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AN IMPLEMENTATION OF PARALLEL GMRES SOLUTION METHOD ON A 3-D UNSTRUCTURED FLOW SOLVER

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ABSTRACT

A parallel GMRES (Generalized Minimal Residual) solution method is implemented on a 3-D flow solver developed earlier. An open source parallel GMRES software, *pARMS* (parallel Algebraic Recursive Multilevel Solvers), is used. *pARMS* uses MPI library routines to run in a parallel computing environment based on distributed memory. The flow solver, *SET3D*, employs a vertex based finite volume method on hybrid, unstructured grids. It currently has Euler explicit and Gauss-Seidel implicit time integration schemes. In this study, *pARMS* software is integrated into *SET3D*, and validated against certain test cases. The results show that the performance of the *pARMS* integrated flow solver is significantly enhanced.

INTRODUCTION

The flow solver, *SET3D*, has been developed in TÜBİTAK-SAGE for the solution of a wide range flow problems[4, 3, 5, 6]. Earlier versions of the solver was based on a cell-centered Finite Volume method. The cell-centered scheme has an advantage of eliminating the need for the control volume generation affords. However, it also brings the disadvantage of distributing the variables to the nodes which may cause additional numerical errors[5]. Recently, to improve accuracy of the solver, a cell-vertex scheme has been implemented.

In the solver, first or second order accurate inviscid fluxes are evaluated by the Roe type flux difference splitting method. Although the Roe type inviscid fluxes are used in the flux evaluations, the flux Jacobians needed in implicit solutions are based on Steger-Warming type fluxes. The iterative implicit solution algorithm is based on a point Gauss-Seidel (GS) method, which requires considerably long computation times for 3-D flow solutions on high-resolution grids.

In the present study, the node-based version of the solver is used. The GS solution algorithm is replaced by a parallel implementation of GMRES method provided by the open-source software, *pARMS*. Moreover, the flux Jacobians are now evaluated numerically. The integration of *pARMS* and the flow solver, *SET3D* is achieved by a system call. The communication needed for the data exchange between *SET3D* and *pARMS* programs is provided using the shared memory segments.

NUMERICAL SOLUTION METHOD

3-D unsteady viscous or inviscid flows over a solid body are computed by solving the Euler or Navier-Stokes equations on an unstructured grid. The integral form of the 3-D flow equations is solved using the finite volume method based on the cell vertex values. The governing equation for a conservative variable, Q, in a volume, Ω, is given as

$$\frac{\partial}{\partial_t}\int_{\Omega} Q \; d\Omega + \oint_S \hat{\mathbf{F}} \cdot \mathbf{d\hat{S}} = \oint_S \hat{\mathbf{G}} \cdot \mathbf{d\hat{S}} \qquad (1)$$

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where $\hat{\mathbf{F}}$ and $\hat{\mathbf{G}}$ are the convective and viscous flux vectors of the conservative variable, Q. $\hat{\mathbf{S}}$ is the outward directed surface vector of the boundary enclosing the volume, Ω.

The convective fluxes are evaluated using a 2^{nd} order accurate upwind biased flux scheme[6]. A higher order accurate flux limiter is used in the flux computations[2]. Gradients are computed by Galerkin formulations. A first order finite difference approximation is employed for the evaluation of the Jacobian matrix. The discretized implicit equations are solved using Newtonian iterations coupled with the GMRES solver, $pARMS$

GMRES Method

The Generalized Minimal Residual Method[8, 7] is an iterative algorithm for the numerical solution of a system of linear equations. The method generates a sequence of orthogonal vectors, then seeks a linear combination of these vectors to approximate the solution of the equation system.

The GMRES solver used in this study is $pARMS$ $v.2.2$, which is a freely available software with source code included[1]. $pARMS$ offers a large selection of preconditioners and a few of the best known accelerators. In the computations, expensive but high accurate ILU (incomplete lower upper factorization) technique is preferred for preconditioning.

Parallel Processing

In the implicit solution of the 3-D unsteady flows, a parallel algorithm based on process decomposition is implemented in a work-sharing paradigm. The whole computation process of the flow solver is partitioned into three tasks. First, the right hand side of the implicit equation system is constructed as a single process. The Jacobian matrix is evaluated in parallel as the second task. This is achieved using PVM (Parallel Virtual Machine) library routines. Then, the GMRES solver, $pARMS$, is executed in a parallel computing environment communicating through MPI (Message Passing Interface) library. The communication between the flow solver, $SET3D$, and the GMRES solver, $pARMS$, is provided using shared memory segments.

Computations are performed in a cluster of Linux based computers with Intel processors. Two parallelization techniques used in this study are explained below:

Shared Memory Segments: An efficient means of passing data between separate programs is to use shared memory segments. Generated a memory portion by a program can easily be accessed by other processes using shared memory segments. The Jacobian matrix and the right hand side vector produced at each time step by the flow solver, $SET3D$, is sent to the GMRES solver, $pARMS$, using shared memory segments.

Parallel Computing Environment with Message Passing: $pARMS$, the parallel GMRES solver uses MPI for parallel processing. The program spawns a specified number of processes in different processors based on domain decomposition paradigm. First, the local preconditioning matrix is generated on each processor, then, the local solution vector is constructed using GMRES method. Finally, all the local solutions are collected through MPI to give the global solution.

PVM is the other message passing library for parallel computing environment used in the solver. Construction of the Jacobian matrix at each time step is parallelized using PVM routines.

RESULTS

In this study, a previously developed serial running Euler solver is modified to run in a parallel computing environment using shared and distributed memory. The supersonic flow over a generic fuselage, and the transonic flow over a wing are computed as test studies.

The supersonic flowfield is computed at a Mach number of 2.0. In this computation, the number of the node points in the unstructured grid is 34075, which is also the number of the unknowns per conservative variable. The Jacobian matrix has more than two millions non-zero element. About 20 MB memory is allocated in the shared memory segment for double precision data communication between the flow solver, $SET3D$, and the GMRES solver, $pARMS$.

For the supersonic computation, three cases are studied. In the first case, the serial flow solver and the parallel GMRES solver are communicated with each other by reading and writing data files. In the second case, data communication between the solvers are provided using shared memory segments. In both cases, the parallel GMRES solver used 4 processors to solve the system of linear equations. In the third case, the explicit solution algorithm is used. Table 1 shows the computation wall clock time for the cases considered. As seen from the table, Case 2 in which shared memory segments are used, requires about 30% less time than Case 1 does. Higher performance of the implicit solution algorithm over that of the explicit algorithm in terms of the computing duration is also read from the table. Case 3 requires 8 and 12 more time than Cases 1 and 2 for a converged solution. The variation of the residual along the unsteady time cycles is given in Figure 1 for Case 2.

As a second test study, the transonic flowfield over the ONERA M6 wing is computed at a Mach number of 0.84. This problem is previously studied and solved using the explicit version of $SET3D$[3]. An earlier implicit solution using $SET3D$ is not available due to the divergence of the Gauss-Seidel algorithm for this problem. Therefore, the present implicit solution based on GMRES algorithm is compared to the explicit solution.

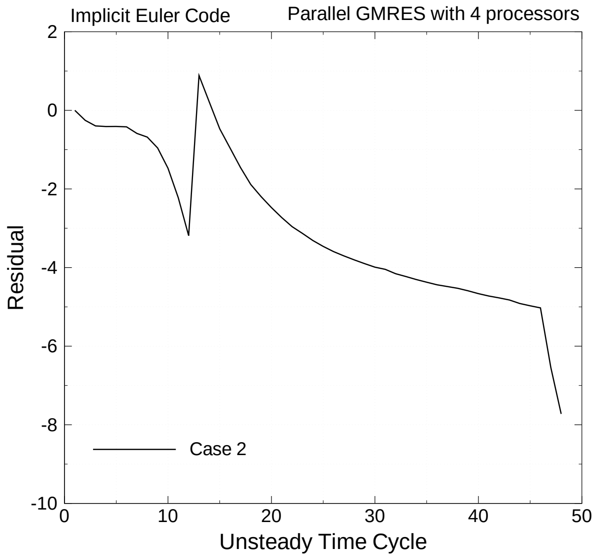

Figure 1: Residual variation along unsteady time cycles for the first test study

Table 1: Computation wall clock time for the first test study

	CPU Time (sec)
Case 1	**105**
Case 2	**70**
Case 3	**810**

Table 2: Comparison of the different solver strategies used in the second test study

	Number of Iteration	CPU Time (minute)	Residual Order
Parallel SET3D - Parallel GMRES by pARMS	–	–	-
Serial SET3D - Parallel GMRES by pARMS	48	**11**	7.2
Serial and Parallel SET3D - Gauss-Seidel	*Not Converged*	-	-
Parallel SET3D - Explicit	–	–	-
Serial SET3D - Explicit	5000($max.$)	**168**	4.7

For this transonic computation, the number of the node points in the unstructured grid is 90696. The Jacobian matrix has about thirty three millions non-zero element. Approximately 350 MB memory is allocated in the shared memory segment. As the total program requirement, more than 1 GB memory is used.

The GMRES based implicit algorithm needs about 10 minutes for a converged solution with a seven order reduced residual. The computation using the explicit version of *SET3D* takes almost three hours for a converged solution with a five order reduced residual. The performance of the GMRES based implicit solution is clearly seen in terms of both the computation duration and the accuracy(Table 2).

Figures 2 and 3 give the flowfield over the ONERA M6 wing computed using respectively the GMRES based implicit algorithm and the explicit algorithm. Although the solution algorithms are different in the computations, the results are in a good agreement with each other as observed from the figures.

Preliminary results show that the performance of the GMRES based implicit flow solver is superior when compared to the previous versions of the solver. More cases is required to asses the final conclusion.

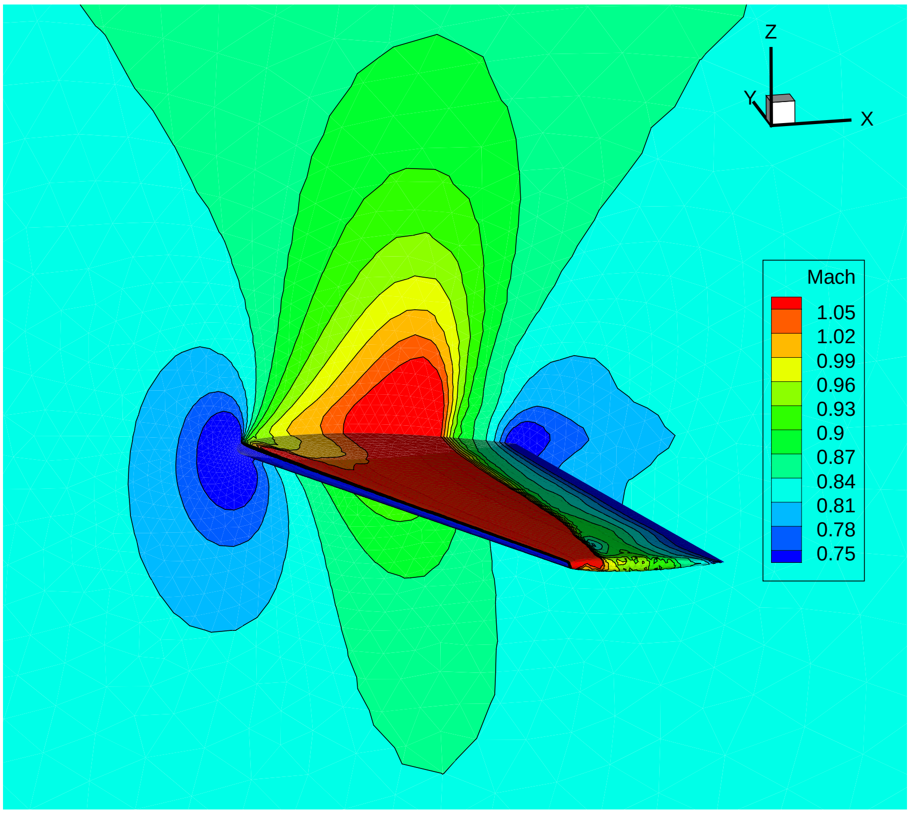

Figure 2: Mach number lines by GMRES based implicit *SET3D*

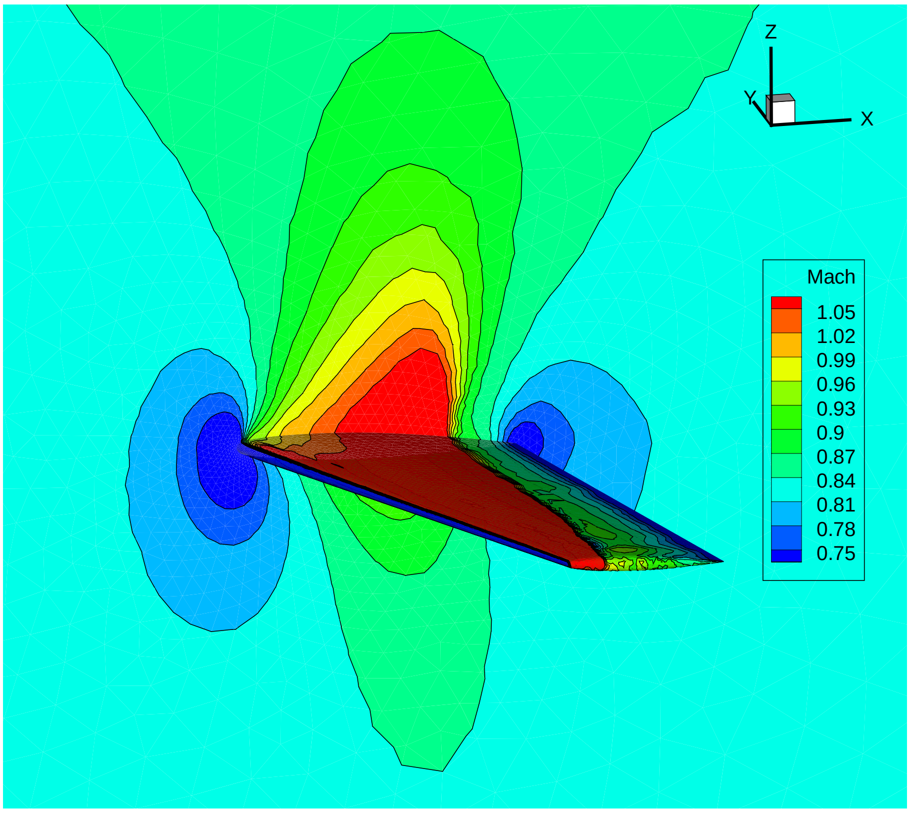

Figure 3: Mach number lines by explicit *SET3D*

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