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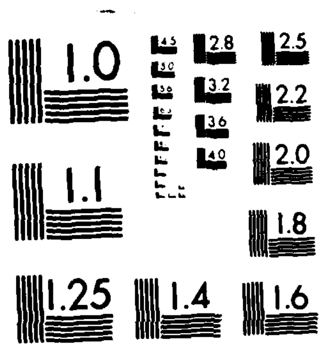

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EXPLICIT SMOOTH VELOCITY KERNELS FOR VORTEX METHODS

J. T. Beale and A. J. Majda

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

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ABSTRACT

Recently the authors showed the convergence of a class of vortex methods for incompressible, inviscid flow in two or three space dimensions. These methods are based on the fact that the velocity can be determined from the vorticity by a singular integral. The accuracy of the method depends on replacing the integral kernel with a smooth approximation. The purpose of this note is to construct smooth kernels of arbitrary order of accuracy which are given by simple, explicit formulas.

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* Department of Mathematics, Tulane University, New Orleans, LA 70118.

** Department of Mathematics, University of California, Berkeley, CA 94720.

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SIGNIFICANCE AND EXPLANATION

Vortex methods simulate incompressible, inviscid flow by a system of ordinary differential equations for the paths of representative particles in the fluid. They have the advantage that the computational elements are automatically concentrated in the region of vorticity and errors like the numerical diffusion of difference methods are avoided. The use of modified velocity kernels ensures the accuracy and stability of the method. Explicit formulas for these kernels make it possible to implement this method as directly and efficiently as if no smoothing were used.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

EXPLICIT SMOOTH VELOCITY KERNELS FOR VORTEX METHODS

J. T. Beale* and A. J. Majda**

Recently the authors proved the convergence of a class of vortex methods for the simulation of incompressible, inviscid flow in two or three space dimensions without boundaries (see [1,2]). The principle of such methods is to reduce the calculation of the flow to a system of ordinary differential equations for the paths of representative particles. The velocity field is given by the convolution of a singular kernel with the vorticity distribution. In the class of methods treated, the stability and discretization error are controlled by a distortion of the nearby interaction of the particles. This is accomplished by convolving the integral kernel with a smooth approximation to the delta function. The choice of this function determines the order of accuracy of the method for smooth flows. The purpose of this note is to produce a class of functions which lead to smooth kernels given by simple, explicit formulas. With these choices, the method can be implemented with essentially no more effort than would be necessary if the original kernel were used. In each case treated here, kernels of high order accuracy are obtained easily from ones of low order by scaling or other modification.

A general description of various vortex methods in use can be found in the survey article of Leonard [6]. A summary of theoretical results is contained in [7], and complete proofs are given in [1,2,5]. Numerical

* Department of Mathematics, Tulane University, New Orleans, LA 70118.

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experiments of Hald and Del Prete [4] for two-dimensional methods as in [2] are in general agreement with the predictions of the convergence results, and further experiments, including tests of higher order accuracy, are currently under way. A three-dimensional method similar to that of [1], but with significant differences, has been used by Chorin [3].

Vortex methods are based on the fact that, for incompressible flow, the velocity is determined from the vorticity by a convolution,

$$u(z,t) = (K*\omega)(z,t) = \int K(z-z')\omega(z',t)dz' \quad . \tag{1}$$

(We will use notation consistent with [1,2]. This formula is interpreted differently in two or three dimensions; see below.) In the methods of [1,2], as in earlier work, the velocity kernel K is replaced by

$$K_\delta = K * \psi_\delta, \qquad \psi_\delta(z) = \delta^{-N}\psi(z/\delta) \quad . \tag{2}$$

Here $N = 2$ or 3 is the space dimension and δ is a parameter to be chosen in conjunction with the linear spacing h of the particles introduced at time zero. The smoothing of the kernel by the function ψ_δ can be interpreted as the approximation of the vorticity distribution by a sum of "blobs" of prescribed shape (see [5] or [7]).

We will choose the function ψ subject to the conditions

(i) ψ is smooth and rapidly decreasing, i.e.,

$$|D^\beta\psi(z)| \le C_{\beta j}(1 + |z|^2)^{-j}$$

for every multi-index β and every integer j;

(ii) $\int \psi(z)d^Nz = 1$;

(iii) $\int z^\beta\psi(z)d^Nz = 0, \quad 1 \le |\beta| \le p-1$,

where p is an integer.

The results of [1,2] imply that vortex methods satisfying (i) - (iii) converge provided the relation between δ and h is properly chosen. If $\delta = h^q$, q any fixed number with $0 < q < 1$, the error is of the order of

$\delta^p = h^{pq}$, i.e. the method is essentially pth order. Our object here is to choose ψ so that K_δ has a simple expression consistent with these requirements. As we shall see, choices of ψ with $p = 2$ easily lead to choices with $p \geq 4$.

Condition (i) implies that the Fourier transform of ψ, as well as ψ itself, is smooth and rapidly decreasing. We will always take $\psi = \psi(r)$, $r = |z|$. In this case (iii) holds by symmetry for $|\beta|$ odd, so that p may be assumed even. For radial ψ, (iii) is always satisfied with $p = 2$. This set of conditions is more stringent than those in the general theory of [1,2]. (In the earlier language we are assuming ψ to be in the class $F \in S^{-\infty,p}$.) The condition (i) can be relaxed somewhat to allow a ψ which is not very smooth at $z = 0$. Indeed, our simplest choice in three dimensions has this property. With a weaker condition replacing (i), a similar convergence result holds, but q is restricted to an interval $0 < q < q_0$ for some $q_0 < 1$. (See [1] for precise statements.)

Two-dimensional Flows

In the 2-D case the vorticity is the scalar function $\omega = u_{2,x} - u_{1,y}$. The distinguishing property of two-dimensional flows is that the vorticity is conserved along particle paths:

$$\omega_t + u \cdot \nabla\omega = 0 \quad . \tag{3}$$

Suppose an initial velocity field is prescribed with vorticity ω_0 nonzero only within a bounded set. To simulate the flow, we cover this set with a square grid of size h and introduce a particle at the center of each square. We take the coordinates of a typical particle to be ih, where $i = (i_1, i_2)$ is a pair of integers; the ith particle is assigned the vorticity $\omega_i = \omega_0(ih)$. To compute approximate paths of the particles, we discretize (1), with K replaced by K_δ, remembering (3), and arrive at the system of ordinary differential equations

$$\tilde{z}_i' = \sum_j K_\delta(\tilde{z}_i - \tilde{z}_j)\omega_j h^2, \qquad \tilde{z}_i(0) = ih \quad . \tag{4}$$

The area-preserving property of incompressible flow is used implicitly here. Once the $\tilde{z}_i$'s have been determined, an expression for the veloc be obtained by setting

$$\tilde{u}^h(z,t) = \sum_j K_\delta(z-\tilde{z}_j)\omega_j h^2 \quad .$$

To apply this method it is best to have an explicit formula for K_δ. If G is the Green's function for $-\nabla^2$, $G(z) = -(2\pi)^{-1} \log r$, then with $z = (x,y)$

$$K(z) = (\partial_y, -\partial_x)G = \frac{(-y,x)}{2\pi r^2} \quad .$$

A natural choice of ψ is the Gaussian $\psi^{(2)}(r) = e^{-r^2}/\pi$. The necessary conditions (i) - (iii) are satisfied with $p = 2$. If $K_\delta = K * \psi_\delta$ then

$$K_\delta = (\partial_y, -\partial_x)G_\delta \quad , \quad G_\delta = G * \psi_\delta \quad . \tag{5}$$

Since ψ is radial, G_δ is also, and

$$\nabla^2 G_\delta = \nabla^2(G * \psi_\delta) = -\psi_\delta \quad \text{or}$$

$$\frac{1}{r} D_r(rD_r G_\delta) = -\psi_\delta(r) = -\frac{1}{\pi\delta^2} e^{-r^2/\delta^2} \quad .$$

after integration we have

$$D_r G_\delta = \frac{1}{2\pi r}(e^{-r^2/\delta^2} - 1) \quad .$$

The constant of integration is determined by the fact that G_δ must be smooth. The corresponding velocity kernel K_δ may now be found from (5):

$$K_\delta^{(2)}(z) = \frac{(-y,x)}{2\pi r^2}(1 - e^{-r^2/\delta^2}) \quad .$$

The superscript (2) has been inserted to indicate the order of the kernel.

Next we will obtain a fourth order kernel by choosing $\psi = \psi^{(4)}$ as a combination of two Gaussians with different scalings,

$$\psi^{(4)}(r) = c_1\psi^{(2)}(r) + c_2\psi^{(2)}(r/a)$$

where a is arbitrary except that $a \neq 1$. To satisfy condition (ii) we must have

$$c_1 + a^2c_2 = 1 \quad .$$

This leaves us with one constraint to impose moment conditions. Because of symmetry, condition (iii) will hold with $p = 4$ provided

$$\int \psi^{(4)}(r)r^2 \cdot rdr = 0 \quad .$$

This in turn holds if

$$c_1 + a^4c_2 = 0 \quad ,$$

and the two equations determine $\psi^{(4)}$ in terms of a. We can now find $K_\delta^{(4)}$ just as in the previous case:

$$K_\delta^{(4)}(z) = \frac{(-y,x)}{2\pi r^2}\,(1 - c_1e^{-r^2/\delta^2} - c_2a^2e^{-r^2/a^2\delta^2}) \quad .$$

For example, the choice $a^2 = 2$ leads to

$$K_\delta^{(4)}(z) = \frac{(-y,x)}{2\pi r^2}\,(1 - 2e^{-r^2/\delta^2} + e^{-r^2/2\delta^2})$$

$$= \frac{(-y,x)}{2\pi r^2}\,(1 - e^{-r^2/2\delta^2})(1 + 2e^{-r^2/2\delta^2}) \quad .$$

It should be clear that higher order kernels can be constructed by adding further terms with Gaussians of different scalings in the expression for ψ. A typical sixth order kernel is

$$K_\delta^{(6)}(z) = \frac{(-y,x)}{2\pi r^2}\,(1 - \frac{8}{3}\,e^{-r^2/\delta^2} + 2e^{-r^2/2\delta^2} - \frac{1}{3}\,e^{-r^2/4\delta^2}) \quad .$$

Of course, care must be taken in evaluating any version for r small, since the factor due to the smoothing vanishes at $z = 0$.

Even simpler high order kernels can be obtained by choosing ψ in the form $\psi(r) = P(r)e^{-r^2}$, where P is a polynomial in even powers of r. Then as in the argument above

$$rD_rG_\delta(r) = -\delta^{-2} \int rP(r/\delta)e^{-r^2/\delta^2}dr$$

$$= (2\pi)^{-1}\{Q(r/\delta)e^{-r^2/\delta^2} - Q(0)\} \quad ,$$

where Q is another even polynomial of the same degree. For condition (ii) to hold we must have $rD_rG_\delta(r) \to -1/2\pi$ as $r \to \infty$, so that $Q(0) = 1$. Finally

$$D_rG_\delta(z) = \frac{1}{2\pi r}\,(Q(r/\delta)e^{-r^2/\delta^2} - 1) \quad ,$$

and according to (5),

$$K_\delta(z) = K(z)(1 - Q(r/\delta)e^{-r^2/\delta^2}) \quad .$$

To satisfy the moment conditions (iii) we need to have

$$\int_0^\infty r^{2j}P(r)e^{-r^2}r\,dr = 0, \qquad 1 < j < (p-2)/2 \quad ,$$

or after integrating by parts,

$$\int_0^\infty r^{2j-1}Q(r)e^{-r^2}dr = 0 \quad .$$

The moment conditions are thus reduced to linear equations for the coefficients of Q. With $p = 4$ we find $Q(r) = 1 - r^2$, corresponding to the fourth order kernel

$$K_\delta^{(4)}(z) = \frac{(-y,x)}{2\pi r^2}\{1 + (-1 + r^2/\delta^2)e^{-r^2/\delta^2}\} \quad .$$

For order p a polynomial of degree $p - 2$ is sufficient. For example, with $p = 6$ we have

$$K_\delta^{(6)}(z) = K(z)\{1 - Q(r/\delta)e^{-r^2/\delta^2}\}$$

with $-Q(r) = -1 + 2r - r^4/2$.

Three-dimensional flows

In the three-dimensional case the vorticity $\omega = \nabla \times u$ is a vector quantity, and the velocity is expressed in the form (1) by the Biot-Savart Law. We will approximate the particle paths by an analogue of (4), but now the vorticity must be updated as well as the position. A natural way to do this is to use the direct generalization of (3)

$$\omega_t + u \cdot \nabla\omega = \omega \cdot \nabla u \quad ;$$

this is essentially the method used by Chorin [3]. However, the derivative on the right must be computed by differences based on the current particle locations, which already contain errors. To avoid this difficulty, we use instead a Lagrangian expression for the vorticity evolution due to Cauchy. Let α be the Lagrangian position and $\phi^t : \alpha \to z$ the coordinate mapping induced by the flow. Then

$$\omega(z,t) = \nabla\phi^t(\alpha) \cdot \omega_0(\alpha)$$

where ω_0 is the initial vorticity and $z = \phi^t(\alpha)$. Thus the vorticity is carried along particle paths but distorted by the Jacobian matrix of the flow. Differentiating in t, with α fixed, we have

$$\frac{d\omega}{dt}(z,t) = \nabla_\alpha u(z,t) \cdot \omega_0(\alpha) \quad ,$$

with a Lagrangian, rather than Eulerian, gradient of the velocity. This derivative can easily be implemented by a difference operator on the initial grid. We are thus led to the following method: given current values of $\{\tilde{z}_j\}$, $\{\tilde{\omega}_j\}$, we can compute

$$\tilde{u}^h(z,t) = \sum_j K_\delta(z - \tilde{z}_j(t))\tilde{\omega}_j(t)h^3 \quad .$$

The updates are then defined by the system of ordinary differential equations

$$\tilde{z}_i' = \tilde{u}^h(\tilde{z}_i,t), \qquad \tilde{z}_i(0) = ih$$

$$[illegible] \quad \nabla^{h} [illegible] (z_i,t) \cdot \omega_0(ih), \qquad \tilde{\omega}_i(0) = \omega_0(ih) \quad ,$$

where ∇^h is an anti-symmetric difference operator whose order is at least the intended order of accuracy. (See [1] for more details.)

The three-dimensional realization of (1) is

$$u = K * \omega = \nabla\times(G * \omega) \quad ,$$

where G is the Green's function for $-\nabla^2$, $G = 1/4\pi r$, and the convolution is componentwise. As before we set $G_\delta = G * \psi_\delta$ and $K_\delta = K * \psi_\delta$. It is easy to see that

$$(K_\delta * \omega)(z) = \int \frac{\partial G_\delta}{\partial r}(|z-z'|)\,\frac{z-z'}{|z-z'|} \times \omega(z')dz'$$

or more briefly

$$K_\delta(z) = \frac{\partial G_\delta}{\partial r}(|z|)\,\frac{z}{|z|} \times \quad .$$

Thus K_δ will have a simple expression provided $\partial G_\delta/\partial r$ does so.

In this case it is less clear how to choose ψ than in the two-dimensional case, and it is best to proceed in the opposite direction from before. For simplicity we assume at first that $\delta = 1$. We suppose that

$$\frac{\partial G_1}{\partial r} = -\frac{f(r)}{4\pi r^2}$$

with f to be determined; this form is convenient since we expect $\partial G_1/\partial r \sim \partial G/\partial r = -1/4\pi r^2$ as $r \to \infty$. Then

$$-\psi = \nabla^2 G_1 = r^{-2}D_r\{r^2 D_r G_1\}$$

so that

$$\psi(r) = \frac{f'(r)}{4\pi r^2} \quad . \tag{6}$$

We can now list the conditions which must be satisfied by f so that conditions (i) - (iii) hold for ψ. Since ψ should be smooth we require

(C1) $f'(r)$ is a smooth function of r^2;

(C2) $f(r) = O(r^3)$ as $r \to 0$.

It is easily seen that the total weight of ψ is $f(\infty)$, and our last condition is therefore

(C3) $f(r) \to 1$ as $r \to \infty$, and f' is rapidly decreasing.

If (c1) - (c3) hold, then ψ, defined by (6), satisfies (i) - (iii) with $p = 2$. Two choices of f meeting our requirements are

$$f(r) = 1 - e^{-r^3}, \qquad f(r) = \tanh r^3 \quad ,$$

corresponding to $\psi(r) = (3/4\pi)e^{-r^3}$ and $\psi(r) = (3/4\pi)\mathrm{sech}^2 r^3$, respectively. The first choice is simpler and is analogous to the Gaussian function in two dimensions. Actually, in this case (C1) does not hold in the strictest sense at the origin because $f(r)$ has terms r^6 and higher in the Taylor expansion. However, the general theory of [1,2] applies to this choice, and we do not expect the difference to be significant in practice. Having chosen f, we define ψ_δ from (2) and reverse our steps to find

$$\frac{\partial G_\delta}{\partial r} = - \frac{f(r/\delta)}{4\pi r^2}$$

so that

$$K_\delta(z) = - \frac{1}{4\pi r^3} f(r/\delta) z \times \quad .$$

The kernels just constructed are second order accurate with respect to δ. If f' is arbitrarily smooth, as is true for $f(r) = \tanh r^3$, then we have convergence with $\delta = h^q$, $q = 1-\varepsilon$, and the errors are essentially second order in h as well. For the "cubic Gaussian", the results of [1] require $q < 5/8$, so that the order of convergence in h is $5/4 - \varepsilon$. (See Theorem 1 in [1] and the remarks following Theorem 2; the number M is 6 in this case. The predicted order of convergence is not sharp and can be improved at least to $3/2 - \varepsilon$.)

To obtain kernels with $p = 4$ we can combine two different scalings as before. Let $\psi^{(4)}(r) = c_1\psi(r) + c_2\psi(r/a)$, where ψ is one of the two choices specified above. The conditions that $\psi^{(4)}$ have weight one and satisfy the second order moment conditions lead to the equations

$$c_1 + a^3 c_2 = 1$$

$$c_1 + a^5 c_2 = 0 \quad .$$

Again reversing the steps we have

$$\psi_\delta^{(4)}(r) = \frac{1}{4\pi r^2 \delta} \{c_1 f'(r/\delta) + c_2 a^2 f'(r/a\delta)\}$$

$$\frac{\partial G_\delta}{\partial r}(r) = -\frac{1}{4\pi r^2} \{c_1 f(r/\delta) + c_2 a^3 f(r/a\delta)\}$$

$$K_\delta(z) = -\frac{1}{4\pi r^3} \{c_1 f(r/\delta) + c_2 a^3 f(r/a\delta)\} z\times \quad .$$

For example, with $f(r) = 1-e^{-r^3}$ or $\tanh r^3$ it would be convenient to choose $a^{-3} = 2$. In the first case this gives

$$K_\delta(z) = -\frac{1}{4\pi r^3} \{1 - c_1 e^{-r^3/\delta^3} - c_2 e^{-2r^3/\delta^3}\} z\times$$

so that only one exponentiation is necessary.

An alternative method can be used to produce kernels of fourth order in δ from the ones of second order already obtained. Suppose a function $f(r)$ has been found as above meeting conditions (C1) - (C3). We will choose

$$f_4(r) = c_1 f(r) + c_2 r f'(r) \tag{7}$$

with appropriate constants and check that the corresponding kernel

$$K_\delta^{(4)}(z) = -\frac{1}{4\pi r^3} f_4(r/\delta) z\times$$

is fourth order.

If f satisfies (C1) and (C2), then f_4 does also, and (C3) will hold provided $c_1 = 1$. We need to impose the moment condition (iii) with $|\beta| = 2$. The correspondence between f_4 and $\psi^{(4)}$ is given by (6), and we can convert the condition on $\psi^{(4)}$ to a similar one for f_4:

$$0 = 4\pi \int_0^\infty \psi^{(4)}(r)r^2 \cdot r^2 dr = \int_0^\infty f_4'(r)r^2 dr$$

$$= \int_0^\infty g_4'(r)r^2 dr = -2 \int_0^\infty g_4(r)r \, dr \quad ,$$

where $g_4(r) = f_4(r) - 1$, so that $g_4(\infty) = 0$. If we now substitute from (7) with $f = 1 + g$ and $c_1 = 1$, our condition becomes

$$0 = \int_0^\infty \{g(r)r + c_2 g'(r)r^2\}dr$$

$$= (1 - 2c_2) \int_0^\infty g(r)r \, dr \quad ,$$

after integrating by parts. This holds if $c_2 = \frac{1}{2}$, and therefore the choice

$$f_4(r) = f(r) + \frac{1}{2} rf'(r)$$

satisfies all our requirements.

We can apply this result directly to the two choices of f made above. If $f(r) = 1 - e^{-r^3}$, then

$$f_4(r) = 1 + (-1 + \frac{3}{2} r^3)e^{-r^3} \quad .$$

For $f(r) = \tanh r^3$, we have

$$f_4(r) = \tanh r^3 + \frac{3}{2} r^3 \operatorname{sech}^2 r^3$$

or

$$f_4(r) = T + \frac{3}{2} r^3(1 - T^2), \qquad T = \tanh r^3 \quad .$$

Again, either of these two methods can be extended to produce higher order kernels. Similar arguments could be used in the 2-D case and would lead to the Gaussian kernels found before and additional ones as well. Although convergence proofs for vortex methods have been given only in the circumstances of [1,2,5], the smooth kernels obtained here could be applied to other versions of these methods, for example the three-dimensional method of [3]. It should be noted, however, that for a vorticity distribution on a set of lower dimension, such as an interface between two potential flows, the formulas for modified kernels are somewhat different. Of course, optimal choices of the parameters will have to be determined through detailed numerical experiments.

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