Journal of Computational Physics 229 (2010) 527–540

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Interface curvature via volume fractions, heights, and mean values on nonuniform rectangular grids

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ARTICLE INFO

Article history:
Received 12 May 2009
Received in revised form 7 October 2009
Accepted 13 October 2009
Available online 21 October 2009

Keywords:
Volume-of-fluid
Curvature
Height function
Mean value
Nonuniform grids
Numerical differentiation

ABSTRACT

Estimating the local curvature of an interface involves the local determination of normals to the interface, and the rates that they turn along the interface. This is challenging in volume-of-fluid type methods since the interface between materials is 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 this work, we generalize the height function method to nonuniform rectangular grids. We demonstrate analytically and numerically that—using three successive (adjacent) integral mean values (or "column" heights)—interface curvature can be estimated to second-order accuracy, the first derivative (interface normal) to third-order accuracy, and the curve location to fourth-order accuracy—each at its own special points. We also show that there are special points where the curvature can be estimated to fourth-order accuracy when using five successive mean values instead.

Underlying all this is a result about the accuracy of the jth-derivative of the kth-degree polynomial that interpolates 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 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.) The special points 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.

In our case, let $F(x)$ be an indefinite integral of the unknown interfacial curve $f(x)$. Then $F(x_i)$ at $k+1$ successive stencil points x_i is calculated using cumulative sums of the k successive integral mean values of f, weighted by the successive interval sizes. The $k+1$ points $(x_i, F(x_i))$ are now interpolated by a kth degree polynomial $(PF)(x)$. It's first derivative $(PF)^{(1)}$ approximates the unknown curve f; while $(PF)^{(2)}$ and $(PF)^{(3)}$, respectively, approximate $f^{(1)}$ and $f^{(2)}$. Thus, the results above using three successive mean values correspond to $k=3$ and $j=3,2,1$. The curvature result using five successive mean values correspond to $k=5$ and $j=3$. For this last case, since the curvature $\kappa = f^{(2)}/(1+(f^{(1)})^2)^{3/2}$, we use the facts that $f^{(1)} = F^{(2)} = (PF)^{(2)} + O(h^4)$ on the whole stencil interval, not just at the three special points having $O(h^4)$ accuracy for $f^{(2)}$.

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doi:10.1016/j.jcp.2009.10.022

1. Introduction

In volume-of-fluid methods the interface between regions is specified by the relative amount the interface cuts off from the computational cells that it crosses, rather than by a discrete set of points lying on the interface itself. But estimating the local curvature of an interface involves the local determination of normals to the interface, and the rates that they turn along the interface. This might seem problematic using such locally smeared information as fractional amounts cut off from interfacial cells. Nevertheless, for a two-dimensional uniform grid of square mesh cells with corners $(x_i, y_j)_{i=1}^{m}\,{}_{j=1}^{n}$, one may first choose a local vertical direction (say, the increasing y direction) from the four possibilities available (x or y—increasing or decreasing). Then, one may define a local height for the interface in each of three neighboring "vertical" columns of cells—columns associated with, say,

$$x_i \leqslant x \leqslant x_{i+1}, \quad x_{i+1} \leqslant x \leqslant x_{i+2}, \quad \text{and} \quad x_{i+2} \leqslant x \leqslant x_{i+3}$$

by summing all partial areas in a column below the interface but above a horizontal floor common to the three intervals. Dividing by the column width, this succeeds in defining a local piecewise-constant interfacial "height function" for the interface:

$$H(x) = H_{i+1/2}, \quad x_i \leqslant x < x_{i+1}, \quad i = 2, \ldots, N-1. \tag{1}$$

The two derivatives in the relevant expression for the local curvature of the interface, namely,

$$\kappa := \frac{d^2y/dx^2}{[1 + (dy/dx)^2]^{3/2}} \tag{2}$$

are now estimated by applying centered difference formulas to the related discrete function

$$(x_{m+1/2}, H_{m+1/2}), \quad x_{m+1/2} := (x_m + x_{m+1})/2, \quad m = i, i+1, i+2. \tag{3}$$

The estimate is demonstrably second-order accurate at the mid-point of the intersection of the interface with the middle column, see e.g. Cummins et al. [3].

The "height function" method [15,7] has mainly been used on uniform rectangular meshes. For such grids, it has been demonstrated to yield second-order accuracy using three successive heights $H_{i+1/2}$ (or columns) for both interface curvatures [13,10,3,5] and interface normals [4]. The method has also been extended to compute fourth-order accurate curvature using five successive heights $H_{i+1/2}$ (or columns) [14]. Recent studies on the height function method have focused on improving the estimation of the height function itself by choosing the best local rectangular set of mesh squares [16,8,1,12]. The focus of this note is not on the choice of the optimum set of mesh squares for estimating the height function.

Instead, this note focuses on showing, both analytically and numerically, that given (integral) mean values (or column heights) associated with three adjacent columns of a nonuniform grid, we can compute second-order accurate curvature associated with the average location of the four successive grid points. For the case of a uniform grid this four-point average location is the location of the mid-point of the middle interval. We also find locations in each stencil interval where third-order accurate approximate first derivatives, and fourth-order accurate points on the curve, can be (and are) calculated. Finally, we extend a recent fourth-order accurate curvature result of Sussman and Ohta [14], based on five adjacent uniform columns, to nonuniform rectangular grids.

2. Nonuniform rectangular grids

This note extends the height function result to nonuniform"tensor product" grids; that is to say, to grids of mesh points

$$(x_i, y_j)_{i=1}^{m}\,{}_{j=1}^{n}, \quad x_0 < x_1 < \cdots < x_m, \quad y_0 < y_1 < \cdots < y_n$$

that are not necessarily uniformly spaced (see Fig. 1). The result is more clearly stated and analyzed in terms of the single-valued function $(x, f(x))$, presumed to describe the interface locally, along with f's integral mean values

$$\bar{f}_{i+1/2} := \frac{\int_{x_i}^{x_{i+1}} f(t)\,dt}{(x_{i+1} - x_i)}. \tag{4}$$

The sequence $\bar{f}$ is the present analog of the "height function", and is presumed to be known data.

We now suppose that the (unknown) interfacial curve $(x, f(x))$ crosses four successive vertical mesh lines $x = x_i, \ldots, x = x_{i+3}$. Let now $F(x)$ be an indefinite integral of the interfacial curve function $f(x)$. Then

$$\left(\frac{dF}{dx}\right)(x) = f(x), \quad \text{and} \quad \left(\frac{\Delta F}{\Delta x}\right)_{i+1/2} := \frac{[F(x_{i+1}) - F(x_i)]}{(x_{i+1} - x_i)} = \bar{f}_{i+1/2} \tag{5}$$

are the (unknown) derivative and the (known) first difference quotient of F, respectively. More important for curvature estimates of the curve are the (unknown) second and third derivatives of F and its (known) second and third difference quotients: