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CONSTRUCTION OF HIGHER ORDER ACCURATE VORTEX AND PARTICLE METHODS

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# CONSTRUCTION OF HIGHER ORDER ACCURATE VORTEX AND PARTICLE METHODS

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Dedicated to Milton E. Rose on Occasion of his 60th Birthday

## **ABSTRACT**

The standard point vortex method has recently been shown to be of high order of accuracy for problems on the whole plane, when using a uniform initial subdivision for assigning the vorticity to the points. If obstacles are present in the flow, this high order deteriorates to first or second-order. This paper introduces new vortex methods which are of arbitrary accuracy (under regularity assumptions) regardless of the presence of bodies and the uniformity of the initial subdivision.

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#### 1. INTRODUCTION

There has been a growing interest recently in the theory and application of point vortex methods to the numerical solution of the incompressible Euler and Navier-Stokes equations. The impetus for the Euler case stems from the basic work of Dushane [6], Hald and Del Prete [7], and Hald [8], the Fourier analysis of Beale and Majda [1], [2], [3], and the Sobolev space approach of Raviart [12] and Cottet [4]. A recent paper by Cottet and Gallic [5] extends the latter approach to linear Burger's type equations with "viscosity" accounted for by splitting the convection and viscous parts and using a Green's function for the viscous computation. A method for introducing viscosity into particle methods for compressible flows is given by Monaghan and Gingold [9]. See also [10] and [11]. Apart from the first three of these references, the authors all obtain high order of accuracy error estimates, limited mainly by the regularity of the exact solution of the continuous equations. Unfortunately, the possibility of obtaining this accuracy is dependent on the existence of expansions similar in nature to the Euler-MacLaurin sum formula. If, for any reason, it is not possible to assert the existence of such expansions, the accuracy drops to first- or second-order, depending on the exact details of the algorithm and which errors are being estimated. If general boundaries (bodies) are present in the flow field, or if the initial subdivision of the flow field is not uniform, the necessary expansions will most likely cease to exist. Then questions arise as to how higher-order schemes may be constructed, and more important whether it is worthwhile to use them in view of the extra expense which is involved. The purpose of the paper is to give some possible answers to these questions.

In Section 2, the basic equations are given, and the simplest particle method is defined for comparison with some higher-order schemes. These schemes are introduced in Section 3. There, three methods for generating schemes of arbitrary accuracy are provided. An appendix contains some technical results about solving scalar hyperbolic equations with distributional data.

This paper is of an algorithmic nature and does not contain numerical results or precise error estimates. These will appear elsewhere.

## MODEL PROBLEM

The incompressible Euler Equations in vorticity-velocity form are

$$\omega_{t} + (u\omega)_{x} + (v\omega)_{y} = 0$$

$$\text{in } \mathbb{R}^{2}$$

$$\text{div}(u,v) = 0 : \text{curl}(u,v) = \omega$$

$$(2.1)$$

with initial condition

$$\omega(x,y,0) = \omega_0(x,y). \tag{2.3}$$

The basic ideas for constructing higher-order schemes will be shown for (2.1) and (2.3), with (u,v) assumed given. For these linear problems it is not necessary to assume that (u,v) is solenoidal.

In this setting, we will now define the basic particle (or point vortex) method. Subdivide the plane into squares of side h, number the squares 1, 2, 3,5.6. in some convenient way and define a distributional approximation

to  $\omega_0(x,y)$  by

$$\omega_{0h}(x,y) = \sum_{i} h^{2} \omega(x_{i},y_{i}) \delta(x-x_{i}, y-y_{i})$$
 (2.4)

where  $(x_i, y_i)$  denotes the center of the i<sup>th</sup> mesh square, and  $\delta(x-x_i, y-y_i)$  denotes the Dirac delta function with pole at  $(x_i, y_i)$ . Now solve (2.1) and (2.2) with  $\omega_0(x,y) + \omega_{0h}(x,y)$ . The well known solution to the latter problem is the distribution

$$\omega_{h}(x,y,t) \equiv \sum_{i} h^{2} \omega(x_{i},y_{i}) \delta(x-X(x_{i},y_{i};t), y-Y(x_{i},y_{i};t))$$
 (2.5)

where  $X(x_i, y_i, t)$  denotes the solution of the characteristic equation

$$dX/dt = u(X,Y,t) X(0) = x_i$$

and correspondingly for Y.

No use is made of the uniformity of the mesh in deriving (2.5). For a nonuniform mesh,  $h^2$  in (2.5) is the area of the appropriate mesh square. In the error formulas below, h denotes the largest mesh length.

It is immediately clear from this definition that the particle approximation is <u>non-dissipative</u>, in the sense that no artificial viscosity is introduced because after the discretization of the initial condition is made (2.1) is solved exactly. In practice some ODE solver must be used to compute the trajectories, but in theory its error can be made arbitrarily small. This principle, of solving the exact equation with approximate data, seems to be common to particle methods generally and distinguishes them from finite

difference and finite element methods. The latter, at least, solves an approximate equation with exact data.

A rigorous error analysis of the method just defined can be found in [12]. This analysis is too complicated to reproduce here. Nevertheless, we need some simple guide to compare the accuracy of various schemes. It seems reasonable to look at the difference  $\omega_0 - \omega_{0h}$  against a test function as a measure of "truncation error" since it is the only error made. Thus we define, for a given method of approximation and a given function  $\omega_0$  with compact support  $\overline{\Omega}$  (where area  $(\overline{\Omega}) = 1$  say)

$$\tau_{h}(\phi) = \iint (\omega_{0} - \omega_{0h}) \phi dx dy. \qquad (2.6)$$

Here, the integration is performed over  $\mathbb{R}^2$ . The restriction that  $\omega_0$  has compact support is a matter of convenience rather than necessity and could be replaced by sufficiently rapid decay at large distances from the origin.

As an example, consider (2.4). Then we find

$$\tau_{h}(\phi) = \iint \omega_{0} \phi dxdy - \int_{i}^{\infty} h^{2}(\omega_{0} \phi)(x_{i}, y_{i}). \qquad (2.7)$$

This shows that a midpoint rule numerical integration is being used to approximate the integral, and under smoothness conditions it follows that as  $h\, \div\, 0$ 

$$\tau_h(\phi) = 0(h^2).$$

Clearly, higher-order integration formulas can be compared with each other on this basis. For a 2  $\times$  2 product Gauss rule in each element, for example, we have  $\tau_h = 0(h^4)$ .

Next, recall the important fact that in the nonlinear case it is necessary to compute the velocity field at each timestep by solving (2.2). Assume that this is to be done using the Green's function. Let W denote the number of arithmetical operations required to compute the velocity field at each particle position. If there are N particles, then  $W \simeq CN^2/2$ , for some constant C. Below, we will use W as a standard unit of work to compare various new algorithms. For the Gauss case therefore we have a work count of 16W. From this we see that use of a higher-order rule does not necessarily assure a greater computational efficiency for typical values of h. In the next section, methods for obtaining high-order accuracy without such a large increase in the cost of the computation are defined.

## 3. HIGHER ORDER METHODS

The preceding remarks suggest that increasing the order of accuracy by adding more integration nodes may not be a good idea. It is natural to try to do the same thing by increasing the amount of information associated with each node. Specifically, in this section we shall associate with  $(x_i, y_i)$ ,  $m^{th}$  order distributions of the form

$$M_{\mathbf{i}}(\mathbf{x},\mathbf{y}) \equiv \sum_{\alpha \in \mathbf{w}_{\mathbf{i}\alpha}} w_{\mathbf{i}\alpha} \, b^{\alpha} \, \delta(\mathbf{x}-\mathbf{x}_{\mathbf{i}}, \mathbf{y}-\mathbf{y}_{\mathbf{i}}). \tag{3.1}$$

In (3.1), which generalizes the simple  $\delta$  functions in (2.4),  $\alpha$  denotes a multi-index, and  $(x_i,y_i)\in\mathbb{R}^2$ . Choice of the weights  $w_{i\alpha}$  and the nodes  $(x_i,y_i)$  can be made in many ways. We shall give three methods in this section.

# Method 1 (Direct Integration):

In this method,  $(x_i,y_i)$  are the corners of the elements, each of which has associated with it an expansion of the form (3.1). The weights in the expansion are chosen so that when  $\omega_{0h}$  is substituted into (2.6), the second term gives a rule for integration of the function  $(\omega_0,\phi)$ , involving its values along with those of its derivatives through order m at the nodes. We shall consider the cases m=0 and m=1 in more detail.

Let m = 0. A rule for a square of side h with corners at P, Q, R, S which is exact for bilinear functions is

$$\iint f \, dxdy \approx (h^2/4) \, (f(P) + f(Q) + f(R) + f(S)). \tag{3.2}$$

Using this as a composite rule implies the choice  $w_{i00} = h^2 \omega(x_i, y_i)$  so that we define

$$M_{i}(x,y) \equiv h^{2}\omega(x_{i},y_{i}) \delta(x-x_{i}, y-y_{i}).$$
 (3.3)

Since this gives a rule which is locally exact for linear functions but not for all quadratics its accuracy is  $0(h^2)$  in the sense of (2.6) while the work is IW. This is essentially no different from the mid-point rule. In fact this rule is clearly analogous to the trapezoidal rule.

For a quadrilateral mesh, a bilinear mapping can be used to map the quadrilaterals onto a standard square in which (3.1) can be used. In some circumstances it may be desirable to use a triangular mesh instead of the quadrilateral one. An  $O(h^2)$  rule for triangles analogous to (3.1) can then be used, avoiding the need to map the domains.

Now let m = 1. Analogous to (3.2) we have the formula

$$\iint f \, dxdy \approx A(f(P) + f(Q) + f(R) + f(S)) 
+ B(-f_x(P) + f_x(Q) + f_x(R) - f_x(S)) 
+ C(-f_y(P) - f_y(Q) + f_y(R) + f_y(S))$$
(3.4)

where  $A = h^2/4$ ,  $B = C = h^3/24$ , and P, Q, R, S denote the corners of the square  $-h/2 \le x$ ,  $y \le h/2$  labelled counterclockwise starting from the top right. Analogous to (3.3) there is the expression

$$M_{\mathbf{i}}(\mathbf{x},\mathbf{y}) \equiv \sum_{|\alpha| \leq 1} w_{\mathbf{i}\alpha} D^{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\mathbf{i}}, \mathbf{y}-\mathbf{y}_{\mathbf{i}}). \tag{3.5}$$

In (3.5), the coefficients are computed from the composite rule based on (3.4). For the uniform square mesh we are using for illustration, the weights are

$$w_{i00} = A \omega_0(x_i, y_i) + B \omega_0(x_i, y_i) + C \omega_0(x_i, y_i)$$

$$w_{i10} = -B^{\prime}\omega_0(x_i, y_i)$$

$$w_{i01} = -C'\omega_0(x_i, y_i).$$

(3.4) is exact for cubic polynomials. It follows that this method is accurate in the sense of (2.6) to  $O(h^4)$ . To compute work units for this scheme, we observe that although there are only  $\approx N$  particles there is some extra work associated with computation of derivatives of the velocity kernel. It turns

out that for this scheme the work units are  $< 2\frac{1}{2}$  W, a satisfactory figure. There is also some additional work required for computing the coefficients of the derivatives in (3.1). This amounts to having to integrate two more systems each of two odes, in addition to the characteristic odes (see appendix).

As in the previous case, rather than use a quadrilateral mesh it might sometimes be better to use a triangular one.

For a square mesh, the m=1 scheme just discussed has an interesting property in the uniform case. This is the following: due to cancellations, the composite rule has weights of zero attached to the derivative unknowns at interior vertices. Hence the higher accuracy is achieved by corrections at the boundary. But this implies the use of a Euler-Maclaurin type expansion. Thus, if  $\omega \varphi$  has a continuous derivatives in  $\mathbb{R}^2$  and compact support, by using nodal derivatives up to this order we can get accuracy  $O(h^{s+1})$  merely by using the m=0 scheme, since this is what the composite scheme reduces to on a uniform mesh in that case. This is another way to look at the results of [1]-[3].

# Method 2 (Finite Element Approach):

The approach here uses a nodal finite element basis in the following way: let  $\{\psi_{i\alpha}\}$   $|\alpha| \leq m$ ,  $i=1,2,\cdots$ , be the standard nodal basis functions associated with the  $i^{th}$  node  $(x_i,y_i)$  of a triangulation of the plane with maximum edge length h. These functions satisfy conditions of the form

$$D^{\beta} \psi_{i\alpha}(x_{i},y_{i}) = \Delta_{ii}^{\alpha\beta},$$

where  $\Delta_{\mbox{ij}}^{\alpha\beta}$  is a Kronecker delta. Then we define  $\mbox{w}_{\mbox{i}\alpha}$  as

$$w_{i\alpha} = (-1)^{|\alpha|} \iiint \psi_{i\alpha}(x,y) \ \omega_0(x,y) dx dy$$
 (3.6)

where the integration is over the whole plane. We now have

$$\iint_{\mathbf{i}} \omega_{0h}(\mathbf{x}, \mathbf{y}) \rho(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = \iint_{\mathbf{i}} \sum_{|\alpha| \le m} w_{\mathbf{i}\alpha} D^{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\mathbf{i}}, \mathbf{y} - \mathbf{y}_{\mathbf{i}})$$

$$\times \phi(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}, \quad \forall \phi \in C^{m} (\mathbb{R}^{2})$$

$$= \sum_{\mathbf{i}} \sum_{|\alpha| \le m} (-1)^{|\alpha|} w_{\mathbf{i}\alpha} D^{\alpha} \phi(\mathbf{x}_{\mathbf{i}}, \mathbf{y}_{\mathbf{i}})$$

$$= \iint_{\mathbf{i}} \omega_{0}(\mathbf{x}, \mathbf{y}) \phi^{h}(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$
(3.7)

where  $\phi^h$  is the finite element interpolant of  $\phi$  on the given triangulation. Equation (2.6) then becomes

$$\tau_{h}(\phi) = \iint \omega_{0}(\phi - \phi^{h}) dxdy. \tag{3.8}$$

Since the error  $|\phi-\phi^h|$  is formally  $0(h^{r+1})$  where r is the degree of the highest order full polynomial space used, we can say here that  $\tau_h$  is of this order.

This type of scheme differs from direct integration schemes in that no approximation of  $\omega_0$  is made. The test function only (often a convolution kernel in practice) is approximated and the result is integrated exactly. Because of this property, the rigorous error estimates for these methods

require minimal regularity on  $\omega_0$  unlike the direct integration methods where to achieve high accuracy requires  $\omega_0$  to have several smooth derivatives throughout  $\mathbb{R}^2$ . The  $O(h^{r+1})$  estimate is in fact valid even if we know only  $\omega_0 \in L^1(\mathbb{R}^2)$ . If  $\omega_0$  has extra regularity it can be exploited to get higher accuracy by going to negative norm estimates of the finite element error. Smoothness of  $\phi$ , however, is certainly required.

Two examples analogous to those considered above are the case of continuous linear elements on triangles, for which we can expect  $O(h^2)$  accuracy with IW work units, and full cubics - defined in terms of derivative unknowns at vertices, and function values at vertices and centroid for which the work will be somewhat larger than the values used so far (about  $10 \ \frac{1}{2} \ W$  units).

In general, the full range of finite element spaces is available for use.

# Method 3 (Taylor/Moment Expansions):

Here we begin by subdividing the plane into arbitrary elements with midside nodes and arbitrary element shapes allowed in principle. Next, we define

$$\alpha_1! \alpha_2! w_{i\alpha} = (-1)^{|\alpha|} \int \int (x-x_i)^{\alpha_1} (y-y_i)^{\alpha_2} \omega_0(x,y) dxdy$$
 (3.9)

in which  $(x_i,y_i)$  is an arbitrary point within the i<sup>th</sup> element, and the integration is over the ith element. The  $w_{i\alpha}$  are proportional to the moments of  $\omega_0$  restricted to the i<sup>th</sup> element, about  $(x_i,y_i)$ . It follows as above, that

$$\iint \omega_{0h}(x,y) \phi(x,y) dxdy = \iint \omega_{0}(x,y) \phi^{[m]}(x,y) dxdy$$
 (3.10)

where  $\phi^{[m]}(x,y)$  is the piecewise polynomial function, in general discontinuous, equal in the i<sup>th</sup> element to the Taylor expansion of  $\phi(x,y)$  through m<sup>th</sup> order terms, about the point  $(x_i,y_i)$ . In this sense the local moment expansion defined by (3.1) and (3.9) "dualizes" into the local Taylor expansion about  $(x_i,y_i)$ .

To get the accuracy of this scheme, we substitute into (2.6) to find that

$$\tau_h(\phi) = \iint \omega_0(\phi - \phi^{[m]}) dxdy$$

so that denoting by h the largest linear dimension of the elements, we obtain accuracy  $O(h^{m+1})$ .

The moments method also needs only minimal regularity on  $\omega_0$  for full accuracy to be obtained. In practice, if m=1 the point  $(x_1,y_1)$  should be chosen to be the center mass of  $\omega_0$  because then  $w_{i\alpha}=0$  for  $|\alpha|=1$ , so we get second-order accuracy for the same work as with the lowest-order scheme. Using quadrilaterals for elements, with N vertices there are approximately N elements and so N particles. For  $O(h^3)$  accuracy the interaction work count is 5W, and for  $O(h^4)$  is 8W.

#### 4. FURTHER REMARKS

There should be no difficulty in extending the ideas of Section 3 to three-dimensional particle methods of the kind suggested in [1] - [3] and [12].

Rigorous analysis using the Sobolev space setting has been carried out for both the finite element and moment expansion methods.

So far an insufficient amount of computation has been done to verify the error estimates and decide about the efficiency of the various methods.

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#### APPENDIX

A framework for finding distributional solutions of (2.1) with initial condition  $\omega_{0h} = D^{\alpha} \delta(x-x_0, y-y_0) |\alpha| \leq m$  can be obtained starting from the following considerations. Let  $X(x_0,y_0;t)$  and  $Y(x_0,y_0;t)$  denote the characteristic curves of the equation (2.1); here, t parameterizes the curve and the generic point  $(x_0,y_0)$  denotes its origin at time t=0. X and Y are computed by solving the ordinary differential equations

$$dX/dt = u(X,Y,t)$$
  $dY/dt = v(X,Y,t)$ 

$$X(0) = x_0$$
  $Y(0) = y_0.$ 

At time t, let  $J(x_0, y_0; t)$  denote the Jacobian of the flow map  $\Phi: (x_0, y_0) + (X, Y)$ . The (nonlinear) case of most interest from the fluids viewpoint has  $u_x + v_y = 0$ , in which case  $J(x_0, y_0; t) = 1$ . We can obtain a formal analytical solution to (2.1) and (2.3) by writing the equation in terms of the material derivative as  $d\omega/dt = 0$ , integrating this equation over an arbitrary domain moving with the velocity field (u,v), say  $\Omega(t)$ , and then using the transport theorem to write

$$d/dt \iint_{\Omega(t)} \omega(X,Y,t)dXdY = 0,$$

from which it follows immediately that

$$\iint\limits_{\Omega(t)} \omega(X,Y,t) dXdY = \iint\limits_{\Omega(0)} \omega_0(x,y) dxdy.$$

Changing the variables on the right-hand side to  $\, X \,$  and  $\, Y \,$  respectively and recalling the arbitrariness of  $\, \Omega(t) \,$  now gives

$$\omega(X,Y;t) = \omega_0(x(X,Y,t), y(X,Y,t))J^{-1}(X,Y;t)$$
 (A.1)

where (x(X,Y,t), y(X,Y,t)) is by inverting the equations X = X(x,y;t), Y = Y(x,y;t). The existence of a unique solution to these equations follows from ode theory provided u and v are smooth. Reversing the steps, it follows that (A.1) satisfies (2.1) given the required regularity of u, v, and  $\omega_0$ .

Let  $\phi \in C^m(\mathbb{R}^2)$ ; multiplying (A.1) by  $\phi$ , integrating and changing the variables on the right to x and y we have

$$\iint \omega(X,Y,t) \phi(X,Y)dXdY = \iint \omega_0(x,y) \phi(X(x,y;t), Y(x,y,t))dxdy, \tag{A.2}$$

or alternatively

$$\langle \omega, \phi \rangle = \langle \omega_0, \phi \circ (X,Y) \rangle$$
 (A.3)

where  $\circ$  denotes composition. If  $X(\cdot,\cdot,t)$  and  $Y(\cdot,\cdot,t)$ ,  $Y(\cdot,\cdot,t) \in W^{m+1,\infty}(\mathbb{R}^2)$  (or  $\in \mathfrak{C}^{(m)}(\mathbb{R}^2)$ ),  $\forall \ 0 \leq t \leq T$ , then the right-side of (A.3) makes sense even if  $\omega_0 + \omega_{0h} = D^\alpha \delta(x-x_0, y-y_0)|\alpha| \leq m$ . Thus a distribution  $\omega$  is defined on  $\mathfrak{C}^{(m)}(\mathbb{R}^2)$  by (A.3). Therefore, we can pose the problem of finding  $\omega_h$  satisfying

$$\langle \omega_{h}, \phi \rangle = \langle \omega_{0h}, \phi_{o}(X,Y) \rangle \quad \forall \phi \in C^{(m)}(\mathbb{R}^{2}). \quad (A.4)$$

A solution  $\omega_h$  to (A.4) is given by

$$\omega_{h}(X,Y) = D^{\alpha} \delta(X - X(x,y;t), Y - Y(x,y;t))\Big|_{x=x_{0}, y=y_{0}},$$
 (A.5)

the purely formal differentiations being performed w.r.t. x and y. Proof that (A.5) satisfies (A.4) is by direct computation.

If  $|\alpha| = 0$  we recover the solution given in Section 2. Consider the case with  $|\alpha| = 1$ . Equation (A.5) gives

$$\begin{split} \omega_{\text{h}10} &= \delta_{\text{X}} \big( \text{X-X}_0, \ \text{Y-Y}_0 \big) \ \text{X}_{\text{x}} \big( \text{x}_0, \text{y}_0, \text{t} \big) + \delta_{\text{Y}} \big( \text{X-X}_0, \ \text{Y-Y}_0 \big) \ \text{Y}_{\text{x}} \big( \text{X}_0, \text{y}_0, \text{t} \big) \\ \omega_{\text{h}01} &= \delta_{\text{X}} \big( \text{X-X}_0, \ \text{Y-Y}_0 \big) \ \text{X}_{\text{y}} \big( \text{x}_0, \text{y}_0, \text{t} \big) + \delta_{\text{Y}} \big( \text{X-X}_0, \ \text{Y-Y}_0 \big) \ \text{Y}_{\text{y}} \big( \text{x}_0, \text{y}_0, \text{t} \big) \end{split}$$

using the abbreviation  $X_0$  for  $X(x_0,y_0;t)$  and similarly  $Y_0$ . If the initial condition is

$$\omega_{h0} = a_{10} \delta_{x}(x-x_{0}, y-y_{0}) + a_{01} \delta_{y}(x-x_{0}, y-y_{0}),$$

then the solution to (A.4) of the required form as given by (A.6) is

$$\omega_h = a_{10}(t) \delta_X(X-X_0, Y-Y_0) + a_{01}(t) \delta_Y(X-X_0, Y-Y_0)$$

where

$$a_{10}(t) = a_{10} \quad X_{x}(x_{0}, y_{0}, t) + a_{01} \quad X_{y}(x_{0}, y_{0}, t)$$

$$a_{01}(t) = a_{10} \quad Y_{x}(x_{0}, y_{0}, t) + a_{01} \quad Y_{y}(x_{0}, y_{0}, t).$$
(A.7)

Letting M denote the matrix

$$\begin{bmatrix} x_x & x_y \\ y_x & y_y \end{bmatrix}$$

differentiation of the characteristic equations shows that

$$dM/dt = \nabla(u,v)M$$

and the initial condition for this system is M(0) = 1, the identity matrix. It will be necessary to solve this and analogous systems for the higher-order cases in order to compute the numerical approximations. Having solved it,  $a_{10}(t)$  and  $a_{01}(t)$  are given by (A.7).

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16. Abstract

The standard point vortex method has recently been shown to be of high order of accuracy for problems on the whole plane, when using a uniform initial subdivision for assigning the vorticity to the points. If obstacles are present in the flow, this high order deteriorates to first or second-order. This paper introduces new vortex methods which are of arbitrary accuracy (under regularity assumptions) regardless of the presence of bodies and the uniformity of the initial subdivision.

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