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Computational Fluid Dynamics and Reacting Gas Flows

With 124 Illustrations, 2 in Full Color

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Bjorn Engquist
Department of Mathematics
University of California
Los Angeles, CA 90024, USA

Mitchell Luskin
School of Mathematics
University of Minnesota
Minneapolis, MN 55455, USA

Andrew Majda
Department of Mathematics
Princeton University
Princeton, NJ 08544, USA

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FOREWORD

This IMA Volume in Mathematics and its Applications

COMPUTATIONAL FLUID DYNAMICS AND REACTING GAS FLOWS

is in part the proceedings of a workshop which was an integral part of the 1986-87 IMA program on SCIENTIFIC COMPUTATION. We are grateful to the Scientific Committee: Bjorn Engquist (Chairman), Roland Glowinski, Mitchell Luskin and Andrew Majda for planning and implementing an exciting and stimulating year-long program. We especially thank the Workshop Organizers, Bjorn Engquist, Mitchell Luskin and Andrew Majda, for organizing a workshop which brought together many of the leading researchers in the area of computational fluid dynamics.

George R. Sell

Hans Weinberger

PREFACE

Computational fluid dynamics has always been of central importance in scientific computing. It is also a field which clearly displays the essential theme of interaction between mathematics, physics, and computer science. Therefore, it was natural for the first workshop of the 1986-87 program on scientific computing at the Institute for Mathematics and Its Applications to concentrate on computational fluid dynamics. In the workshop, more traditional fields were mixed with fields of emerging importance such as reacting gas flows and non-Newtonian flows. The workshop was marked by a high level of interaction and discussion among researchers representing varied "schools of thought" and countries.

This volume contains 15 papers that were presented at the workshop on computational fluid dynamics and reacting gas flows during September, 1986. Numerical problems connected with weather prediction are presented in a paper by H.-O. Kreiss and G. Browning. Recent progress in vortex methods for incompressible flows is described in papers by J. T. Beale and P.-A. Raviart, G. Cottet, and S. Mas-Gallic, and new finite element techniques for compressible and incompressible fluid flow are given and analyzed by C. Johnson. O. Pironneau and F. Hecht have contributed a paper on the necessity and limitations of turbulence modeling for the numerical solution of the Navier-Stokes equations, and new computational research in aerodynamical fluid dynamics is given in the papers by E. Krause and A. Rizzi and E. Murman.

The field of reacting gas flows is represented by papers by A. Kapila and P.L. Jackson, J.H.S. Lee, J. Nunziato and M. Baer, E. Oran, A. Majda and V. Roytburd, and J. Sethian; and the field of non-Newtonian flows is represented by D. Joseph and D. Malkus and M. Webster. G. Baker has contributed a paper on the instabilities of free surface flows.

Let us point out that research in computational fluid dynamics was also presented at other workshops during the program of the year on scientific computing at the IMA, in particular during the mini-symposium on numerical simulation in oil recovery. Proceedings of these workshops appear in the same series.

The conference committee would like to thank the directors of the IMA, Professors H. Weinberger, G. Sell, and W. Miller, and the staff of the IMA, Mr. R. Copeland, Mrs. P. Kurth, Mrs. C. McAree, and Mrs. M. Saunders for their assistance in arranging the workshop. Special thanks are due to Mrs. K. Smith and Mrs. P. Brick for their preparation of the manuscripts. We gratefully acknowledge the support of the National Science Foundation and the Cray Research Foundation.

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TWO-FREQUENCY RAYLEIGH-TAYLOR AND RICHTMYER-MESHKOV INSTABILITIES

G. R. Baker

Exxon Research and Engineering Company

Route 22 East

Annandale, NJ 08801

1. Abstract

When a flat interface between an incompressible, inviscid fluid and vacuum is driven by a pressure gradient in the direction opposite to that of the density gradient, it is linearly unstable to any sinusoidal perturbation. The nonlinear evolution of a single frequency has been studied in the past using boundary integral methods. In practice, the interface is usually randomly perturbed, but this case presents great difficulty to numerical studies because the interface soon becomes severely distorted. However, it is possible to study the evolution of two modes long enough to gain some understanding of their interaction in the nonlinear regime. The behavior is different depending on whether the pressure gradient is externally imposed (Rayleigh-Taylor instability) or internally present (Richtmyer-Meshkov instability).

2. Introduction

Attempts to design fusion reactors by using laser implosion of deuterium-tritium targets have generate recent interest in the Rayleigh-Taylor instability. As the shell of the target is heated and imploded, several complicated physical processes take place, one of which is the Rayleigh-Taylor instability of one of the shell surfaces which causes turbulent mixing and degradation of target performance[1]. Consequently, studies of the Rayleigh-taylor instability have been undertaken in simpler circumstances [2] in order to gain a basic understanding that may be extrapolated to the conditions applicable to laser fusion research. The simplest manifestation of the Rayleigh-Taylor instability is when the pressure in a light gas accelerates a liquid interface. If a perturbation to the flat interface has a fixed wavelength and large enough initial amplitude, then a regular pattern of spikes and bubbles form in time [3]. New experiments [4] show that even when the initial perturbations are small, but random, clear structures still emerge in time, although they are not necessarily in a regular pattern.

The simplest mathematical model to describe this phenomena comprises of Euler's equations for the incompressible flow of the liquid and the requirements that the pressure is continous across the surface and the normal velocity of the liquid is the normal velocity of the surface. The motion of the light gas is ignored and surface tension is neglected. Linear analysis of the perturbations to a flat interface, dictate that all sinusoidal modes grow and that the growth rate is proportional to the square root of the wavenumber. Thus the motion is linearly ill-posed. However, it is possible that the nonlinear motion is well-posed and it is towards clarifying this issue that several numerical calculations have been performed.

The most successful numerical studies have used boundary integral methods [5-7]. The results all show that for a range of initial amplitudes, the perturbation to a flat interface containing a single Fourier mode grows into a pattern of freely falling spikes and steadily rising bubbles. The spikes appear to be stable, whereas different numerical methods exhibit stable bubbles for one method and unstable bubbles for others. Unfortunately, analytic studies [8,9] have not fully clarified the nature of the stability of the bubble. The stretching of the interface as the bubble rises has a stabilizing effect, but whether it stabilizes all modes is difficult to tell. The nonlinear stability of the numerical methods is also unknown in general, although it has been pointed out [10] that nonlinear resonances between modes, that are introduced artificially by a numerical method, will cause instabilites. It is only by careful numerical studies that these issues may be clarified.

While there is debate about the stability of the bubble when the liquid is penetrated by a very light gas, there is no doubt that the interface between two immiscible fluids of comparable densities does become singular in finite time. The interface may be represented by a vortex sheet whose strength is modified by the baroclinic generation of vorticity. Along the sides of the spikes, fairly uniform distributions in strength of the vortex sheet are developed which subsequently undergo Kelvin-Helmholtz instability. Systematic attempts [5] to refine the interface fail; the motion of the interfacial points become chaotic.

It is now widely believed that the motion is ill-posed; the interface develops a curvature singularity in finite time. This belief is founded on several studies [11,12,13] on the behavior of vortex sheets.

Nevertheless, the hope exists that this singularity does not prevent some meaningful interpretation to the motion of the vortex sheet beyond the time of formation of the singularity. In particular, the possibility of an infinitely long spiral, initially small but growing rapidly in time, has been proposed [14]. In the next section of this paper, I summarize some numerical evidence that this may not be so, that in fact the vortex sheet loses its meaning in the classical sense.

Such a conclusion is a pessimistic one for vortex sheet representations of interfacial flow. The reason is embedded in mathematical studies of the weak limit to hyperbolic systems of partial differential equations. In short, near the singularity time, interfacial motion will be strongly susceptible to the slightest amounts of viscosity or surface tension. Unfortunately, the behavior will be very different depending on whether viscosity or surface tension dominates. Consequently, the nature of the error in a numerical method, either dissipative or dispersive, may seriously affect the numerical results. There have been several attempts [15,16] to simply modify the numerical methods so that calculations will continue beyond the singularity time, but no attention has been given to the type of numerical error that is introduced. So the results may be method dependent. Even attempts to explicitly include surface tension [7] have failed to produce reliable results, possibly because the interface was not adequately resolved to capture important small-scale effects. Presently, it is the lack of understanding of the mathematical properties of interfacial flows that prevent the development of reliable numerical methods.

In the final section of this paper, attention is again focussed on the nature of the classical Rayleigh-Taylor intstability, that is, where the motion of the gas may be neglected compared to that of the liquid. To gain a better understanding of the nonlinear stability of the pattern of spikes and bubbles, another higher mode is introduced in to the initial perturbation. If the initial amplitude of the higher mode is small enough, there is almost no change to the pattern of bubbles and spikes. When this approach is applied to the Richtmyer-Meshkov instability, the curvature of the spike tip is sharpened in the presence of a higher mode, and this effect may lead to the development of a curvature singularity in finite time.

3. Vortex Layers and Vortex Sheets

When the densities of the fluids on either side of the interface are comparable, the regions of the interface adjacent to the spike are Kelvin-Helmholtz unstable. Unfortunately, a vortex sheet develops a curvature singularity in finite time as it deforms as a consequence of the Kelvin-Helmholtz instability

[11,12]. Unless there is some meaningful interpretation to the motion of the vortex sheet beyond the singularity time, there is no possibility of continuing the calculation of the interfacial motion for the Rayleigh-Taylor instability without the inclusion of viscosity or surface tension. Some [14,15,16] have speculated that a spiral forms at or just beyond the singularity time. However, there have been no studies that show this is mathematically feasible.

Instead, the observations [5] of the motion of a thin layer of fluid of intermediate density have led to a study in which the vortex sheet is replaced by a thin layer of vorticity. In two-dimensional flow, the motion of a thin layer of uniform vorticity may be calculated by the method of contour dynamics [17]. Clearly, a thin layer of vorticity is a more realistic model for the shear layer. Mathematically, the limit of an infinitely thin layer is a vortex sheet [18], and so by studying the motion of several layers of various thickness, it is possible to extrtapolate the behavior of a vortex sheet.

The method of contour dynamics has already been applied to a periodic thin layer [19], but the results reported are phenomenological in nature. New results, to be reported in detail elsewhere, have concentrated on the analytical properties of the motion of the thin layer and its limit of vanishing thickness. Here, only a summary is given of the appropriate reults.

In order to conduct this study, the following set of equations for the motion of the bounding curves were solved numerically;

$$\frac{\partial z_j^*}{\partial t}(\sigma) = \frac{U}{H\pi i}\sum_{k=1}^{2}\int_0^{2\pi} \frac{y_j(\sigma)-y_k(\sigma')}{z_j(\sigma)-z_k(\sigma')}\frac{\partial z_k}{\partial \sigma}(\sigma')d\sigma',\ j=1,2,$$

where the complex field point $z=x+iy$ has been introduced for convenience and the lower and upper bounding curves for the layer are $z_1(\sigma)$ and $z_2(\sigma)$ respectively. The curves are parametrised by their initial location through the variable σ. The horizontal velocity reaches a constant U, -U far above, below the layer respectively and the mean thickness of the layer is H. Finally, z^* is the complex conjugate of z. These equations are different from the standard ones for the method of contour dynamics, but are easier to treat numerically [20].

The initial conditions must be chosen carefully if a comparison is to be made with the motion of a vortex sheet. In particular,the simplest manifestation of the curvature singularity occurs when the vortex sheet is initially flat, $z=\sigma$, but its strength varies as 1 - a cos(σ), The limit of a layer, specified initially by

$z_1 = \sigma - i\frac{H}{2}(1 - a\,cos(\sigma))$ and $z_2 = \sigma + i\frac{H}{2}(1 - a\,cos(\sigma))$, as H $\rightarrow$ 0 will be such a vortex sheet. Calculations with these initial conditions and various H all show the same basic behavior. At first, vorticity is advected towards those regions where roll-up should take place and the layer thickens there as a consequence of incompressiblity. At times beyond the singularity time of the vortex sheet, the bulge in the layer reorganises itself into a structure that appears elliptical with thin attached arms. Such structures have been seen before [19,21] and may be canonical for patches of vorticity in two-dimensional flow. In Figure 1, a typical result is shown. Since the flow is 2π-periodic, the bounding curves that lie only in a 2π-periodic window are drawn for a layer of mean thickness 0.1 at a time of 4.0. Here $a=0.5$, so the time of singularity for the vortex sheet would be $t_c \approx 1.45$.

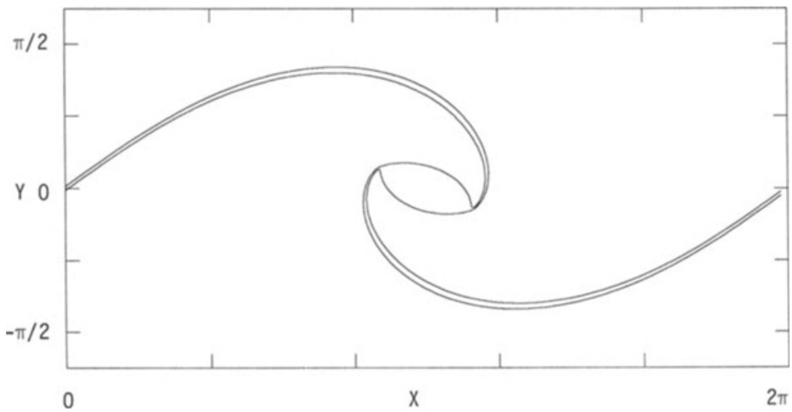

Figure 1. The location of the vortex layer of mean thickness H = 0.1 at time t = 4.0. The initial amplitude a = 0.5.

At first sight, it appears that a curvature singularity might form where the arms attach to the vortex core. If this is so, it would bear directly on the nature of the singularity of the vortex sheet, but careful calculations show that this is not the case. In fact, the bounding curves appear to have a Fourier representation of the form,

$$z(\sigma,t) = \sum a_n(t)\, e^{in\sigma},$$

where for large n

$$|a_n(t)| \approx C\, n^{-\beta(t)} e^{-\alpha(t)n}$$

In Figure 2, $\beta(t)$ is shown as a function of time for various H. Once the vortex core is established, β is almost constant. In Figure 3, α is shown as a function of time for various H, and in each case α decays to zero asymptotically. For $\alpha > 0$, The Fourier series converges and so we may speculate that the motion of a finite layer is well-defined for all time, a result that is stronger than present theory [22].

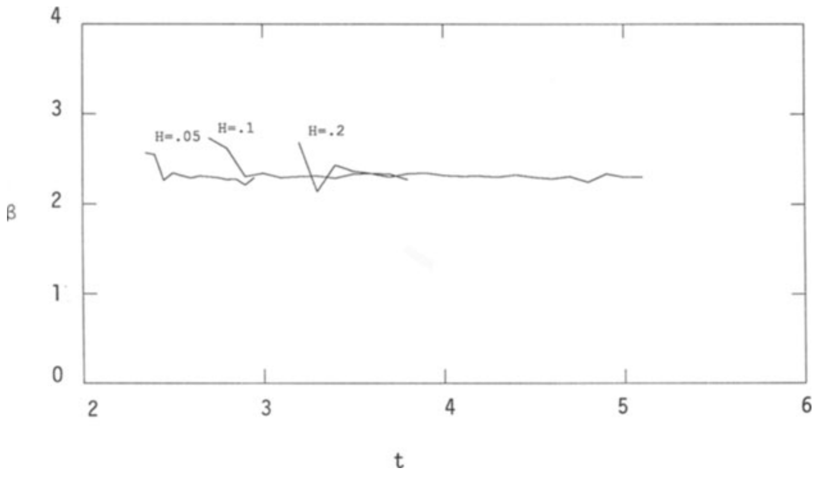

Figure 2. β as a function of time for various mean thicknesses H.

The area of the vortex core varies as H^p with $p \approx 1.6$ for small H. The aspect ratio of the core appears to be independent of H and so its thickness, T, scales as H^q with $q \approx 0.8$. Since the vortex sheet strength is approximately $2UT/H$, it becomes infinite as H vanishes. If this result is true (clearly one can never be absolutely sure that the thickness is small enough in these numerical studies to have obtained the correct asymptotic behavior), there can only be two possibilities. There is a non-classical interpretation to the vortex sheet that allows a motion in which its strength is infinite at a point for a period of time or the motion of the vortex sheet is not defined beyond the singularity time.

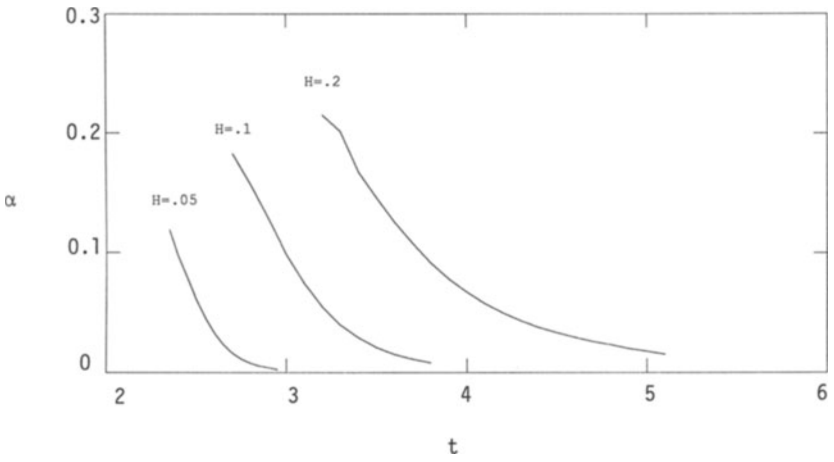

Figure 3. α as a function of time for various thicknesses H.

In conclusion, fundamental questions remain about interfacial flow of two immiscible fluids of comparable densities. Viscosity and surface tension can be expected to play important, but different roles when the curvature at some part of the interface approaches a singularity in time.

4. Two-Frequency Studies

The difficulties that are experienced numerically in the calculation of the evolution of a Rayleigh-Taylor unstable interface between immiscible fluids disappear when the density of the lower fluid is negligible, for then there is no Kelvin-Helmholtz instability present. Numerical results show convergence as the resolution of the interface and its motion is improved [1,5]. While one may speculate that the motion is well-posed, it is best to check the variartion in behavior for a variety of initial conditions. In particular, the flow will be assumed to be 2π-periodic, the wavelength of a Fourier mode setting the spatial scale. In addition, a higher mode will be superimposed initially to test the sensitivity of the motion to initial conditions. Of course, one would prefer to select random initial conditions, but the complexity of the subsequent

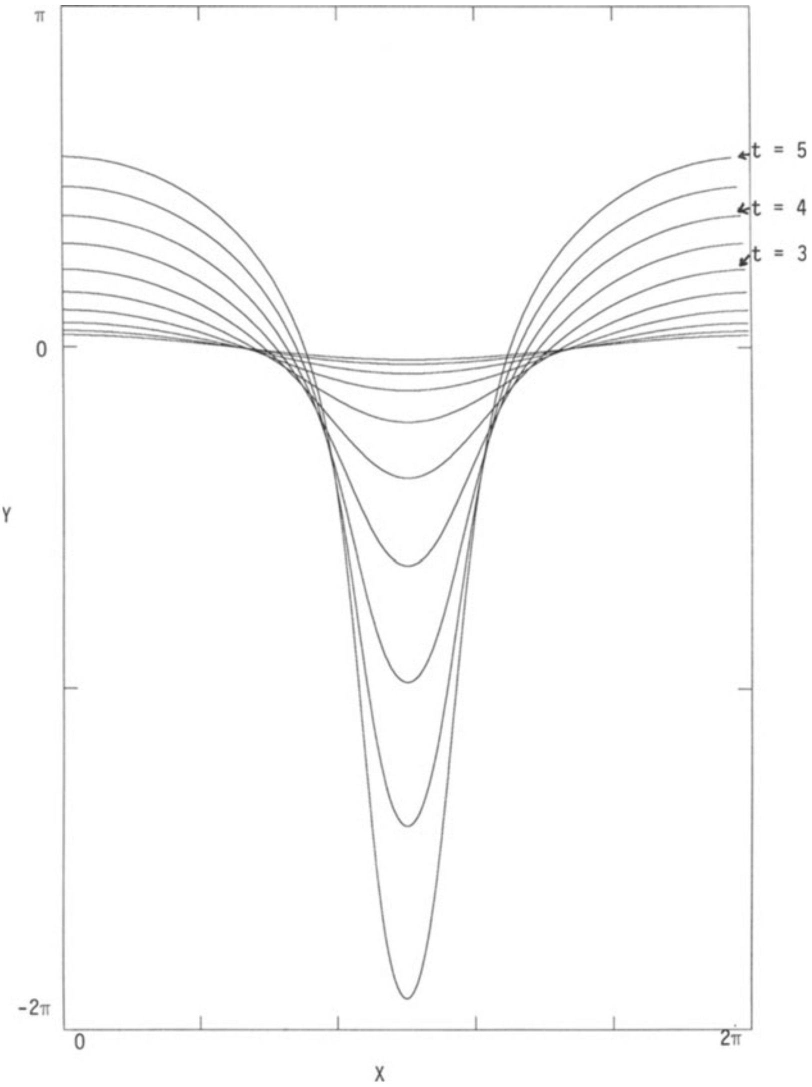

Figure 4. Location of the interface in time steps of 0.5, for $a = 0.1$ and $a_m = 0$

motion is beyond present numerical methods (actually, beyond present day computers). The hope is that a study of the interaction between two modes will shed light on the more general case.

Consider first the Rayleigh-Taylor instability. The flow is initially at rest. The interface is perturbed as

$$z(\sigma) = \sigma + ia\, cos(\sigma) + ia_m\, cos(m\sigma).$$

Linear stability analysis gives the result,

$$z(\sigma) = \sigma + ia\, cosh(t) cos(\sigma) + ia_m\, cosh(\sqrt{m}\, t) cos(m\sigma),$$

where the constant of gravity has been set to 1 (thus defining the time scale). The higher mode grows faster, illustrating the linear ill-posedness of the motion. To study the nonlinear stability of the main mode, the amplitude, a_m of the higher mode must be chosen small enough so that it is still small when the main mode has reached its nonlinear regime. In Figure 4, the location of the interface for the single mode (i. e. $a_m = 0$) with a= 0.1 is shown in increments of 0.5 in time. Nonlinear effects can be seen to be important when t $\approx$ 3.0. Thus one may estimate the critical amplitude a_{mc} for which the higher and main modes reach nonlinearity more or less together, as

$$a_{mc} = \frac{1}{m\, cosh(3\sqrt{m}\,)}$$

In figure 5, the interfacial location is shown in increments of 0.5 in time for the two modes with a = 0.1 and various a_3. In Figure 5a, $a_3 = 0.02$, which is bigger than $a_{3c} \approx 0.004$, and the higher mode dominates the evolution of the interface. In Figure 5b, $a_3 = 0.004$, which is comparable to a_{3c}, and the presence of the modes appear more or less equal when the calculations stopped for lack of spatial resolution. Finally, in Figure 5c, $a_3 = 0.0008$, less than a_{3c}, and the higher mode fails to make any appreciable appearance. Incidentally, 128 points were used in the spatial discretization and the time step was 0.002 in the method that is described in detail elsewhere [23]. The behavior of the interface evolution for m= 3 is consistent with linear analysis with one important exception. In any numerical calculation, truncation and roundoff errors will introduce many modes. Even if their amplitudes are small, the higher modes will have amplitudes that exceed a_{mc} and they should have grown quickly enough to influence the numerical calculations. Despite changes in the spatial resolution, no evidence surfaced that high modes, introduced numerically, were destablising. Perhaps, for large m, a_{mc} asymptotes to a small, but constant value rather than the expression given above. Further calculations with m= 5 continue to support the predicted trend in a_{mc} but many more calculations are needed before there can be any certainty about the behavior of a_{mc} for large m. Unfortunately, the computations are expensive and will take time to complete.

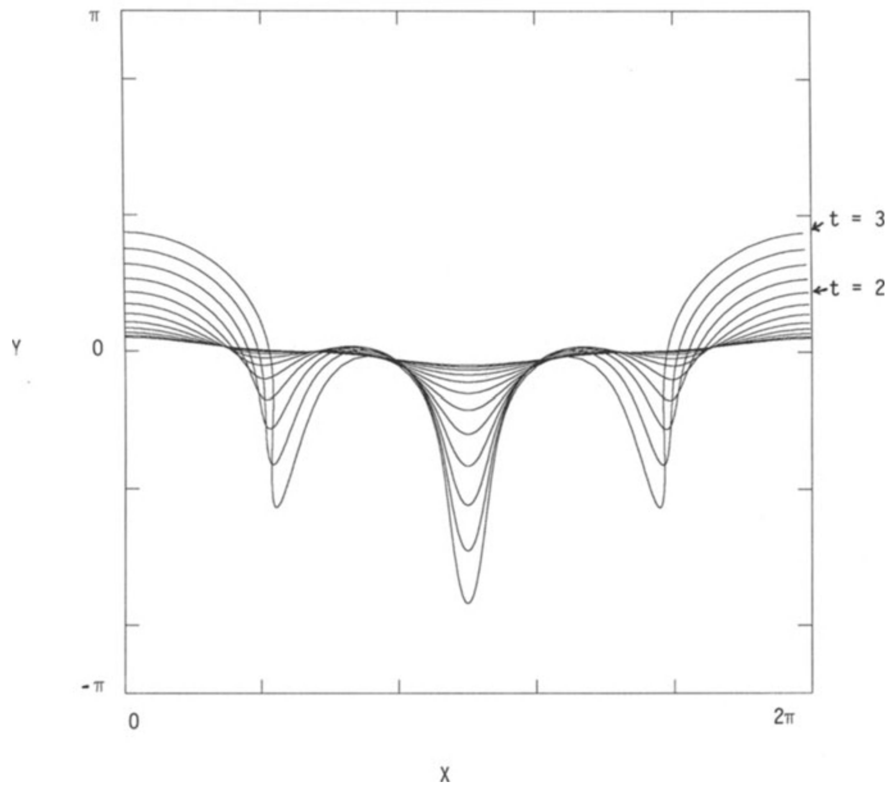

Figure 5a. Location of the interface in time steps of 0.25, for a = 0.1 and a_3 = 0.02.

The same approach can be applied to the Richtmyer-Meshkov instability. For this study, the constant of gravity, g= 0, but the fluid is given an impulsive start. As before, the length scale is determined by setting the wavelength of the main mode to be 2π. The initial velocity potential is chosen to be

$$\phi = -\frac{1}{2} e^{-y} \cos(x),$$

and the interface is flat, $z(\sigma) = \sigma$. Consequently, the dipole sheet strength is initially $\mu = \cos(\sigma)$. In

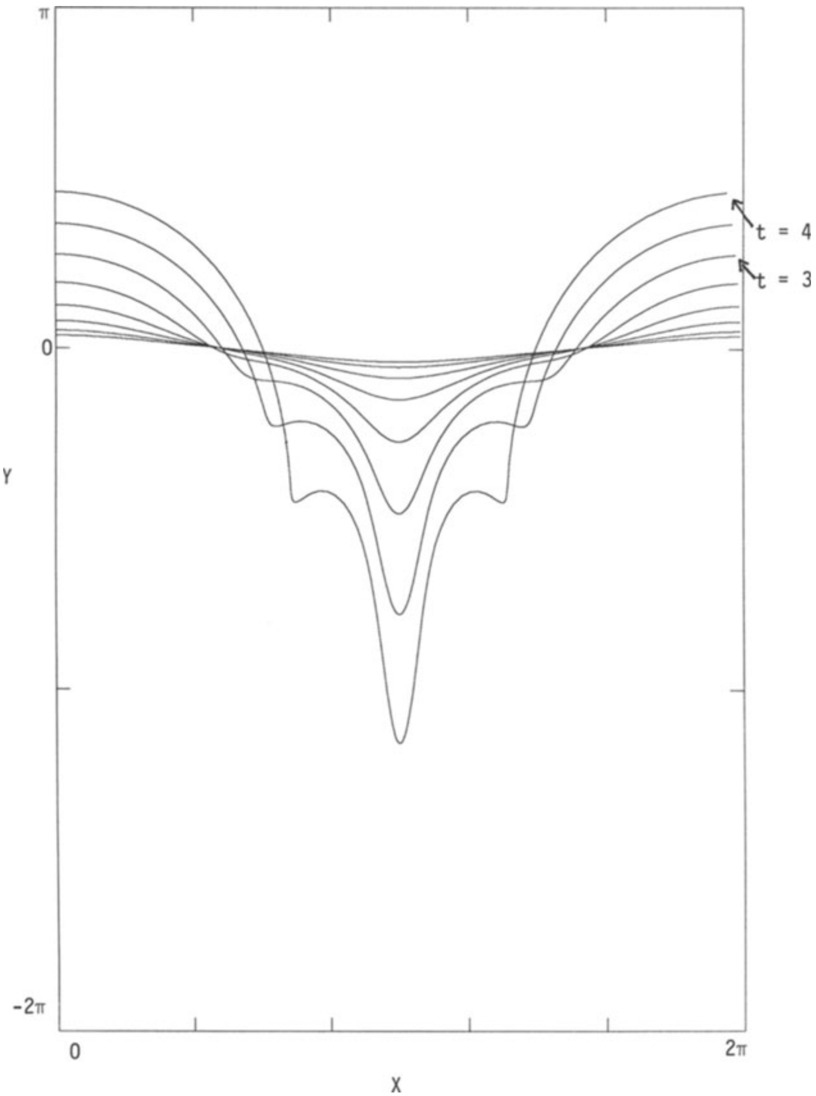

Figure 5b. Location of the interface in time steps of 0.5, for $a = 0.1$ and $a_3 = 0.004$.