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High order numerical quadratures for layer potentials over curved domains in $\mathbb{R}^3$

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Abstract

High order numerical quadratures for approximating layer potentials over curved domains in $\mathbb{R}^3$ are given. More generally, these numerical quadratures are shown to be useful for evaluating surface integral involving kernels which are pseudo-homogeneous of degree -1. A numerical application is presented.

1. Introduction

A large class of linear physical problems can be solved by means of boundary integral equations. Stokes flows, potential flows, the Helmholtz problem, and linear elasticity problems are examples in this list. Usually the mathematical problem consists of finding a scalar- or vector-valued function s, which is solution to a first-kind or second-kind Fredholm equation involving a.e. x on the boundary of the physical domain Ω (e.g. see [5,6] for a review on this technique). Let $K(x,y)$ be the scalar- or matrix-valued kernel of the physical problem. Then, whatever method is chosen for solving the boundary integral equation, the domain boundary is usually represented by a regular atlas $(\Gamma_i,\psi_i)_{i\in I}$, and one is always obliged to evaluate the influence of the panel set $(\Gamma_i)_{i\in I}$ on a finite set of points $(x_j)_{l\in J}$. That is to say, the following integrals have to be evaluated:

$$\int_{\Gamma_i} K(x,y).s(y)\,\mathrm{d}\sigma_y := \mathcal{K}[s,x,i]. \tag{1.1}$$

If the degree of approximation of s is high and if the panels Γ_i are curved, (1.1) must be numerically evaluated (see [4] for an example of such a numerical evaluation).

The objective of this paper is to present numerical quadratures which are suitable for approximating surface integrals of type (1.1). Emphasis is put on kernels which are pseudo-homogeneous of degree -1. An application of the technique presented here is shown at the end of the paper.

2. Regularity hypotheses

It is assumed that $\partial\Omega$ is piecewise C^k and Ω is locally on one side of its boundary. The panels Γ_i may be curved at will; it is only assumed that they are defined by regular mappings $\psi_i : \widehat{S} \longrightarrow \Gamma_i$, where $\widehat{S}$ is the reference simplex in $\mathbb{R}^2$. Such an atlas may be provided by a standard CAD system. Let J_i be the Jacobian determinant of ψ_i and denote by $\tilde{h}_i$ the diameter of Γ_i, then we have the following classical bounds [4,5]:

$$|\psi_i|_{j,\infty,\widehat{S}} \leqslant c\tilde{h}_i^j, \quad \text{and} \quad |J_i|_{j,\infty,\widehat{S}} \leqslant c\tilde{h}_i^{j+2}. \tag{2.1}$$

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$K(x,.)$ is assumed to be pseudo-homogeneous of degree -1 according to the definition as follows. Consider $x \in \mathbb{R}^3$, introduce the polar coordinates (r,θ) for y in $\mathbb{R}^3 - \{x\}$ so that $r := \| y - x \|$, and $\theta := (y-x)/r$. $K(x,.)$ is pseudo-homogeneous of degree -1 at x up to order k, if there is an open neighbourhood U of x so that for all y in $U \cap \partial\Omega - \{x\}$, $rK(x,r,\theta)$ is differentiable with respect to the polar variables up to order k, and the derivatives in question are bounded.

Consider x on $\partial\Omega$ and Γ_i a panel. Even though $K(x,.)$ is locally integrable on $\partial\Omega - \{x\}$, $K(x,y)$ may not be bounded when y approaches x. Hence, any numerical approximation of $\mathcal{K}[s,x,i]$ must take into account this possible singular behavior. In order to tackle this difficulty, $\mathbb{R}^3$ is divided into three domains. The point x is said to belong to the near field of Γ_i if $x \in \text{int}(\Gamma_i)$. If x is at a distance from Γ_i which is equivalent to $\tilde{h}_i := \text{diam}(\Gamma_i)$, *i.e.* $a\tilde{h}_i \leqslant \text{dist}(x,\Gamma_i) \leqslant b\tilde{h}_i$, where a and b are positive constants which are yet to be specified, then x is said to belong to the intermediate field of Γ_i. If the distance from Γ_i to x is larger than $b\tilde{h}_i$, x is said to be in the far field of Γ_i.

3. Near field

Consider $x \in \text{int}(\Gamma_i)$, define $\hat{x} := \psi_i^{-1}(x)$, and introduce the polar coordinates $(\hat{r},\hat{\theta})$ in the reference simplex. Let $\hat{S}_1$, $\hat{S}_2$, and $\hat{S}_3$ be the three vertices of $\hat{S}$, and define $\hat{\theta}_k$, $(k = 1,2,3)$, as the angles between the axis $\hat{x}\hat{x}_1$ and axes $\hat{x}\hat{S}_k$, $(k = 1,2,3)$. Divide $\hat{S}$ into 3 sectors $\hat{S}_k\hat{x}\hat{S}_{k+1}$, where $\hat{S}_4 = \hat{S}_1$. Then, (1.1) can be cast into the form:

$$\mathcal{K}[s,x,i] = \sum_{k=1}^{3} \int_{\hat{\theta}_k}^{\hat{\theta}_{k+1}} \int_{0}^{\hat{r}(\hat{\theta})} \hat{r}K(x,\hat{r},\hat{\theta}) \cdot \hat{s}_i(\hat{r},\hat{\theta}) J_i(\hat{r},\hat{\theta}) \, d\hat{r} \, d\hat{\theta}, \tag{3.1}$$

where $\hat{\theta}_4 := \hat{\theta}_1 + 2\pi$, $\hat{r}(\hat{\theta})$ is the distance from $\hat{x}$ to $\partial\hat{S}$ along the direction $\hat{\theta}$, and J_i is the Jacobian determinant of ψ_i; $s \circ \psi_i$ has been replaced by $\hat{s}_i$ for short. Note that since $K(x,.)$ is pseudo-homogeneous of degree -1, the term $\hat{r}K(x,\hat{r},\hat{\theta})$ in (3.1) is controlled as long as $\hat{r}/r$ is smooth and bounded from above. Introduce the new variable $\xi_1 \in [0,1]$ so that $d\xi_1 = d\hat{r}/\hat{r}(\hat{\theta})$; it is reasonable to think that the integral with respect to ξ_1 can be approximated by using a Gaussian quadrature. As a result, the measure $d\hat{\theta}$ is replaced by $\hat{r}(\hat{\theta})\, d\hat{\theta}$, where $\hat{r}(\hat{\theta})$ may have large variations if $\hat{x}$ is close to the boundary $\hat{S}_k\hat{S}_{k+1}$. Denote by $\hat{z}_k$ the orthogonal projection of $\hat{x}$ onto $\hat{S}_k\hat{S}_{k+1}$ and let $\hat{h}_k = |\hat{z}_k - \hat{x}|$. Let $\hat{\alpha}_k$ be the angle $(\hat{x}\hat{x}_1, \hat{S}_{k+1}\hat{S}_k)$, then $\hat{r}(\hat{\theta}) = \hat{h}_k/\sin(\hat{\theta} - \hat{\alpha}_k)$; that is to say, the measure which is adapted to the situation is $\hat{h}_k\, d\hat{\theta}/\sin(\hat{\theta} - \hat{\alpha}_k)$. Hence, in each sector $\hat{S}_k\hat{x}\hat{S}_{k+1}$ we introduce the new variable $\xi_2 \in [-1,+1]$ so that $d\xi_2 = 2\, d\hat{\theta}/\Delta_k \sin(\hat{\theta} - \hat{\alpha}_k)$ where

$$\Delta_k := \ln\left[\tan\left((\hat{\theta}_{k+1} - \hat{\alpha}_k)/2\right) / \tan\left((\hat{\theta}_k - \hat{\alpha}_k)/2\right)\right].$$

Then, each integral in (3.1) can be approximated by using the tensor product of Gauss–Legendre quadratures on the rectangle $(\xi_1,\xi_2) \in [0,1] \times [-1,+1]$. Let L and N be the number of quadrature points in directions ξ_1 and ξ_2, respectively, we have

$$\mathcal{K}[s,x,i] \approx \sum_{k=1}^{3} \frac{\hat{h}_k}{2}\Delta_k \sum_{n=1}^{N}\sum_{l=1}^{L} \omega_{2n}\omega_{1l}\hat{r}_{ln}K(x,\hat{r}_{ln},\hat{\theta}_n) \cdot \hat{s}_i(\hat{r}_{ln},\hat{\theta}_n) J_i(\hat{r}_{ln},\hat{\theta}_n), \tag{3.2}$$

where ω_{1l}, ω_{2n} are the weights of the quadratures, and we have set $\hat{r}_{ln} := \hat{r}_l(\hat{\theta}_n)$.

Let $\Delta := \max_{k=1,2,3}\{\Delta_k\}$ and assume $\hat{s}_i$ is a polynomial of degree $p \leqslant \min(2L-1, 2N-1)$, then we have the following error estimate:

THEOREM 3.1. If N is great enough, there are positive constants c, c', and $\gamma > \Delta/2$ so that the quadrature error in the near field is bounded from above by

$$c\tilde{h}_i^{2L-p+1} \| \hat{s}_i \|_{p,q,\hat{S}} + c' h (\Delta/2\gamma)^{2N} \| \hat{s}_i \|_{p,\infty,\hat{S}}. \tag{3.3}$$

PROOF. We give a sketch of the proof; for technical details the reader is referred to [3]. Since (3.2) is the tensor product of two one-dimensional quadratures, the quadrature error can be bounded from above by

$$\sum_{k=1}^{3} \hat{h}_k \frac{\Delta_k}{2} \left[\sup_{\xi_1 \in]0,1[} (E_{1k}(\xi_1)) + \sup_{\xi_2 \in]-1,1[} (E_{2k}(\xi_2)) \right],$$

where E_{1k} and E_{2k} are the elementary quadrature errors. A bound on $E_{1k}(\xi_1)$ is given by the classical theory of Gaussian quadratures (see Ref. [1, p. 344]); that is to say, there are two constants c and $\gamma > (\Delta/2)$ such that

$$E_{1k}(\xi_1) \leqslant c(\Delta/2\gamma)^{2N} \| J_i \|_{0,\infty,\widehat{S}} \| \hat{s}_i \|_{p,\infty,\widehat{S}} \| \hat{r} K(x, \psi_i(\hat{r}, \hat{\theta})) \|_{2N,\infty,\widehat{S}}.$$

The key point here is that due to pseudo-homogeneity $\| \hat{r} K(x, \psi_i(\hat{r}, \hat{\theta})) \|_{2N,\infty,\widehat{S}}$ is bounded from above by $c/\tilde{h}_i$.

A bound on E_{2k} is given by the Bramble Hilbert lemma together with various forms of Hölder inequality

$$E_{2k}(\xi_2) \leqslant \sum_{j=0}^{p} | \hat{s}_i |_{j,q,S_\theta} \sum_{l=0}^{2L-j} c_{jl} | \hat{r} K(x, \psi_i(\hat{r}, \hat{\theta})) |_{l,\infty,S_\theta} | J_i |_{2L-j-l,\infty,S_\theta},$$

where S_θ is the segment $\hat{r} \in]0, \hat{h}_k / \sin(\hat{\theta} - \hat{\alpha}_k)[$. The desired result is obtained by using pseudo-homogeneity which yields

$$| \hat{r} K(x, \psi_i(\hat{r}, \hat{\theta})) |_{l,\infty,S_\theta} \leqslant c \tilde{h}_i^{l-1}.$$

Note that error estimate (3.3) is consistent with that of Johnson and Scott's Lemma 3.1, p. 1365 [4]. The present approach, though, emphasizes the polar coordinates' role.

Assume the quadrature error must be of $\mathcal{O}(h^k)$ so that it is of the same order as that induced by the approximation, by some particular scheme, of the solution to the boundary integral equation referred to in the introduction. Then, integers L and N must be chosen so that

$$L = \max\{(p+1)/2, (k+p-1)/2\} \quad \text{and} \quad N = \max\{(p+1)/2, (k-1)\ln(1/h)/\ln(2\gamma/\Delta)\}.$$

If h is small enough the ratio of N/L behaves like $\ln(1/h)$; that is to say, more quadrature points must be put in the azimuthal direction than in the radial direction. This fact has been well observed on numerical tests (cf. [2]).

4. Far field

Assume now that x is in the far field of Γ_i. The integral in (1.1) is approximated by means of a quadrature rule that is exact on $\widehat{S}$ for polynomials of degree $t \geqslant p$. In other words, an approximation of $\mathcal{K}[s, x, i]$ is given by:

$$\mathcal{K}[s, x, i] \approx \sum_{q=1}^{Q(t)} \omega_q^{\text{far}} K(x, \psi_i(\hat{x}_q)) \cdot \hat{s}_i(\hat{x}_q) J_i(\hat{x}_q), \tag{4.1}$$

where ω_q^{far} and $\hat{x}_q$ are the weights and the quadrature points of the quadrature rule in question. An evaluation of the quadrature error is given by:

THEOREM 4.1. Let $\alpha = 1$ (resp. $\alpha = 2$) if $K(x,.)$ is a single (resp. double) layer kernel; then, if $\tilde{h}_i$ is small enough, there is $\gamma > 1$ so that for $q \in [1, \infty]$ the quadrature error, E_t, satisfies:

$$E_t \leqslant c \tilde{h}_i^{2-\alpha} (\gamma b)^{p-t-1-\alpha} \| \hat{s}_i \|_{p,q,\widehat{S}}. \tag{4.2}$$

PROOF. From the Bramble Hilbert lemma we infer that

$$E_t \leqslant c \mid K(x,\psi_i)\cdot \hat{s}_i J_i \mid_{t+1,q,\widehat{S}}.$$

Using the fact that $\hat{s}_i$ is a polynomial of degree p, where $p \leqslant t$, and applying various forms of Hölder inequality yields:

$$E_t \leqslant \sum_{j=0}^{p} \mid \hat{s}_i \mid_{j,q,\widehat{S}} \sum_{l=0}^{t+1-j} c_{jl} \mid K(x,\psi_i) \mid_{l,\infty,\widehat{S}} \mid J_i \mid_{t+1-j-l,\infty,\widehat{S}},$$

where c_{jl} are positive constants which do not depend on i. Furthermore, it can be shown that if $K(x,.)$ is a single or double layer type kernel and if $\tilde{h}_i$ is small enough there exists a constant $\gamma_l \geqslant 1$, independent of i, so that:

$$\mid K(x,\psi_i) \mid_{l,\infty,\widehat{S}} \leqslant c\frac{\tilde{h}_i^{-\alpha}}{(\gamma_l b)^{l+\alpha}}.$$

As a result, we have

$$E_t \leqslant \sum_{j=0}^{p} \mid \hat{s}_i \mid_{j,q,\widehat{S}} \sum_{l=0}^{t+1-j} c_{jl}(\tilde{h}_i\gamma_l b)^{-l-\alpha}\tilde{h}_i^{t+1-j+2}.$$

Setting $\gamma := \inf\{\gamma_l\}$ and using the equivalence of norms in finite dimensional, normed vector spaces, we obtain the desired result. □

Assume as in the previous section that the quadrature error must be of $\mathcal{O}(h^k)$ so that it is of the same order as that induced by the approximation of the solution to (1.1) by some particular scheme. Then, the integer t and the far field constant b must be chosen so that:

$$t = \sup\left\{p, p-1-\alpha+(k+\alpha-2)\frac{\ln(1/h)}{\ln(\gamma b)}\right\}. \tag{4.3}$$

The constant b must be chosen great enough so that $\gamma b > 1$. Numerical tests performed on the simple and double layer potentials of the Laplace equation have shown that for $0 \leqslant p \leqslant 4$, an optimal choice for b may be $0.2 \leqslant b \leqslant 0.4$ (see numerical tests below and [2]).

5. Intermediate field

When x is in the intermediate field of Γ_i, $\widehat{S}$ is divided into N^2 simplexes which are geometrically similar to $\widehat{S}$. On each sub-simplex one uses a quadrature rule which is of the same type as that which has been used in the far field. More precisely, let $\hat{\psi}_n$ be the unique linear mapping which maps $\widehat{S}_n$ into $\widehat{S}$ and which Jacobian determinant is positive. Let t be an integer, yet to be specified, so that $p \leqslant t$. Consider on $\widehat{S}$ a quadrature rule $(\omega_q^{\text{inter}}, \hat{x}_q)_{1\leqslant q\leqslant Q(t)}$ which is assumed to be exact for polynomials of degree less than or equal to t. This quadrature rule is applied on each elementary simplex $\widehat{S}_n$ as follows:

$$\mathcal{K}[s,x,i] \approx \sum_{n=1}^{N^2}\sum_{q=1}^{Q(t)} \frac{1}{N^2}\omega_q^{\text{inter}} K(x,\psi_i(\hat{x}_q^n))\cdot \hat{s}_i(\hat{x}_q^n) J_i(\hat{x}_q^n), \tag{5.1}$$

where we have set $\hat{x}_q^n := \hat{\psi}_n(\hat{x}_q)$ for short.

THEOREM 5.1. Assume x is in the intermediate field and K is a single or double layer type kernel. There is a constant $\beta \geqslant 1$ so that, if $\tilde{h}_i$ is small enough, the quadrature error is bounded by:

$$c\tilde{h}_i^{2-\alpha}(\beta a N_t)^{p-t-1-\alpha} \parallel \hat{s}_i \parallel_{p,q,\widehat{S}}, \tag{5.2}$$

where $N_t := N^{t+3/t+1-p+\alpha}$.

PROOF. Divide the error into N^2 terms, one for each sub-simplex; then, proceed as in the far field. □

Assume that the quadrature error must be of $\mathcal{O}(h^k)$, and that N is chosen so that $N_t \beta a$ is greater than a specified constant C_N. Then, the integer t must be chosen so that:

$$t = \sup\left\{p, p - 1 - \alpha + (k + \alpha - 2)\frac{\ln(1/h)}{\ln(C_N)}\right\}. \tag{5.3}$$

We have yet to specify N and the intermediate field constant a. Note that

$$N = \left(\frac{C_N}{\beta a}\right)^{t+1-p+\alpha/t+3} \tag{5.4}$$

Furthermore, x belongs to a finite set of control or quadrature points. Let Q_{lp} be the set in question. The intermediate field constant can be chosen so that:

$$a = \inf\left\{\frac{\operatorname{dist}(x, \Gamma_i)}{\tilde{h}_i} \;:\; x \in Q_{lp} - \Gamma_i, \quad i \in I\right\}. \tag{5.5}$$

Note that the present scheme is of interest only if we can be sure that N is bounded as h converges to zero. For this matter we have to verify that a does not converge to zero as h decreases to zero. Actually, it can be shown that, provided a quasi-uniformity hypothesis on the atlas $(\Gamma_i, \psi_i)_{i\in I}$ is satisfied, a is bounded below when h converges to zero [3].

6. A numerical application

The quadrature formulae above have been used for approximating the solution to the following boundary integral equation:

$$u(x) - \frac{1}{2\pi}\int_{\partial\Omega} u(y)\frac{\partial}{\partial n_y}\frac{1}{|x-y|}\,\mathrm{d}\sigma_y = -\frac{1}{2\pi}\int_{\partial\Omega} g(y)\frac{1}{|x-y|}\,\mathrm{d}\sigma_y. \tag{6.1}$$

The unknown function $u(x)$ may be interpreted as the trace on $\partial\Omega$ of the solution to an exterior Neumam problem for the Laplace equation. The reader is referred to e.g. [5] or [6] for further details on the mathematical aspect of this problem. This equation is the model equation for external potential flows in aerodynamics.

The solution to (6.1) is approximated by means of a discontinuous Galerkin method [2]. The numerical method of solution has been tested on an ellipsoid of semi-axes $a_1 = 0.5$, $a_2 = 0.25$, and $a_3 = 0.25$. For this class of domain, the analytical solution to (6.1) is known. The atlas $(\Gamma_i, \psi_i)_{i\in I}$ has been provided by a CAD system. Three series of tests have been performed for three different mesh sizes h corresponding to three types of discretization of $\partial\Omega$. The first atlas is composed of 76 panels ($h \approx 1/5$), the second one is composed of 304 panels ($h \approx 1/10$), and the last one is composed of 684 panels ($h \approx 1/15$). In Fig. 1 is plotted the base-10 logarithm of the error $\|u - u_{hp}\|_{L^2(\partial\Omega)}$, for the three values of h defined above, as a function of the polynomial degree of the approximation p. The computations were made in single precision on an Alliant FX80. It may verified that the error is $\mathcal{O}(h^{p+1})$. This suggests, and it has been verified in practice, that for a fixed precision one minimizes the computational cost as one works with a "coarse" panelling and a "high" polynomial degree of approximation. Coarseness of the panelling is understood in the sense that $\partial\Omega$ is approximated by a "small" number of curved panels whose degree of approximation is at least larger than that chosen for approximating the solution, that is p. The panelling coarseness is bounded below by regularity criteria, namely, the panels must not be too far from flat panels.

To fully illustrate the present method, it has been applied on an industrial case. In Fig. 2 is shown the pressure coefficient distribution on a test submarine. The surface consists of 824 curved elements directly obtained from a CAD representation of $\partial\Omega$. No symmetry was assumed. The computation was made with a linear approximation of the potential, $p = 1$. The 2472×2472 order influence matrix takes some thirty minutes

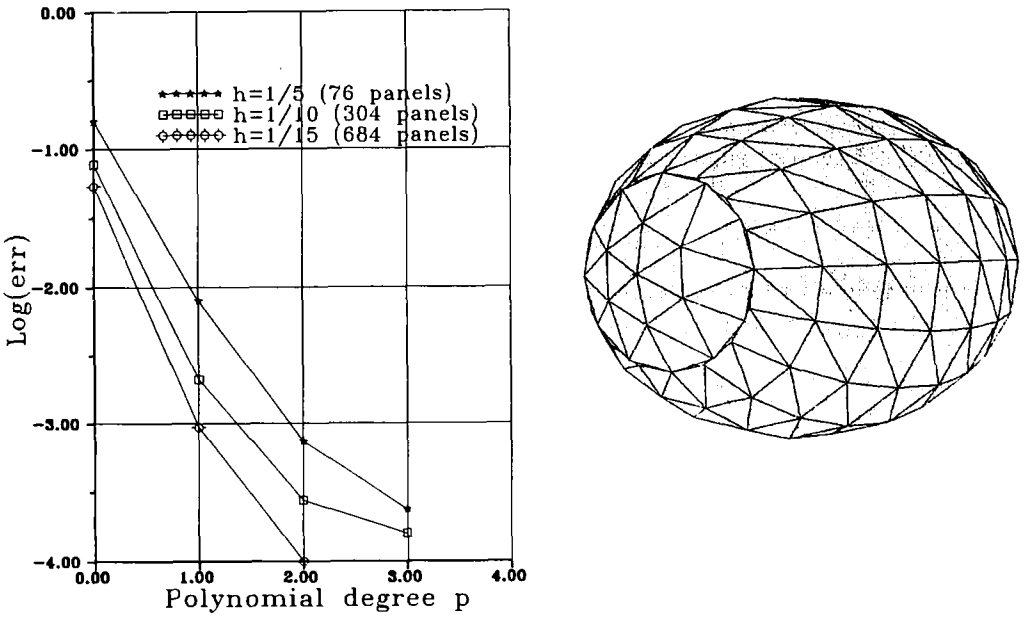

Fig. 1. (left) $L^2(\partial\Omega)$ error as a function of h and p; (right) example of atlas generated by a CAD system (304 panels).

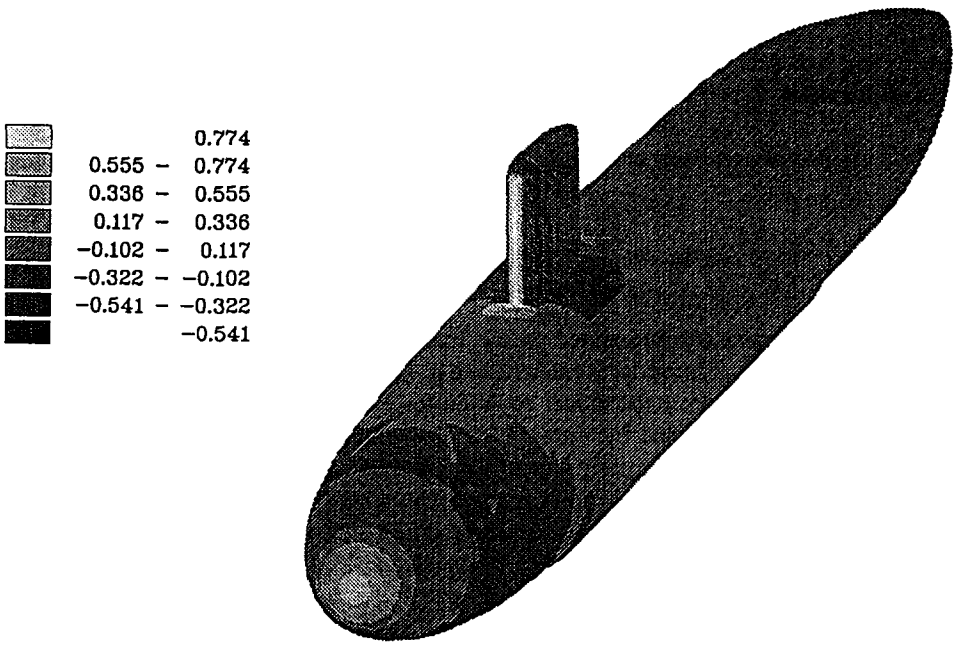

Fig. 2. Pressure coefficient distribution on a test submarine.

of CPU time to construct on an Alliant FX80 computer; using an LU method resident on the computer, the system is solved in a few seconds.

7. Conclusions

A definition of pseudo-homogeneity that emphasizes the role of polar coordinates has been given. Numerical quadratures for approximating integrals of type (1.1) over curved domains in $\mathbb{R}^3$ along with estimates on the quadrature errors have been presented in Eqs. (3.2), (4.1), and (5.1). The error estimate (3.3) is consistent

with that obtained by Johnson and Scott [4] by a different approach. The numerical quadratures are suitable whenever the kernel of the physical problem, which is considered, is pseudo-homogeneous of degree -1. The simple layer potentials of Laplace and Helmholtz equations along with that of the Stokes flow problem and the linear elasticity problem are pseudo-homogeneous of degree -1. The same conclusion holds for the double layer potentials of Laplace and Helmholtz equations. The numerical quadrature presented here may be useful when an approximation of the solution to integral equation of type (6.1) is sought. No approximation of the surface $\partial\Omega$ is needed. The present approach only requires that $\partial\Omega$ is defined by a regular chart of the form $(\Gamma_i, \psi_i)_{i\in I}$ which may be provided by a standard CAD system.

An important problem that has yet to be addressed consists of defining an algorithm that would automatically refine a "coarse" chart of the form $(\Gamma_i, \psi_i)_{i\in I}$ or automatically control the local degree of approximation p in order to attain a fixed precision. Such a strategy would take full advantage of the present method.

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