

A Vortex Method for Flows with Slight Density Variations*

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We present a grid-free numerical method for solving two-dimensional, inviscid, incompressible flow problems with small density variations. The method, an extension of the vortex method, is based on a discretization of the equations written in the vorticity-stream formulation. The method is tested on an exact solution and is found to be both stable and accurate. An application to the motion of a two-dimensional line thermal is also presented.

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INTRODUCTION

In the presence of an external force, density variations can cause fluid motion. For example, in thermal convection the effect of gravity is to cause warm, less dense, fluid to rise when surrounded by cool, more dense, fluid. In the vorticity formulation of the equations of motion one finds an explanation for this phenomenon. The effect of a force acting on density variations is to cause the growth of vorticity in the interior of the fluid. This vorticity then induces the fluid to move. The numerical method we present in this paper is based upon this observation. Specifically, we approximate flows induced by the action of external forces on density variations by calculating the evolution of the vorticity of the fluid.

We assume that the flow is two dimensional, incompressible, inviscid, and that the density variations are small. (We make the Boussinesq approximation [34, 36].) This latter assumption is not a severe restriction since it is often satisfied in many important applications, e.g., thermal convection. By making this assumption the approximation of the equations is much easier to accomplish. Our method is a discretization of the vorticity formulation of the equations of motion, and hence the resulting algorithm can be considered a vortex method. The underlying approximation techniques are based on the vortex method for incompressible flows as implemented by Chorin [12] and analyzed by Hald [23] and Beale and

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Majda [6, 7]. (For a review of vortex methods see Leonard [27] or Chorin [14].) It is a Lagrangian or grid-free method and uses an approximation which is composed of a sum of vortices of finite core size or vortex "blobs." Since the vorticity growth is caused by the presence of density gradients, it is necessary to calculate their evolution in time. Usually this is done by calculating the evolution of the density and numerically differentiating the result. Early tests proved this approach to be somewhat unsatisfactory [1], so we consider the density derivatives as primitive variables and calculate a solution to an equation which describes their evolution. We mention that many of the ideas contained in the convergence proofs for three-dimensional vortex methods [3, 6] can be used with a little modification to obtain a convergence proof for the method presented here [1].

Previous work using the vorticity formulation to study motions induced by density variations has mainly concentrated on the problem of calculating the motion of an interface which separates two fluids of different densities. In this case the vorticity is confined to the interface and the problem reduces to one of calculating the motion of a vortex sheet whose strength changes in time [9]. Numerical experiments on this problem have been carried out by Baker *et al.* [4, 5], Meng and Thompson [29], and others. The method that we present is derived under different assumptions, namely, that the density is continuously varying. Our method is therefore applicable to problems that do not have sharply defined interfaces. (One application might be the calculation of the motion of a continuously stratified fluid.)

However, there is a natural extension of our method to flows that have density discontinuities. The resulting method is similar to the method presented by Meng and Thompson [29]. Both methods use essentially the same formula for the growth of vorticity. The methods differ in the way in which the normals to the interface (necessary to calculate the growth of vorticity) are approximated. Meng and Thompson calculate the normals by finding a normal to a curve that passes through a set of points representing the interface. In our method we approximate the solution of an equation that describes the evolution of the normals to the interface. For comparison purposes we consider the problem of calculating the motion of a two-dimensional thermal. Using our method on this problem we are able to calculate the roll-up of the interface in a numerically consistent manner. This is an improvement on the results that were obtained by Meng and Thompson. The computational results are rather startling, and we find evidence that the magnitude of the vorticity of the solution and the length of the interface become infinite in finite time.

In the implementation of our method one needs to specify the initial interparticle spacing, h , and a value of the smoothing parameter δ (roughly equal to the core radius of the "blobs"). As is typical of this type of vortex method, improvement in accuracy is obtained by letting $h \rightarrow 0$ and $\delta \rightarrow 0$ simultaneously. (For smooth solutions this follows from the convergence theory [1], and for non-smooth solutions one hopes this is true.) It was found that the manner in which the limit $h \rightarrow 0$ and $\delta \rightarrow 0$ was taken had an important effect on the computational results. If

h was reduced too rapidly relative to δ then the calculations became inconsistent upon further refinement. In the two-dimensional thermal problem the effect was to cause the interface of the thermal to "tangle." To overcome this difficulty we formulated an empirical procedure for determining the proper approach to the limit. This procedure was very successful, and it may be of value in other vortex calculations which suffer from the same type of problem.

In Section 1 we consider a simple model problem to illustrate some of the features of the numerical approximations used in our scheme. Section 2 contains a presentation of the equations that we use to describe the motion of a fluid with small density variations. As mentioned earlier, we treat the density derivatives as primitive variables and in this section we derive equations for them and give a formula which can be used to reconstruct the density from a solution of such equations. We prove that the density constructed in such a fashion is equivalent to that obtained by solving the continuity equation. In Section 3 we discretize the equations of motion to derive our numerical scheme. We present in Section 4 an exact solution to the equations of motion and use this solution to verify the accuracy and stability of the method. In Section 5 we apply our method to calculate the motion of a two-dimensional thermal. The problem involves the calculation of an interface and we describe how to adapt the method to deal with this complication. We describe our empirical procedure for choosing the two parameters h and δ , and present the computational results obtained with these choices.

1. MODEL PROBLEM

Two important aspects of our numerical scheme are that it is Lagrangian and it uses "blob"-type approximation. To illustrate some of the features of this type of numerical approximation we consider a Lagrangian method for calculating the motion of a quantity being transported by an incompressible flow. This problem is useful not only for demonstrating some features of our method but also for demonstrating some features of vortex methods in general.

Let $\mathbf{u}(x, t) = (u_1(x, t), u_2(x, t))$ be a given velocity field defined on R^2 such that $\text{div } \mathbf{u} = 0$. Let $f(x, t)$ be some quantity passively transported by the velocity field \mathbf{u} , i.e., f satisfies the partial differential equation

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \text{grad } f = 0 \quad (1.1)$$

$$f(x, 0) = f_0(x). \quad (1.2)$$

We assume that the support of $f_0 \subseteq \Omega$, Ω a bounded set in R^2 . The problem is to calculate an approximation to $f(x, t)$ for times $t \geq 0$.

Our starting point is to write (1.1) and (1.2) in Lagrangian form as

$$\frac{dx(\alpha, t)}{dt} = \mathbf{u}(x(\alpha, t), t), \quad x(\alpha, 0) = \alpha \quad (1.3)$$

$$\frac{df(x(\alpha, t), t)}{dt} = 0, \quad f(x(\alpha, 0), 0) = f_0(\alpha) \quad (1.4)$$

where $\alpha = (\alpha_1, \alpha_2) \in \mathbb{R}^2$. The solution to (1.3), $x(\alpha, t)$, is the trajectory of a fluid particle which at time $t=0$ is located at the point α . Equation (1.4) describes the evolution of f along the particle trajectory $x(\alpha, t)$. In particular, (1.4) expresses the fact that the quantity f does not change along particle paths. For a discussion of the equivalence of (1.1)–(1.2) with (1.3)–(1.4), see [18].

We approximate the solutions to (1.1) and (1.2) by constructing discrete approximations to Eqs. (1.3) and (1.4). Let A^h denote the set of nodes of a grid of mesh width h , and define Ω^h as the intersection of Ω with A^h . The discrete approximation to (1.3) and (1.4) is obtained by computing the solution to the set of ordinary differential equations

$$\frac{dx(jh, t)}{dt} = \mathbf{u}(x(jh, t), t), \quad x(jh, 0) = jh \quad (1.5)$$

$$\frac{df(x(jh, t), t)}{dt} = 0, \quad f(x(jh, 0), 0) = f_0(jh) \quad (1.6)$$

for all $jh = (j_1 h, j_2 h) \in \Omega^h$.

Thus, the computed approximation to $f(x, t)$ for $t \geq 0$ consists of the values of the function f at the set of points $\{x(jh, t) \mid jh \in \Omega^h\}$.

What is attractive about such a scheme is that the values of the function f at the points $x(jh, t)$ are not smoothed by this process. It is for this reason that we are justified in calling the method non-diffusive. We are computing the exact solution at the points $x(jh, t)$; hence the method is similar to the Random Choice Method [13, 22] where a solution is constructed as a superposition of locally exact solutions. We expect that the most prominent feature of the Random Choice Method, the ability to compute accurately the evolution of sharp fluid discontinuities, will also be a feature of this method. This property is not shared by conventional finite difference schemes for solving (1.1) and (1.2).

One unattractive feature of such a scheme is the difficulty in approximating the function $f(x, t)$ at points other than the particle trajectories, $\{x(jh, t) \mid jh \in \Omega^h\}$, or approximating differential and integral operators applied to f . This difficulty arises because the points at which the approximate solution is computed, $x(jh, t)$, are not necessarily distributed uniformly in space. Interpolation or differentiation formulas tend to be computationally unstable or of low accuracy. An approximation procedure that has proven successful in overcoming this difficulty is that which is implicitly used in the vortex method. We now describe this approximation scheme.

For this approximation we need to define a class of approximate delta functions which we denote by $M^{L,p}$. This class of functions is introduced in [3] and is similar to the class of functions $FeS^{L,p}$ considered by Beale and Majda in [7], and to Cotlet's class C'_p in [17].

DEFINITION. The class $M^{L,p}$ is the collection of functions $\psi: R^2 \rightarrow R$ which satisfy all of the following conditions:

- (i) $\int_{R^2} \psi(x) dx = 1$;
- (ii) $\int_{R^2} x^\alpha \psi(x) dx = 0$, for all multi-indices α such that $1 \leq |\alpha| \leq p-1$, $\int_{R^2} |x|^p |\psi(x)| dx < \infty$;
- (iii) $\psi \in C^L(R^2)$;
- (iv) $|x|^{2+|\beta|} |D^\beta \psi(x)| \leq C$ for some C , and all β s.t. $|\beta| \leq L$;
- (v) $|x|^{p+4} |\psi(x)| \leq C$ for some constant C .

Examples of functions in this class will be given in Section 4. (See also [8].)

For a ψ in $M^{L,p}$ we define $\psi_\delta = (1/\delta^2) \psi(x/\delta)$ where δ is a given parameter. We take as our approximation to f the function f^h defined by

$$f^h(x, t) = \sum_{jh \in \Omega^h} \psi_\delta(x - x(jh, t)) f(x(jh, t), t) h^2. \quad (1.7)$$

In the vortex method this type of approximation is used to approximate the vorticity. (In some versions of the vortex method, however, the function ψ is not chosen to be in $M^{L,p}$.) An interpretation of (1.7), due to Chorin [12], is that we are approximating $f(x, t)$ by a sum of "blobs" of common shape ψ_δ with strength $f(x(jh, t), t) h^2$ located at the points $x(jh, t)$. We also mention that such an interpolation is nearly identical to kernel estimation as discussed by Monaghan and Gingold [21] and Monaghan [30]. An interesting observation due to Monaghan [30] is that kernel estimation and hence "blob" approximation can be viewed as a generalization of more standard approximation techniques, i.e., polynomial or Fourier approximation.

Rather than give a proof of convergence for this scheme, we give a brief description of the ideas behind the proof. (For a proof see [1].) The proof is based on techniques that are used in the analysis of the vortex method [3, 6, 7, 17, 23]. However, the velocity field is given in this problem rather than determined as part of the solution, so the analysis is simpler.

There are two basic estimates to make in order to obtain a convergence proof. The first is a consistency, or accuracy, estimate of the approximation (1.7) to $f(x, t)$. The second is a stability estimate, in essence an estimate of the behavior of the approximation (1.7) when its calculated components (in this case the $x(jh, t)$'s) are perturbed. We will use the letter C to denote a generic constant. Its dependence upon components of the estimate, if important, will be explicitly mentioned.

Fix an x' in R^2 and a time T . For the consistency estimate, we assume that the particle trajectories $x(jh, t)$ are computed exactly and estimate

$$f(x', t) - f^h(x', t) = f(x', t) - \sum_{jh \in \Omega^h} \psi_\delta(x' - x(jh, t)) f(x(jh, t), t) h^2.$$

for all t , $0 \leq t \leq T$. We estimate this expression by adding and subtracting $f_\delta = \psi_\delta * f$, and estimating each term in

$$\{f(x', t) - f_\delta(x', t)\} + \{f_\delta(x', t) - \sum_{jh \in \Omega^h} \psi_\delta(x' - x(jh, t)) f(x(jh, t), t) h^2\} \quad (1.8)$$

separately.

The first term, $f - f_\delta$, represents the error introduced in approximating the function f by its mollification with ψ_δ . Since the Fourier transform changes convolution into products, this term is estimated using Fourier analysis. Denoting the Fourier transform of $f(x)$ by $\hat{f}(\omega)$, and using the fact that $\max_{x \in R^2} |g(x)| \leq \int |\hat{g}(\omega)| d\omega$, we have

$$\begin{aligned} |f(x', t) - f_\delta(x', t)| &\leq \int_{R^2} |\hat{f}(\omega) - \hat{f}(\omega) \hat{\psi}_\delta(\omega)| d\omega \\ &\leq \int_{R^2} |\hat{f}(\omega)| |1 - \hat{\psi}_\delta(\omega)| d\omega. \end{aligned}$$

The conditions (i), (ii), and (iv) on the function ψ imply that

$$|1 - \hat{\psi}_\delta(\omega)| \leq C\delta^p |\omega|^p$$

where the constant is independent of ω and δ . This last inequality reveals in part why ψ is an approximate delta function; its Fourier transform closely approximates the Fourier transform of the delta function. Using this inequality and assuming that f decays sufficiently fast we find

$$|f(x', t) - f_\delta(x', t)| \leq C\delta^p. \quad (1.9)$$

To estimate the second term in (1.8), we first change variables in the convolution using the flow map $x(\alpha, t)$ defined by the solution to (1.3). The velocity field is incompressible so that the Jacobian of this flow map is identically one. Thus the second term in (1.8) can be expressed as

$$\int \psi_\delta(x' - x(\alpha, t)) f(x(\alpha, t), t) d\alpha - \sum_{jh \in \Omega^h} \psi_\delta(x' - x(jh, t)) f(x(jh, t), t) h^2.$$

As Cottet [17] recognized, this difference is the error involved in using the trapezoidal rule for approximating the integral of the function

$$g(x', \alpha) = \psi_\delta(x' - x(\alpha, t)) f(x(\alpha, t), t) \quad (1.10)$$

with respect to α . The trapezoidal rule is normally considered to be accurate to order h^2 , however, by using the Poisson summation formula and the fact that f is of compact support, one can show [3] that the error for the trapezoidal rule applied to the function $g(x', \alpha)$ has a bound of the form

$$\left| \int_{R^2} g(x', \alpha) d\alpha - \sum_{jh \in \Omega^h} g(x', jh) h^2 \right| \leq Ch^k \max \{ \|D_{\alpha_1}^k g\|_{L^1(R^2)}, \|D_{\alpha_2}^k g\|_{L^1(R^2)} \}. \quad (1.11)$$

By finding L^1 estimates for the derivatives of the function (1.10) and using (1.11) one obtains the estimate

$$\left| \int \psi_\delta(x' - x(\alpha, t)) f(x(\alpha, t), t) d\alpha - \sum_{jh \in \Omega^h} \psi_\delta(x' - x(jh, t)) f(x(jh, t), t) h^2 \right| \leq C \frac{h^k}{\delta^k}. \quad (1.12)$$

What limits the size of k is the smoothness of the flow and the smoothness of the functions f and ψ , i.e., the number of derivatives of $g(x', \alpha)$ in L^1 . In our use of this estimate we assume that the smoothness of the function ψ is the limiting factor and so take $k = L$ where L is that of M^{L-p} . We remark that the initial placement of the computational points in Ω^h is intimately related to the accuracy estimate given above. However, one need not consider only rectangular distributions of initial computational points. In [3], other initial distributions are discussed. (Non-rectangular distributions may be useful for constructing methods which preserve some special symmetry of a given problem.)

The estimates (1.9) and (1.12) hold uniformly for $x' \in R^2$ and $0 \leq t \leq T$ so that we have

$$\max_{x \in R^2} \left| f(x', t) - \sum_{jh \in \Omega^h} \psi_\delta(x' - x(jh, t)) f(x(jh, t), t) h^2 \right| \leq C \left(\delta^p + \left(\frac{h}{\delta} \right)^k \right) \quad (1.13)$$

where the constant depends only on T , properties of ψ , and bounds for a finite number of derivatives of the function f and velocity field u .

The second estimate for the convergence proof is an estimate of the stability of the approximation (1.7). This is an estimate of the error introduced in (1.7) by using approximate solutions of (1.5). Since (1.6) can be solved exactly, $f(x(jh, t), t) = f_0(jh)$, we do not estimate the effects of using approximate solutions of (1.6) in (1.7). However, in more general circumstances, i.e., when there are source terms, this latter effect cannot be neglected.

Define the discrete L^2 norm for functions defined on Ω^h by $\|v\|_h = (\sum_{jh \in \Omega^h} |v(jh)|^2 h^2)^{1/2}$. Assume that the perturbed solutions of (1.5), which we denote by $\tilde{x}(jh, t)$, satisfy

$$\|\tilde{x}(jh, t) - x(jh, t)\|_h \leq h\delta \quad (1.14)$$

for all $0 \leq t \leq T$. Then by using the mean value theorem, Taylor's theorem, and bounds for the derivatives of (1.10) up to time T one obtains an estimate,

$$\left\| \sum_{jh \in \Omega^h} \psi_\delta(x - \tilde{x}(jh, t)) f(x(jh, t), t) h^2 - \sum_{jh \in \Omega^2} \psi_\delta(x - x(jh, t)) f(x(jh, t), t) h^2 \right\|_{L^2(\bar{R})} \leq C \delta^{-1} \|\tilde{x}(ih, t) - x(ih, t)\|_h \tag{1.15}$$

for $0 \leq t \leq T$. The requirement (1.14) reveals the fact that we are not able to get estimates for all perturbations of the trajectories; only for sufficiently small perturbations. For the details of this estimate see [1].

The convergence of (1.7) to the solution of (1.1) follows easily from the consistency and stability estimates (1.13) and (1.15). We have

THEOREM 1. *Assume the velocity field \mathbf{u} and the function f are sufficiently smooth for $0 \leq t \leq T$. Assume that the support of the initial function f_0 is contained in a bounded set Ω and that $\psi(x)$ is in $M^{l,p}$ for some $p > 0$ and $L \geq 3$. If h is sufficiently small, $\delta = h^q$ for $q < 1$, and if $\|\tilde{x}(ih, t) - x(ih, t)\|_h \leq Ch^s$ where $s > q + 1$ then we have for $0 \leq t \leq T$ and any bounded set \bar{R} ,*

$$\max_{0 \leq t \leq T} \|\tilde{f}^h(x, t) - f(x, t)\|_{L^2(\bar{R})} \leq C(h^{pq} + h^{L(L-1-q)} + h^{s-q}) \tag{1.16}$$

where

$$\tilde{f}^h(x, t) = \sum_{jh \in \Omega^h} \psi_\delta(x - \tilde{x}(jh, t)) f(x(jh, t), t) h^2$$

and $\tilde{x}(jh, t)$ is a computed solution to (1.5). The assumptions on p, q, L , and s imply that as $h \rightarrow 0$ the right-hand side of (1.16) tends to zero. Here the constant depends on p, L, \bar{R}, Ω , and a finite number of derivatives of the velocity and the function f .

Proof. The proof follows easily from the triangle inequality. We have

$$\tilde{f}^h(x, t) - f(x, t) = \{\tilde{f}^h(x, t) - f^h(x, t)\} + \{f^h(x, t) - f(x, t)\}. \tag{1.17}$$

The first term of (1.17) is estimated using the stability estimate (1.15), and the second term using the consistency estimate (1.13). Thus

$$\|\tilde{f}^h(x, t) - f(x, t)\|_{L^2(\bar{R})} \leq C \delta^{-1} \|\tilde{x}(ih, t) - x(ih, t)\|_h + C \left(\delta^p + \left(\frac{h}{\delta} \right)^L \right) \leq C(h^{s-1} + h^{pq} + h^{L(L-1-q)}).$$

We note that the trajectories $\tilde{x}(jh, t)$ need to be computed with increasing accuracy as $h \rightarrow 0$ to assure convergence. This is not an unreasonable requirement. We expect that the errors committed in the calculation of $\tilde{x}(jh, t)$ will be largely in

the numerical solution of the ordinary differential equations (1.5) and therefore uniformly of order $(\Delta t)^l$ for some $l > 1$. The requirement that

$$\|\tilde{x}(ih, t) - x(ih, t)\|_h \leq Ch^s$$

implies that we need $(\Delta t)^l \leq C'h^s$ or $(\Delta t)^l/h^s \leq C'$ for some $C' \geq C$. Thus, this requirement is very similar to the stability requirement for explicit finite difference schemes for the approximation of solutions of hyperbolic equations.

In summary, a numerical method for approximating the solution to (1.1) and (1.2) consists of solving the ordinary differential equations (1.5) and (1.6). We construct an approximation of the solution at points other than $x(jh, t)$ using the approximation scheme (1.7). The consistency and stability estimates of the approximation can be combined to establish the convergence of this approximation to the exact solution.

We will use a technique similar to that described above for the construction of approximate solutions of the equations for a fluid of variable density. In particular, our approximation will consist of computing the trajectories of a finite number of fluid particles and the values of the flow quantities (density, vorticity, etc.) associated with them. In our approximation it will be necessary to find approximations, based on this computed information, to derivative and integral operators applied to the flow quantities. We will construct the approximations by applying the particular operators to approximations of the form (1.7). For example, we would use

$$f_x^h(x, t) = \sum_{jh \in \Omega^h} \frac{\partial \psi_\delta}{\partial x} (x - x(jh, t)) f(x(jh, t), t) h^2$$

as an approximation to the x derivative of f .

2. EQUATIONS OF MOTION

In this section we present the equations which we use to describe the motion of an ideal inviscid incompressible fluid with small density variations.

The equations of motion of an ideal inviscid incompressible fluid are

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \text{grad } \rho = 0 \quad (2.1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \text{grad } \mathbf{u} = -\frac{\text{grad } P}{\rho} + \mathbf{F} \quad (2.2)$$

$$\text{div } \mathbf{u} = 0. \quad (2.3)$$

The initial conditions are

$$\rho(x, y, 0) = \rho_0(x, y), \quad \mathbf{u}(x, y, 0) = \mathbf{u}_0(x, y).$$

Here ρ is the density, $\mathbf{u} = (u_1, u_2)$ is the velocity, P is the pressure, and $\mathbf{F} = (F_1, F_2)$ is the external force. We assume that the force \mathbf{F} is conservative, i.e., $\text{curl } \mathbf{F} = 0$. For a derivation see [15, 26].

If the variations in density are small we can make the Boussinesq approximation [34, 36] to (2.1)–(2.3). Consider the following steady solution to Eqs. (2.1)–(2.3):

$$\bar{u}(x, y, t) = 0$$

$$\bar{\rho}(x, y, t) = \rho_c$$

with \bar{P} chosen so that

$$\text{grad } \bar{P} = \rho_c \mathbf{F}$$

where ρ_c is a constant.

Define ρ' , P' , and \mathbf{u}' by

$$\rho' = \rho - \bar{\rho}, \quad P' = P - \bar{P}, \quad \mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}}.$$

We substitute these expressions into (2.1)–(2.3) and find, after some simplification,

$$\frac{\partial \rho'}{\partial t} + \mathbf{u}' \cdot \text{grad } \rho' = 0 \quad (2.4)$$

$$\left(1 + \frac{\rho'}{\rho_c}\right) \left(\frac{\partial \mathbf{u}'}{\partial t} + \mathbf{u}' \cdot \text{grad } \mathbf{u}'\right) = \frac{\text{grad } P'}{\rho_c} + \frac{\rho'}{\rho_c} \mathbf{F} \quad (2.5)$$

$$\text{div } \mathbf{u}' = 0 \quad (2.6)$$

with initial conditions

$$\rho'(x, y, 0) = \rho'_0(x, y), \quad \mathbf{u}'(x, y, 0) = \mathbf{u}'_0(x, y).$$

For small variations in the density about the state ρ_c , $\rho' \ll \rho_c$, we make the Boussinesq approximation,

$$1 + \frac{\rho'}{\rho_c} \approx 1. \quad (2.7)$$

Thus (2.5) becomes

$$\frac{\partial \mathbf{u}'}{\partial t} + \mathbf{u}' \cdot \text{grad } \mathbf{u}' = \frac{\text{grad } P'}{\rho_c} + \frac{\rho'}{\rho_c} \mathbf{F}. \quad (2.8)$$

For the sake of simplicity we will drop the primes and refer to \mathbf{u}' , ρ'/ρ_c , and P' in (2.4)–(2.8) as the velocity, density, and pressure, respectively. In this notation the equations now become

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \text{grad } \rho = 0 \tag{2.9}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \text{grad } \mathbf{u} = \frac{\text{grad } P}{\rho_c} + \rho \mathbf{F} \tag{2.10}$$

$$\text{div } \mathbf{u} = 0 \tag{2.11}$$

$$\rho(x, y, 0) = \rho_0(x, y), \quad \mathbf{u}(x, y, 0) = \mathbf{u}_0(x, y).$$

Equations (2.9)–(2.11) are the equations that we shall be using.

It is convenient for numerical work to put (2.9)–(2.11) into a vorticity-stream form. Let ω be the vorticity, $\omega = \text{curl}(\mathbf{u})$, and let Ψ be the stream function. Then these equations can be written as

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \text{grad } \rho = 0 \tag{2.12}$$

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \text{grad } \omega = \text{curl}(\rho \mathbf{F}) \tag{2.13}$$

$$\Delta \Psi = -\omega, \quad u_1 = \Psi_y, \quad u_2 = -\Psi_x \tag{2.14}$$

where Δ is the Laplace operator. If we use the fact that $G = (1/2\pi) \log(r)$ is the Green's function for Δ , and $r = (x^2 + y^2)^{1/2}$, we find

$$\Psi = -G * \omega$$

where $*$ represents convolution. Thus, if we use (2.14), we obtain the following expression for the velocity in terms of the vorticity;

$$u_1 = -\frac{\partial G}{\partial y} * \omega, \quad u_2 = \frac{\partial G}{\partial x} * \omega$$

or

$$\mathbf{u} = K * \omega \tag{2.15}$$

where $K = (1/2\pi r^2)(-y, x)$.

We mention that the pressure P does not occur in Eqs. (2.12)–(2.15). This is a result of using the vorticity formulation and the Boussinesq approximation. The elimination of the pressure from the equations greatly simplifies our computational task and is our primary motivation for using this approximation.

Equation (2.13) expresses the fact that in a fluid of variable density the vorticity grows where there are density gradients. To calculate the effect of this term we need to compute density derivatives. One method is to find an approximation to the density derivatives by numerically solving (2.12) and then differentiating the resulting solution. This was tried and found to be somewhat unsatisfactory. Another approach is to find an equation of evolution for the density derivatives and solve that equation, i.e., treat the density derivatives as the primary variables. This latter approach is the one which we use here.

If we make the assumption that the support of the initial density distribution is contained in a bounded set, then we can express (2.12) in the following equivalent form:

$$\frac{\partial \rho_x}{\partial t} + \mathbf{u} \cdot \text{grad } \rho_x = -u_{1x} \rho_x - u_{2x} \rho_y \quad (2.16)$$

$$\frac{\partial \rho_y}{\partial t} + \mathbf{u} \cdot \text{grad } \rho_y = -u_{1y} \rho_x - u_{2y} \rho_y \quad (2.17)$$

$$\rho = G_x * \rho_x + G_y * \rho_y \quad (2.18)$$

$$\rho_x(x, y, 0) = \rho_{0x}(x, y), \quad \rho_y(x, y, 0) = \rho_{0y}(x, y).$$

Here ρ_x and ρ_y are the derivatives of the density and $G = (1/2\pi) \log(\mathbf{r})$, $\mathbf{r} = (x^2 + y^2)^{1/2}$. Equation (2.16) is obtained by differentiating Eq. (2.12) with respect to x and using the condition that $\text{div } \mathbf{u} = 0$. Equation (2.17) is obtained similarly. Equation (2.18) is derived from Poisson's formula [25] and integration by parts,

$$\rho = G * \Delta \rho = G_x * \rho_x + G_y * \rho_y.$$

We use (2.18) to reconstruct the density from its gradients because it has an easily implementable numerical analogue. Our numerical method will be based on approximations to the solutions of (2.13)–(2.15) and (2.16)–(2.18).

To demonstrate the equivalence of (2.12) and (2.16)–(2.18); if \mathbf{u} and ρ are sufficiently smooth, and $\text{div } \mathbf{u} = 0$, then it is easily seen that any solution of (2.12) is also a solution of (2.16)–(2.18). The fact that a sufficiently smooth solution of (2.16)–(2.18) is a solution of (2.12) is the content of the following theorem.

THEOREM 2. *Assume that for any time t , $0 \leq t < T$, \mathbf{u} and its derivatives are continuous and bounded for $x \in \mathbb{R}^2$ and $\text{div } \mathbf{u} = 0$. Also assume $\bar{\rho}_x$ and $\bar{\rho}_y$ have compact support and are twice continuously differentiable (in both \mathbf{x} and t) solutions of (2.16) and (2.17). If we define ρ by*

$$\rho = G_x * \bar{\rho}_x + G_y * \bar{\rho}_y \quad (2.19)$$

where G is the fundamental solution of Laplace's equation, then

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \text{grad } \rho = 0 \quad \text{and} \quad \frac{\partial \rho}{\partial x} = \bar{\rho}_x, \quad \frac{\partial \rho}{\partial y} = \bar{\rho}_y.$$

The equivalence of these equations is most likely true under less restrictive assumptions, but such a result is not needed for our work, so we do not pursue the matter. To prove the theorem we need the following lemma:

LEMMA 1.1. *Under the hypothesis of Theorem 2 we have*

$$(\bar{\rho}_x)_y = (\bar{\rho}_y)_x.$$

Proof. If we differentiate (2.16) with respect to y and then subtract from it Eq. (2.17) differentiated with respect to x we find, after some simplification through the use of the condition $\text{div } \mathbf{u} = 0$ and equality of cross partials, that the quantity $\tilde{w} = (\bar{\rho}_x)_y - (\bar{\rho}_y)_x$ satisfies the equation

$$\frac{\partial \tilde{w}}{\partial t} + \mathbf{u} \cdot \text{grad } \tilde{w} = 0 \tag{2.20}$$

with initial data

$$\tilde{w}(x, y, 0) = \rho_{0_{xy}} - \rho_{0_{yx}} = 0.$$

Using the fact that \tilde{w} is a C^1 solution of (2.20) with vanishing initial data, one can show, using energy estimates [18], that $\tilde{w} = 0$ for all $t, 0 \leq t < T$.

This completes the proof. We now prove Theorem 2.

Proof. Let ρ be given by (2.19). We first show that $\partial \rho / \partial x = \bar{\rho}_x$. Using integration by parts and equality of cross partials, we find

$$\begin{aligned} \frac{\partial \rho}{\partial x} &= (G_x * \bar{\rho}_x + G_y * \bar{\rho}_y)_x \\ &= G * (\bar{\rho}_x)_{xx} + G * (\bar{\rho}_y)_{xy}. \end{aligned}$$

If we use Lemma 1.1 and Poisson's formula, then we have

$$\begin{aligned} &= G * (\bar{\rho}_x)_{xx} + G * (\bar{\rho}_x)_{yy} \\ &= \bar{\rho}_x. \end{aligned}$$

Similarly we have that $\partial \rho / \partial y = \bar{\rho}_y$.

Assume $\sigma(x, y)$ is a solution of (2.12) with initial data $\sigma_0(x, y) = \rho_0(x, y)$. Then σ_x and σ_y satisfy (2.16) and (2.17), respectively, with initial data given by the derivatives of ρ_0 . By assumption, $\bar{\rho}_x$ and $\bar{\rho}_y$ and hence $\partial \rho / \partial x$ and $\partial \rho / \partial y$ also satisfy

(2.16) and (2.17). From the uniqueness of solutions to Eqs. (2.16) and (2.17), we conclude that $\sigma_x = \partial\rho/\partial x$ and $\sigma_y = \partial\rho/\partial y$. Thus $\sigma = \rho + c$, where c is a constant. In particular we find that ρ of (2.19) satisfies the same equation as σ , namely, (2.12). This completes the proof.

3. DISCRETIZATION OF THE EQUATIONS OF MOTION

In this section we describe an approximation scheme for Eqs. (2.13)–(2.18). Our technique is to write the equations in Lagrangian form and then discretize them. Unlike the model problem in which the velocity field that moves the fluid quantities is given, in these equations the velocity field must be calculated as part of the solution. However, the numerical procedure that forms the basis of the vortex method is applicable and will be used to determine the velocity field. In Lagrangian form Eqs. (2.13)–(2.18) are

$$\frac{dx(\alpha, t)}{dt} = \mathbf{u}(x(\alpha, t), t) \quad (3.1)$$

$$\frac{d\omega(x(\alpha, t), t)}{dt} = \rho_x(x(\alpha, t), t) F_2 - \rho_y(x(\alpha, t), t) F_1 \quad (3.2)$$

$$\frac{d\rho_x(x(\alpha, t), t)}{dt} = -u_{1x}(x(\alpha, t), t) \rho_x(x(\alpha, t), t) - u_{2x}(x(\alpha, t), t) \rho_y(x(\alpha, t), t) \quad (3.3)$$

$$\frac{d\rho_y(x(\alpha, t), t)}{dt} = -u_{1y}(x(\alpha, t), t) \rho_x(x(\alpha, t), t) - u_{2y}(x(\alpha, t), t) \rho_y(x(\alpha, t), t) \quad (3.4)$$

$$\rho(x(\alpha, t), t) = G_x * \rho_x(x(\alpha, t), t) + G_y * \rho_y(x(\alpha, t), t) \quad (3.5)$$

with initial conditions

$$\begin{aligned} x(\alpha, 0) &= \alpha, & \omega(x(\alpha, 0), 0) &= \omega_0(\alpha) \\ \rho_x(x(\alpha, 0), 0) &= \rho_{0x}(\alpha), & \rho_y(x(\alpha, 0), 0) &= \rho_{0y}(\alpha). \end{aligned}$$

Here $\alpha = (\alpha_1, \alpha_2) \in R^2$, \mathbf{u} is defined by (2.15), and G is the fundamental solution of Laplace's equation. The solution to (3.1), $x(\alpha, t)$, is the trajectory of a fluid particle which at time $t=0$ is located at the point α . Equations (3.2) and (3.3)–(3.4) describe the evolution of the vorticity and the density derivatives along the particle trajectory $x(\alpha, t)$.

Assume the support of ω_0 , ρ_{0x} , and ρ_{0y} are contained in some bounded set Ω . Let A^h denote the set of nodes of a grid of mesh width h , and define Ω^h as the intersection of Ω with A^h . Let ψ be in $M^{L,p}$, where $M^{L,p}$ is defined as in Section 1. We will approximate the solution to (3.1)–(3.5) by solving approximations to these

equations for all points which are initially in Ω^h . For notational simplicity we denote by $x_j(t)$ the trajectory starting at jh , i.e., $x_j(t) = x(jh, t)$. Using this notation and also using $\tilde{\cdot}$ to denote computed quantities, the method consists of solving the equations

$$\frac{d\tilde{x}_j(t)}{dt} = \tilde{u}^h(\tilde{x}_j(t), t) \tag{3.6}$$

$$\frac{d\tilde{\omega}(\tilde{x}_j(t), t)}{dt} = \tilde{\rho}_x(\tilde{x}_j(t), t) F_2 - \tilde{\rho}_y(\tilde{x}_j(t), t) F_1 \tag{3.7}$$

$$\frac{d\tilde{\rho}_x(\tilde{x}_j(t), t)}{dt} = -\tilde{u}_{1x}^h(\tilde{x}_j(t), t) \tilde{\rho}_x(\tilde{x}_j(t), t) - \tilde{u}_{2x}^h(\tilde{x}_j(t), t) \tilde{\rho}_y(\tilde{x}_j(t), t) \tag{3.8}$$

$$\frac{d\tilde{\rho}_y(\tilde{x}_j(t), t)}{dt} = -\tilde{u}_{1y}^h(\tilde{x}_j(t), t) \tilde{\rho}_x(\tilde{x}_j(t), t) - \tilde{u}_{2y}^h(\tilde{x}_j(t), t) \tilde{\rho}_y(\tilde{x}_j(t), t) \tag{3.9}$$

with initial conditions

$$\begin{aligned} \tilde{x}_j(0) &= jh, & \tilde{\omega}(\tilde{x}_j(0), 0) &= \omega_0(jh) \\ \tilde{\rho}_x(\tilde{x}_j(0), 0) &= \rho_{0x}(jh), & \tilde{\rho}_y(\tilde{x}_j(0), 0) &= \rho_{0y}(jh) \end{aligned}$$

for all points $jh \in \Omega^h$. The velocity $\tilde{u}^h(\tilde{x}_j(t), t)$ is computed by

$$\tilde{u}^h(\tilde{x}_j(t), t) = \sum_{ih \in \Omega^h} (K * \psi_\delta)(\tilde{x}_j(t) - \tilde{x}_i(t)) \tilde{\omega}(\tilde{x}_i(t), t) h^2 \tag{3.10}$$

and the derivatives of the velocity field in (3.8) and (3.9) are computed by

$$\tilde{u}_x^h(\tilde{x}_j(t), t) = \sum_{ih \in \Omega^h} \left(K * \frac{\partial \psi_\delta}{\partial x} \right) (\tilde{x}_j(t) - \tilde{x}_i(t)) \tilde{\omega}(\tilde{x}_i(t), t) h^2 \tag{3.11}$$

$$\tilde{u}_y^h(\tilde{x}_j(t), t) = \sum_{ih \in \Omega^h} \left(K * \frac{\partial \psi_\delta}{\partial y} \right) (\tilde{x}_j(t) - \tilde{x}_i(t)) \tilde{\omega}(\tilde{x}_i(t), t) h^2. \tag{3.12}$$

The density is approximated by

$$\begin{aligned} \tilde{\rho}(x, t) &= \sum_{ih \in \Omega^h} (G_x * \psi_\delta)(x - \tilde{x}_i(t)) \tilde{\rho}_x(\tilde{x}_i(t), t) h^2 \\ &+ \sum_{ih \in \Omega^h} (G_y * \psi_\delta)(x - \tilde{x}_i(t)) \tilde{\rho}_y(\tilde{x}_i(t), t) h^2. \end{aligned} \tag{3.13}$$

We remark that the expression for the velocity \mathbf{u} is obtained, as in the vortex method, by applying the kernel K to the approximation of the vorticity given by

$$\tilde{\omega}^h(x, t) = \sum_{ih \in \Omega^h} \psi_\delta(x - \tilde{x}_i(t)) \tilde{\omega}(\tilde{x}_i(t), t) h^2.$$

We also note that the approximations to the velocity derivatives given by (3.11) and (3.12) are obtained by differentiating the approximation to the velocity (3.10). The density approximation (3.13) is obtained by using the approximations to the density derivatives

$$\begin{aligned} \tilde{\rho}_x^h(x, t) &= \sum_{ih \in \Omega^h} \psi_\delta(x - \tilde{x}_i(t)) \tilde{\rho}_{x_i}(x_i(t), t) h^2 \\ \tilde{\rho}_y^h(x, t) &= \sum_{ih \in \Omega^h} \psi_\delta(x - \tilde{x}_i(t)) \tilde{\rho}_{y_i}(x_i(t), t) h^2 \end{aligned}$$

in (3.5).

For functions ψ which depend only on r , the convolution of the kernels K and G with ψ_δ can be computed explicitly. (See [8].)

The accuracy of these schemes is dependent upon the initial grid spacing h , the smoothing parameter δ , and the functions ψ . Error estimates for the approximation scheme (3.6)–(3.13) given in [1] can be used to select the parameters.

As in the model problem, the initial points need not be the nodes of a rectangular grid. If one does not use a rectangular distribution of points, then the approximation scheme is essentially unchanged. However, in the approximations (3.10)–(3.13) the factor h^2 should be replaced by a factor p_i , where the p_i are weight factors depending on the distribution of the computational points and accuracy considerations. (See [3].)

4. TEST PROBLEM

Given the force function

$$\mathbf{F}(x, y, t) = 2t\bar{F} \left(\frac{-y}{r^2}, \frac{x}{r^2} \right)$$

where $r^2 = (x^2 + y^2)$, t is the time variable, and \bar{F} is a constant, then a C^7 solution to (2.12)–(2.15) with initial conditions

$$\begin{aligned} \rho(x, y, 0) &= \frac{\alpha}{16} - \frac{\alpha}{16} \left(1 - \frac{r^2}{\alpha} \right)^8, & r^2 \leq \alpha \\ &= \frac{\alpha}{16}, & r^2 > \alpha \\ \omega(x, y, 0) &= 0 \end{aligned} \tag{4.1}$$

is

$$\begin{aligned} \rho(x, y, t) &= \rho(x, y, 0) \\ u_1(x, y) &= \frac{-y\rho(x, y, 0)}{r^2} \bar{F}t^2, & r^2 \leq \alpha & \quad u_2(x, y) = \frac{x\rho(x, y, 0)}{r^2} \bar{F}t^2, & r^2 \leq \alpha \\ &= \frac{-y(\alpha/16) \bar{F}t^2}{r^2}, & r^2 > \alpha & \quad = \frac{x(\alpha/16) \bar{F}t^2}{r^2}, & r^2 > \alpha. \end{aligned} \tag{4.2}$$

The smoothness of the density follows from the definition of $\rho(x, y, 0)$. For $r^2 \leq \alpha$, the term $\rho(x, y, 0)$ occurring in (4.2) is a polynomial in r^2 with no constant term, so $\rho(x, y, 0)/r^2$ is a polynomial in r^2 . Thus the velocities are infinitely differentiable for $r^2 < \alpha$. The non-smoothness of the velocity occurs at the points for which $r^2 = \alpha$.

The flow is a radially symmetric body of fluid rotating about the origin. What makes the flow interesting is that fluid particles at different distances from the origin move at different rates, i.e., there is local shear. Typically, flows with shear present the greatest challenge to Lagrangian schemes [31] and we therefore believe that this problem is a non-trivial test of the method.

The parameters to be chosen are h , the initial mesh width, δ , the smoothing parameter, and the function ψ used in (3.10)–(3.13). We allowed h to take on three values, $h = 0.0886$, $h = 0.0728$, and $h = 0.0626$, corresponding to 200, 300, and 400 points, respectively. The error estimates of the convergence results given in [1] suggest that we should choose $\delta = h^q$ for some $q < 1$. We therefore let $\delta = h^q$ for $q = 0.95$, $q = 0.85$, and $q = 0.75$. The functions ψ used in the approximations (3.10)–(3.13) were chosen to be in $M^{L,p}$ and one of

$$(p = 2, L = \infty) \quad \psi(r) = \frac{e^{-r^2}}{\pi} \tag{4.3}$$

$$(p = 4, L = \infty) \quad \psi(r) = \frac{1}{\pi} \left(2e^{-r^2} - \frac{1}{2} e^{-r^2/2} \right) \tag{4.4}$$

$$(p = 6, L = \infty) \quad \psi(r) = \frac{1}{\pi} \left(8e^{-r^2} - \frac{27}{4} e^{-(3/4)r^2} + e^{-r^2/2} \right). \tag{4.5}$$

These functions are suggested by Beale and Majda in [8]. The integration of the ordinary differential equations (3.6)–(3.9) was performed using fourth-order Runge–Kutta. The time step, $\Delta t = 0.1$, was chosen sufficiently small so that a decrease in the time step did not significantly effect the results.

We measured the relative error in the first component of the velocity. This error is computed by

$$\frac{[\sum_{ih \in \Omega^h} |\tilde{u}_1^h(\tilde{x}_i(t), t) - u_1(\tilde{x}_i(t), t)|^2 h^2]^{1/2}}{[\sum_{ih \in \Omega^h} |u_1(\tilde{x}_i(t), t)|^2 h^2]^{1/2}}$$

where \tilde{u}_1^h is the computed velocity, u_1 is the exact velocity, and $\tilde{x}_i(t)$ are the computed point positions.

We found that for all values of the parameters tried the errors grew at a rate which was independent of the number of time steps, i.e., the method was stable. We present in Tables I and II the errors for the various choices of the parameters at times $t = 1.0$ and $t = 1.6$. These times correspond to a maximum point rotation of $\pi/4$ and 2π radians, respectively.

TABLE I
Errors in Velocity (%) at Time $t = 1.0$

	$p = 2$	$p = 4$	$p = 6$
$h = 0.0886$			
$\delta = h^{0.95}$	5.3	0.82	0.25
$\delta = h^{0.85}$	8.3	1.8	0.32
$\delta = h^{0.75}$	12.0	3.9	1.0
$h = 0.0723$			
$\delta = h^{0.95}$	3.7	0.40	0.14
$\delta = h^{0.85}$	6.1	1.0	0.12
$\delta = h^{0.75}$	9.8	2.4	0.49
$h = 0.0628$			
$\delta = h^{0.95}$	2.8	0.24	0.10
$\delta = h^{0.85}$	4.8	0.67	0.061
$\delta = h^{0.75}$	8.1	1.7	0.29

TABLE II
Errors in Velocity (%) at Time $t = 1.6$

	$p = 2$	$p = 4$	$p = 6$
$h = 0.0886$			
$\delta = h^{0.95}$	5.7	3.7	5.4
$\delta = h^{0.85}$	8.3	2.7	3.5
$\delta = h^{0.75}$	12.0	3.9	2.1
$h = 0.0723$			
$\delta = h^{0.95}$	3.9	2.4	3.7
$\delta = h^{0.85}$	6.0	1.5	2.1
$\delta = h^{0.75}$	9.7	2.3	1.1
$h = 0.0628$			
$\delta = h^{0.95}$	3.0	1.6	2.7
$\delta = h^{0.85}$	4.8	1.0	1.4
$\delta = h^{0.75}$	8.0	1.6	0.78

From these results we see that using higher-order blob functions ($p \geq 2$) is beneficial. This effect can be quite substantial, as one sees by comparing the results for different blob functions at time $t = 1.6$ with $h = 0.0626$. For a blob function with $p = 2$ the error is 8 % while for a function with $p = 6$ the error is 0.78 %. The theoretical estimates given in [1] support this result. We also see that there is a pronounced effect on the error when the relations between h and δ are varied. However, the effect is not uniform with respect to time or blob function. We note that by choosing a large value of δ with respect to h the growth of error in time is diminished. This is most clearly seen with the higher-order functions, where it appears that more smoothing is necessary to preserve accuracy. In experiments on the vortex method [8, 32] similar conclusions about the relative size of h and δ have been obtained.

Since the effect of the choice of the relative size of h and δ on the error is unclear, it is difficult to abstract from these results what the correct relation should be. To overcome this difficulty we have devised an empirical procedure for determining it. This procedure is described and tested in the next section.

5. APPLICATION TO A 2-D THERMAL

A 2-D thermal is that object which is initially a cylindrical body of buoyant fluid having its axis of symmetry perpendicular to the gravitational force and which has moved under the effect of gravity. We model the motion of a line thermal by computing the solution to Eqs. (2.12)–(2.14) with initial data of the form

$$\rho_0(x, y) = \rho_1 \quad \text{for } r \leq \bar{r}$$

$$= 0 \quad \text{for } r > \bar{r}$$
(5.1)

$$\omega_0(x, y) = 0.$$
(5.2)

Here $r = (x^2 + y^2)^{1/2}$ and ρ_1 is a constant such that $\rho_1 \leq 0$. For the external force, \mathbf{F} , we used $\mathbf{F} = -(0, g)$ where g is a constant. In all of our calculations we used $\rho_1 = -0.1$, $g = 10.0$, and $\bar{r} = 0.5$.

Due to the presence of gravity, the circular region of lighter fluid will rise in time. The problem is to calculate the motion of this lighter fluid. For a more detailed description of line thermals and of theoretical and experimental studies of their motion see [20, 33, 35, 36]. An earlier numerical study of the motion of a 2-D thermal is presented in [29]. Our interest in this problem is to gain an understanding of the behavior of the method when it is applied to more realistic problems, i.e., problems closer to those which our numerical method is intended to be useful for.

The problem we are solving has singular initial data. This presents difficulties since the numerical scheme as described in Section 3 and tested in Section 4 is based on assumptions of continuous density distributions. However, the general approach that we take, that of calculating the evolution of the vorticity and the density

gradients, suggests a reasonable discretization and we are able to formulate a numerical scheme.

To construct a numerical scheme we need to choose an initial distribution for the computational points and the initial conditions for the equations describing the evolution of the vorticity and the density derivatives. The initial points we used were those uniformly distributed along the interface $\{(x, y) \mid x^2 + y^2 = \bar{r}^2\}$. This is a reasonable choice because the density derivatives, and hence the vorticity, of the solution to (2.12)–(2.14) will be non-zero only on this set. Thus, letting α_k denote the computational points we used

$$\alpha_k = \bar{r}(\cos(kh), \sin(kh)) \quad \text{for } k = 1, \dots, N$$

where

$$h = \bar{r} \frac{2\pi}{N}.$$

Using this choice of computational points we must determine the weights occurring in the approximation for the velocity (3.10) and density (3.13). (Since the initial points are not on a rectangular grid, the factor h^2 is not appropriate.) We must also determine appropriate initial values for the density and vorticity. As the important components in the approximations (3.10)–(3.13) are the products of the values of the vorticity times the weight factors and density derivatives times weight factors, it is convenient in this problem to consider these products as single quantities. The differential equations describing the evolution of the vorticity and the density derivatives can be transformed (upon multiplication by the weight factors) into equations for these combined quantities. For the initial conditions for the products involving the density derivatives we used

$$\tilde{\rho}_x(\alpha_k, 0) p_k = \rho_{0y}(\alpha_k) p_k = \gamma \cos(\alpha_k)$$

$$\tilde{\rho}_y(\alpha_k, 0) p_k = \rho_{0x}(\alpha_k) p_k = \gamma \sin(\alpha_k).$$

Here p_k is the weight factor used in place of h^2 in the approximations (3.10)–(3.13). The constant γ is chosen so that when we construct the density using (3.13) the total mass of the lighter fluid is identical to the mass of the lighter fluid in the initial condition (5.1). Specifically, we choose γ so that

$$\begin{aligned} \int_{|x| \leq \bar{r}} \tilde{\rho}^h(x, 0) dx &= \gamma \int_{|x| \leq \bar{r}} \sum_{k=1}^N G_x(x - \alpha_k) \cos(\alpha_k) dx \\ &\quad + \gamma \int_{|x| \leq \bar{r}} \sum_{k=1}^N G_y(x - \alpha_k) \sin(\alpha_k) dx \\ &= -\rho_1 \pi \bar{r}^2. \end{aligned}$$

For the initial conditions of the products involving the vorticity we used

$$\tilde{\omega}(\alpha_k, 0) p_k = \tilde{\omega}_0(\alpha_k) p_k = 0 \quad \text{for } k = 1, \dots, N.$$

There is a second technique which would lead one to a numerical scheme for this problem. This consists of modifying the initial conditions (5.1)–(5.2) so that the procedure described in Section 3 will work. Specifically, one would first smooth the initial data, i.e., change the jump discontinuity into a smoothly varying transition, and then approximate the solution of this smoothed problem. The usefulness of such an approach has been demonstrated in conjunction with the Fourier method [28]. A disadvantage of using this technique is that it uses more computational points than that described above. However, the possibility of using the latter approach demonstrates an attractive feature of our method. In particular, when one smooths out the interface (which entails thickening it) there is a natural discretization of the smoothed problem that is consistent with our numerical method. This feature is not present in vortex sheet or integral equation approaches. Computations involving this second technique to calculate the motion of a thermal are currently being carried out.

The other parameters that need to be selected are the function ψ and the parameter δ . We chose the function ψ used in (3.10) and (3.11) to be

$$\psi(r) = \frac{1}{\pi} e^{-r^2} \quad (5.3)$$

where $r = (x^2 + y^2)^{1/2}$

The last parameter to be specified is the parameter δ . We found that the proper choice of δ was a critical factor in obtaining consistent numerical results. Our first, and unsuccessful, technique was to let $\delta = h^q$ for some $q < 1$. With these choices we then solved the equations (3.6)–(3.9) using a fourth-order Runge–Kutta scheme with a step size of $\Delta t = 0.1$. We monitored the quality of the computation by computing the mass of the thermal at each time step. Typically, for the values of q that we tried, $q = 0.95$, $q = 0.75$, and $q = 0.5$, it was found that there was a time \bar{T} , depending on q , such that the solution failed to conserve mass for $t \geq \bar{T}$. Furthermore, decreasing h (increasing the number of computational points) did not improve the results. Sample results for the calculations for $\delta = h^{0.75}$ are shown in Figs. 6.1(a)–(c). In these figures the interface position at $t = 3.0$ for different values of h is shown. We see that as $h \rightarrow 0$ the results are not consistent.

We believe the inconsistency of the results is due to the manner in which we are approaching the solution of Eqs. (2.9)–(2.11) with the numerical approximation. We expect that as $h \rightarrow 0$ and $\delta \rightarrow 0$ the numerical approximation will approach the solution. However, there is no reason a priori to assume that approaching the limit $h = 0$ and $\delta = 0$ using the relation $\delta = h^q$ is appropriate for this problem. The solutions were numerically unstable and we concluded that for a given value of h , the smoothing parameter δ determined by the relation $\delta = h^q$ was not large enough to suppress the instability.

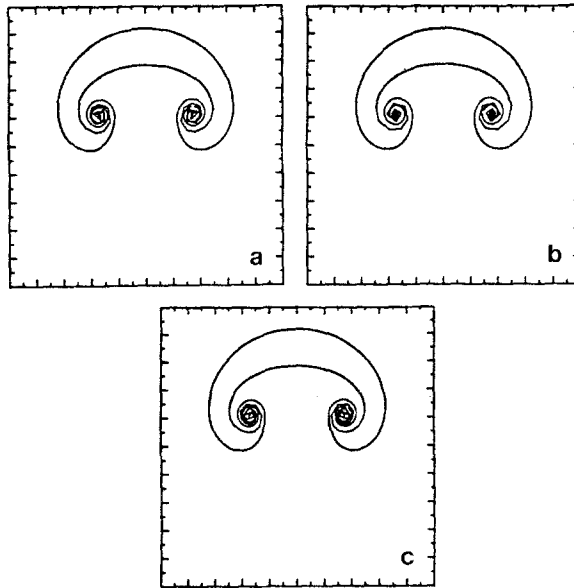


Fig. 6.1. Interface position at time $t=3.0$ with $\delta=h^{0.75}$ and $h=\pi/N$. N is 200, 300, and 400 in (a)–(c), respectively.

To overcome the difficulty in choosing the proper relation between h and δ we used the following procedure. We fixed a value of δ , say, δ_1 , and then determined an h_1 , so that for all $h < h_1$ the computational results did not significantly change for $0 \leq t \leq \tilde{T}$. (\tilde{T} is selected arbitrarily.) We then selected another δ , say, δ_2 , with $\delta_2 < \delta_1$. Again, we found an h_2 such that for $h < h_2$ the results did not significantly change over $0 \leq t \leq \tilde{T}$. We continued in this manner and thus constructed a sequence (h_1, δ_1) , $(h_2, \delta_2), \dots, (h_i, \delta_i)$. Our hope was that as the sequence $(h_i, \delta_i) \rightarrow (0, 0)$ the corresponding numerical solutions approach the solutions of (2.9)–(2.11) with data (5.1)–(5.2). One can view the above procedure as empirically determining the appropriate approach to the limit.

This procedure worked well. Our assessment of convergence was obtained by considering three features of the computation.

- (1) The conservation of mass of the lighter fluid for $0 \leq t \leq \tilde{T}$.
- (2) The convergence of the length of the interface.
- (3) The convergence of the position of the interface.

As an example of the convergence behavior, the results for $\delta = 0.07$ are presented in Table III and Figs. 6.2(a)–(c). Table III shows the variation with respect to h at time $\tilde{T} = 3.0$ of the mass and of the arc length. Figures 6.2(a)–(c) show the position of the interface at time $\tilde{T} = 3.0$ as h is varied. We mention that the time step, $\Delta t = 0.1$, was chosen small enough so that it had an insignificant effect on the results.

TABLE III
Fixed Delta Convergence at $t = 3.0$

N	Mass	Arc length
150	7.641×10^{-2}	9.768
250	7.855×10^{-2}	9.824
350	7.854×10^{-2}	9.839
450	7.854×10^{-2}	9.846

Note. $\delta = 0.07$. Initial mass = 7.8539×10^{-2} .

We computed the solution to the above problem for several different values of δ . We limited ourselves to $\delta \geq 0.04$ because for smaller δ 's the number of points necessary to obtain convergence was very large (> 800). In Fig. 6.3 we plot the position of the interface for times $t = 0.0$ to $t = 3.0$ and for $\delta = 0.1$. (These figures represent the converged solution with respect to the parameter h .) It was observed that the computed solutions for smaller values of δ were similar to the solution presented in Fig. 6.3. The overall shape and the distance traveled were essentially independent of the size of δ used. This demonstrates an attractive feature of the method, specifically that one need not choose exceptionally small δ in order to obtain the gross features of the flow. This is important because the numerical

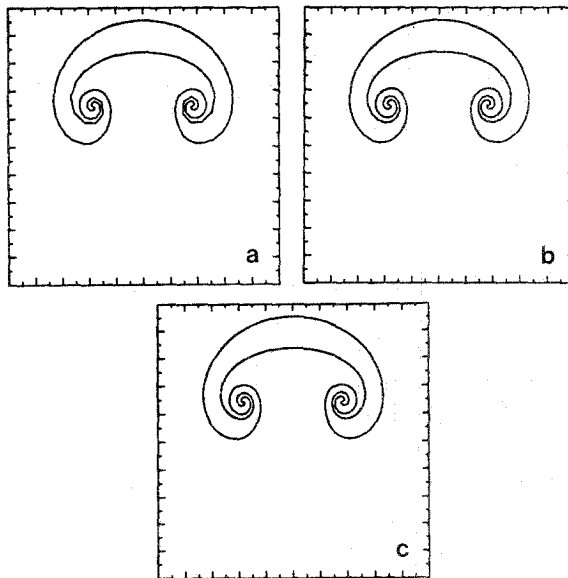


FIG. 6.2. Interface position at time $t = 3.0$ with $\delta = 0.07$ and $h = \pi/N$. N is 200, 300, and 400 in (a)-(c), respectively.

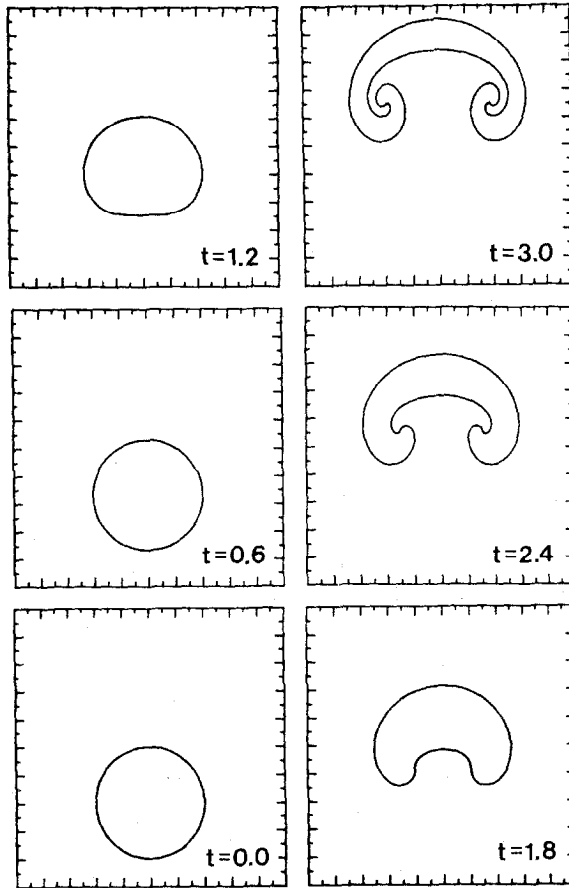


FIG. 6.3. Interface as a function of time. $\delta = 0.1$.

method requires more computational points, i.e., more computational labor, the smaller the value of δ . The change in the numerical solutions with δ was in the small-scale features of the solutions; notably in the eye of the curl. This aspect of the solutions can be seen in Figs. 6.4(a)–(f) in which the solutions for different δ 's at time $t = 3.0$ are presented. For a more revealing picture of the interface at small δ 's, we present in Fig. 6.5 the result at time $t = 3.0$ of the interface location for $\delta = 0.04$.

As stated in the Introduction, we find evidence that the solution has a singularity in finite time. The evidence that suggests this is the behavior of the arc length of the interface and the magnitude of the vorticity of the solution in time. In Fig. 6.6 we plot the arc length versus time for the values of δ tested. Up to time $\bar{T} = 1.0$ the arc length is approximately constant. After that time the arc length grows at a rate which is approximately proportional to $\delta^{-0.105}$. Thus it appears that as δ tends to zero the length of the interface becomes infinite, and that this occurs around time \bar{T} .

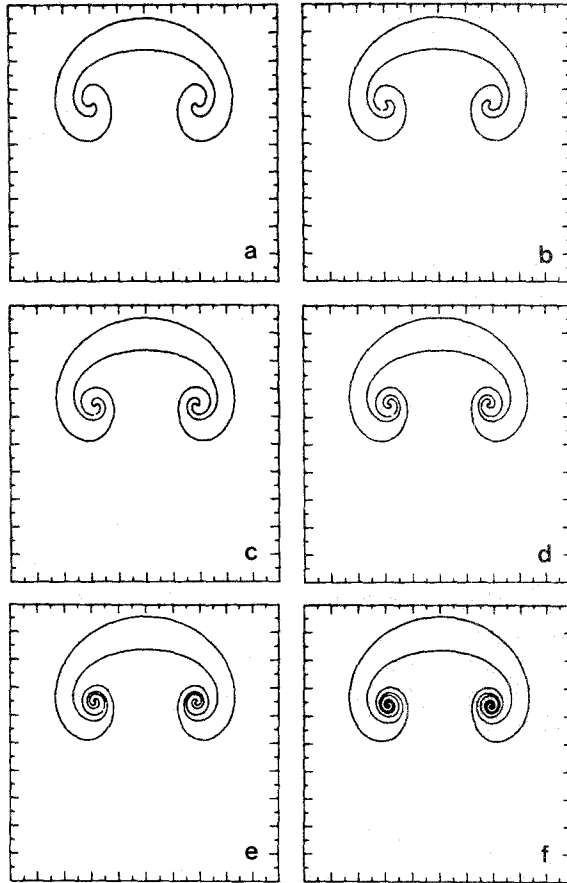


FIG. 6.4. Interface position at time $t = 3.0$. δ values 0.1 to 0.05 in increments of 0.01 for (a)-(f), respectively.

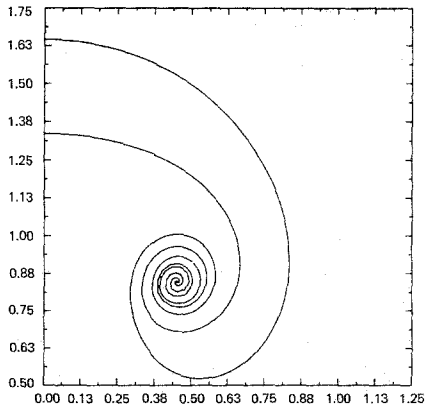


FIG. 6.5. Interface position at $t = 3.0$. $\delta = 0.04$.

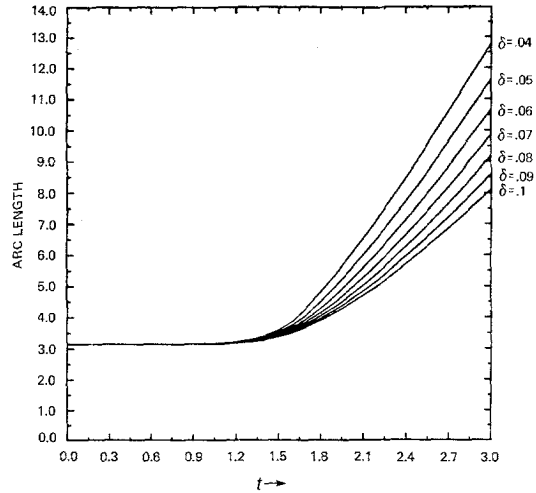


FIG. 6.6. Arc length as a function of time.

The singularity of the solution is also evident in the magnitude of the vorticity. As the thermal evolved the vorticity became concentrated in the “eye” of the thermal. As δ was reduced, the magnitude of this vorticity appeared to grow without bound. Specifically, we found that the maximum vorticity at time 3.0 is approximately described by the equation

$$\max|\omega| = A + B\delta^{-k}$$

where $k = 2.028$ and A and B are two constants independent of δ .

This behavior suggests that a singularity of the flow occurs at about time \bar{T} . However, there are some aspects of the calculation that deserve further study. In particular, the validity of the approach to the singular solution (if it indeed exists) as the limit of our computed solutions as $\delta \rightarrow 0$ remains to be studied. It also remains to be seen whether or not the computational results are the same if the limiting solution is obtained as the limit of solutions of thermals with thickened interfaces. We believe that this is the case, but it must be checked.

6. CONCLUSIONS

We have presented a numerical method for calculating the motion of an incompressible fluid of slightly varying density. The method is grid free and, in view of the method’s ability to resolve the roll-up of the 2-D thermal, is capable of representing very complicated fluid motion. Although the method gives “smoothed” approximations to the solutions of the fluid equations, this smoothing does not accumulate and contaminate the numerical approximation. It is this property that is the distinctive advantage of this method over finite difference methods.

As for the efficiency of our method, it requires $O(n^2)$ operations for each time step, where n is the number of computational points. Compared to grid techniques which usually require $O(m)$ or $O(m \log m)$, where m is the number of grid points, the method presented here may seem to be inefficient. Such a conclusion is not necessarily valid since one typically needs many fewer computational points using our method than with grid techniques to resolve the fine-scale structures of the flow. We mention that the operation count of the method presented here may be reduced if one uses particle-grid techniques such as Cloud In Cell [16] or its variants [2, 10, 11, 24]. (For a review of particle-grid methods see [19].) Although using such algorithms leads to a loss of accuracy in the calculation, their use can reduce the amount of computational labor enormously.

An aspect of the implementation of our method is the choice of the "blob" function ψ and the smoothing parameter δ . From the results presented in Section 4 we conclude that for smooth problems using higher-order functions, ψ in $M^{L,p}$ with $p > 2$, is likely to be beneficial. Also, letting the core parameter $\delta = h^q$ for $0 < q < 1$, where h is the initial mesh width, seems a proper choice. For non-smooth problems the results of Section 5 indicate that the proper relation between h and δ is a crucial factor for obtaining consistent numerical results. Since there are no theoretical estimates that can be used to indicate what this relation might be, we recommend determining the relation between h and δ by the empirical procedure described in Section 5. This procedure may also be of use for determining the proper relation of h and δ in other vortex calculations, especially when the smoothness of the solution is not known.

Possible future applications of the method include the study of the instabilities of continuously stratified fluids and the study of the roll-up of an interface separating two fluids of slightly different densities.

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