PRECONDITIONING METHODS FOR LOW MACH NUMBER COMPRESSIBLE FLOW SIMULATIONS WITH AN OPTMIZED PSEUDO SPEED OF SOUND

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Abstract. This study establishes a new procedure for selecting the control parameters in preconditioning methods used to simulate low Mach number compressible flows. The main parameter studied here is the pseudo speed of sound. Its formula is derived in the literature from an analysis of the governing equations at low Mach numbers, making sure their respective eigenvalues have the same order of magnitude. However, preconditioning is simply a mathematical tool used to remove stiffness from ill-conditioned systems of equations. Hence, one could obtain the optimal value of the pseudo speed of sound by minimizing the condition number of this system. In order to validate this novel methodology, several steady-state simulations were performed with explicit and implicit pseudo-time marching schemes as well as approximations for spatial derivatives with different accuracy orders. The results obtained were compared to the ones generated with the standard pseudo speed of sound used in the literature. Significant improvements in numerical stability and computer time are observed.

Keywords: *Preconditioning Methods, Compressible Flows, Low Mach Number, Optimized Pseudo Speed of Sound*

1. INTRODUCTION

In fluid mechanics, the Navier-Stokes equations provide the most complete model for the study of compressible flows of Newtonian fluids. However, the main difficulty associated with the numerical simulation of these unsteady equations is the degradation of convergence at very low flow speeds. Whenever the Mach number is very small, there is a huge disparity between the convective and acoustic eigenvalues in this system of equations because the speed of sound is much larger than the convective velocity. Hence, time step size in time marching schemes is limited by acoustics instead convection, even though the former is not relevant in most low Mach number flows (Turkel, 1987). The significant increase in computational cost that follows is not the only problem that must be dealt with. Pressure gradients are inversely proportional to the Mach number square. Hence, pressure round-off errors are amplified at low Mach numbers, causing accuracy problems as well (Merkle and Choi, 1988). A few different techniques have been developed to minimize the problem of numerical stiffness and accuracy of compressible flow simulations at low Mach numbers. They enable the development of robust methods capable of dealing with flows at arbitrary Mach number. The present paper focuses on Preconditioned Density-Based methods.

These methods deal with the problems mentioned above in two steps. First, they solve a set of primitive variables instead of the standard conservative ones. This set always contains pressure and velocity components but there are different possibilities regarding the last dependent variable, although it is usually temperature. Furthermore, pressure is split into hydrodynamic and thermodynamic contributions. The latter is usually constant whereas the former is the actual dependent variable. In doing so, round-off error propagation is dramatically reduced. This variable transformation follows a simple chain rule and generates a Jacobian matrix that multiplies the physical-time derivative. The second and final step modifies this matrix, forcing all eigenvalues to have the same order of magnitude. Hence, it essentially eliminates all stiffness issues related to the differences in acoustic and convective flow speeds. There are several different ways of specifying this modified matrix (Turkel, 1993; Turkel, 1999), known as preconditioning matrix, which introduces a few control parameters. They are the subject of the present paper.

1.1. Low Mach Number Stiffness

The eigenvalue disparity of the Navier-Stokes equations at low Mach numbers may be checked algebraically if one considers an inviscid and one-dimensional unsteady compressible flow, written as

$$\frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x} = 0 \,, \tag{1}$$

where Q represents the standard conservative variables and E_i the inviscid fluxes, given by

$$Q = \{\rho, \rho u, \rho E\} \quad \text{and} \quad E_i = \{\rho u, \rho u^2 + p, (\rho E + p)u\} \,, \tag{2}$$

and ρ is the density, u the flow velocity in the direction x and p is the pressure. Only perfect gases are considered in this study. Their equation of state is

$$p = \rho RT = (\gamma - 1)\rho e\,, \tag{3}$$

where e is the internal thermal energy per unit mass, obtained with

$$e = C_v T\,, \tag{4}$$

and T is the temperature, C_v the specific heat of gas at constant volume, k the coefficient of thermal conductivity, R the gas constant and γ is the ratio of specific heats. Finally, the total internal energy per unit mass E is given by

$$E = e + \frac{u^2}{2}\,. \tag{5}$$

Using the chain rule allows one to re-write equation (1) as

$$\frac{\partial \mathrm{Q}}{\partial \mathrm{t}} + \frac{\partial \mathrm{E_i}}{\partial \mathrm{Q}}\frac{\partial \mathrm{Q}}{\partial \mathrm{x}} = \frac{\partial \mathrm{Q}}{\partial \mathrm{t}} + \mathrm{A}\frac{\partial \mathrm{Q}}{\partial \mathrm{x}} = 0\,, \tag{6}$$

where A is the inviscid flux Jacobian matrix defined as

$$A = \frac{\partial \mathrm{E_i}}{\partial \mathrm{Q}} = \begin{bmatrix} 0 & 1 & 0 \\ \dfrac{\partial \mathrm{p}}{\partial \rho} - \mathrm{u}^2 & 2\mathrm{u} + \dfrac{\partial \mathrm{p}}{\partial(\rho \mathrm{u})} & \dfrac{\partial \mathrm{p}}{\partial(\rho \mathrm{E})} \\ \mathrm{u}\left(\dfrac{\partial \mathrm{p}}{\partial \rho} - \mathrm{H}\right) & \mathrm{u}\dfrac{\partial \mathrm{p}}{\partial(\rho \mathrm{u})} + \mathrm{H} & \mathrm{u}\left(1 + \dfrac{\partial \mathrm{p}}{\partial(\rho \mathrm{E})}\right) \end{bmatrix}, \tag{7}$$

and, according to Fedkiw *et al.* (1997), the pressure derivatives above for thermally perfect gases are

$$\frac{\partial p}{\partial \rho} = (\gamma - 1)\left(\frac{u^2}{2} - h\ + C_p T\right),\ \frac{\partial p}{\partial(\rho u)} = -(\gamma - 1)u \quad \text{and} \quad \frac{\partial p}{\partial(\rho E)} = (\gamma - 1)\,, \tag{8}$$

with h representing the enthalpy per unit mass and H the total enthalpy per unit mass, defined as

$$H = e + \frac{p}{\rho} + \frac{u^2}{2}\,. \tag{9}$$

The eigenvalues of matrix A provide the direction in which characteristic waves propagate information in this particular flow model given by equation (1). They are given by

$$A \rightarrow \{\lambda_1,\ \lambda_2,\ \lambda_3\} = \{u,\ u + c,\ u - c\}\,, \tag{10}$$

where c is the speed of sound.

Now it is clear why low Mach number flows, where $u << c$ and the flow is dominated by convective time scales instead of acoustic ones, yield eigenvalues with vastly different magnitudes. These differences are responsible for the stiffness faced by time marching schemes, since the time step utilized is calculated with expressions such as

$$\Delta \mathrm{t} = \mathrm{CFL} \times \min\left\{\frac{\mathrm{L}}{|\lambda_1|}, \frac{\mathrm{L}}{|\lambda_2|}, \frac{\mathrm{L}}{|\lambda_3|}\right\}, \tag{11}$$

where L is a characteristic length, usually given by the local grid spacing, and CFL is the Courant-Friedrich-Lewy number, which relates the physicals velocities with the numerical ones ($\mathrm{L}/\Delta \mathrm{t}$). Hence, time steps are going to be

dictated by acoustic scales even though the convective scales are the most important ones at low Mach numbers. In other words, they are going to be dictated by numerical stability instead of accuracy considerations, drastically increasing computer times since the former imposes values that much smaller than the latter.

1.2. Low Mach Number Preconditioning

It is well known that density becomes independent of pressure at low Mach numbers. In the zero Mach number limit when the flow is incompressible, pressure gradients are important but not the pressure itself. Therefore, as previously mentioned, it is important to obtain pressure directly from the conservation equations rather than indirectly from an equation of state. This can be achieved by using the chain rule to re-write equation (1) as

$$\frac{\partial \mathrm{Q}}{\partial \hat{\mathrm{Q}}}\frac{\partial \hat{\mathrm{Q}}}{\partial \mathrm{t}}+\frac{\partial \mathrm{E_i}}{\partial \mathrm{x}}=\mathrm{T}\frac{\partial \hat{\mathrm{Q}}}{\partial \mathrm{t}}+\frac{\partial \mathrm{E_i}}{\partial \mathrm{x}}=0 \tag{12}$$

where the Jacobian matrix T that achieves this transformation is given by

$$\mathrm{T}=\frac{\partial \mathrm{Q}}{\partial \hat{\mathrm{Q}}}=\begin{bmatrix} \dfrac{\partial \rho}{\partial \mathrm{p}} & 0 & \dfrac{\partial \rho}{\partial \mathrm{T}} \\ \mathrm{u}\dfrac{\partial \rho}{\partial \mathrm{p}} & \rho & \mathrm{u}\dfrac{\partial \rho}{\partial \mathrm{T}} \\ \mathrm{H}\dfrac{\partial \rho}{\partial \mathrm{p}}-\left(1-\rho\dfrac{\partial \mathrm{h}}{\partial \mathrm{p}}\right) & \rho\mathrm{u} & \mathrm{H}\dfrac{\partial \rho}{\partial \mathrm{T}}+\rho\dfrac{\partial \mathrm{h}}{\partial \mathrm{p}} \end{bmatrix}, \tag{13}$$

and the chosen primitive variable vector $\hat{Q}$ is

$$\hat{\mathrm{Q}}=\{\mathrm{p_H},\mathrm{u},\mathrm{T}\}\,, \tag{14}$$

with $p = p_T + p_H$, where the new dependent variables p_T and p_H are the thermodynamic and hydrodynamic pressure contributions, respectively, with the former assumed constant in the present work. Hence, the spatial derivatives in the momentum equation depend only on p_H. This additional modification is justified by the fact that $p_T \sim O(\rho c^2)$ and $p_H \sim O(\rho u^2)$ and is crucial to reduce the pressure round-off error propagation.

The second necessary step to enable low Mach number simulations using the original conservation equations requires reducing the stiffness caused by eigenvalue disparity, as discussed previously. This can be better understood by looking at the thermally perfect gas relations

$$\frac{\partial \rho}{\partial p}=\frac{1}{RT}\,,\ \frac{\partial \rho}{\partial T}=\frac{-\rho}{T}\,,\ \frac{\partial h}{\partial p}=0\quad\text{and}\quad\frac{\partial h}{\partial T}=C_p\,, \tag{15}$$

or, more specifically, at the density dependence on pressure. For an arbitrary real fluid, it is given by

$$\frac{\partial \rho}{\partial \mathrm{p}}=\frac{1}{\mathrm{c}^2}-\frac{\partial \rho}{\partial \mathrm{T}}\left(1-\rho\frac{\partial \mathrm{h}}{\partial \mathrm{p}}\right)\Bigg/\left(\rho\frac{\partial \mathrm{h}}{\partial \mathrm{T}}\right), \tag{16}$$

according to Merkle and Choi (1987). Equation (12) still contains eigenvalues with vastly different values because the speed of sound c is still much larger than the convection speed u. This problem can be minimized if we replace the sound speed by a preconditioning velocity V_p in relation (16), effectively re-writing it as

$$\rho_{\mathrm{p}}=\frac{1}{\mathrm{V_p^2}}-\frac{\partial \rho}{\partial \mathrm{T}}\left(1-\rho\frac{\partial \mathrm{h}}{\partial \mathrm{p}}\right)\Bigg/\left(\rho\frac{\partial \mathrm{h}}{\partial \mathrm{T}}\right), \tag{17}$$

which changes the Jacobian matrix T into the preconditioning matrix Γ given by

$$\Gamma = \begin{bmatrix} \rho_p & 0 & \rho_T \\ u\rho_p & \rho & u\rho_T \\ H\rho_p - \left(1 - \rho\dfrac{\partial h}{\partial p}\right) & \rho u & H\rho_T + \rho\dfrac{\partial h}{\partial p} \end{bmatrix}, \tag{18}$$

where ρ_T is obtained from

$$\rho_T = \delta\frac{\partial \rho}{\partial T} \tag{19}$$

and was introduced only to generate the preconditioning matrixes used by Venkateswaran and Merkle (1999), with $\delta = 0$, and Weiss and Smith (1995), with $\delta = 1$.

The impact caused by preconditioning the governing equations can be evaluated through the calculation of their new eigenvalues. In order to do this, one must re-write equation (12) as

$$\boldsymbol{\Gamma}\frac{\partial \hat{\mathrm{Q}}}{\partial \tau} + \frac{\partial \mathrm{E_i}}{\partial \mathrm{x}} = \boldsymbol{\Gamma}\frac{\partial \hat{\mathrm{Q}}}{\partial \tau} + \hat{A}\frac{\partial \hat{\mathrm{Q}}}{\partial \mathrm{x}} = \frac{\partial \hat{\mathrm{Q}}}{\partial \tau} + \boldsymbol{\Gamma}^{-1}\hat{A}\frac{\partial \hat{\mathrm{Q}}}{\partial \mathrm{x}} = 0, \tag{20}$$

where τ represents a pseudo-time, since the correct physical-time t is lost upon preconditioning, and the new inviscid flux Jacobian matrix $\hat{\mathrm{A}}$ is given by

$$\hat{\mathrm{A}} = \frac{\partial E_i}{\partial \hat{\mathrm{Q}}} = \begin{bmatrix} u\dfrac{\partial \rho}{\partial p} & \rho & u\dfrac{\partial \rho}{\partial T} \\ 1 + u^2\dfrac{\partial \rho}{\partial p} & 2\rho u & u^2\dfrac{\partial \rho}{\partial T} \\ u\dfrac{\partial(\rho H)}{\partial p} & \rho\left(H + u^2\right) & u\dfrac{\partial(\rho H)}{\partial T} \end{bmatrix}, \tag{21}$$

noting that the total enthalpy derivatives can be obtained by combining relations (9) and (15). The eigenvalues of equation (20), in either one of its forms, are obtained from matrix $\Gamma^{-1}\hat{\mathrm{A}}$ to yield

$$\lambda_1 = u,\ \lambda_2 = \frac{u}{2}\left(1 + \frac{V_p^2}{c^2}\right) + \sqrt{V_p^2 + \left(\frac{u}{2}\left(1 - \frac{V_p^2}{c^2}\right)\right)^2} \quad \text{and} \quad \lambda_3 = \frac{u}{2}\left(1 + \frac{V_p^2}{c^2}\right) - \sqrt{V_p^2 + \left(\frac{u}{2}\left(1 - \frac{V_p^2}{c^2}\right)\right)^2}, \tag{22}$$

clearly showing that as long as $\mathrm{V_p} << \mathrm{c}$, low Mach number stiffness will be negligible.

2. STANDARD PSEUDO SPEED OF SOUND

The derivation above follows what is arguably the most used preconditioning method used in the literature, the one by Venkateswaran and Merkle (1999). According to this method, one should use

$$\mathrm{V_p} = \min\{\mathrm{V_{inv}}, \mathrm{c}\}, \quad \text{where} \quad \mathrm{V_{inv}} = \sqrt{\mathrm{u}^2}, \tag{23}$$

for steady inviscid flows. This formula guarantees two important features. First, V_P is always positive, which means the mathematical nature of a flow will not be modified. In other words, if a flow is originally either parabolic or hyperbolic, it will remain so under preconditioning. Furthermore, it is not possible for compressible flows to be elliptic since a time derivative, with or without preconditioning, is always present. Second, this formula has a switch that reverts V_P back to its original value when the flow is transonic. Nevertheless, it must be modified whenever stagnation points are present since the flow velocity approaches zero in such regions. For this reason, a stagnation velocity is defined as

$$V_{st} = \sqrt{\frac{|\Delta p|}{\rho}}, \tag{24}$$

where Δp is the local pressure difference. Relation (23) is then re-written as

$$\mathrm{V_p} = \min\{\max\{\mathrm{V_{inv}},\ \mathrm{V_{st}}\},\ \mathrm{c}\}. \tag{25}$$

3. OPTIMIZED PSEUDO SPEED OF SOUND

The solution of algebraic systems can be obtained by different methods. Each one requiring multiplications between scalars and/or vectors and/or matrixes. These are composed of integer and/or real numbers that must be approximated by a finite number of digits, giving it what is commonly called machine precision. The propagation of these round-off errors is related to the number of basic algebraic operations performed by each method and, specially, to the condition number of the associated matrixes. The first source of error is minimized by an efficient implementation of each method, which reduces the number of basic operations, most importantly multiplications and divisions. The second one is problem dependent and is the main focus of the current paper.

Given a generic algebraic system such as $A \cdot \mathrm{x} = \mathrm{b}$, its condition number with respect to an infinity norm is

$$\kappa_\infty(A) = \left\|A\right\|_\infty \times \left\|A^{-1}\right\|_\infty, \tag{26}$$

which essentially measures the sensitivity of a system to small perturbations. The values of $\kappa_\infty(A)$ go from one to infinity. One represents perfect conditioning, where perturbations will not be amplified at all throughout the algebraic operations. As this number gets higher, the system becomes more and more ill-conditioned. In extreme cases, round-off errors will be amplified to such an extent that accuracy degrades severely. The same happens to convergence whenever iterative or marching schemes are utilized. As the Mach number gets smaller, the discrete version of the compressible governing equations, obtained after applying a numerical solution method to it, becomes more and more ill-conditioned. This relationship between a numerical property and its physical origin arguably led all studies found in the literature to define control parameters for low Mach preconditioning methods, such as the pseudo speed of sound, following a dimensional analysis of the governing equations under different flow conditions. These studies always had the same basic goal: select the control parameters in such a way to force the well known eigenvalues of the compressible Euler equations to have the same order of magnitude. However, this problem is a numerical one and no relationship with the original physical properties of the flow should be necessary, only its mathematical nature must be maintained. Hence, this basic goal can be refined: select the value of V_P that minimizes the condition number κ_∞.

An algebraic system of equations is obtained at each grid point whenever explicit time marching schemes are chosen. Its size depends only on the number of differential equations being solved. This leads to

$$\kappa_\infty(\mathbf{\Gamma}) = \left\|\mathbf{\Gamma}\right\|_\infty * \left\|\mathbf{\Gamma}^{-1}\right\|_\infty, \tag{27}$$

where Γ is the same preconditioning matrix defined in (18). An analysis of κ_∞ shows a single global minimum that varies little throughout the grid, giving V_P a smooth spatial distribution.

Even though multigrid strategies and parallelization are easier to implement with explicit marching schemes, implicit ones should be used instead because they are more efficient at driving a solution to steady-state. Whenever doing so, the algebraic system ceases to be decoupled and one should look at all grid points simultaneously. Hence, their size depends on the number of grid points utilized. This usually leads to block tri-diagonal systems for one-dimensional problems because they can be solved more efficiently. However, minimizing equation (26) for such a system is very inefficient and an alternative path must be followed. This starts with the fact that these tri-diagonal systems are very often diagonally dominant. Furthermore, a block diagonal system would be obtained in the theoretical limit of maximum diagonal dominance. The condition number of such a system is simply the maximum value among the condition numbers of each block diagonal element. It will be minimized whenever the condition number of each element is minimized. Hence, one could say that equation (27) is still a valid approximation for multi-diagonal systems as long as they are diagonally dominant.

4. NUMERICALS EXPERIMENTS

Preliminary results were generated for a quasi-1D flow inside a diffuser. Explicit and implicit Euler methods were used for pseudo-time marching from an initial condition consisting of a uniform flow with $M = 10^{-3}$. Spatial resolution was obtained with a first-order upwind scheme based on preconditioned flux difference splitting. Our novel methodology is compared with the one derived by Venkateswaran and Merkle (1999) and widely used in the literature. These curves were generated with their respective optimal *CFL* numbers in terms of computer time.

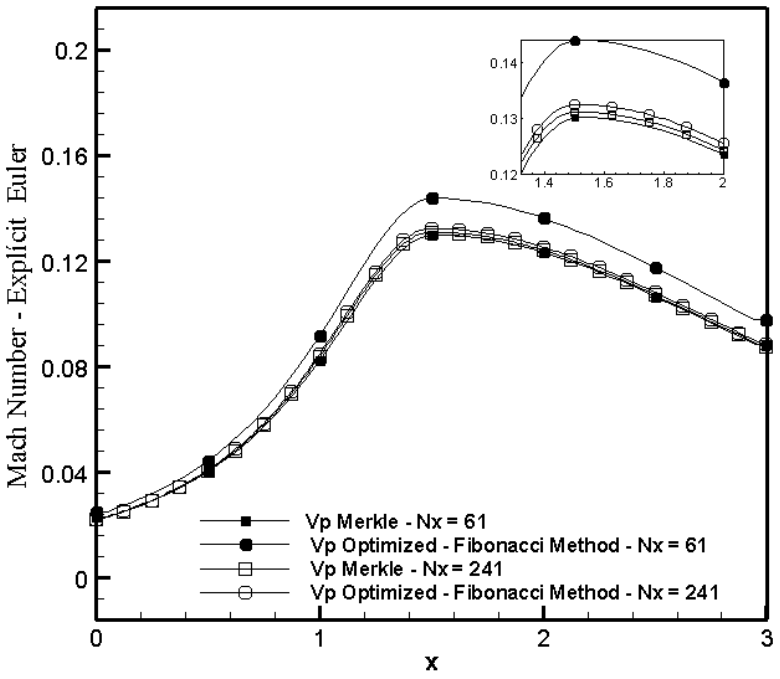

Figure 1. Mach Numbers inside diffuser for the explicit Euler scheme with different grid sizes: Nx = 61 and 241.

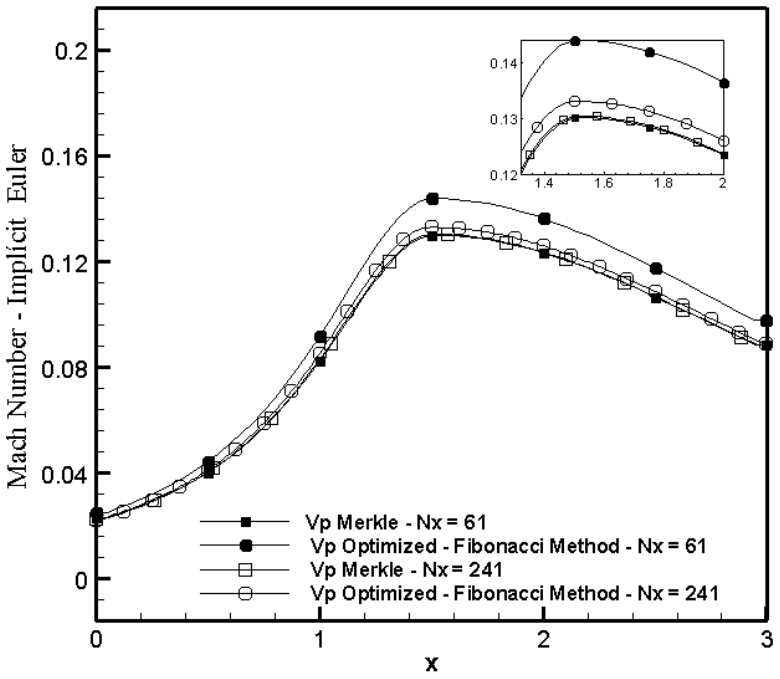

Figure 2. Mach Numbers inside diffuser for the implicit Euler scheme with different grid sizes: Nx = 61 and 241.

First, steady-state solutions for the Mach number spatial variation are shown in Figures 1 and 2, obtained with the explicit and implicit Euler method, respectively. These figures show differences, although very small, between the solutions generated with traditional and novel pseudo speeds of sound. This is somewhat expected since first-order schemes are used in space. Their high levels of numerical dissipation have a significant impact on solution accuracy through the magnitude of the preconditioned eigenvalues.

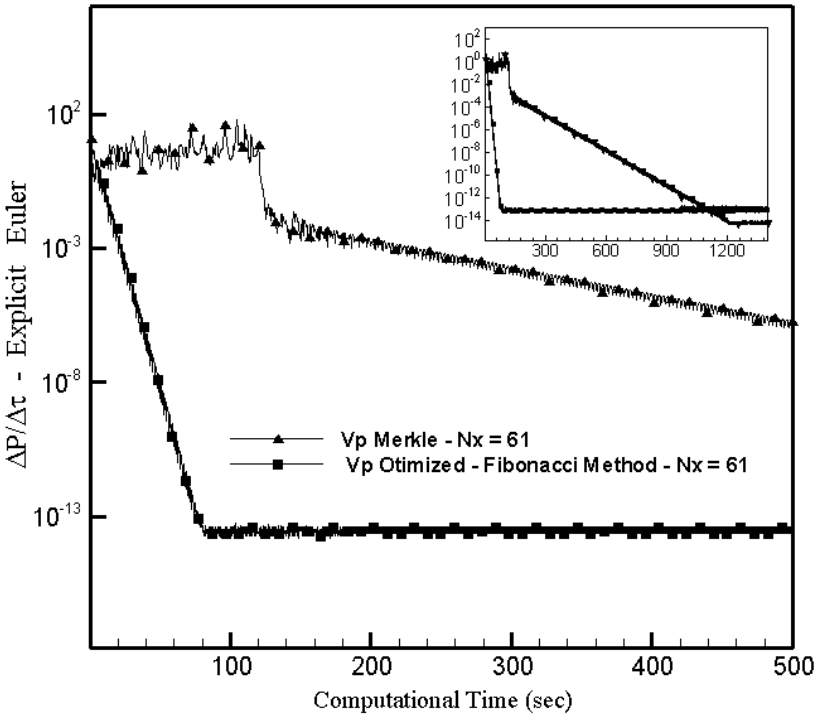

Figure 3. Pressure increment decay with computational time for the explicit Euler scheme with Nx = 61.

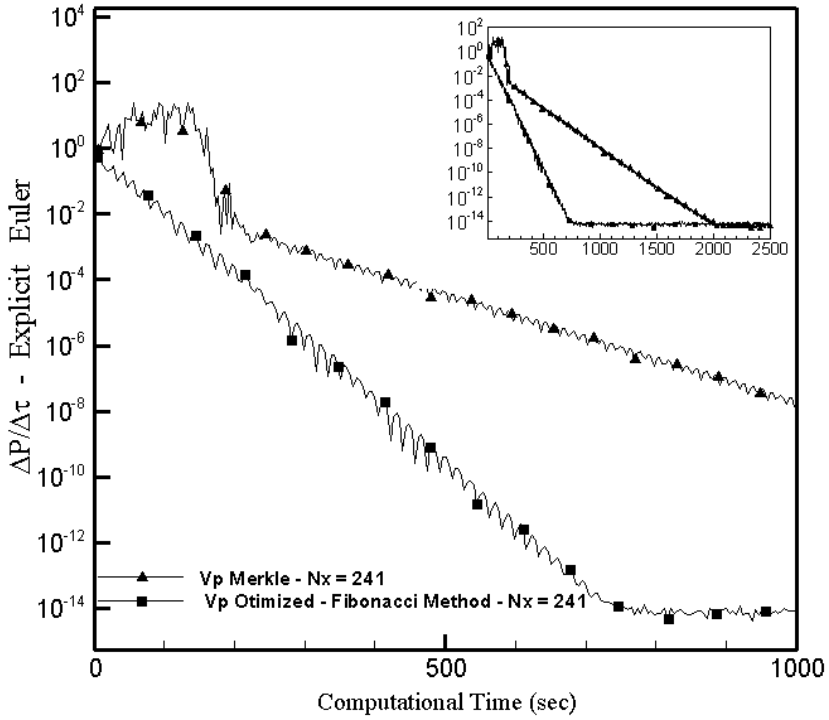

Figure 4. Pressure increment decay with computational time for the explicit Euler scheme with Nx = 241.

Now it is possible to compare convergence rates from both methodologies when explicit Euler marching in pseudo-time is utilized. This is an important test since the optimized pseudo speed of sound was derived for this particular scheme. Results are shown in Figures 3 and 4, generated with Nx = 61 and 241, respectively. Enhanced numerical stability is clear, specially at the initial transient, and leads to higher CFL numbers and, hence, dramatic improvement of convergence rates. They also increase as error tolerances decrease but decrease as grid size decreases.

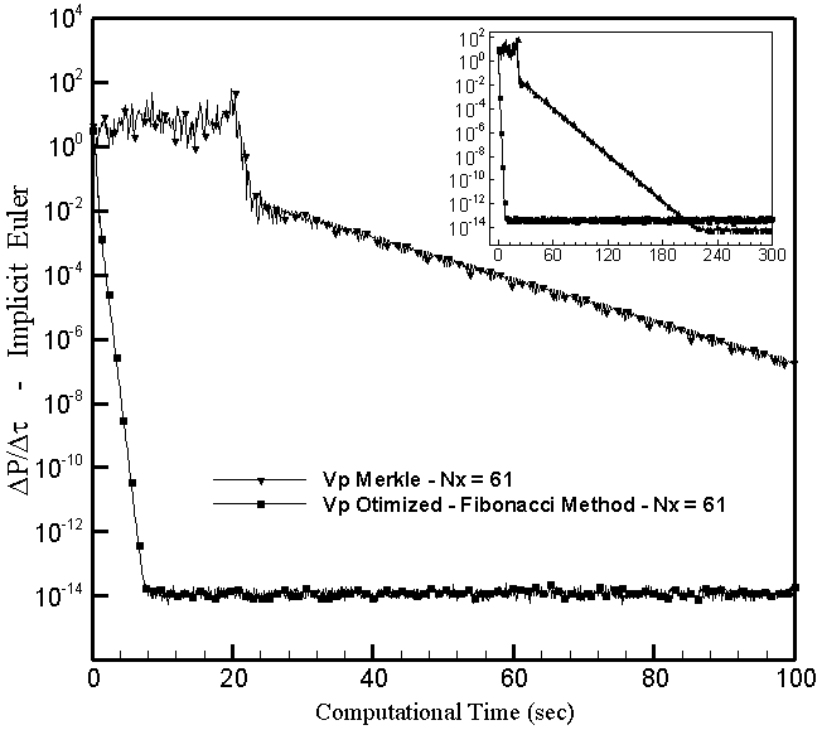

Figure 5. Pressure increment decay with computational time for the implicit Euler scheme with Nx = 61.

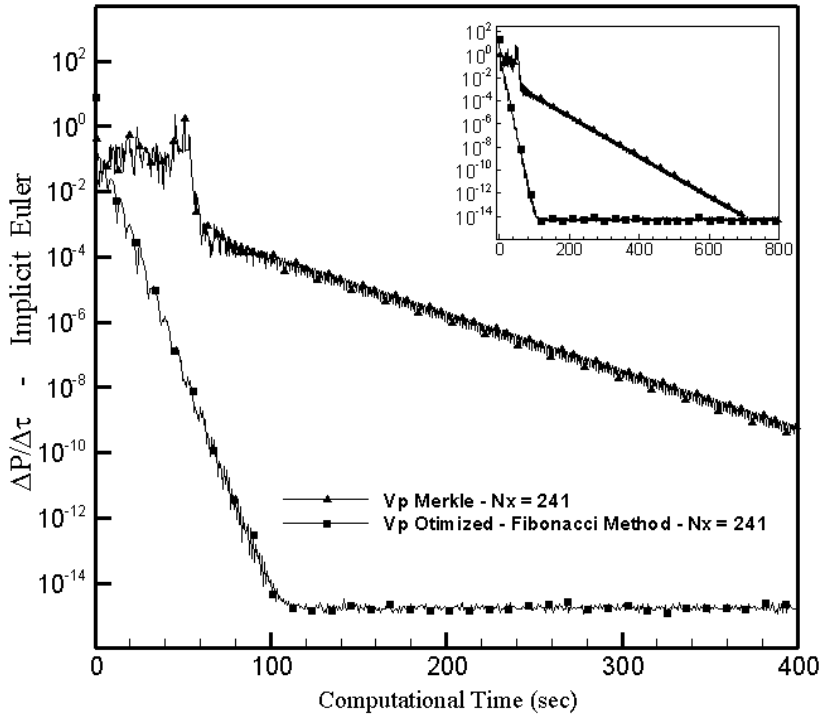

Figure 6. Pressure increment decay with computational time for the implicit Euler scheme with Nx = 241.

Finally, these same comparisons are made when implicit Euler marching in pseudo-time is utilized. This is an important test because implicit marching is the usual choice in the literature because it leads to faster convergence towards steady-state, when compared to explicit marching schemes. However, it should be noted again that the optimal pseudo speed of sound calculation in only approximate for this scheme. Despite this shortcoming, the novel

methodology actually performs better with this implicit marching scheme than with its explicit counterpart. Lets consider machine precision error tolerance results. The optimized pseudo speed of sound leads to an approximate 1000% decrease in computer time when compared to its traditional formulation for explicit marching with Nx=61. This number increases to approximately 2400% when implicit marching is used instead. When the number of grid points used increases to Nx = 241, this improvement is decreased by about 3 times for both marching schemes. Furthermore, there is a small difference between machine precision errors generated with both methodologies with a smaller grid. This is likely due to the excessive dissipative errors introduced by the first-order scheme in space, since it disappears when the number of grid points used increases to Nx = 241.

4. CONCLUSION

This paper presented a novel formulation for the pseudo speed of sound used in low Mach number preconditioned density-based methods. Significant improvements in performance were obtained when compared to a traditional and well known formulation commonly used in the literature. These preliminary studies show that it is worth pursuing this approach and extending it to different test cases, such as transient and viscous problems not only in one but also more spatial dimensions.

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