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NOTE

Analytical Relations Connecting Linear Interfaces and Volume Fractions in Rectangular Grids

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The computational-geometric problems arising when a linear interface cuts a cube are considered. They are of interest in particular for the calculation of volume fractions or interface positions in three-dimensional interface calculations in the Volume of Fluid (VOF) methods. Typically, the normal vector is known. One then wants to compute the volume fraction knowing the interface position, or conversely the interface position knowing the volume fraction. Explicit expressions of general use are given, and the algorithms used to search for solutions are described in detail. Explicit formulas for cubic roots are found to be less than two thirds as time consuming as Newton–Raphson iterations.

Key Words: interfaces; VOF methods.

1. INTRODUCTION

The reconstruction of a boundary between two materials in a numerical computation is of interest in many different domains, ranging from scientific topics such as combustion, two-phase flows, and computer graphics to applications such as ink-jet printers, nozzles, and other technologies. Among the approaches which have been proposed and have undergone continual improvement we can mention markers [1], level sets [2], and volume tracking [3–5].

In this note we focus on one of the basic steps in these algorithms: the computation of the intersection of a planar interface with a right hexahedron or a cube, as a function of the volume below the interface. More precisely, the available data in the computation comprise the volume fraction V_f in each cell of the grid: cells cut by an interface have V_f

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between zero and one; those without an interface have V_{f} equal to zero or one. We initially approached this problem from the point of view of volumetric tracking methods and specifically a piecewise linear interface calculation (PLIC), although the results are useful in a more general context. In PLIC methods, the boundary between materials is approximated in each computational cell with a linear interface defined by the equation $\mathbf{m} \cdot \mathbf{x} = \alpha$, where $\mathbf{m}$ is given. (Indeed the problem of finding the normal vector $\mathbf{m}$ is complex and nonlocal and is discussed independently in the references.) We distinguish the "forward" problem, that is, to find the volume fraction V_{f} occupied by one species given α, from the "inverse" problem, which consists of finding α given the volume fraction. The relation between V_{f} and α is continuous and one-to-one but in PLIC the overall reconstruction is not in general continuous at the cell boundary. Both the inverse and forward problems can occur several times, according to the chosen numerical schemes, during the reconstruction and propagation of the interface.

As stated, the problem is essentially geometric in nature. Several implementations use extensively embedded *if-else if-endif* constructs. In some cases, the large number of levels in these contructs and the number of cases make the code difficult to compile optimally and to maintain. In this note, a careful investigation of the geometry and of the analytical expression connecting V_{f} and α produces a significant reduction in the number of possible cases and a corresponding streamlining of the numerical algorithm, increasing in this way the efficiency and clarity of the resulting code.

2. THE STANDARD PROBLEM

In three-dimensional (3D) space with Cartesian coordinates (x_1, x_2, x_3) we consider a rectangular parallelepiped of sides Δx_1, Δx_2, Δx_3 and a plane with normal vector $\mathbf{m} = (m_1, m_2, m_3)$ given by the equation

$$m_1 x_1 + m_2 x_2 + m_3 x_3 = \alpha, \tag{1}$$

where the plane constant α is a parameter related to the smallest distance from the origin. In the standard forward problem we assume that the three coefficients m_i are all positive and we need to determine the "cut volume" *ABGHKNML* of the rectangular cell which is also below the given plane, as shown in Fig. 1. Then the function $f(x_1, x_2, x_3) = m_1 x_1 + m_2 x_2 + m_3 x_3 - \alpha$ is negative at point A and positive at point F, while the vector $\mathbf{m}$ is pointing toward the region where f is positive. If we interchange the two species the normal vector reverses its orientation, the coefficients m_i are now negative, and the volume of interest becomes *DCFEKNML*. In Ref. [6] we have shown that the volume *ABGHKNML* is given by the expression

$$V = \frac{1}{6\, m_1 m_2 m_3} \left[\alpha^3 - \sum_{i=1}^{3} F_3(\alpha - m_i \Delta x_i) + \sum_{i=1}^{3} F_3(\alpha - \alpha_{\max} + m_i \Delta x_i) \right], \tag{2}$$

with $\alpha_{\max} = \sum_{i=1}^{3} m_i \Delta x_i$ and the function $F_n(y)$ defined as

$$F_n(y) = \begin{cases} y^n & \text{for } y > 0 \\ 0 & \text{for } y <= 0. \end{cases}$$

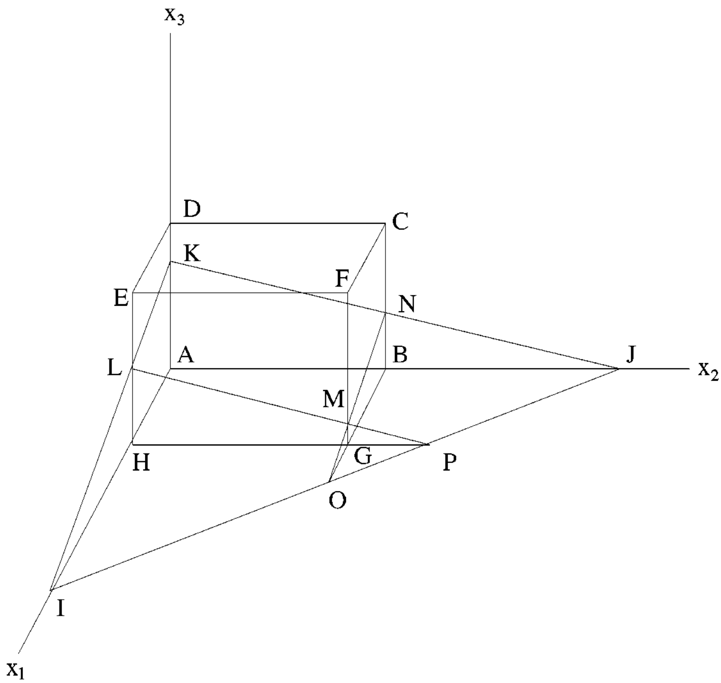

FIG. 1. The "cut volume" is the region inside the parallelepiped *ABCEFGH* and below the plane *IJK*.

We recall that the first term ($\alpha^3/6m_1m_2m_3$) is the volume of the tetrahedron *AIJK*, the first sum removes tetrahedra such as *HIPL*, when the vertices I, J, and K move beyond the cell faces, and the second sum adds back the volumes of the smaller tetrahedra such as *GOPM*, when the lines *IJ*, *JK*, and *KI* are completely outside the cell boundary. The functions $F_3(y)$ make sure that these terms are algebraically added only when the above-mentioned conditions are satisfied. The function V varies from zero, when $\alpha = 0$, to the volume of the parallelepiped $V_0 = \Delta x_1 \Delta x_2 \Delta x_3$, when $\alpha = \alpha_{\max}$. The volume fraction V_{f} is defined as $V_{\mathrm{f}} = V/V_0$ and varies correspondingly from zero to one. In two dimensions (2D), expression (2) simplifies to

$$V = \frac{1}{2m_1m_2}\left[\alpha^2 - \sum_{i=1}^{2} F_2(\alpha - m_i\Delta x_i)\right], \tag{3}$$

where, as shown in Fig. 2, the contributions to V represent respectively the areas of the three triangles *AEH*, *BFE*, and *DGH*, which are geometrically similar. Again, the function $F_2(y)$ makes sure that the last two triangles are considered only when the vertices E and H move outside the cell. For the moment, we restrict our analysis to a unitary cube, $\Delta x_i = 1$; then the volume V and the volume fraction V_{f} coincide. We also normalize the plane equation (1) by dividing it by ($\sum_{i=1}^{3} m_i$); then $\alpha_{\max} = \sum_{i=1}^{3} m_i = 1$. The normalization of the two-dimensional problem is similar. Later, we will generalize this procedure to negative m_i and to a rectangular parallelepiped. We can now summarize some useful properties:

(1) V is a continuous, one-to-one, monotonically increasing function of α with continuous first derivative.

(2) Both V and α vary in the range [0, 1].

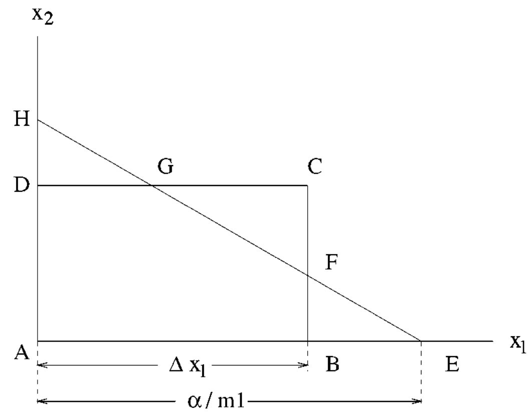

FIG. 2. The "cut volume" refers to the region within the rectangle *ABCD* which also lies below the straight line *EH*.

(3) The expression for V is invariant with respect to a permutation of the indices, so we need to consider only one case, say $m_1 \leq m_2 \leq m_3$ in 3D and $m_1 \leq m_2$ in 2D.

(4) The graph of V has odd symmetry with respect to the point $(V, \alpha) = (1/2, 1/2)$, so we restrict the analysis to the range $0 \leq \alpha \leq 1/2$.

(5) In 3D we let $m_{12} = m_1 + m_2$ and $m = \min(m_{12}, m_3)$; then V varies cubically in the region $0 \leq \alpha \leq m_1$, quadratically in $m_1 \leq \alpha \leq m_2$, again cubically in $m_2 \leq \alpha \leq m$, and finally in $m \leq \alpha \leq 1/2$ cubically if $m = m_3$ and otherwise linearly if $m = m_{12}$; in 2D with $m = m_1$, V varies quadratically in the region $0 \leq \alpha \leq m$ and linearly in $m \leq \alpha \leq 1/2$.

(6) In the interval $0 \leq \alpha \leq 1/2$ and for arbitrary m_i there is a lower bound for $V(\alpha)$. In 3D this line is realized for $m_1 = m_2 = m_3 = 1/3$, corresponding to a plane cutting each coordinate plane with a 45°-angle line. The volume V is a cubic function of α in the whole domain and it is given by the expressions $V = 9\alpha^3/2$ for $0 \leq \alpha \leq 1/3$ and $V = (-18\alpha^3 + 27\alpha^2 - 9\alpha + 1)/2$ for $1/3 \leq \alpha \leq 1/2$. In 2D the lower bound is realized for $m_1 = m_2 = 1/2$, corresponding to a 45°-angle line, and it is a quadratic function of α: $V = 2\alpha^2$.

(7) In the same region there is also an upper bound. In 3D this is the line with $m_1 = m_2 = 0$ and it represents a plane parallel to one of the three coordinates planes. The function $V(\alpha)$ is linear: $V = \alpha$. In 2D the same linear function is obtained with $m_1 = 0$, representing a line parallel to one of the two coordinate axes.

(8) In 3D, the limit $m_1 \to 0$ is smooth: the lines become those of the two-dimensional problem. In particular, the first cubic region collapses into the origin, the quadratic one extends itself to $0 \leq \alpha \leq m_2 = m$, the next cubic region collapses to the point of the line at $\alpha = m$, and finally the straight line, since now $m_3 = (1 - m) \geq m_{12} = m$, extends itself to the interval $m \leq \alpha \leq 1/2$. The further limit $m_2 \to 0$ is also smooth with the quadratic region collapsing into the origin.

The two limiting curves are shown in Figs. 3 and 4 for the 2D and 3D cases, respectively, together with two other intermediate lines. The full circles in the two figures denote the points where the function $V(\alpha)$ changes its behaviour.

A direct numerical implementation of formula (2) becomes unstable when $m_1 \to 0$ or both $m_1, m_2 \to 0$. In the 2D problem one must face only the first limit. This is because

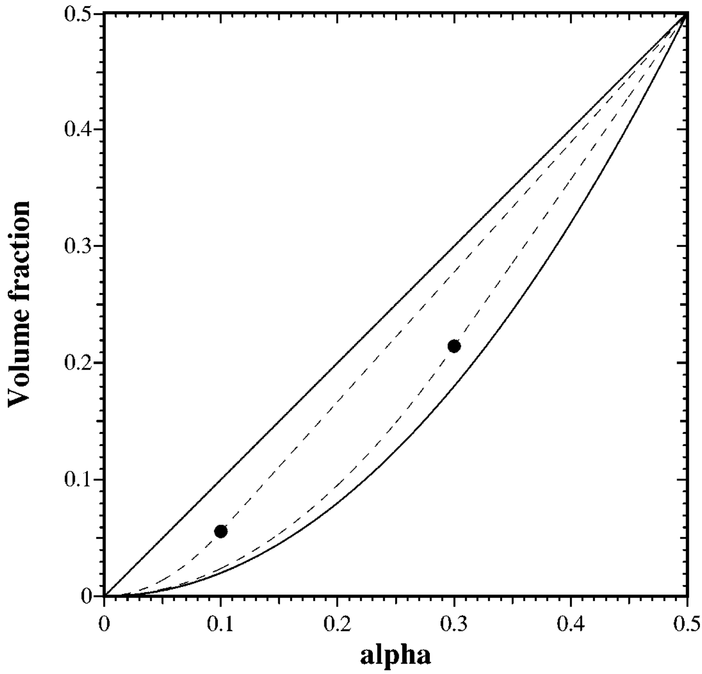

FIG. 3. The upper and lower limiting curves (solid lines) for the two-dimensional problem are shown together with two intermediate lines (dashed lines). The function $V(\alpha)$ changes from quadratic to linear behaviour at the points denoted by the full circles.

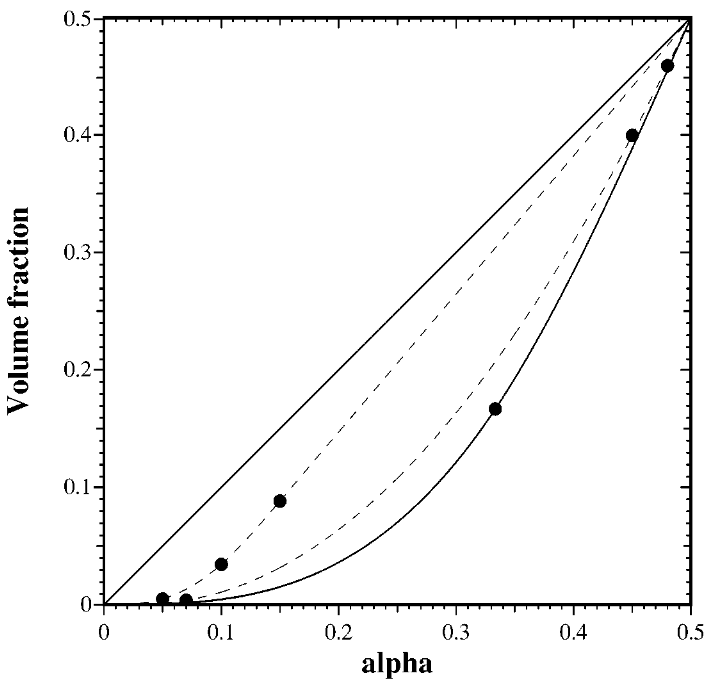

FIG. 4. The upper and lower limiting curves (solid lines) for the three-dimensional problem are shown together with two intermediate lines (dashed lines). For these two lines, the top one has $(m_1 + m_2) < m_3$; the reverse is true for the lower one. The full circles denote points where the function $V(\alpha)$ changes behaviour.

$V \to 1$ as $\alpha \to 1$ and when m_1 becomes very small the numerator of expression (2) must be $\mathcal{O}(m_1)$. However, this small number is obtained as an algebraic sum of $\mathcal{O}(1)$ numbers and this is the source of a numerical instability due to roundoff errors. The oscillations become wilder and wilder as $m_1 \to 0$. A simple, but efficient solution is to artificially set to zero m_1 (or both m_1 and m_2, if necessary), when it is smaller than a prescribed value, and to use the finite limit of formula (2). The error introduced in the direction of the normal vector is then very small. Elsewhere formula (2) can be used safely. However, from the point of view of a numerical implementation this is not much cheaper than expanding analytically equation (2) in each region and implementing a simple *if-else if-endif* construct. The analytical expressions for both the forward and inverse problems, restricted to the ranges $0 \le V \le 1/2$ and $0 \le \alpha \le 1/2$, can be derived with some straightforward algebra from relations (2) and (3).

Two-Dimensional Forward Problem

For the 2D forward problem we have

$$
\begin{aligned}
V &= \frac{\alpha^2}{2m(1-m)} && \text{for } 0 \le \alpha < m,\\
V &= \frac{\alpha}{(1-m)} - V_1 && \text{for } m \le \alpha \le 1/2.
\end{aligned}
$$

Two-Dimensional Inverse Problem

The 2D inverse problem is specified by

$$
\begin{aligned}
\alpha &= \sqrt{2m(1-m)V} && \text{for } 0 \le V < V_1,\\
\alpha &= V(1-m) + \frac{m}{2} && \text{for } V_1 \le V \le 1/2,
\end{aligned}
$$

with $V_1 = m/2(1-m)$. Notice that the limit $m = 0$ is correctly described by these expressions.

Three-Dimensional Forward Problem

In 3D the forward problem is

$$
\begin{aligned}
V &= \frac{\alpha^3}{6m_1m_2m_3} && \text{for } 0 \le \alpha < m_1,\\
V &= \frac{\alpha(\alpha - m_1)}{2m_2m_3} + V_1 && \text{for } m_1 \le \alpha < m_2,\\
V &= \frac{\alpha^2(3m_{12} - \alpha) + m_1^2(m_1 - 3\alpha) + m_2^2(m_2 - 3\alpha)}{6m_1m_2m_3} && \text{for } m_2 \le \alpha < m;
\end{aligned}
$$

for the fourth interval there are two possible cases, one for $m = m_3 < m_{12}$ and the other for $m = m_{12} < m_3$:

$$
\begin{aligned}
V &= \frac{\alpha^2(3 - 2\alpha) + m_1^2(m_1 - 3\alpha) + m_2^2(m_2 - 3\alpha) + m_3^2(m_3 - 3\alpha)}{6m_1m_2m_3} && \text{for } m_3 \le \alpha \le 1/2,\\
V &= \frac{2\alpha - m_{12}}{2m_3} && \text{for } m_{12} \le \alpha \le 1/2.
\end{aligned}
$$

Three-Dimensional Inverse Problem

The 3D inverse problem is given by

$$\begin{aligned} \alpha &= \sqrt[3]{6m_1m_2m_3V}, && \text{for } 0 \le V < V_1, \\ \alpha &= \frac{1}{2}\left(m_1 + \sqrt{m_1^2 + 8m_2m_3(V - V_1)}\right), && \text{for } V_1 \le V < V_2, \\ P(\alpha) &= a_3'\,\alpha^3 + a_2'\,\alpha^2 + a_1'\alpha + a_0' = 0, && \text{for } V_2 \le V < V_3; \end{aligned}$$

again there are two cases in the fourth interval, one for $V_3 = V_{31} < V_{32}$ and the other for $V_3 = V_{32} < V_{31}$:

$$\begin{aligned} P(\alpha) &= a_3''\,\alpha^3 + a_2''\,\alpha^2 + a_1''\,\alpha + a_0'' = 0, && \text{for } V_{31} \le V \le 1/2, \\ \alpha &= m_3V + \frac{m_{12}}{2}, && \text{for } V_{32} \le V \le 1/2\,. \end{aligned}$$

In the previous relations $V_1 = m_1^2/(\max(6m_2m_3, \epsilon))$, which is an approximation of the value $m_1^2/6m_2m_3$. This approximation is needed because the limit for V_1 as $m_1, m_2 \to 0$ is zero; however, numerically we must prevent the denominator of V_1 from becoming zero, so ϵ is an arbitrary small number. Aside from that, the above set of expressions for V and α is well behaved numerically for all possible m_i. The other limiting values of the range of validity of each relation are given by the following expressions: $V_2 = V_1 + (m_2 - m_1)/2m_3$, $V_3 = V_{31} = [m_3^2(3m_{12} - m_3) + m_1^2(m_1 - 3m_3) + m_2^2(m_2 - 3m_3)]/(6m_1m_2m_3)$ when $m = m_3$ or $V_3 = V_{32} = m_{12}/2m_3$ when $m = m_{12}$. For the coefficients of the two cubic polynomials we have $a_3' = -1$, $a_2' = 3m_{12}$, $a_1' = -3(m_1^2 + m_2^2)$, $a_0' = m_1^3 + m_2^3 - 6m_1m_2m_3V$, $a_3'' = -2$, $a_2'' = 3$, $a_1'' = -3(m_1^2 + m_2^2 + m_3^2)$, and $a_0'' = m_1^3 + m_2^3 + m_3^3 - 6m_1m_2m_3V$.

In the third and fourth region, where $V_{31} \le V \le 1/2$, we need to find the roots of the cubic polynomial $P(\alpha)$ that has the following properties:

(1) $P(\pm\infty) = \mp\infty$.

(2) For a given V in these two regions, there are three real roots of $P(\alpha)$ and the proper one is the middle one. For this root, $P(\alpha)$ is an increasing function of α, as shown in Fig. 5, consistent with properties (1) and (5) of formula (2).

An analytical solution can now be found easily [7, 8]. We first divide by a_3 the third-degree polynomial in α, so that $a_3 = 1$, and let

$$p_0 = \frac{a_1}{3} - \frac{a_2^2}{9}; \quad q_0 = \frac{a_1a_2 - 3a_0}{6} - \frac{a_2^3}{27};$$

then the discriminant $\Delta = p_0^3 + q_0^2$ is negative, which is the condition for having three real roots. Finally by letting [9] $\cos(3\,\theta) = q_0/\sqrt{-p_0^3}$, it follows that the root of interest is

$$\alpha = \sqrt{-p_0}\,(\sqrt{3}\sin\theta - \cos\theta) - \frac{a_2}{3}.$$

While all previous analytical relations for V and α involve at most the calculation of a square or a cubic root, here we need to evaluate a few square roots and trigonometric functions. It is then questionable if for this case a direct root-finding routine is computationally less expensive. We have implemented such a routine based on the Newton–Raphson (NR) method in conjunction with the secant method [10]. In the case where the NR iteration sends

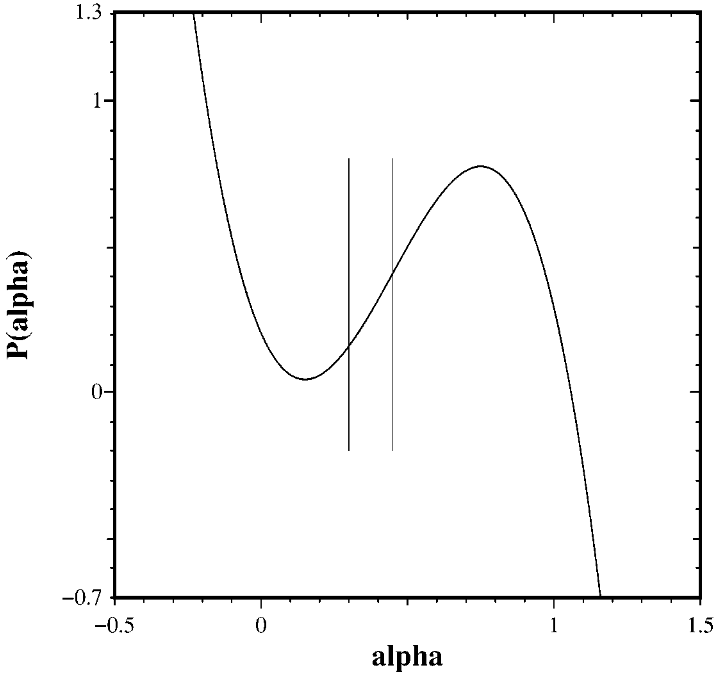

FIG. 5. Typical behaviour of the cubic polynomial $P(\alpha)$. The region of validity of the expression is that within the two vertical segments.

the point outside the α-interval, we make a linear interpolation instead of a simple bisection of the interval. This is motivated by the smooth behaviour of the function V (as seen in Figs. 4 and 5), and we have found that this consistently reduces the number of iterations when the NR forecast goes out of range. An optimal initial guess for α is calculated with a linear average from the α and V values that delimit the region where $V(\alpha)$ is cubic. We run the problem for several millions of different situations by randomly changing the coefficients m_i and the points inside the proper range in volume fraction. We need an average number of less than four iterations to achieve a convergence of $<10^{-16}$ (in double precision); nevertheless the direct use of the analytical expressions (in our case the gcc math library functions) is less than two-thirds as time consuming as the numerical approach.

3. THE GENERAL PROBLEM

We are now in the condition to generalize both the forward and inverse problems to rectangular grids and negative m_i. For the extension to rectangular grids we consider formula (2) for the volume V and divide it by the cell volume $V_0 = \Delta x_1 \Delta x_2 \Delta x_3$. We then obtain the following expression for the volume fraction $V_f = V/V_0$:

$$V_{\mathrm{f}} = \frac{1}{6\prod_{i=1}^{3} m_i \Delta x_i}\left[\alpha^3 - \sum_{i=1}^{3} F_3(\alpha - m_i\Delta x_i) + \sum_{i=1}^{3} F_3(\alpha - \alpha_{\max} + m_i \Delta x_i)\right]. \quad (4)$$

We observe that with the linear transformation $m_i' = m_i \Delta x_i$ formula (4) reduces to expression

(2) with $\Delta x_i = 1$, as long as the plane equation (1) is normalized with $\alpha_{\max} = 1$. All the results obtained in the previous section can then be easily extended to a rectangular cell. This observation applies to the two-dimensional case as well.

If one or more of the m_i are negative, the geometry can be brought to the standard case depicted in Figs. 1 and 2, with the linear transformation $x_i' = \Delta x_i - x_i$, which describes a simple mirror reflection with respect to the plane $x_i = \Delta x_i/2$. After the calculation of V_{f} or α with the given analytical expressions, the configuration is brought back to the actual position with similar reflections.

Finally, it is often necessary to calculate the volume V cut by the linear interface relative to a right parallelepiped that is different from the grid cell. This is the case if, for example, it is necessary to calculate the volume fraction in neighbouring cells in an iterative scheme which tries to optimize the value of the normal vector $\mathbf{m}$ [3, 5] or in the propagation of the interface, in particular with split schemes, where the volume V represents the fluid flux across the cell boundary. This problem can be easily solved by moving the origin of the local Cartesian coordinate system (in our case point A of Figs. 1 and 2) to one vertex of the parallelepiped. The translation is clearly described by the linear transformations $x_i' = x_i - x_{0i}$, where the vertex (x_{01}, x_{02}, x_{03}) is such that all sides $\Delta x_i'$ of the right tetrahedron are positive.

4. CONCLUSION

We have presented a unified and general approach to the problem of connecting the nonhomogeneous term α of a linear equation representing the interface to the volume fraction V_{f} of a cell of a rectangular grid divided in two parts by the interface. The forward relation $V_{\mathrm{f}}(\alpha)$ is at most a polynomial of degree 2 and 3, in two and three dimensions respectively. The behaviour of V_{f} changes a few times in the range of variation of α, and we have given expressions valid in each interval for all values of the coefficients of the linear equation. We have shown that the analytical solution for the inverse relation $\alpha(V_{\mathrm{f}})$ is computationally cheaper than a fast root-finding technique, even when the root is one of a third-order polynomial. Finally we have extended our approach to the more general situation of negative coefficients and rectangular grids. The solution we have proposed consists of a sequence of simple linear geometrical transformations, translations, and mirror reflections and of an *if-else if-endif* construct containing the analytical expressions we have derived, which can be easily implemented in a numerical routine.

REFERENCES

1. S. Popinet and S. Zaleski, A front tracking algorithm for the accurate representation of surface tension, *Int. J. Numer. Meth. Fluids*, 775–793 (1999).
2. J. A. Sethian, *Level Set Methods* (Cambridge Univ. Press, Cambridge, UK, 1996).
3. W. J. Rider and D. B. Kothe, Reconstructing volume tracking, *J. Comput. Phys.* **141**, 112–152 (1998).
4. R. Scardovelli and S. Zaleski, Direct numerical simulation of free-surface and interfacial flow. *Annu. Rev. Fluid Mech.* **31**, 567–603 (1999).
5. J. E. Pilliod, Jr., and E. G. Puckett, Second-order accurate volume-of-fluid algorithms for tracking material interfaces. Technical report, Lawrence Berkeley National Laboratory, 1997. No. LBNL-40744.
6. D. Gueyffier, A. Nadim, J. Li, R. Scardovelli, and S. Zaleski, Volume of fluid interface tracking with smoothed surface stress methods for three-dimensional flows, *J. Comput. Phys.* **152**, 423–456 (1999).

7. J. Li, Résolution numérique de l'équation de Navier–Stokes avec reconnexion d'interfaces. Méthode de suivi de volume et application à l'atomisation. Ph.D. thesis, Université Pierre et Marie Curie, 1996.
8. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, DC, 1964).
9. W. H. Beyer, *CRC Standard Mathematical Tables*, 26th Ed. (CRC Press, Boca Raton, FL, 1982).
10. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge Univ. Press, Cambridge, UK, 1986).