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Accurate Estimation of Geometrical Properties of a Volume-of-Fluid Interface on Nonuniform Rectangular Grids

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Estimating the local curvature of an interface involves the local determination of normals (lines perpendicular) to the interface, and the rates that they turn as one moves along the interface. This is challenging for volume-of-fluid type methods of interface approximation because the interface between materials is then specified by the relative amount it cuts off from the computational cells that it crosses (also referred to as volume fraction data), rather than by a discrete set of points lying on the interface itself. In our work [1], we have generalized a volume-of-fluid method, called the height function method, to nonuniform grids of rectangular cells (see Fig. 1). First, for each vertical column of mesh cells, the volume fractions determine an (integral) mean value (or column height) for the portion of the interfacial curve that crosses that column. We then demonstrate analytically and numerically that three successive (adjacent) mean values suffice to estimate interfacial curvature to second-order accuracy, the interfacial slope to third-order accuracy, and the interfacial curve's location to fourth-order accuracy–each at its own special points as one crosses the three columns (see Fig. 2). Second-order accurate curvature can be estimated anywhere by linearly interpolating the second-order accurate curvatures between two successive special points. And finally, we have determined the special locations where the curvature can be estimated to fourth-order accuracy when using five successive mean values instead.

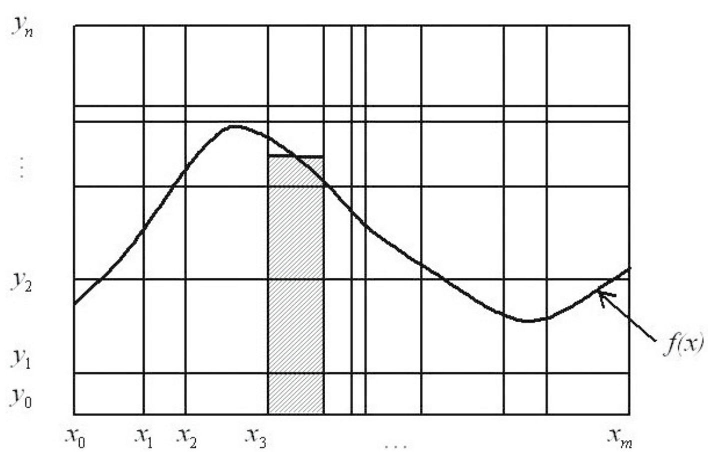

Fig. 1. Illustration of an irregular rectangular grid and a known (integral) mean value of the unknown interfacial curve between the sides of one of the grid's columns.

Underlying all this is a result about the accuracy of the jth-derivative of the kth-degree polynomial that interpolates (matches) a function F at $k + 1$ "stencil points" placed irregularly in an interval of width h. Namely, for all smooth-enough functions F and for k fixed and h getting small, there are $k + 1 - j$ special points in the interval at which the error in the polynomial's jth derivative is of order $O(h^{k+2-j})$. This is one order higher than the usual $O(h^{k+1-j})$ error holding over the whole interval for that derivative. Increasing a method's order of accuracy has consequences for computational efficiency. For example, the error in a third-order $O(h^3)$ accurate method goes to zero at least as fast as the third power h^3 of the interval width h. Then, cutting the width by a factor of 2 would cut the error by a factor of $2^3 = 8$.

These special points of accuracy in the interval are the $k + 1 - j$ (real) zeroes of certain F-independent polynomials, of degree $k + 1 - j$, with coefficients depending on the interval's stencil points. For example, take $j = k$, the polynomial's degree. It is classic that the interpolating polynomial's kth derivative is a first-order $O(h)$ accurate estimate of the kth derivative of F anywhere in the h-sized interval containing the stencil points. But it is second-order $O(h^2)$ accurate only at one special point; namely, at the average location of the $k + 1$ stencil points.

In the context of the first paragraph, suppose the (unknown) interfacial curve $f(x)$ crosses k adjacent columns of cells. The edges of the columns determine $k + 1$ successive points $x_1, x_2, \ldots, x_{k+1}$. Let $F(x)$

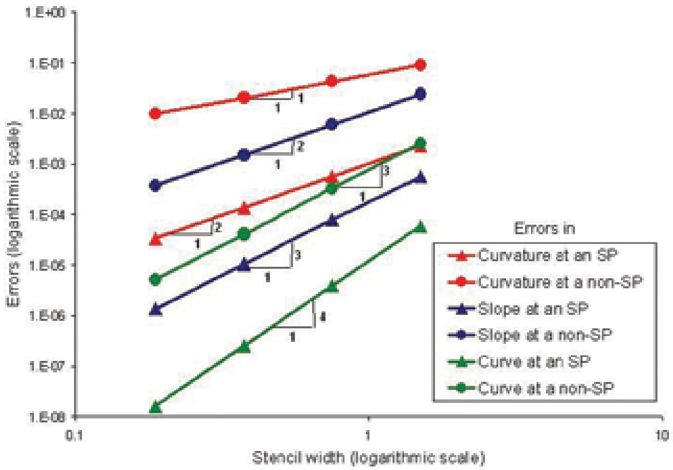

Figure 2. Log-log plots of the errors in interfacial curvature, interfacial slope or the interfacial curve's location–at an appropriate special point (SP) of accuracy or at a point that is not a special point of accuracy–using a cosine test function and a shrinking stencil of four nonuniformly distributed mesh points. The indicated slope of a plot gives the error's order of accuracy.

be an indefinite integral of the function $f(x)$. Then $F(x_i)$ at the $k + 1$ successive locations x_i is calculated using cumulative sums of the k known successive integral mean values of f, weighted by the successive distances between the x_i. The $k + 1$ points $(x_i, F(x_i))$ are now interpolated by a kth degree polynomial $(PF)(x)$. Its first derivative $(PF)^{(1)}$ approximates the unknown curve $f = (F^{(1)})$, while $(PF)^{(2)}$ and $(PF)^{(3)}$, respectively, approximate $f^{(1)}$, and $f^{(2)}$. Then the results in Fig. 2, for the curvature $f^{(2)}/(1+(f^{(1)})^2)^{3/2}$, the slope $f^{(1)}$, and the curve's location f, are obtained using $k = 3$ successive mean values and the derivatives $j = 3, 2, 1$. The $O(h^4)$ accurate curvature using five successive mean values involves $k = 5$ and $j = 3, 2$.

For more information contact Marianne Francois at mmfran@lanl.gov.

[1] M.M. Francois, B.K. Swartz, *J. Comp. Phys.* **229,** 527 (2010).

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