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AN APPROXIMATE FACTORIZATION SCHEME APPLIED TO THE SEGREGATED FINITE-VOLUME METHODS

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SUMMARY

The approximate factorization (AF) scheme is largely employed in the methods in which the equation systems are solved simultaneously, like the well known Beam and Warming method. The advantage of the AF procedure is that two and three dimensional problems can be solved as a sequence of one dimensional problems.. The extension of the AF scheme, applied to the conventional segregated methods, realized in this work, demonstrates that the procedure works well for small time steps. For large time steps the procedure can be applied only to the momentum conservation equations.

INTRODUCTION

The numerical prediction of fluid flow and heat transfer phenomena normally leads to the solution of linear systems of algebraic equations. When the discretization is done using a structured grid the resulting matrix possesses a well defined structure. Using the finite volume approach, the matrices have, in problems defined in simply connected domains or without repetitive boundary conditions, a number of non zero diagonals equals to: i) five, in 2D problems employing a orthogonal discretization; ii) nine, in 2D problems with nonorthogonal discretization; iii) seven, in 3D problems with orthogonal discretization and iv) nine in 3D problems with a nonorthogonal discretization. These numbers increases if high order schemes are used to evaluate the convective and diffusive terms at the interfaces of the elemental control volume and decreases if some terms are explicitly evaluated, that is, they are added to the independent vector. In real problems when the discretization needs to be very fine the direct solutions of these equation systems is unfeasible.

In the methodologies which follow the procedure outlined in [1], the solution of the linear system of equations is generally done using iterative methods. These methods can be classified as implicit or semi-implicit, depending on the number of terms of the matrix which are removed from the matrix coefficients and introduced in the independent vector. In these methodologies, since the linear systems originated from each conservation principle are solved in a segregated manner, other iterative levels are needed for updating the coefficients and the source terms.

In the other hand, in the numerical schemes similar to the one proposed by Beam and Warming [2], where the equations are linearized using a Newton-Raphson procedure and are solved simultaneously, the only source of iteration is related to the solution of the linear system involved. It is wise to point out that, in these schemes, to each element in a matrix originated from a segregated approach corresponds to a 4X4 or 5X5 sub-matrix, depending wether the problem is 2D or 3D. This difficulty, however, is partially removed by the use of the approximate factorization process, where 2D and 3D problems are solved as a sequence of one dimensional ones. In this manner the matrices assume a block tridiagonal structure, to which efficient solvers can be applied [3] making the process, as a whole, non iterative.

The main goal of the present work is the development of an approximate factorization scheme applied to the solution of linear systems originated from methods which uses the segregated approach.

THE APPROXIMATE FACTORIZATION (AF) SCHEME APPLIED TO THE SIMULTANEOUS SOLUTION

In the solution of compressible flows the partial differential equations are linearized expanding the non linear terms about a known solution in time. The procedure is analogous to the Newton-Raphson method applied for the solution of non linear algebraic equations. Due to this linearization process the governing differential equations need to be solved simultaneously.

Consider, as an example, the 2D compressible flow of an inviscid fluid. The governing equations written in delta form [2][3], after the linearization process and time discretization assume the following form

$$\Delta U + \Delta t \left[\frac{\partial}{\partial x} (A\Delta U) + \frac{\partial}{\partial y} (B\Delta U) \right] = RHS \qquad (1)$$

where [A] and [B] are the jacobian matrices originated from the linearization process. ΔU is the time variation of the vector U, whose components are ρ, ρu, ρv and E_t, where E_t is the total energy by volume. After the spatial discretization of the derivatives, Eq.(1) gives rise to a block pentadiagonal linear system, where each block is a 4X4 matrix. The solution of this linear system is not trivial. Consider now the Eq.(1) written in the form of a differential operator applied to a unknown vector ΔU, resulting

$$\left[I + \Delta t \left[\frac{\partial A}{\partial x} + \frac{\partial B}{\partial y} \right] \right] \Delta U = RHS \qquad (2)$$

To avoid the solution of a block-pentadiagonal matrix, the differential operator is split in the product of two onedimensional operators, resulting in

$$\left[I + \Delta t \frac{\partial A}{\partial x} \right] \left[I + \Delta t \frac{\partial B}{\partial y} \right] \Delta U = RHS \qquad (3)$$

If one defines an auxiliary vector ΔU^* as

$$\Delta U^* = \left[I + \Delta t \frac{\partial B}{\partial y} \right] \Delta U \qquad (4)$$

and substitutes Eq.(4) in Eq.(3), ΔU^* can be found through the solution of a block tridiagonal matrix. Since ΔU^* is known, the ΔU vector can be found in the same manner using Eq.(4). In this way a 2D problem was solved through a solution of two 1D problems.

Obviously, the product of one-dimensional operators does not reproduce the original 2D operator, introducing an error in the ΔU vector. This error, however, is of order Δt^2, which is the same order of the errors introduced in the time discretization of the governing differential equations. Therefore, the approximate factorization process does not alter the order of the approximation errors of the whole solution, and the scheme can be considered as non-iterative. Recall that when the steady state is reached, the RHS of Eq.(2) vanishes and the only distribution of U which produces ΔU equal to zero is the distribution which satisfies the steady part of the discretized differential equations. Therefore, if the procedure converges, the solution obtained will be the correct solution for the steady state.

The approximate factorization scheme is widely used in the solution of compressible flows where the governing equations are solved simultaneously. The observed drawback of the process is the slow convergence when Δt increases, specially in 3D problems [4].

THE SOLUTION METHODS EMPLOYED IN THE CONVENTIONAL SEGREGATED FORMULATION

In the segregated formulation using finite-volume methods the differential equations are represented, for a 2D problem for example, as

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x}(\rho u\phi) + \frac{\partial}{\partial y}(\rho v\phi) = -P^{\phi} + \Gamma^{\phi}\left[\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right] \qquad (5)$$

where ϕ plays the role of ρ, u, v, T, etc. The appearence of the diffusive terms, not included when the simultaneously formulation was described, and the exclusion of source terms are immaterial for the purpose of what follows. Eq.(5) discretized using finite volume method results in

$$a_P\phi_P - a_e^*\phi_E - a_w^*\phi_W - a_n^*\phi_N - a_s^*\phi_S = b \qquad (6)$$

or, in matrix form, as

$$[A]\{\phi\} = \{b\} \qquad (7)$$

As already pointed out, the direct solution of Eq.(7) is unfeasible. So, iterative procedures are employed, like the point-by-point Jacobi, Gauss-Seidel and SOR methods or the line-by-line methods, which requires the aplication of the TDMA [1] solver in lines and columns. Strongly implicit techniques are also used, like SIP [5], MSI [6] and the SIP version proposed in [7]. The point-by-point and line-by-line techniques, although easy in programing and efficient in coarse meshes are too time consuming in refined grids. Besides that, because of the explicit nature of the procedures, they require the positivity of the coefficients for achieving convergence [1][8]. This requirement is very strong since, for assuring the positivity of the coefficients, it is necessary to introduce some form of upwinding in the evaluation of the fluxes at the interfaces, with the consequent degradation of the solution due to numerical diffusion. One of the characteristics of the methodologies just mentioned is the capability of eliminating high frequency errors in the solution during the iterative procedure. The use of block correction schemes or multi-grid techniques speeds up the convergence process because they actuate in the damping of low frequency errors [9]. In the other hand, the strongly implicit procedures, based on the LU decomposition of the matrix of coefficients, although iterative, possess a high rate of convergence.

THE SEGREGATED FINITE-VOLUME METHOD IN DELTA FORM

If the exact solution of Eq.(7) is obtained, the errors in the distribution during the transient will be due solely to the spatial and temporal discretization. If the solution is iterative, another error is introduced depending on the truncation of the iterative cycles (convergence criterion). Even when the interest lies in the steady state solution if Eq.(7) is not solved subjected to a very strong convergence criterion, the resulting steady state solution will be wrong. It is well known the irrealistic solutions obtained when only few Jacobi iterations are performed.

Recently [8] the authors developed a segregated formulation in delta form. The main characteristic of this formulation is that the dependent variables are the time variations of the conserved properties. In delta form Eq.(6) assumes the following form

$$a_P\Delta\phi_P - a_e^*\Delta\phi_E - a_w^*\Delta\phi_W - a_n^*\Delta\phi_N - a_s^*\Delta\phi_S = RHS \qquad (8)$$

where

$$\Delta\phi = \phi^{t+\Delta t} - \phi^{t} \qquad (9)$$

Details of the development and a few tests can be found in [8]. By now it suffices to say that the term RHS is evaluated using known variables from the previous time level and it corresponds to the discretization of the steady state part of the governing differential equation, Eq.(5). Therefore, when the steady state is reached the RHS and, of course, $\Delta\phi$ vanish.

AN APPROXIMATE FACTORIZATION SCHEME APPLIED TO THE SEGREGATED FINITE VOLUME METHOD

The solution of Eq.(8) can be obtained by the same methods employed in the solution of Eq.(6). However, the delta form has the advantage that when the steady state is reached the RHS is zero, implying in a zero time variation for ϕ, even if approximate methods are used in the solution of Eq.(8). Therefore, the basic idea is, following what is done in the simultaneous solution methods, to develop a direct method for the solution of Eq.(8) whose errors introduced in the transient solutions be acceptable. To this end, consider Eq.(8) divided by a_P, resulting

$$\Delta\phi_P - a_e\Delta\phi_E - a_w\Delta\phi_W - a_n\Delta\phi_N - a_s\Delta\phi_S = RHS \qquad (10)$$

For simplicity, consider the case in which the domain have been discretized by a 3X3 grid, without the use of fictitious points, shown in Fig.1.

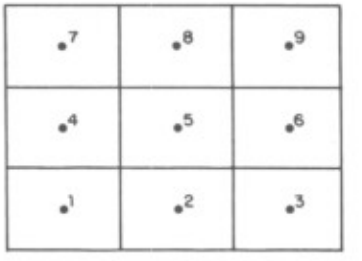

Fig. 1 A 3X3 grid.

The system of equations given by Eq.(10) can be represented by the following equation

$$[A]\{\Delta\phi\} = \{RHS\} \qquad (11)$$

and the matrix [A] assumes the form

$$[A] = \begin{bmatrix} 1 & a_e & & a_n & & & & & \\ a_w & 1 & a_e & & a_n & & & & \\ & a_w & 1 & & & a_n & & & \\ a_s & & & 1 & a_e & & a_n & & \\ & a_s & & a_w & 1 & a_e & & a_n & \\ & & a_s & & a_w & 1 & & & a_n \\ & & & a_s & & & 1 & a_e & \\ & & & & a_s & & a_w & 1 & a_e \\ & & & & & a_s & & a_w & 1 \end{bmatrix} \quad (12)$$

An approximate factorization process to this problem can be established if one replaces the original problem, Eq.(11), by the problem

$$[A_x]\,[A_y]\,\{\Delta\phi\} = \{RHS\} \quad (13)$$

where

$$[A_x] = \begin{bmatrix} 1 & a_e & & & & & & & \\ a_w & 1 & a_e & & & & & & \\ & a_w & 1 & & & & & & \\ & & & 1 & a_e & & & & \\ & & & a_w & 1 & a_e & & & \\ & & & & a_w & 1 & & & \\ & & & & & & 1 & a_e & \\ & & & & & & a_w & 1 & a_e \\ & & & & & & & a_w & 1 \end{bmatrix} \quad (14)$$

and

$$[A_y] = \begin{bmatrix} 1 & & & a_n & & & & & \\ & 1 & & & a_n & & & & \\ & & 1 & & & a_n & & & \\ a_s & & & 1 & & & a_n & & \\ & a_s & & & 1 & & & a_n & \\ & & a_s & & & 1 & & & a_n \\ & & & a_s & & & 1 & & \\ & & & & a_s & & & 1 & \\ & & & & & a_s & & & 1 \end{bmatrix} \quad (15)$$

If one defines $\{\Delta\phi^*\}$ by

$$\{\Delta\phi^*\} = [A_y]\,\{\Delta\phi\} \quad (16)$$

Eq.(13) results

$$[A_x]\,\{\Delta\phi^*\} = \{RHS\} \quad (17)$$

Eq.(17) is a one-dimensional problem and can be easily solved through a TDMA-like procedure. In the sequence, Eq.(16) allows the calculation of $\{\Delta\phi\}$ in a similar fashion. Obviously, the approximate factorization procedure given by Eq.(13) does not reproduce the original problem given by Eq.(11). New terms, involving the product of two of the coefficients of the original system of equations, are present and are analogous to that which appears in Eq.(2) in excess to Eq.(2), related to the simultaneous scheme. Therefore, the problem actually solved by the aproximate factorization scheme is

$$\Delta\phi_P - a_e\Delta\phi_E - a_w\Delta\phi_W - a_n\Delta\phi_N - a_s\Delta\phi_S - a_n a_e\Delta\phi_{NE} + - a_s a_e\Delta\phi_{SE} - a_n a_w\Delta\phi_{NW} - a_s a_w\Delta\phi_{SW} = RHS \quad (18)$$

SOME NUMERICAL EXPERIMENTS

As a test, the well known problem of the lid-driven cavity was chosen. The solution was obtained for several values of the dimensionless time step defined as $\Delta t.L/u_{wall}$, with Reynolds number equal to 1000. The cavity was discretized using a 10X10 grid uniformely spaced, and the SIMPLEC [10] method was used to deal with the pressure-velocity coupling. The solution was considered converged when

$$\frac{|\Delta\phi|}{u_{wall}} \leq 10^{-6} \quad (19)$$

for ϕ equal to u and v, in every cell of the domain. For the purpose of the test, a problem involving only a scalar field, like a conduction problem, could be solved. However, the chosen problem is far more complex, because it is a nonlinear problem with a strong coupling between the equations. Table 1 shows the number of iterations and the CPU effort in seconds to reach convergence, as a function of the dimensionless time step for three different situations, as i) the approximate factorization is not applied; ii) it is applied in the solution of the momentum equations, and iii) it is applied to all three linear systems, comprising momentum and mass conservation. When the approximate factorization process is not applied the equations are solved using the MSI [6] procedure. For the evaluation of ϕ at the interfaces of the control volumes the UDS scheme [1] was applied.

Table 1. Performance of the AF process with UDS.

Δt^*	MSI		AF in u,v		AF in u,v,P	
	IT	CPU	IT	CPU	IT	CPU
0.2	266	15.1	268	11.9	270	9.7
0.4	148	8.6	151	6.9	156	5.7
0.6	107	6.4	111	5.2	120	4.6
0.8	87	5.2	92	4.4	103	4.0
1.0	75	4.5	80	3.9	101	3.9
1.2	68	4.2	74	3.6	106	4.0
1.4	64	4.0	70	3.5	114	4.3
1.6	62	3.8	67	3.3	120	4.5
1.8	61	3.6	66	3.2	129	4.8
2.0	61	3.6	66	3.1	138	5.1

The results obtained demonstrate the savings in the computer effort when the approximate factorization is applied in the solution of the momentum equations, although the number of iterations is a little higher. The results of the third column, however, show that for Δt^* higher than 1.2 the application of the factorization process does not help in the convergence rate. Such results were expected since the errors introduced in the solution varies with Δt^2 and the errors are specially damaging when related to the mass conservation equation.

Table 2 shows the results of a more severe test where the UDS scheme is replaced by the CDS scheme. Because the CDS scheme is non dissipative the convergence rate is slower even solving the linear systems using MSI. The stars in the table indicate that the convergence was not reached in 1000 iterations. The results shown that for small values of Δt^* the approximate factorization is always of benefit. However, the global performance is more susceptible to the increase of the time step. Such a behaviour is easily explained. The coefficients a_e, a_w, a_n e a_s in Eq.(10) obey the following equation

$$a_e + a_w + a_n + a_s + M_p/(a_p^* \Delta t + M_p) = 1 \quad (20)$$

where Δt is the time step and M_p is the mass inside the control volume. When the UDS scheme is applied the coefficients are all positives, and of course, all of them less than unity (and smaller as smaller the time step is). Therefore, the additional terms originated by the approximate factorization, resulting from product of two coefficients, are also small. By its turn, in the CDS scheme the coefficients can be negative with absolute value larger than unity. In this case the additional terms are harmful to the performance of the method for smaller Δt than are for the UDS scheme. It is important to point out that the use of point-by-point and line-by-line solvers would bring the procedure to divergence due to the presence of negative coefficients.

Table 2. Performance of the AF process with CDS.

Δt^*	MSI		AF in u,v		AF in u,v,P	
	IT	CPU	IT	CPU	IT	CPU
0.2	549	30.7	549	24.2	571	20.1
0.4	313	17.7	313	14.0	364	12.9
0.6	236	13.4	236	10.7	317	11.3
0.8	202	11.6	201	9.2	314	11.2
1.0	187	10.7	183	8.4	509	17.8
1.2	182	10.5	175	7.9	*	*
1.4	182	10.5	180	7.8	*	*
1.6	187	10.6	578	23.8	*	*
1.8	195	10.9	*	*	*	*
2.0	205	11.3	*	*	*	*

In order to have more informations about the behaviour of the AF procedure, few more tests were conducted using the lid-driven cavity problem, where the grid, the Reynolds number and the dimensionless time step were changed. The outcome of the tests are as follow. Keeping the same grid and the same Reynolds number but reducing the dimensionless time step, the performance of the AF procedure is superior of the MSI irrespective of using UDS or CDS, confirming the tendencies of Table 1 and 2. In these cases the number of iterations necessary for convergence is pratically the same for the three cases, requiring less CPU effort for the AF since the time per iteration of the AF scheme is smaller. This result was expected since smaller Δt^* imply in smaller coefficients a_e, a_w, a_n and a_s according to Eq.(20).

If the grid is refined the value of Δt^* for keeping the AF procedure advantageous reduces when compared with the Δt^* values for the 10X10 grid, regardless if the UDS or CDS is used. This result is surprisingly since the grid refinement increases the diffusive part of the coefficients, improving the stability characteristics. Probably, due to the fact that the grid refinement diminishes the quantity of mass M_p inside the control volumes, this would cause larger coefficients, according to Eq.(20). Despite this fact, for small values of Δt^*, the AF procedure performs better than the MSI method. The minimum CPU effort is, however, obtained with the MSI using larger time steps, and large enough to cause divergence of the AF procedure.

Finally, tests realized with a 20X20 grid indicated that the performance of the AF, when compared with the MSI, is independent of the Reynolds number. Using CDS the number of iterations for convergence increases with the Reynolds number, but this behaviour is also present in the MSI and in the AF for the two situations analyzed.

Partial Cancellation of the Additional Terms. The solution of the linear systems of equations through the AF procedure is an approximated process due to the presence of the additional terms shown in Eq.(18). The influence of these terms can be reduced if in the algebraic equation the partial cancellation of these terms is realized before the solution is carried out. Eq.(10) is then substituted by

$$\Delta\phi_p - a_e\Delta\phi_E - a_w\Delta\phi_W - a_n\Delta\phi_N - a_s\Delta\phi_S + \alpha\,(a_n a_e\Delta\phi_{NE} + a_s a_e\Delta\phi_{SE} + a_n a_w\Delta\phi_{NW} + a_s a_w\Delta\phi_{SW}) = RHS \qquad (21)$$

where α is a relaxation parameter. In order to mantain the pentadiagonal structure the ϕ values in NE, NW, SE and SW are expressed as a function of ϕ in P, E, W, N and S by expressions like

$$\phi_{NE} = \phi_N + \phi_E - \phi_P \qquad (22)$$

Similar procedure is also used in [6]. The use of this procedure to the test case with Reynolds number equal to 1000 and a 10X10 grid gives rise to good results when the AF was applied in the solution of the momentum equations. Even adopting the CDS scheme the solution was always obtained with almost the same number of iterations as when using MSI, but with 30% less computer effort for the whole range of Δt^* examined. Unfortunatelly the time step limitation continued to restrict the application of the AF to the solution of the mass conservation equation.

CLOSURE

The main goal of the present work was the development of a non-iterative scheme using the approximate factorization concept applied to pentadiagonal systems in the segregated framework. The tests carried out to illustrate the procedure demonstrated that it performs better than the MSI scheme when solving the momentum equations employing the UDS approximation. Still using the UDS approximation but now solving the mass conservation equation the performance deteriorates requiring smaller time steps in order to converge faster than the MSI. For the CDS approximation the time steps required are even more resctritive for the AF procedure to show better performance. However, the results obtained encourages further developments of the procedure in the context of the segregated methods of solution.

Finally, the analysis of the AF process proposed in the present work when compared with the AF in the context of simultaneous solution contributes for a better understanding of the latter and its known difficulty in handling transients with large time steps.

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