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Note

A Computational Method for Determining Curvatures

1. INTRODUCTION

Interface curvature has a significant influence on the behavior of many physical problems, such as flame propagation [1], free surface flows [2, 3], and crystal growth [4, 5]. In numerical studies involving interfaces, it is common to use partial volume in the cells to indicate the location of the interface. Subsequent calculation of the curvature of the interface based on these partial volumes, however, is not a trivial task. Intuitively we can simply add up the partial volumes in the cells to represent the so-called liquid height and utilize a central finite difference scheme to find the first and second derivatives of the interfaces. This approach can result in substantial errors when there are large variations in the interface curvature.

More accurate methods of finding the curvature from a given partial-volume field are proposed in Nichols *et al.* [6], Smith [7], and Chorin [8]. In Nichols *et al.* [6], a line segment is fitted into each interfacial cell and, therefore, the first derivative is found readily. The second derivative is then calculated by the change in the first derivatives. Smith [7], has also used the line-segment approach to find the first derivatives. For the second derivatives, however, midpoints of the neighboring line segments are selected and a circle is made to pass through these points. The above two methods lead to difficulties because the second derivatives are found after the line segments are calculated. For an interface which is not well behaved the two methods could lead to large errors. Another more comprehensive approach is proposed by Chorin [8]. An osculating-circle is to be found, which will give the correct partial-volume field in the neighborhood of the cell under consideration. This method was tested on circles and on one sine wave and it was shown to be satisfactory for circles but not as good for the sine wave. In this paper, we present a new method, utilizing a second-order polynomial curve fitting, which is capable of giving an averaged curvature within an interfacial cell in a 2-dimensional space. This method is tested on several circles with different radii and sine waves with different frequencies.

2. SOLUTION ALGORITHM

Consider a 5×5 square cell unit as shown in Fig. 1 and an arbitrary curve which passes through it. Let us assume that this curve is the interface between the black region, below the curve, and the white region, above the curve. We introduce an

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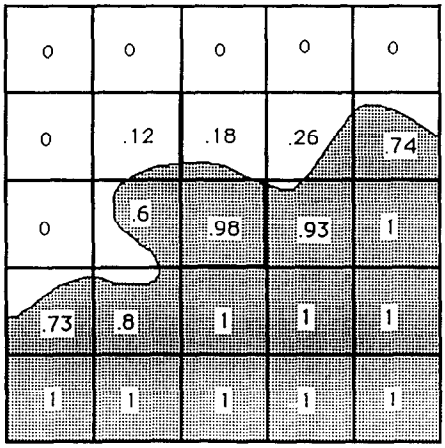

FIG. 1. Interface between two regions, with representative area fractions.

area fraction, f_{ij}, for each cell, c_{ij}, where i increases from left to right and j increases from bottom to top. Then, f_{ij} lies between zero (for an all white cell) and one (for an all black cell). Our objective is to solve the following inverse problem; that is, given the area fractions in a 5×5 cell unit, what is the equation for the curve that cuts through the middle 3×3 cell unit? The curvature can then be calculated for the center cell knowing the equation that best describes the interface curve. The basic assumptions of the method are: (1) In a 3×3 cell unit there can at most be one connected interface; (2) the grid spacing is small enough to resolve the interface to such an extent that a second-order polynomial can be a good approximation of the interface.

In order to find the interface curve, first a standard base for the 5×5 cell unit is chosen. This is achieved by adding the partial areas in the three cells at each side of the middle 3×3 cell unit and determining the side with the largest value. Then, this cell unit, with c_{33} at the center, is re-oriented with the largest value side at the bottom. By examining the area fractions, f_{ij}, in cells c_{25}, c_{45}, c_{52}, and c_{12} the appearance of the interface can then be categorized as comprised of 13 different cases as shown in Fig. 2. For example, if the area fractions f_{45}, f_{52}, and f_{12} are non-zero, f_{25} is zero, and $f_{42}+f_{43}+f_{44}<3.0$, the interface will resemble the curve given in case 9.

Denote the sum of f_{22}, f_{23}, and f_{24} by f_a, the sum of f_{32}, f_{33}, and f_{34} by f_b, and the sum of f_{42}, f_{43}, and f_{44} by f_c. In the 3×3 cell unit, the interface is to be represented by $z = ax^2 + bx + c$. The area under this curve is then $A = a(x_2^3 - x_1^3)/3 + b(x_2^2 - x_1^2)/2 + c(x_2 - x_1)$, where x_1 and x_2 are the boundaries of the curve. By solving a set of simultaneous equations, which will be discussed later, the coefficients of the second-order polynomial can be found. Hence, the first derivative, $z_x = 3a + b$, and the second derivative, $z_{xx} = 2a$, can be obtained immediately. Note that the derivatives are evaluated at the center of the center cell,

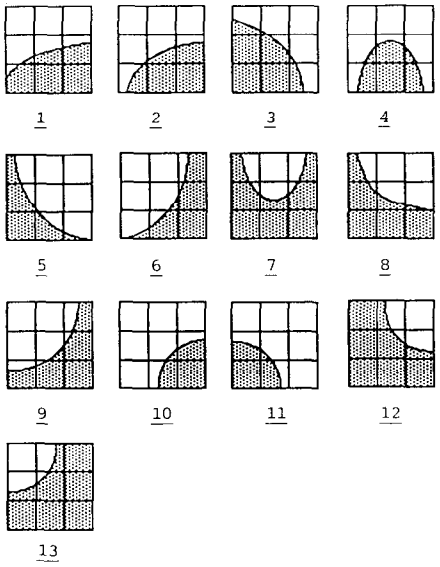

FIG. 2. Possible cases for the interface curve.

c_{33}, where $x = 3h/2$ and they are normalized with the grid spacing, h. Finally, the curvature of the curve in the center cell is computed from

$$\frac{1}{R} = \frac{-z_{xx}}{(1+z_x^2)^{1.5}}. \tag{1}$$

For case one, the three equations, after being normalized by the grid spacing, h, for solving a, b, and c are

$$f_a = \frac{a}{3} + \frac{b}{2} + c$$

$$f_b = \frac{7}{3}a + \frac{3}{2}b + c$$

$$f_c = \frac{19}{3}a + \frac{5}{2}b + c.$$

Upon solving for a and b we get: $a = (f_a - 2f_b + f_c)/2$ and $b = 3f_b - f_c - 2f_a$, which when substituted into Eq. (1) yields the basic liquid-height approximation. For case two, there are four equations needed, namely,

$$f_a = \frac{a}{3}(1-x_1^3) + \frac{b}{2}(1-x_1^2) + c(1-x_1)$$

$$f_b = \frac{7}{3}a + \frac{3}{2}b + c$$

$$f_c = \frac{19}{3}a + \frac{5}{2}b + c$$

$$0 = ax_1^2 + bx_1 + c,$$

where x_1 is the interception point of the curve with the x-axis. The equations are arranged to give a fourth-order equation of x_1,

$$\tilde{c}_1 x_1^4 + \tilde{c}_2 x_1^3 + \tilde{c}_3 x_1^2 + \tilde{c}_4 x_1 + 1 = 0$$

where $\tilde{c}_1, \tilde{c}_2, \tilde{c}_3$, and $\tilde{c}_4$ are functions of f_a, f_b, and f_c. Upon solving for an x_1 between zero and one, the coefficients can be expressed as

$$a = ((f_a - f_b)\, x_1 + \tfrac{1}{2}(3f_a - f_b))/(2x_1 - x_1^2 - \tfrac{2}{3})$$
$$b = (f_b - f_a) - 2a.$$

For case 4, the necessary five equations are

$$f_a = \frac{a}{3}(1-x_1^3) + \frac{b}{2}(1-c_1^2) + (1-x_1)\, c$$

$$f_b = \frac{7}{3}a + \frac{3}{2}b + c$$

$$f_c = \frac{a}{3}(x_2^3 - 8) + \frac{b}{2}(x_2^2 - 4) + (x_2 - 2)\, c$$

$$0 = ax_1^2 + bx_1 + c$$
$$0 = ax_2^2 + bx_2 + c,$$

where x_1 and x_2 are the interception points of the curve with the x-axis. The five equations are again arranged to give the solutions of x_1 and x_2 first, then a and b are given by:

$$a = f_b/(x_1 x_2 + \tfrac{7}{3} - \tfrac{3}{2}(x_1 + x_2))$$
$$b = -a(x_1 + x_2).$$

All the other cases can be easily converted into case one, two, and four and solved in the same way, respectively.

3. Numerical Examples for Circles and Sine Waves

A program is written to implement the above method. The sequence of events in the program are as follows: (1) Given the fractional area field; (2) pick up a surface cell in the domain; (3) determine the heaviest side of a 3×3 cell unit with the cell under consideration in the center; (4) pick up the parametric cells c_{25}, c_{45}, c_{52}, and c_{12}, and determine the case to be computed; (5) establish the set of simultaneous equations; (6) solve for the coefficients and then the curvatures.

The program was tested on sine waves of different magnitudes and frequencies and circles with different radii. The results are shown in Figs. 3 to 6. Figure 3 presents a typical situation in the test of a sine wave. The sine wave, $z = 0.5 \sin(2\pi x)$, is seen to cut through the computational grid. In one vertical column of cells, the curve can run through many cells, which are to be called "interface cells" in the following text. The curvature in an interface cell is calculated by the use of the present curve fitting scheme if at least one of its neighboring cells is com-

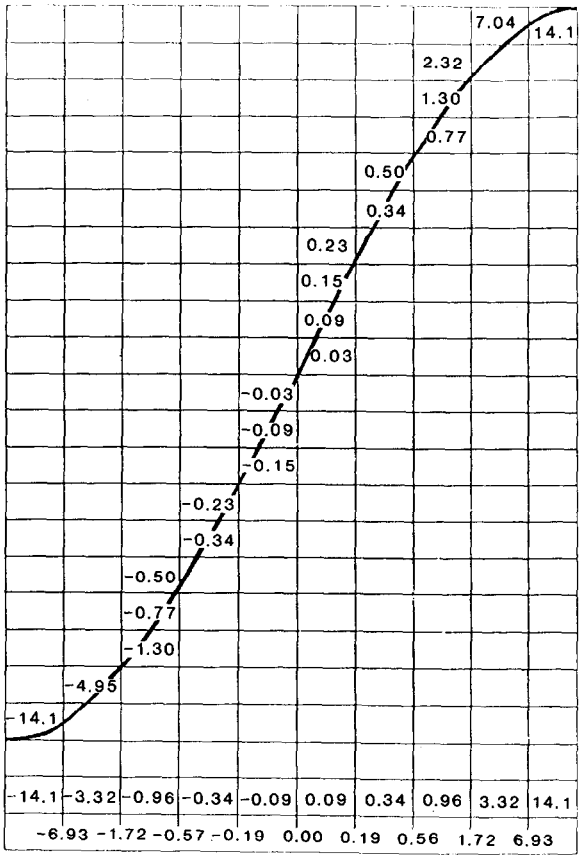

FIG. 3. Typical curvature calculation method for an interface using a sine wave represented by $z = 0.5 \sin(2\pi x)$.

pletely white; otherwise, its curvature is taken to be the average of those of the neighboring interface cells. In Fig. 3 only the calculated curvatures along the sine wave are shown. At the bottom of this figure theoretical values of the curvature, which is a function of x, are shown both in the center of a vertical column of cells and at the lattices. In order to compare the computed values with the theoretical values, an approximation must be made to assign an x value to an interface cell. If there is only one interface cell in a vertical column, then the x value is assigned at the center. If there is more than one interface cell, the interface within each of these cells is assumed vertical. Each vertical interface will then specify a particular x value. By the use of this approximation, the computed set of data are plotted on the curve of the theoretical curvature, and are shown in Figs. 4 and 5.

In Fig. 4, the computed curvature along the sine wave, $z = 0.3 \sin(2\pi x)$, is shown. In this figure the theoretical values of the curvature are shown as the solid line. The data sets of open circles and plus signs are essentially the same except that the grid system for the set of plus signs is shifted by half spacing to the right. The purpose of doing this is to show the adaptability of the present method as well as to demonstrate the difficulty of obtaining the original curvature. As can be inferred from the two figures, if the curves were not known theoretically these two figures would lead to two different curvature readings for the interface. This is, however, an inherent problem of the partial volume approach. When the field is represented by partial volumes, the information of the true location or the equation of the interface is given up; therefore, all subsequent computations will suffer from this lack of information.

In Fig. 5, two sine waves are tested. One is $z = 0.5 \sin(\pi x)$; the other is $z = 0.5 \sin(2\pi x)$. The results are generally satisfactory, with the understanding that the calculated curvature is the averaged curvature in the cell. Also due to the finite size

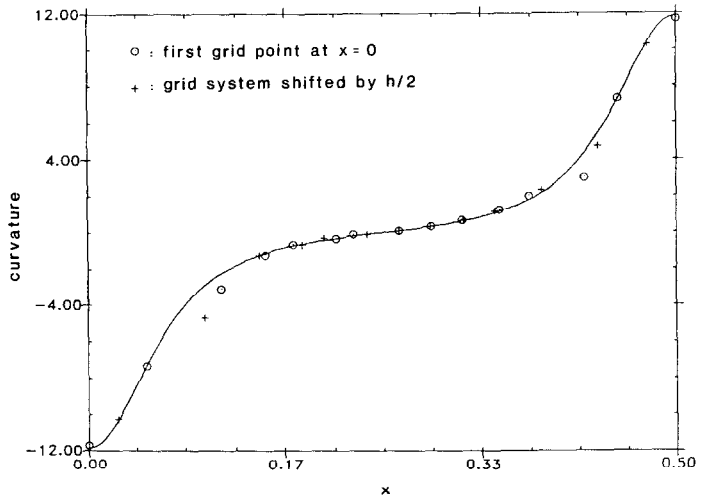

FIG. 4. Effect of grid shift on the calculated curvatures of a sine wave represented by $z = 0.3 \sin(2\pi x)$.

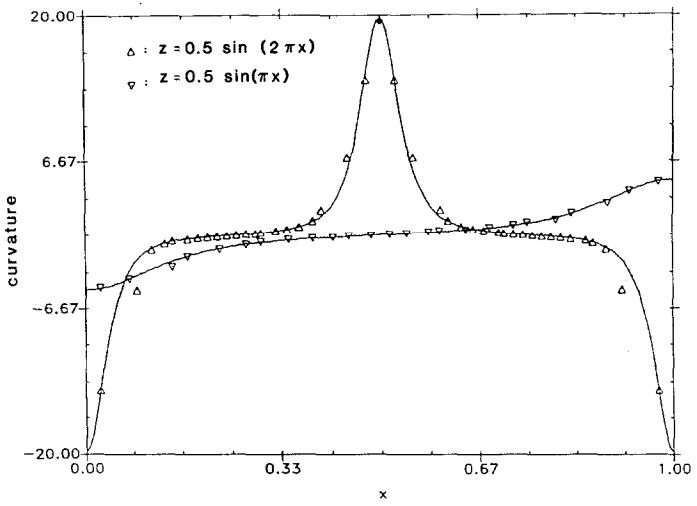

FIG. 5. Testing the accuracy of the curvature computation using sine waves with different frequencies.

of the cell, there is no way to pinpoint what the x value should be. On the curve of $z = 0.5 \sin(2\pi x)$ there is one data point which is seen to be significantly lower than the theoretical value. There are two reasons for this to happen: one is that the interface at this location is oriented at a relatively large angle with respect to one of the grid lattices; the other is, due to the grid location, the center cell of the 5×5 cell unit under consideration has a very small area fraction compared to the neighboring cells. Note that it is not possible to reduce the effect of these two factors by reducing the cell size.

Another observation from Fig. 5 is that, at the midpoint of the curve, where the maximal curvature reaches 20.0, the computed data are unable to predict this value. One reason for this is that the maximum point is located on the lattice so that it cannot be computed. The grid location can be altered to make the maximum point at the center of the cell, then it can be predicted fairly well. In fact, the grid shift is tried and a value of 19.5 is obtained (in Fig. 5 this point is shown by a diamond sign). Here again we see the dependence of the calculated curvature on the grid location. If the grid location is not to be altered, then another way to approach this maximal value is to reduce the grid size.

In Fig. 6 several circles of different sizes are tested. Due to the symmetry only the results in the first quadrant are shown. In all cases, the grid size, h, is uniform and equal to 0.025. From cases (1) to (4) the radius of the circles are decreased from 0.5 to 0.2. The true curvatures are presented at the last column of the table in Fig. 6. One general feature is that the maximum error always occurs around $\pi/4$ of the polar angle, which is due to the orientation of the interface relative to the grid system. The other feature is that the maximum error does not seem to increase monotonically with the curvature. This is again due to the location of the center cell

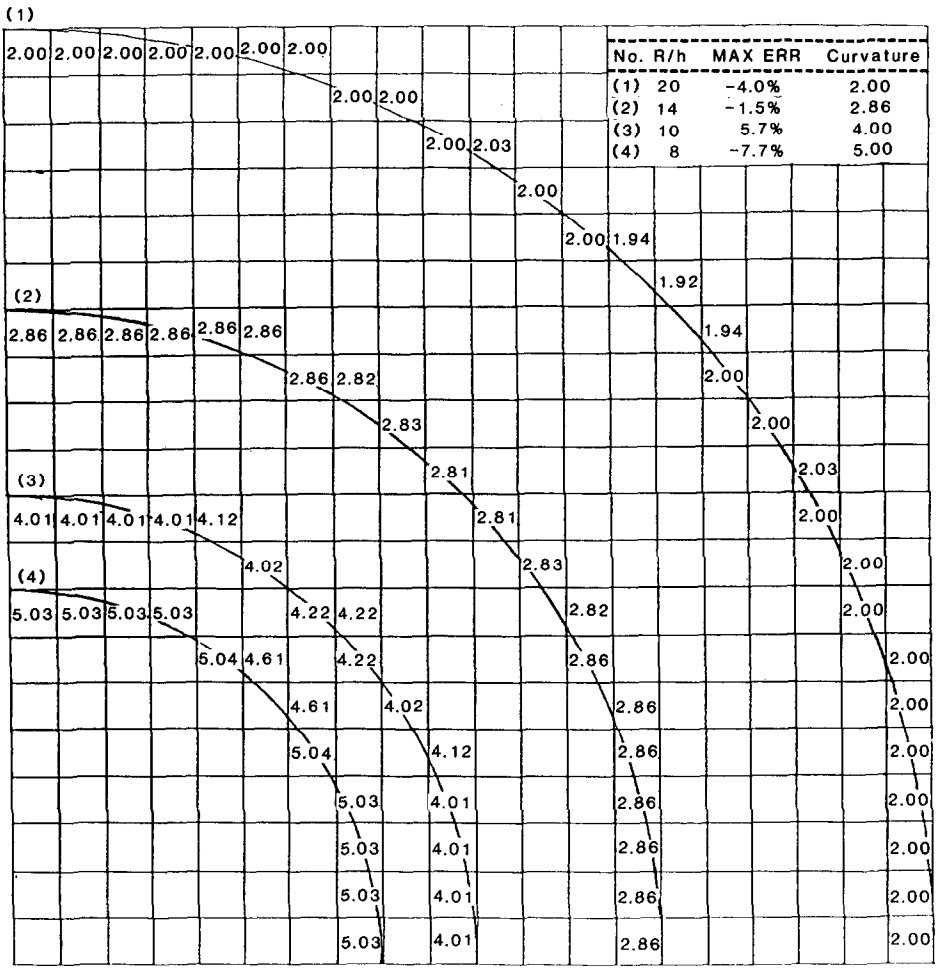

FIG. 6. Computed curvatures for circles with radius-grid spacing ratio, R/h, from 8 to 20.

under consideration. As it was mentioned earlier, large errors are obtained when the grid system is located in such a way that the center cell contains very little area fraction. The general trend is, however, that greater curvature induces greater errors.

4. CONCLUSION

A new method is developed for computing the interfacial curvature and is tested on various size circles and different sine waves. This method is simple and fast because a large portion of it is the simple liquid-height method, which is the first-order approximation of the shape of the interface. The general conclusions are that

greater curvatures induce greater errors and that the computed curvatures depend on the grid locations if there is a radius of curvature smaller than the grid spacing.

It must be pointed out that a partial volume field, if viewed locally, can be fitted into numerous interfacial equations, which would give different curvatures in the desired cell. No one method should be considered more "exact" than the other methods. A suitable method is the one which is easy to use and proved correct for known curves. The method reported in this article serves this purpose well and is proven to be capable of computing a workable curvature field for numerical studies of interfacial problems.

APPENDIX: NOMENCLATURE

c: a cell, the subscript indicate the location
f: the area fraction, defined as the black area divided by the cell area
h: the grid spacing
a, b, c: the coefficients of the second-order polynomial
z: the vertical position
x: the horizontal coordinate on the 3×3 cell unit
x_1, x_2: the interception points of the curve with the grid lattice.

REFERENCES

1. G. H. MARKSTEIN, *Non-steady flame propagation* (Pergamon Press, New York, 1964).
2. P. G. DRAZIN AND W. H. REID, *Hydrodynamic Stability* (Cambridge Univ. Press, London, 1981).
3. J. J. STOKER, *Water Waves* (Interscience, New York, 1957).
4. J. S. LANGER, *Rev. Mod. Phys.* **52**, 1 (1980).
5. B. R. PAMPLIN, *Crystal Growth* (Pergamon, New York, 1975).
6. B. D. NICHOLS, C. W. HIRT, AND R. S. HOTCHKISS, *Report LA-8355*, Los Alamos Scientific Lab., 1980 (unpublished).
7. J. SMITH, *J. Comput. Phys.* **39**, 112 (1981).
8. A. J. CHORIN, *J. Comput. Phys.* **57**, 472 (1985).

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J. Y. POO AND N. ASHGRIZ

Department of Mechanical and Aerospace Engineering
State University of New York at Buffalo
Buffalo, New York 14260