximum convergence acceleration will be obtained when the CFL time step becomes of the order of the other limiting time steps, namely the chemical time step and the Fourier time step. Note that there is no such limitation as low-Mach number or low density ratio, which is the case for low-Mach formulations, as long as only steady solutions are looked for. The application of the proposed method to unsteady computations is however restricted to low-Mach number flows for which the speed of sound has a negligible impact.

3. IMPLEMENTATION

Usually CFD compressible codes solve for density, momentum, total energy, and mass fractions in conservative dimensional or non-dimensional form. Due to the unchanged continuity equation, the conservative form of the momentum equation introduces a new term when using convergence acceleration, leading to

$$\left(\frac{\partial \rho U_i}{\partial t}\right)^* = -\frac{1}{\alpha^2}\frac{\partial \rho U_i U_j}{\partial x_j} - \frac{\partial P^*}{\partial x_i} + \frac{1}{\alpha^2}\frac{\partial \tau_{ij}}{\partial x_j} + \left(\frac{1}{\alpha^2} - 1\right) U_i \frac{\partial \rho U_j}{\partial x_j}.$$

The total energy is calculated normally, $\rho e_t^* = e_c + P^*/(\gamma - 1)$, and the total energy equation, in conservative form, can be directly written from the momentum and pressure equations. We obtain

$$\left(\frac{\partial \rho e_t^*}{\partial t}\right)^* = -\frac{1}{\alpha^2}\frac{\partial U_j e_c}{\partial x_j} - \frac{\gamma}{\gamma - 1}\frac{\partial U_j P^*}{\partial x_j} + \frac{1}{\alpha^2}\left[\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + \frac{\partial U_j \tau_{ij}}{\partial x_i} + \dot{Q}\right] + \left(\frac{1}{\alpha^2} - 1\right) U_i^2 \frac{\partial \rho U_j}{\partial x_j}.$$

Note that the additional term in both equations is proportional to the divergence of momentum: this term can be omitted without perturbing the final steady solution.

The practical implementation is very simple: the only changes made to the code are the scaling of the convective terms in the momentum and energy equations and the modification of the equation of state. The diffusion and source terms in the energy and total energy equations can be simply reduced by dividing the viscosity and thermal conductivity as well as heat release Q by α^2. For non-dimensional formulations, the diffusive terms are reduced by multiplying the Reynolds number by α^2. Note that if the species diffusivities are calculated through Schmidt numbers, these numbers have to be divided by α^2 so that the product $Re \cdot Sc$ does not change. Finally one has to keep in mind that the calculations are done at a pressure level artificially lowered, which must be rescaled to get the true pressure level of the final solution. Boundary conditions also have to be rescaled to adapt to the lower pressure.

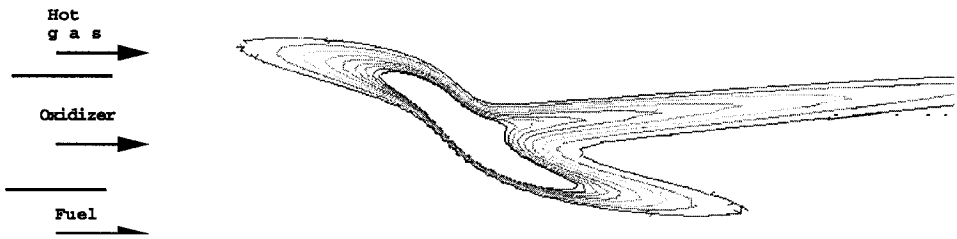

FIG. 1. Configuration and reaction rate contours of the steady two-dimensional diffusion flame.

As the nature of the equations remains unchanged, the numerical discretization schemes and boundary conditions treatment can be applied without modification.

4. VALIDATION

Validation tests have been conducted using a finite volumes, unstructured code (AVBP) developed at CERFACS [8, 9]. One-dimensional and two-dimensional flames have been calculated, with and without convergence acceleration.

A stationary, one-dimensional premixed methane–air flame was calculated with a convergence acceleration factor $\alpha^2 = 100$, then compared to the standard calculation. Both final steady solutions were extremely close, and it took about ten times less iterations to reach the same level of convergence (in terms of residuals).

We show here only the second test case, a two-dimensional stabilized diffusion flame. Figure 1 shows the configuration and the calculated steady solution. Three different streams are injected at inlet: a fuel stream, an oxidizer stream, and a hot products stream. The flame is stabilized by the hot stream, as shown in [10]. The simulation presented here was conducted on a 100×200 grid, refined around the flame location. We used simple chemistry (only two species were computed), and an inlet velocity of 72 cm/s. For convergence acceleration we have used $\alpha^2 = 100$. Residuals of the different variables are plotted versus time in Fig. 2. Both calculations correspond to the same number of iterations. The accelerated calculation goes much further in time than the standard calculation in the same number of iterations (the time step is multiplied by 10): before 600 iterations the accelerated calculation has already seen the flame ignition (corresponding to the peak in all curves), whereas the standard calculation is still in the phase where all profiles are only diffusing. The time evolution

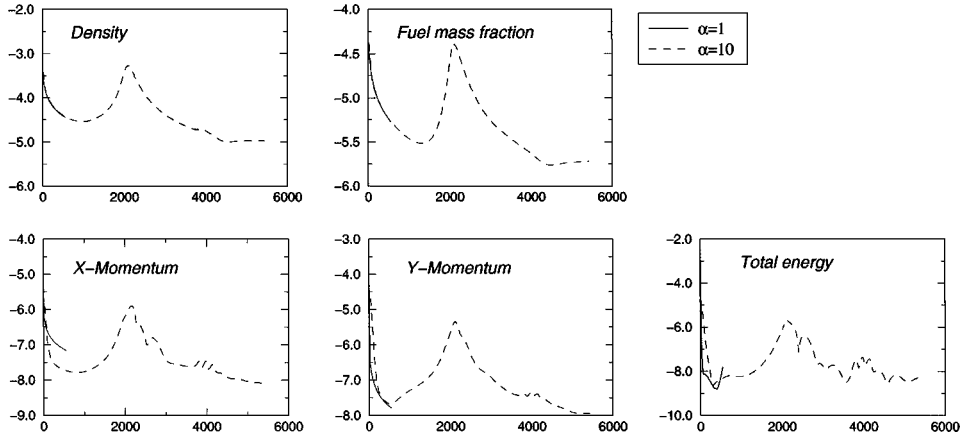

FIG. 2. Log of the residuals of the conservative variables vs time non-dimensionalized with the acoustic time L/c.

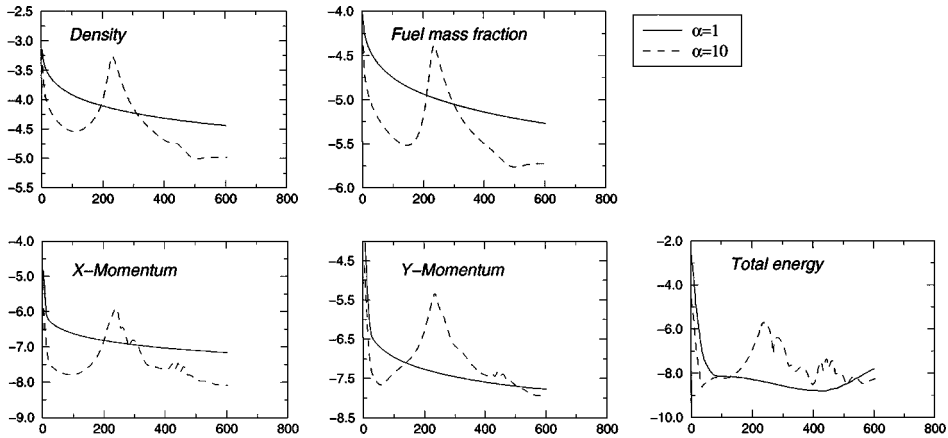

FIG. 3. Log of the residuals of the conservative variables vs the number of iterations.

of the residuals of density and mass fractions is unchanged, as we did not modify the corresponding equations. Residuals for momentum and energy behave quite differently. They can be understood by plotting them against the number of iterations (Fig. 3). The last (600th) iteration of the standard computation corresponds to the same physical time as the 60th iteration of the accelerated computation, so that residuals for all variables differ significantly after iteration 60. Before this point, and as expected from the derivation of the method, residuals for dynamic variables (momentum and energy) are smaller whith convergence acceleration (initially by a factor α^2 for energy and α for momentum), but the slopes are the same: the gain is not here. However, residuals for density and mass fractions, starting at the same level, drop much faster with the accelerated method.

5. CONCLUSION

We have shown that steady combustion simulations can be drastically accelerated by modifying the characteristic time scale of the acoustics, while keeping the full compressible conservation equations. The implementation in codes is very simple and requires only some minor modifications on the convective terms and the boundary conditions. Convergence acceleration has been successfully obtained on one-dimensional and two-dimensional flame calculations, with a speed-up of the order of 10. In theory, typical speed-up can go up to 100, which is the order of magnitude of the ratio of sound speed to usual flame speeds.

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