Mecánica Computacional, Volumen XIX, pp. 373-378
Compilado por: F. Quintana y S. Felicelli
San Carlos de Bariloche, Noviembre de 2000

AN ANISOTROPIC ERROR ESTIMATOR FOR COMPRESSIBLE FLOW PROBLEMS

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ABSTRACT.

In this article, a local anisotropic *a posteriori* error estimator is presented. to solve compressible flow equations using automatic mesh generators. The components of this association were selected among several choices available (Almeida et. al, 1998), (Borges et al, 1998) giving a powerful computational tool. The main aim of this simulation is to capture solution discontinuities (in this case shocks), using the least amount of computational resources (elements) compatible with a solution of good quality. This leads to high aspect ratio elements (stretching). In order to achieve this, a directional error estimator was specifically selected. The numerical results show good behaviour of the error estimator, resulting in strongly adapted meshes in few steps (typically 3 or 4 iterations).

INTRODUCTION

Local *a posteriori* error estimators are the appropriate tool to identify automatically regions of the domain where the solution is inaccurate. When the solution shows a highly unidimensional behaviour with smooth variation in one direction and high gradients in the orthogonal one, isotropic error estimators produce strongly refined meshes in all directions. To overcome this problem, in this work a non-isotropic error estimator is presented. A finite element approximation for Euler equations in compressible flow is employed . A Newtonian, compressible inviscid fluid in thermodynamic equilibrium is supposed and no sinks, sources or internal body forces are considered. Since the first papers by (Babuška and Rheinboldt IJNME, 1978) and (Babuška and Rheinboldt SIAM, 1978) on a posteriori error estimates in the finite element method, the subject has become increasingly important in finite element computations. There are essentially two major types of estimators: I) estimators based on residual considerations, and II) estimators based on averaging techniques. A quite precise mathematical analysis has been presented in some linear and nonlinear problems for estimators based on residual considerations (Babuška et al, 1992)(Verfürth, 1989), (Verfürth, 1994). However, some practical difficulties arise trying to obtain anisotropic meshes based on these kinds of estimators. For this reason, in this work a type II estimator has been chosen. An anisotropic error estimator based on the Hessian matrix is presented here, to get highly distorted meshes to approximate solutions with high gradients in some directions and withsmooth behavior in the rest of the domain. This estimator was combined with a flow solver (Quintana, 1993), (Donea and Giuliani, 1981), and coupled together with an automatic mesh generator (Fancello et al, 1991), (Fancello, Salgado Guimarães and Vénere, 1991).

GOVERNING EQUATIONS

The Euler equations in conservative form are usually preferred for CFD. The set of Euler equations for compressible laminar flow of a perfect gas can be written as follows:

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u_i\\ \rho\varepsilon\end{bmatrix}+\sum_{j=1}^{N}\frac{\partial}{\partial x_j}\begin{bmatrix}\rho u_j\\ \rho u_i u_j+p\delta_{ij}\\ (\rho\varepsilon+p)u_j\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}\qquad i=1,2$$

where, u_i stands for the velocity components, ρ the density p pressure, ϵ total specific energy and δ_{ij} is the Kronecker delta. The state equation for a perfect gas, $p=\rho(\gamma-1)[\varepsilon-0.5u_iu_i]$ has proved to be a good approximation for diatomic gases at moderate temperatures and will be used to complete the set.

Boundary conditions: A weak form of imposing boundary conditions was adopted in this work, because the normal definition is not ambiguous (Dari, 1995). As detailed in (Donea & Giuliani, 1981), the number of boundary conditions to be imposed (Donea and Giuliani, 1981) depends on the number of positive eigenvalues in a characteristic analysis.

Wall boundary condition: The well known *slip condition* is imposed here: $u_n = 0$ where u_n is the normal component of the velocity field and no restriction is imposed on density.

Far-field boundary condition: Inflow ($u_n < 0$): Every variable is here prescribed. $\rho = \rho^\infty$ $u_n = u_n^\infty$ $u_t = u_t^\infty$ $e = \frac{p^\infty}{(\gamma-1)\rho^\infty} + \frac{1}{2}((u_n^\infty)^2 + (u_t^\infty)^2)$

Outflow ($u_n > 0$)

Different strategies are possible for the outflow boundary:
i) Impose p and cancel second derivatives for v.
ii) Cancel normal derivatives. ($\frac{\partial\phi}{\partial\bar{n}} = 0$)(adopted in this work)
iii) No conditions imposed.

Symmetries: On the symmetry plane $u_n = 0$ *(slip condition)* and for the other variables, the condition ($\frac{\partial\phi}{\partial\bar{n}} = 0$) is imposed.

NUMERICAL APPROACH

The Navier-Stokes set of equations is approximated with a stabilized finite element technique using tetrahedra for 3D problems or triangles in two dimensions. No convergence accelleration techniques have been implemented in this job.

THE *A POSTERIORI* ERROR ESTIMATOR

Standard assumption and notation are introduced in this section. Given a polygon $\Omega \subset \mathbb{R}^2$, we consider a family of triangulations $\{\mathcal{T}_h\}$ of Ω such that any two triangles in $\mathcal{T}_h$ share at most a vertex or an edge. In the definition of the error estimator we shall use the standard conforming space

$$V_h = \{v \in H_0^1(\Omega) : v|_T \in \mathcal{P}_k(T)\}$$

where $\mathcal{P}_k(T)$ denotes the space of polynomials of degree not greater than k. With each node N_i, $1 \le i \le M$ of the triangulation, we associate a basis function $\varphi_i \in V_h$ in the usual manner. For each i, we set $S_i = supp\varphi_i$.

DERIVATIVE RECOVERY TECHNIQUES

Gradient recovery operator

As linear elements are being used, a specific procedure must be implemented to recover second-order derivatives. These can be recovered using twice a polinomial expansion algorithm that will be presented to compute first-order derivatives (gradients).

As a first step, we recall the *Clément* interpolation operator: given a function $v \in L^2(\Omega)$, we let $P_i v$ denote the projection of the function $v|_{S_i} \in L^2(S_i)$ over the subspace $\mathcal{P}_k(S_i)$; i.e. one has

$$P_i v \in \mathcal{P}_k(S_i) \text{ and } (v - P_i v, p)_{S_i} = 0, \qquad \forall p \in \mathcal{P}_k(S_i) \tag{1}$$

where $(\cdot,\cdot)_S$ is used to denote the inner L^2-product. We set

$$\Pi_C v = \sum_{i=1}^{M} P_i v(N_i)\varphi_i$$

We define the following gradient recovery operator $\nabla_R : V_h \to (V_h)^2$ given by

$$\nabla_R u_h = \Pi_C(\nabla u_h) := \left(\Pi_C \frac{(\partial u_h}{\partial x)}, \Pi_C \frac{(\partial u_h}{\partial y)}\right)$$

In (1) the Gaussian integration points can be used in the numerical computation of the integral. In this case the technique is called *patch recovery technique* (Zienkiewicz and Zhu, 1992) or integral polynomial expansion as will be referred to here. Integration of (1) with different techniques leads to other gradient recovery alghoritms.

The following points must be remarked on:

a) The matrix of the system is symmetrical and independent of the component i to be recovered.

b) The number of equations to solve simultaneously is very reduced (3 for linear triangular elements). Thus the cost of recovery becomes proportional to the number of nodes in the mesh.

c) Once the parameters a have been calculated, the gradient in the studied node is easily calculated.

d) The number of existent elements in a *patch* can be insufficient to ensure the well-posedness of the least-squares problem. This usually happens on boundary nodes and element side nodes (quadratic elements, for example). In this case the initial *patch* is redefined incorporating the elements in those *patches* associated to the nodes of the elements in the initial *patch*.

e) For high-order polinomial expansion, the matrix $\mathbf{P}_p$ can be ill-conditioned due to the monomials degree and the coordinates of the integration points. To overcome this issue, the original *patch* Ω_p is transformed into another normalized $\hat{\Omega}_p$ and in this normalized domain the polinomial expansion is carried out. For example, in two-dimensional problems we can take $\hat{\Omega}_p = [-1,1] \times [-1,1]$ and the linear transformation which maps Ω_p in $\hat{\Omega}_p$ is given by

$$\hat{x} = \frac{2}{\ell_x}(x - x_m), \quad \hat{y} = \frac{2}{\ell_y}(y - y_m)$$

where $\ell_x = x_{max} - x_{min}$, $\ell_y = y_{max} - y_{min}$, $x_m = \frac{1}{2}(x_{max} + x_{min})$and $y_m = \frac{1}{2}(y_{max} + y_{min})$. In the previous expressions we used the notation (x_{min}, y_{min}) and (x_{max}, y_{max}) to represent the maximum and minimum coordinates of the rectangle which contains the *patch* under study. In the case of meshes generated using automatic techniques,such as the *advancing front technique*, (Peiró, 1989), it is convenient to use a compatible transformation with the one used in the mesh generation algorithm.

The second-order derivatives (Hessian matrix) can be recovered using twice the polinomial expansion algorithm proposed to recover the first-order derivative (gradient). In fact, taking $\nabla_R u_h$ as a new field, on each of its components we can apply the algorithm described, obtaining $H^*(u_h) = \nabla_R(\nabla_R u_h)$. Since this matrix is non symmetric, its symmetrical part is adopted to satisfy the symmetry of the Hessian matrix. Therefore, the recovered Hessian $H_R(u_h) \in V_h^{2\times 2}$ is computed as

$$H_R(u_h) = \frac{H^*(u_h) + (H^*(u_h))^t}{2} \tag{2}$$

It is assumed that $u_h \in V_h$ is a good approximation of u which verifies

$$||u - u_h||_{L^2(\Omega)} \simeq C||H_R(u_h(x))(x - x_0) \cdot (x - x_0)||_{L^2(\Omega)} \tag{3}$$

This shows that the interpolation error at one point x such that $|x - x_0|$ is small enough is governed by the behavior of the second-order derivative at this point. Thus, the interpolation error is not distributed isotropically around point x_0; i.e. the error depends on *direction* $x - x_0$ and the recovered Hessian matrix value at this point, $H_R(u(x))$. Therefore, (3) suggests the use of this expression **as a directional local estimator**. However, the recovered Hessian matrix cannot be used as a metric, because it is not positive definite. Using Peiró's idea (Peiró, 1989), the following tensor is introduced

$$\mathbf{G} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T \tag{4}$$

where $\mathbf{Q}$ is the matrix which has the eigenvectors of the recovered Hessian matrix as columns, and $\mathbf{\Lambda} = diag\{|\lambda_1|, |\lambda_2|\}$ and $|\lambda_i|, i = 1,2$ are the absolute values of the eigenvalues $(|\lambda_1| \leq |\lambda_2|)$ of $H_R(u_h(x))$.

Now, given a partition $\mathcal{T}_h$ of Ω, the anisotropic error estimator of $T \in \mathcal{T}_h$ is defined as

$$\eta_T = \{\int_{\Omega_T} (\mathbf{G}(u_h(x_0))(x - x_0) \cdot (x - x_0))^2 d\Omega\}^{\frac{1}{2}} \tag{5}$$

and the global estimator η by

$$\eta = \{\sum_{T\in\mathcal{T}_h} \eta_T^2\}^{\frac{1}{2}} \tag{6}$$

where x_0 is the baricenter of T. The definition of η_T can be used to obtain the following upper bound

$$
\begin{aligned}
\eta_T^2 &= \int_{\Omega_T} (\mathbf{G}(u_h(x_0))(x-x_0)\cdot(x-x_0))^2 d\Omega = \\
&= \int_{\Omega_T} (\sum_{i=1,2} |\lambda_i(x_0)| [e_i(x_0)\otimes e_i(x_0)](x-x_0)\cdot(x-x_0))^2 d\Omega = \\
&= \int_{\Omega_T} \{\sum_{i=1,2} |\lambda_i(x_0)| [e_i(x_0)\cdot(x-x_0)]^2\}^2 d\Omega \leq \\
&\leq \int_{\Omega_T} \{\sum_{i=1,2} |\lambda_i(x_0)| h_i^2\}^2 d\Omega
\end{aligned}
\qquad (7)
$$

where $\mathbf{e}_i(N), i = 1, 2,$ are the eigenvectors of the recovered Hessian matrix.

It is expected that the *shape* of the element be such that the local error in any direction yields the same value. This is equivalent to stating that the local error in the principal directions of curvature yields the same constant in each element, i.e. $|\lambda_1| h_1^2 = |\lambda_2| h_2^2 = constant$ and therefore, the *stretching* of element T is defined as $s_T := \frac{h_1}{h_2} = \sqrt{\frac{|\lambda_2|}{|\lambda_1|}}$ and combining s_T with (7) it follows that $\eta_T^2 \leq \text{area}_T\{2\,|\lambda_2(x_0)|\,h_2^2\}^2$ Which leads to the following upper bound of the local error estimator

$$\eta_T \leq 2\,\text{area}_T{}^{\frac{1}{2}}\,|\lambda_2(x_0)|\,h_2^2.$$

This inequality shows that the local estimator is bounded by the maximum of the second-order derivative in the baricenter of the element multiplied by the square of the element length in this direction.

NUMERICAL RESULTS

Some numerical results obtained by applying the proposed methodology on the solution of compressible Euler equations are presented here. As a vector field of unknowns is computed, and a scalar field indicator is needed to evaluate the Hessian matrix, density has been selected. Mach number and velocity moduli have alternatively been used with similar results. In a forthcoming paper, we shall consider the idea of generalizing our error estimator (5-6) to account for all vector field components simultaneously.

Compression corner

This problem deals with an inviscid supersonic flow ($M = 2$) over a wedge at an angle $\theta = 10^o$. The domain is shown in figure 1. At the inflow ($x = 0$) the values of the variables are: $\rho = 1.0$(density), $\|v\| = 1.0$(velocity), $p = 0.17857$(pressure), and the slip condition was set along the wedge ($y = 0$). The outflow exact solution yields $\rho = 1.45843, v_x = 0.88731, v_y = 0.0, p = 0.30475, M = 1.64$. Density was used as the key scalar field to compare with the previous test. Figure 1 shows the last adapted mesh (step 3, 1354 elements and $s_T \in [1; 30]$). Comparing density contours of fig. 1 with the exact values, a good agreement can be verified.

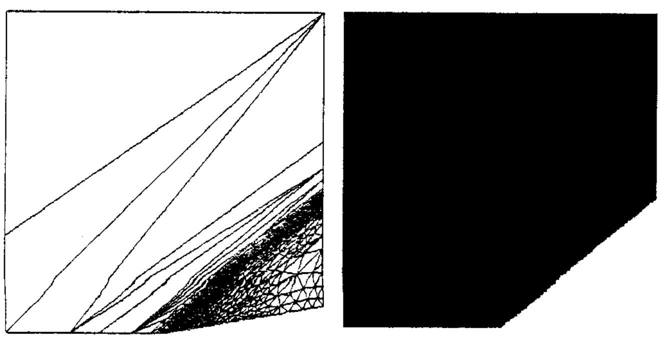

Figure 1. Final finite element mesh (1391 elements, 738 nodes) and corresponding solution (density contours)using density as the key variable

Supersonic flow over a blunt body
This second example has been selected to study the estimator behaviour in the vicinity of strong shocks and the quality of meshes in regions where the body shape is convex. A two-dimensional Mach 2 inviscid flow over a blunt body at zero angle of attack is studied. Due to the problem symmetry we consider only one half of the domain. The undisturbed flow is set at the inflow and at the top of the domain, and is given by: $\rho = 1.0, \|v\| = 1.0, p = 0.17857$(pressure). The stagnation streamline has been selected as the symmetry boundary, where velocity is corrected on each step with a slip condition (this is imposing $u_n = 0$). Figure 2 shows the last adapted mesh (786 nodes, 1484 elements, $s_T \in [1;21]$) which was generated using the density the key scalar variable for the error estimator. The corresponding solution (density contours) is also plotted here.

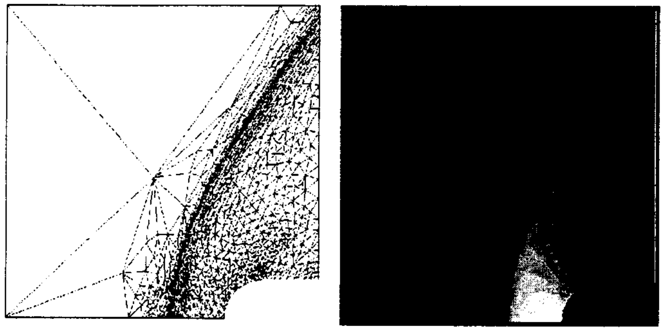

Figure 2. Final finite element mesh (1484 elements, 786 nodes) and corresponding solution (density contours)using density as key variable

Comparing with the previous test, it is evident that a good solution can be found in just three steps (compared with 5 in the previous test) and using a coarser mesh (786 vs. 1597 nodes)with the density as the key variable.

CONCLUSIONS

Based on the recovery of the Hessian matrix, the definition of an anisotropic *a posteriori* error estimator, a mesh-adaptive procedure has been presented. Some numerical applications show that the proposed anisotropic error estimator provides an accurate approximation of the exact error. As a consequence, highly accurate solutions are obtained keeping the number of unknowns affordably low. A further interesting aspect of this mesh-adaptive procedure is that it is *problem independent*, i.e. the algorithm can be easily incorporated to any finite element solver to perform an adaptive analysis. In addition, although an unstructured *advancing front* mesh generator is used, this approach can be employed in association with any unstructured mesh generation that accounts for a local metric defined on the *old* mesh taken as a background mesh during the mesh generation procedure. Future works are under way to extend procedure capabilities to vector unknowns, time-dependent problems and 3-D applications.

ACKNOWLEDGEMENTS

This work was partially supported by PIA 7116 Conicet (Argentina) and PICT 12-03239 of ANPCyT (Argentina).

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