Introduction of Domain Decomposition Techniques in Time-dependent Flow Problems

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ABSTRACT. The purpose of this article is firstly to report on our experience in using domain-decomposition techniques to improve the efficiency of existing time integration solvers employed to compute hypersonic non-equilibrium flows. Secondly, our goal is to analyze alternate overlapped/non-overlapped domain decomposition algorithms for a model parabolic advection-diffusion-production equation in view of implementation on a parallel computer.

1. Introduction

The context of our preliminary experiments is that of hyperbolic systems (Euler equations plus finite-rate chemistry). Hence, in the hypersonic regime, and for steady external flows, the main numerical difficulty resides in the capture of a strong shock, and in the accurate solution of the species dissociation/recombination phenomena. Due to the presence of a strong shock, and the necessity of coupling complex physical phenomena, the issue of efficiency is critical, and it makes the approach of domain-decomposition attractive from two standpoints. The first is to partition geometrically the computational region occupied by the fluid into subdomains, and use the same numerical algorithm in each. The second considers subdomains where the physical modeling is different. We consider both types of experiments in Sections 3 and 4. Before this, we recall the ingredients of our basic method. Finally, in Section 5, we consider parallel algorithms by domain decomposition on an advection-diffusion model problem (with linear source term).

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2. Basic Implicit Algorithm for Hypersonic Steady Non-Equilibrium Flow

Our typical problem is the computation of the hypersonic, steady non-equilibrium flow around a blunt geometry, modeling a reentry vehicle. We consider the flow of air made of 5 reacting species, N, O, NO, N_2 and O_2 . The flow is governed by the Euler equations (omitted here) coupled with a set of species-convection equations of the type: $\partial/\partial t(\rho Y_s) + \operatorname{div}(\rho Y_s \overline{V}) = \Omega(\rho, T, Y_1, \cdots, Y_5)$, where Y_s is a mass fraction. Hence the problem is of hyperbolic type with source terms, and the applications considered involve highly compressible flows.

The equations are approximated by upwind finite-volume schemes applicable to unstructured meshes [1] [2]. For the time-integration (to steady state) our basic algorithm employs a fractional-step approach, in which the Euler equations and the chemistry equations are advanced forward in time by two subsequent separate substeps [3]. Both substeps are implicit, and solved by Gauss-Seidel. The timestep is local and is increased along the convergence process as the inverse of the residual error, sometimes unlimitedly. Many experiments on the efficiency of this basic algorithm are reported in [3] [4].

3. Experiments with several subdomains, a single numerical model

The external, inviscid non-equilibrium flow over a 60 cm-long double-ellipse geometry at zero incidence is considered. The freestream Mach number is 25. A reference calculation has been performed applying the basic algorithm with a single mesh of 2025 points.

The same mesh is partitioned in seven subdomains (see Figure 1). The same algorithm is applied to full convergence to the smaller domain near the nose, and then to the other subdomains in the direction of the flow. At the interface, Dirichlet conditions from the previous computation are enforced. The converged solution is shown on Figure 1 where iso-temperature contours are drawn. Evidently, the whole solution is smooth (and identical to the single-mesh solution). By the partitioning into subproblems, a reduction in computational work by a factor of 1.6 has been observed. Of course, in this example, the procedure works because all the interfaces are supersonic. However, this algorithm realizes in a very simple way a form of global space-marching which is very attractive if unstructured grids are used, because more conventional space-marching techniques are rather complex to implement in such context.

In a next experiment, the first subdomain, in the nose region where the flow is mostly subsonic, is itself subdivided into 3 overlapped subdomains (see Figure 2) and recomputed. Of course, when computing the first subdomain informations are needed from the two other subdomains because the region is subsonic. Thus the computed solution near the boundaries of the new central subdomain is obviously incorrect; however, with sufficient overlapping, the proper information is "evidently" transferred to the lateral subdomains, since the global solution

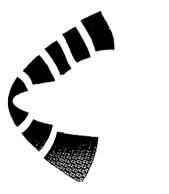




FIGURE 1

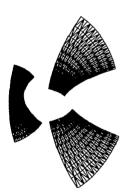




FIGURE 2

is smooth and identical. A minor reduction of the computing time (20%) was realized in this way, but more importantly, the experiment has demonstrated that if the overlapping is sufficiently broad, convergence is maintained even when division is introduced in the elliptic region.

Implementing a multiplicative Schwarz algorithm using the same domain decomposition of the subsonic region resulted in no reduction of CPU time.

Next, the additive Schwarz algorithm (well suited for parallel implementation) was tested. The initial mesh was decomposed into nine overlapped subdomains (see Figure 3). The computation time was observed to be approximately the same as for the reference case. Nevertheless, this result is promising, since each subdomain calculation can be realized independently, perhaps on a separate processor.

In a second calculation, the subsonic region alone was decomposed in both directions in a total of nine overlapped subdomains (see Figure 4). As a result, the computation time was (only) doubled: again, a parallel implementation of this algorithm would be efficient.





FIGURE 3

FIGURE 4

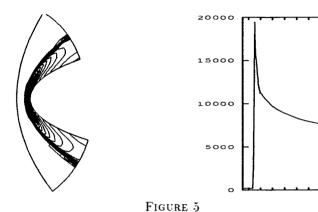
In all the above tests, a general remark can be made: on each subdomain, the robustness of the scheme increases noticeably, due to a better condition of the matrices. Consequently, larger timesteps can be used stably and for steady-state computations fewer time iterations are necessary. For example, in the last example with nine overlapped subdomains, the following CFL numbers could be used on the various subdomains:

no. of the subdomain	1	2	3	-1	-5	6	7	8	9
CFL number	20	40	8	∞	∞.	40	∞	\propto	∞

All these CFL numbers are larger or equal to the value 20 of the reference calculation. Hence, a gain in steady-state convergence is also realized.

4. Experiment with three physical models

We have experimented on the interfacing of three numerical approximations associated with three levels of physical modeling (as in [6]). More precisely, a simpler model is obtained by considering only the Euler equations ("inert gas model"); inversely, a more complex model is obtained by considering in addition thermal non-equilibrium equations (e.g. for N_2 and O_2) of the same mathematical form as the species equations ("chemical and thermal non-equilibrium model"). Typically, this model is redundant in say "half" of the shock layer far from the shock near the body where thermal equilibrium is achieved [5]. Hence, a calculation was made on the previous mesh decomposition (which is a "physical" decomposition). In the three subdomains on the left which contain the freestream region, the inert gas model was used. In the three subdomains on the right and next to the body, the standard chemical non-equilibrium model was used. In the three subdomains in between which contain the shock, the most complex model (chemical and thermal non-equilibrium) was considered. On figure 5, the resulting solution can be observed to be smooth. When employing the most complex model in the shock region only, a reduction in computation time of 48% was measured.



5. Analysis and Implementation of parallel algorithms for a model equation

In view of future applications to the Navier-Stokes equations for non-equilibrium flows, a study is engaged on the following parabolic equation which contains besides the usual advection-diffusion terms, a linear source term to model a typical

production rate :
$$\begin{cases} u_t + \overline{V} . \nabla u - \nu \Delta u = -\lambda u & (\nu, \lambda > 0) \\ u = g & \text{over } \Gamma_{\text{in}} . u_n = 0 & \text{over } \Gamma_{\text{out}} \cup \Gamma_{\text{w}} \end{cases}$$

in which \overrightarrow{V} is a given velocity field. After an implicit time-discretisation, this equation becomes:

$$\alpha u + \overline{V} \cdot \nabla u - \nu \Delta u = f \quad (\alpha > 0)$$

where f contains terms evaluated at the previous time level.

Our first experiment involves overlapped subdomains. If the distributions of u over the boundaries of say two overlapping subdomains Ω_1 and Ω_2 are respectively u_1 and u_2 , and Ω_{12} is the overlap region, the matching condition is realized by driving to zero at each node i of the interface the following quantity

$$J_i = \int_{C_1 \cap \Omega_{12}} (u_1(i) - u_2(i)) \ ds$$

where C_i is the cell around i. The solution of this linear system is carried by a GMRES algorithm. For this test case, this procedure was not found efficient compared with the additive Schwarz algorithm. Of course, fewer time-steps were needed but an increase of the cost by a factor of 3.5 was observed. This is perhaps due to the overly simple context.

An alternative to the above algorithm is to construct a partition of the domain $\Omega = \Omega_1 \cup \Omega_2$ [7] [8]. We denote γ the interface. In such case, one introduces the interface function v, and the target is to calculate this control function so that the index $J(v) = \frac{1}{2} \int_{\gamma} \left(\frac{\partial u_1}{\partial n} + \frac{\partial u_2}{\partial n} \right)^2 ds$ is driven to zero, knowing that

the auxiliary conditions $u_1 = v$ and $u_2 = v$ are enforced at the interface. The index is driven to zero by a descent method whose iteration writes:

$$v(y)^{\alpha+1} = v(y)^{\alpha} - \frac{J \nabla J(y)}{\left\| \nabla J(y) \right\|^2}$$

The gradient is computed from the solution of the adjoint equations [9]:

$$\nabla J(y) = \left(\lambda_x^{(1)} - \lambda_x^{(2)}\right)(0, y)$$

where $\lambda^{(1)}$ and $\lambda^{(2)}$ are two co-states. This procedure was tested on a 1D case :

$$\begin{cases} \alpha u + a u_x - \nu u_{xx} = f : (x, y) \in [0, 1]^2 \\ u(0) = 1, \ u(1) = 0 \end{cases}$$

The partition was made at x = 1/2.

In 1D, this descent method identifies to Newton's method. However, because J and its gradient vanish simultaneously, only linear convergence is achieved. This can be remedied by considering the following alternate index:

$$J(v) = u_x^{(1)}(\frac{1}{2}) - u_x^{(2)}(\frac{1}{2})$$

In this case, quadratic convergence is achieved, and in fact full convergence is realized in two iterations since the index is linear in v.

To extend this elementary concept in 2D, one has to introduce as many such indices, linear in u, as control points, and to solve as many adjoint equations (with different boundary conditions). Hence the alternative is either to use a single quadratic index and face the necessity of identifying an efficient preconditioner, or introduce a large number of linear constraints. The second choice may reveal efficient on a parallel machine, if the various adjoint equations can be solved simultaneously.

6. Conclusions

We have shown with several experiments that domain decompositon techniques were efficient for hypersonic flows, even on a non parallel machine. We have also made a calculation with three different physical models on the subdomains. Simple interface procedures have been proposed in the case of the advection-diffusion model problem. This work permits to envisage certain efficient extensions to the Navier-Stokes equations particularly if a parallel architecture can be exploited.

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