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Note

Relationship between the Truncation Errors of Centered Finite-Difference Approximations on Uniform and Nonuniform Meshes

Two of the major problems facing the numerical analyst when constructing the numerical solution of partial differential equations are (1) the numerical implementation of the boundary conditions along the boundaries of the physical space, and (2) the selection of the finite-difference mesh to represent the continuous physical space.

The careful implementation of boundary conditions is essential. For the more common coordinate systems (i.e., Cartesian, cylindrical, and spherical), the boundaries of the physical space seldom lie along coordinate lines. When only first-order accuracy is required, the implementation of boundary conditions along arbitrary lines in the physical space presents no particular problem. When higher-order accuracy is desired, however, serious problems arise. This has led to the extensive use of coordinate transformations to map the boundaries of the physical space onto coordinate lines of a transformed space. The value of this procedure is well established and well understood, thus it is not discussed further.

Nonuniform meshes in the physical space are commonly employed to space mesh points closely in regions where gradients are large and fine details are desired, and to space mesh points widely in the remainder of the physical space. Computational time is dependent (sometimes exponentially) on the total number of mesh points in the physical space. By the careful choice of a nonuniform mesh, a given number of mesh points can be distributed over the physical space in an optimum manner, thus minimizing computational time. When only first-order accuracy is desired, the use of nonuniform meshes presents no special problems. When higher-order accuracy is desired, serious problems are encountered. This has led to the extensive use of coordinate transformations to map nonuniform meshes in the physical space into uniform meshes in the transformed space. The present discussion is concerned with the relationship between the truncation errors of centered finite-difference approximations applied directly on the nonuniform physical mesh and the truncation errors of the same centered finite-difference approximations applied on the corresponding transformed uniform mesh.

The most common grid generation methods are conformal transformations, algebraic methods, and methods based on the solution of Poisson's equation. The results of applying a grid generation method are two grid systems: the desired nonuniform mesh in the physical space and the corresponding uniform mesh in the transformed space.

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After the two grid systems have been generated, two approaches exist for constructing finite-difference approximations to derivatives. The most common approach is to construct the finite-difference approximations on the uniform mesh in the transformed space. The advantage of this approach is that two- or three-point (for first or second derivatives, respectively) centered finite-difference operators yield second-order accurate approximations. The disadvantage of this approach is that the transformed differential equations must be solved. Those equations are considerably more complicated than the original differential equations since each term is multiplied by a transformation metric, and more terms are present.

An alternate approach is to construct the finite-difference approximations on the nonuniform mesh in the physical space. In this case, the grid generation method is used merely to achieve the desired nonuniform mesh in the physical space. The advantage of this approach is that the original differential equations are solved. The disadvantage of this approach is that the two- or three-point centered finite-difference operators, when appled on a nonuniform mesh, do not yield second-order accurate approximations.

Hirt and Ramshaw [1] and Roache [2] show that finite-difference approximations on a nonuniform mesh have lower-order formal accuracy than finite-difference approximations on a uniform mesh. Hirt and Ramshaw also show that the truncation errors of the two approaches are identical for the algebraic coordinate transformation they employed. Consequently, they chose to construct finite-difference approximations on the nonuniform mesh in the physical space. Roache, on the other hand, concludes that the approach employing the transformed uniform mesh is preferable because of the higher-order formal accuracy.

Which approach is more accurate? What are the relationships between the two approaches? The present discussion examines the two approaches in detail and clarifies the relationships between them.

Consider the function

$$f = \phi(x) \tag{1}$$

The function f is discretized at the points x_i, where the x_i form a nonuniform mesh. A centered finite-difference approximation to f_x at point i is given by

$$\bar{f}_x = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}} \tag{2}$$

Expanding $\phi(x)$ in a Taylor series yields

$$\phi_{i\pm 1} = \phi_i \pm \phi_x|_i \Delta x_\pm + \tfrac{1}{2}\phi_{xx}|_i \Delta x_\pm^2 + O(\Delta x_\pm^3) \tag{3}$$

where $\Delta x_+ = (x_{i+1} - x_i)$ and $\Delta x_- = (x_i - x_{i-1})$. Thus,

$$\phi_{i+1} - \phi_{i-1} = \phi_x|_i (\Delta x_+ + \Delta x_-) + \tfrac{1}{2}\phi_{xx}|_i (\Delta x_+^2 - \Delta x_-^2) + O(\Delta x_\pm^3) \tag{4}$$

For the nonuniform mesh,

$$x_{i+1} - x_{i-1} = (x_i + \Delta x_+) - (x_i - \Delta x_-) = \Delta x_+ + \Delta x_- \tag{5}$$

Combining Eqs. (2), (4), and (5) yields

$$\bar{f}_x = \phi_x|_i + \tfrac{1}{2}\phi_{xx}|_i(\Delta x_+ - \Delta x_-) + O(\Delta x_\pm^2) \tag{6}$$

Equation (6) shows that $\bar{f}_x$ is formally first order in $\Delta x_\pm$. Consequently, for any initial mesh spacing, if the number of grid points is doubled in a manner so that the values of $\Delta x_\pm$ are halved, the truncation error halves.

Consider the coordinate transformation $\xi = \zeta(x)$ and its inverse $x = \eta(\xi)$:

$$\xi = \zeta(x) \qquad \text{and} \qquad x = \eta(\xi) \tag{7}$$

By emplying Eq. (7), Eq. (1) may be transformed to

$$f = \phi(x) = \phi[\eta(\xi)] = \psi(\xi) \tag{8}$$

The first derivative f_x is given by

$$f_x = \psi_\xi \xi_x = \psi_\xi \zeta_x \tag{9}$$

The function $f = \psi(\xi)$ is discretized at the points ξ_i, where the ξ_i form a uniform mesh. A centered finite-difference approximation to f_x at point i is given by

$$\bar{\bar{f}}_x = \zeta_x|_i \frac{\psi_{i+1} - \psi_{i-1}}{\xi_{i+1} - \xi_{i-1}} \tag{10}$$

Expanding $\psi(\xi)$ in a Taylor series yields

$$\psi_{i\pm1} = \psi_i \pm \psi_\xi|_i \Delta\xi + \tfrac{1}{2}\psi_{\xi\xi}|_i \Delta\xi^2 + O(\Delta\xi^3) \tag{11}$$

where $\Delta\xi = \Delta\xi_+ = (\xi_{i+1} - \xi_i) = \Delta\xi_- = (\xi_i - \xi_{i-1})$. Thus,

$$\psi_{i+1} - \psi_{i-1} = 2\psi_\xi|_i \Delta\xi + O(\Delta\xi^3) \tag{12}$$

For the uniform mesh,

$$\xi_{i+1} - \xi_{i-1} = (\xi_i + \Delta\xi) - (\xi_i - \Delta\xi) = 2\Delta\xi \tag{13}$$

Combining Eqs. (10), (12), and (13) yields

$$\bar{\bar{f}}_x = \zeta_x|_i \psi_\xi|_i + O(\Delta\xi^2) \tag{14}$$

Equation (18) shows that $\bar{\bar{f}}_x$ is formally second order in $\Delta\xi$. Consequently, for any initial mesh spacing, if the number of grid points is doubled in a manner so that the values of $\Delta\xi$ are halved, the truncation error quarters.

From Eqs. (6) and (14), it appears that $\bar{f}_x$ has first-order accuracy because of the nonuniform mesh. This is true if the values of $\Delta x_{\pm}$ are halved as the mesh is refined by doubling the number of mesh points. If, however, the values of $\Delta x_{\pm}$ are chosen so that the term $(\Delta x_{+} - \Delta x_{-})$ in Eq. (6) quarters as the number of mesh points is doubled, then the truncation error of $\bar{f}_x$ behaves in a second-order manner.

A procedure for determining the required values of $\Delta x_{\pm}$ to achieve a second-order truncation error for $\bar{f}_x$ is obtained by expanding the coordinate transformation $x = \eta(\xi)$ in a Taylor series. Thus,

$$x_{i\pm 1} = x_i \pm \eta_\xi|_i \Delta\xi + \tfrac{1}{2}\eta_{\xi\xi}|_i \Delta\xi^2 \pm \tfrac{1}{6}\eta_{\xi\xi\xi}|_i \Delta\xi^3 + O(\Delta\xi^4) \tag{15}$$

The term $(\Delta x_{+} - \Delta x_{-})$ can be written as

$$\Delta x_{+} - \Delta x_{-} = (x_{i+1} - x_i) - (x_i - x_{i-1}) = (x_{i+1} - x_i) + (x_{i-1} - x_i) \tag{16}$$

Substituting Eq. (15) into Eq. (16) yields

$$\Delta x_{+} - \Delta x_{-} = \eta_{\xi\xi} \Delta\xi^2 + O(\Delta\xi^4) \tag{17}$$

Consequently, if the values of $\Delta x_{\pm}$ are chosen so that the values of $\Delta\xi$ are halved, the term $(\Delta x_{+} - \Delta x_{-})$ quarters and the truncation error of $\bar{f}_x$ quarters. Thus, the finite-difference approximation $\bar{f}_x$, which is formally first order in $\Delta x_{\pm}$, behaves in a second-order manner. It is not necessary to actually apply the coordinate transformation to the differential equations. All that is required is that the spacing of the nonuniform mesh corresponds to the coordinate transformation.

The relationship between the truncation errors of the two approaches is obtained by considering a particular set of corresponding points in x space and ξ space, where those in ξ space are equally spaced. Thus,

$$f_{i\pm 1} = \phi(x_{i\pm 1}) = \phi_{i\pm 1} = \psi(\xi_{i\pm 1}) = \psi_{i\pm 1} \tag{18}$$

where

$$x_{i\pm 1} = \eta(\xi_{i\pm 1}) \tag{19}$$

From Eq. (15),

$$x_{i+1} - x_{i-1} = 2\eta_\xi|_i \Delta\xi + O(\Delta\xi^3) \tag{20}$$

From Eq. (7),

$$dx = \eta_\xi \, d\xi \qquad \text{and} \qquad d\xi = \zeta_x \, dx \tag{21}$$

For continuous transformations having unique continuous inverses,

$$\eta_\xi = dx/d\xi = 1/\zeta_x \tag{22}$$

Consequently, Eq. (20) may be written as

$$x_{i+1} - x_{i-1} = 2\Delta\xi/(\zeta_x|_i) + O(\Delta\xi^3) \tag{23}$$

Substituting Eqs. (18) and (23) into Eq. (2) and comparing with Eq. (10) gives

$$\bar{f}_x = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}} = \zeta_x|_i \frac{\psi_{i+1} - \psi_{i-1}}{\xi_{i+1} - \xi_{i-1}} + O(\Delta\xi^2) = \bar{\bar{f}}_x + O(\Delta\xi^2) \tag{24}$$

Consequently, $\bar{f}_x$ and $\bar{\bar{f}}_x$ differ by second-order terms in ξ for a particular set of corresponding points in x space and ξ space. For coordinate transformations $x = \eta(\xi)$ that are polynomials of second degree or less, all derivatives of η of higher order than 2 are identically zero, and the $O(\Delta\xi^2)$ terms in Eqs. (20), (23), and (24) are identically zero. In that special case, $\bar{f}_x = \bar{\bar{f}}_x$ exactly, and the two finite-difference approximations have the same truncation error. That is the situation considered by Hirt and Ramshaw [1]. In general, however, the coordinate transformation $x = \eta(\xi)$ is not a second-degree polynomial, and $\bar{f}_x$ and $\bar{\bar{f}}_x$ differ by second-order terms.

The general features demonstarted in the foregoing for centered finite-difference approximations to f_x also apply to f_{xx}.

The above analysis illustrates the effect of coordinate transformations on the accuracy of centered finite-difference approximations. It is seen that a finite-difference approximation in a nonuniform mesh is formally first order and a finite-difference approximation in a uniform mesh is formally second order. The finite-difference approximation in the nonuniform mesh, however, behaves in a second-order manner if the mesh points of the nonuniform mesh are chosen in accordance with the cordinate transformation. The truncation errors of centered finite-difference approximations in the two meshes differ by second-order terms. For f_x, the truncation errors are identical for coordinate transformations $x = \eta(\xi)$ that are second-degree polynomials, and for f_{xx}, the truncation errors are identical for coordinate transformations $x = \eta(\xi)$ that are first-degree polynomials.

In principle, any nonuniform mesh having n points, no matter how nonuniform, may be transformed into a uniform mesh by some coordinate transformation having n free parameters. Centered finite-difference approximations in the nonuniform mesh are then second order with respect to the transformed uniform mesh. However, the coordinate transformations required to transform highly irregular meshes into uniform meshes may have inflection points, large values of the higher-order derivatives, and multivalued regions. Even though these coordinate transformations yield second-order finite-difference approximations, the truncation errors may be quite large. In general, the best results are obtained with smooth coordinate transformations.

The objective of applying a coordinate transformation is to obtain a desired nonuniform mesh in the physical space. The choice between writing finite-difference approximations in the untransformed nonuniform mesh or the transformed uniform mesh should be based on considerations of numerical accuracy and computational efficiency. From the analysis presented herein, it is clear that both approaches can yield second-order finite-difference algorithms. Consequently, both approaches have their uses in the field of numerical analysis, and numerical analysts should be aware of both approaches.

REFERENCES

1. C. W. HIRT AND J. D. RAMSHAW, Prospects for numerical simulation of bluff-body aerodynamics, *in* "Aerodynamic Drag Mechanisms of Bluff Bodies and Road Vehicles" (G. Sovran, T. Morel, and W. Mason, Jr., eds.), pp. 313–355, Plenum, New York, 1978.
2. P. J. ROACHE, "Computational Fluid Dynamics," rev. ptg., p. 295, Hermosa, Albuquerque, N. M., 1976.

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