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Development of an error-minimizing adaptive grid method

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Abstract

We present the first step in the development of a moving adaptive grid technique for flow and transport problems that is based on the approximate minimization in the L_1 norm of the modeling error due to discretization. The technique consists of a second-order accurate discretization scheme designed for error analysis, a filter technique to ensure sufficiently smooth solutions, and an iterative solver for the nonlinear adaptive grid equations. We describe how these elements have been used for the numerical approximation of a given one-dimensional function. This application has been chosen to test and optimize the error-minimizing adaptive grid method. Results are presented for a function having a smooth part, a discontinuity and a uniform part. In comparison with a uniform grid, a gain in accuracy of a factor 10 to almost 1000 was obtained using 40 to 200 grid points.

1. Introduction

The standard approach followed in moving adaptive grid methods is the equidistribution of an error measure over the grid cells. Many different error measures have been proposed in the literature, often chosen heuristically, with little or no justification [6]. However, if error measures do not contain all relevant error information, grid adaptation may not lead to any improvement of the solution [8]. Ideally, error measures should include all important sources of numerical solution errors, i.e., terms that indicate how the quality of the grid affects the accuracy of the numerical simulation. The design of suitable error measures for grid adaptation is still an area of active research [6,7].

Residual-based, a posteriori error estimates for flow and transport problems of practical interest still lack sharpness or are not generally applicable [4,7]. Also, refining the grid in regions where the residual is large does not necessarily lead to an improvement in the solution; local solution errors may be the result of the accumulation during propagation of errors that have been generated elsewhere. We have, therefore, not opted for the development of a grid adaptation method that aims to reduce some upper error bound to a given tolerance level. Instead, our goal is to minimize that part of the

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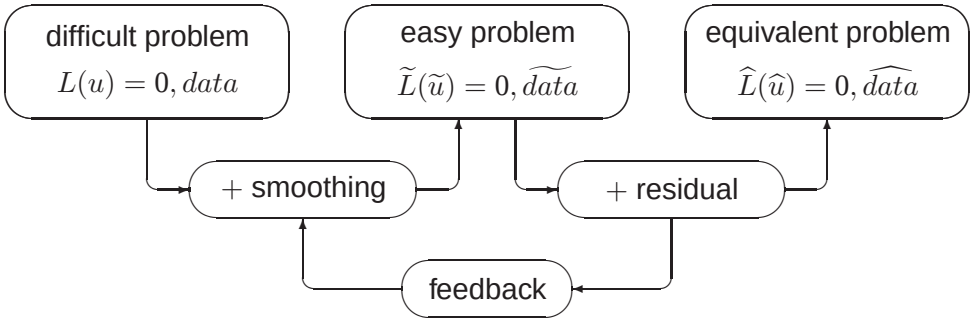
numerical solution error that is generated locally as a result of using a numerical approximation of the model equations. We will refer to this error as the numerical *modeling* error.

The purpose of grid adaptation is the reduction of numerical errors. However, the presence of other modeling errors should be taken into consideration as well (see, e.g., [2]). For example, grid refinement is not useful in regions where the largest errors are due to the applied physical model or caused by unreliable or incomplete input data. In complex applications, the effect of these physical modeling errors on the solution can at best be quantified very roughly. The reduction of the numerical solution error through grid adaptation may, therefore, be of limited practical use. On the other hand, consideration of the numerical modeling error enables a comparison with physical modeling errors. This may be used to assess the relative importance of the latter and hence the usefulness of local adaptive grid refinement. This is an important additional motivation for the present approach.

The local residual will be approximated by means of a truncated Taylor series expansion. Accuracy is obtained only when the series converges rapidly. This requires smoothness in some sense of *all* variables. We will discuss this aspect in Section 2. Smoothing or regularization is used frequently in adaptive grid techniques [1,3,6,7]. The discretization scheme that we apply is presented in Section 3 and has been designed especially for the purpose of error analysis; it allows us to establish the effect of the local residual on the numerical solution. Considering the magnitude of the residual as such is generally not sufficient, since this indicates primarily the approximation error in the discretized equations. The scheme is applied to the problem of determining a numerical approximation of a given one-dimensional function in Section 4, where we also present the error-minimizing adaptive grid method. Some conclusions are given in Section 5.

2. The two-step numerical modeling technique

We propose a numerical modeling technique that consists of two steps: a smoothing step, and a discretization step. The smoothing step ensures that the lowest-order terms of the residual of the discretization step are dominant, so that we can limit ourselves to the analysis of the leading terms of the error expansion. The following diagram shows the different elements of the two-step numerical modeling technique.



The difficult mathematical-physical problem—whose solution u may contain, e.g., steep gradients—consists of differential operator L and an imposed data set $data$ with information about geometry, coefficients, initial and boundary conditions, source terms, etc. It is transformed to an easier differential

problem by adding artificial dissipation terms to L and by smoothing $data$, resulting in a smooth solution $\widetilde{u}$. The discrete approximation of the easy problem, $\overline{L}(\overline{u}) = 0,\ \overline{data}$, is not included in the diagram. The discretization is part of the transformation from the easy problem to the equivalent differential problem, whose solution $\widehat{u}$ is a close and smooth approximation of numerical solution $\overline{u}$. An approach similar to this two-step modeling has been proposed in the context of adaptive grid methods by Eriksson and Johnson [3].

The smoothing is assumed to be such that the easy problem can be discretized accurately on the available grid, and that the leading terms of the residual are dominant. This is obtained by making the smoothing coefficients a function of these leading error components, which in the diagram is indicated by the *feedback* loop. So, writing the equivalent differential problem as

$$\widehat{L}(\widehat{u}) = \widetilde{L}(\widehat{u}) + \text{residual}, \qquad \widehat{data} = \widetilde{data} + \text{residual},$$

we have that the residual can be approximated accurately by its lowest-order components.

Some form of two-step modeling is used in virtually any discretization method that is applied to flow and transport problems of practical interest. Artificial dissipation may be added either explicitly to the equations, in the form of even derivative terms, or implicitly, by incorporating a dissipative mechanism like flux limiters inside the discretization method. Data smoothing is usually not applied, but forms an essential part of the two-step modeling technique. Steep gradients in, e.g., initial and boundary conditions may otherwise create temporarily or locally steep gradients in the solution, thereby reducing the accuracy of the residual approximation and hence the applicability of an error-minimizing adaptive grid algorithm.

3. A discretization method designed for error analysis

We consider the one-dimensional piecewise linear numerical solution $\overline{u}$ and its smooth, equivalent approximation $\widehat{u}$. The difference between $\overline{u}$ and $\widehat{u}$ is $\mathrm{O}(\Delta x^2 \widehat{u}_{xx})$ provided that both functions are sufficiently smooth. Since on a non-uniform grid Δx is discontinuous, it is convenient to express the interpolation error in a parameter space with uniform grid $[\xi_i]$, for which we introduce the two piecewise linear numerical functions

$$\overline{u}(\xi) = u_i + \frac{\xi - \xi_i}{\Delta\xi}(u_{i+1} - u_i), \qquad \overline{x}(\xi) = x_i + \frac{\xi - \xi_i}{\Delta\xi}(x_{i+1} - x_i),$$

with $\xi_i \leqslant \xi \leqslant \xi_{i+1}$ and $\xi_{i+1} - \xi_i = \Delta\xi$, $\forall i$, where ξ is the coordinate of the computational space. When the smooth approximations $\widehat{u}$ and $\widehat{x}$ of $\overline{u}$ and $\overline{x}$ are defined such that $\widehat{u}(\xi_i) = u_i$ and $\widehat{x}(\xi_i) = x_i$, $\forall i$, we have

$$\overline{u}(\xi) = \widehat{u}(\xi) + \frac{(\xi_{i+1} - \xi)(\xi - \xi_i)}{2}\,\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\,\widehat{u}(\xi) + \mathrm{O}\big(\Delta\xi^3\big),$$

$$\overline{x}(\xi) = \widehat{x}(\xi) + \frac{(\xi_{i+1} - \xi)(\xi - \xi_i)}{2}\,\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\,\widehat{x}(\xi) + \mathrm{O}\big(\Delta\xi^3\big).$$

From these expressions we obtain

$$\overline{u}(\overline{x}) = \widehat{u}(\overline{x}) + \alpha(\xi) D_\xi^{u,x} + \mathrm{O}\big(\Delta\xi^3\big), \tag{1}$$

with

$$\alpha(\xi) = \frac{(\xi_{i+1} - \xi)(\xi - \xi_i)}{2\Delta\xi^2} \quad \text{and} \quad D_\xi^{u,x} = \Delta\xi^2 \left[\widehat{u}_{\xi\xi} - \widehat{u}_\xi \frac{\widehat{x}_{\xi\xi}}{\widehat{x}_\xi} \right]. \tag{2}$$

$D_\xi^{u,x}$ is the interpolation error made in physical space expressed in terms of variables defined in computational space, and indicates how the second-order interpolation error depends on solution variation, grid size and grid stretching. It is, however, incorrect to consider $D_\xi^{u,x}$ as a reliable estimate of a second-order discretization error. Second-order accurate discretization schemes are usually built up from a mix of (upwind) extrapolations, (central) interpolations and piecewise constant approximations, which are used for different (combinations of) variables in different terms of a system of PDEs. Although the use of second-order accurate interpolations is consistent with such a scheme, it is also incompatible since other discrete solution approximations have been used in the construction of the scheme as well. This explains why in general it is not possible to reformulate the residual of discretized PDEs in terms of local discretization errors in the numerical solution. It also indicates which discretization scheme may allow such a reformulation: one that is rigorously based on piecewise linear approximations. This has been verified by considering the discrete approximation of the equation

$$\frac{\partial au}{\partial t} + \frac{\partial bu}{\partial x} = \frac{\partial}{\partial x} c \frac{\partial u}{\partial x} + eu + s(u). \tag{3}$$

Flow/transport equation (3) has been discretized on the non-uniform, moving grid $[x_i(\tau), t(\tau)]$. Since piecewise linear approximations do not permit the evaluation of second derivatives, a weak formulation of (3) must be considered. First derivatives can be approximated, but second-order accuracy is obtained only at cell centers. So the space discretization of (3) that ensures maximum compatibility is obtained by the procedure:

- transform (3) to the computational space (ξ, τ),
- define unique linear approximations per grid cell for *all* variables,
- integrate the equation over the volumes $[\frac{1}{2}(\xi_{i-1} + \xi_i), \frac{1}{2}(\xi_i + \xi_{i+1})]$.

The integrals must be evaluated up to at least fourth-order accuracy, so that the second-order components of the residual can be determined with second-order accuracy. A space discretization of (3) is then obtained whose local residual can indeed be expressed up to $\mathrm{O}(\Delta\xi^4)$ in terms of interpolation errors. Its equivalent differential equation can be written as

$$\begin{aligned}
&\frac{\partial}{\partial\tau}\left[\widehat{x}_\xi\left(\widehat{a} + \frac{D_\xi^{a,x}}{12}\right)\left(\widehat{u} + \frac{D_\xi^{u,x}}{12}\right)\right] - \frac{\partial}{\partial\xi}\left[\widehat{x}_\tau\left(\widehat{a} + \frac{D_\xi^{a,x}}{8}\right)\left(\widehat{u} + \frac{D_\xi^{u,x}}{8}\right)\right] \\
&\quad + \frac{\partial}{\partial\xi}\left[t_\tau\left(\widehat{b} + \frac{D_\xi^{b,x}}{8}\right)\left(\widehat{u} + \frac{D_\xi^{u,x}}{8}\right)\right] \\
&= \frac{\partial}{\partial\xi} t_\tau\left(\widehat{c} + \frac{D_\xi^{c,x}}{8}\right)\left[\frac{1}{\widehat{x}_\xi}\frac{\partial}{\partial\xi}\left(\widehat{u} - \frac{D_\xi^{u,x}}{24}\right) + \frac{1}{12}\frac{\partial}{\partial\xi}\left(\frac{D_\xi^{u,x}}{\widehat{x}_\xi}\right)\right] \\
&\quad + t_\tau \widehat{x}_\xi\left[\left(\widehat{e} + \frac{D_\xi^{e,x}}{12}\right)\left(\widehat{u} + \frac{D_\xi^{u,x}}{12}\right) + s\left(\widehat{u} + \frac{D_\xi^{u,x}}{12}\right)\right] + \mathrm{O}\big(\Delta\xi^4\big),
\end{aligned} \tag{4}$$

with the D-terms as in (2).

Eq. (4) is equal to Eq. (3) transformed to computational space, plus the second- and higher-order residual components in space. The second-order error terms are in the form of D-terms only, and show

that the residual has a local effect on solution and other variables that is similar to that of interpolation errors (cf. Eq. (1)). Minimizing the interpolation errors by, e.g., grid adaptation is, therefore, equivalent to the minimization of the local numerical modeling error, i.e., the solution error generated locally by the discretization scheme. Because of the compatibility between discretization and the underlying discrete function approximations we call this scheme *compatible*.

Boundaries are, like the finite volume boundaries, located at cell centers, where both Dirichlet-type and Neumann-type conditions can be discretized in a compatible way. Compatibility in time is no problem either, but requires some care to ensure stability and smoothness. This is presently under study.

4. An adaptive grid test

In this section we address the problem of how to minimize the numerical solution error as a function of the position of the grid points, and how to solve the minimization problem. As an example, we will consider the numerical solution of the simple one-dimensional test problem

$$u(x) = u_{\text{giv}}(x), \quad \text{with } u_{\text{giv}} = \begin{cases} \frac{1}{2} - \frac{1}{2}\tanh(20x - 6), & \text{if } 0 \leqslant x \leqslant 0.65, \\ 1, & \text{if } 0.65 < x \leqslant 1. \end{cases} \tag{5}$$

The non-smoothness of u_{giv} makes this a difficult problem to solve. By adding some form of artificial smoothing, (5) is transformed to the easy problem

$$\widetilde{u} - \frac{\mathrm{d}}{\mathrm{d}x}\,\nu^h\,\frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x} = u_{\text{giv}}, \quad \nu^h = c_\nu \Delta x^2 E. \tag{6}$$

Error feedback is obtained by making artificial smoothing coefficient ν^h a function of discretization error E. Since ν^h itself should be smooth as well, E is taken equal to the smoothed absolute value of $D_\xi^{u,x}$, for which a constant smoothing coefficient is used. The compatible discretization of (6) reads

$$\begin{aligned} &\left[\frac{\Delta x_{i-1/2}}{8} - \frac{\nu^h_{i-1/2}}{\Delta x_{i-1/2}}\right] u_{i-1} + \left[\frac{3\Delta x_{i-1/2} + 3\Delta x_{i+1/2}}{8} + \frac{\nu^h_{i-1/2}}{\Delta x_{i-1/2}} + \frac{\nu^h_{i+1/2}}{\Delta x_{i+1/2}}\right] u_i \\ &\quad + \left[\frac{\Delta x_{i+1/2}}{8} - \frac{\nu^h_{i+1/2}}{\Delta x_{i+1/2}}\right] u_{i+1} = \int_{x_{i-1/2}}^{x_{i+1/2}} u_{\text{giv}}\,\mathrm{d}x, \end{aligned} \tag{7}$$

with $\Delta x_{i-1/2} = x_i - x_{i-1}$, $\nu^h_{i-1/2} = \frac{1}{2}(\nu^h_{i-1} + \nu^h_i)$ and $x_{i-1/2} = \frac{1}{2}(x_{i-1} + x_i)$, $\forall i$.

Eq. (6) is also discretized at the boundaries, using constant extrapolations of Δx, u and E outside the domain and an incompatible finite difference approximation for the second derivative. The effect of this inevitable deviation from the compatible approach is not clear yet.

Error E is determined in an analogous way, by solving the system of equations

$$\left(\tfrac{1}{8} - c_E\right)(E_{i-1} + E_{i+1}) + \left(\tfrac{3}{4} + 2c_E\right)E_i = \frac{1}{\Delta\xi}\int_{\xi_{i-1/2}}^{\xi_{i+1/2}} \left|D_\xi^{u,x}\right| \mathrm{d}\xi, \tag{8}$$

where the integral in the right-hand side is evaluated using central finite differences and a three-point trapezium integration rule. The boundary conditions of (8) are constructed in a way similar to those of Eq. (7).

Contrary to u, the smoothing of E is performed in computational space, using a constant smoothing coefficient c_E. This is a crucial part of the algorithm; non-smoothness of $D_\xi^{u,x}$ indicates the presence of relatively large error terms of $\mathrm{O}(\Delta\xi^4)$, which were assumed to be negligible and have to be suppressed under all circumstances to avoid interaction with the numerical solution. The smoothing procedure of (8) is the same as the one proposed by Dorfi and Drury [1], and has been used frequently in grid adaptation. Here it is used for the adaptive smoothing of the solution as well.

Discretization error $D_\xi^{u,x}$ will be measured in the L_1 norm, so that it behaves like $\mathrm{O}(\Delta x)$ in the vicinity of discontinuities. This ensures a meaningful error behavior as a function of the grid size, and is consistent with the maximum possible local order of accuracy of any discretization method. The error-minimizing adaptive grid problem for discretization (7) can be stated as

$$\text{solve: } \min_{x_j} \left\| D_\xi^{u,x} \right\|_1. \tag{9}$$

Assuming that $D_\xi^{u,x}$ is $\mathrm{O}(\Delta\xi^2)$, we found that L_1 error minimization is approximately equivalent to the equidistribution of the L_1 error per grid cell. The assumption is not valid in the neighborhood of steep gradients, but even then error equidistribution can still be applied when not $|D_\xi^{u,x}|$ but rather its smooth equivalent E is equidistributed. This is because the use of E limits the maximum possible stretching of the grid, and hence avoids the occurrence of extremely high, but unstable local grid refinements [1]. Discretization and approximate linearization of this equidistribution principle leads to the iterative grid process

$$\left[\frac{x_\xi^{m,l-1} E^{m,l-1}}{(\Delta\xi^{m,l})^3}\right]_{i-1/2} - \left[\frac{x_\xi^{m,l-1} E^{m,l-1}}{(\Delta\xi^{m,l})^3}\right]_{i+1/2} = 0, \tag{10}$$

i.e., given the grid, solution and the smoothed discretization error at iteration $m, l-1$, the next grid at iteration m, l is determined in computational space. We then obtain the next grid in physical space $[x_i^{m,l}]$ by means of the coordinate transformation at iteration $m, l-1$. This procedure is repeated 5 times per outer iteration m, by transferring solution $u_i^{m,l-1}$ to the next grid by means of a simple and cheap interpolation, followed by the determination of the next smoothed discretization error $E_i^{m,l}$. It was found that this inner grid iteration loop, indicated by the index l, strongly enhances the stability and convergence speed of the outer iteration. The grid at iteration $m, 5$ defines the new coordinate transformation at level $m+1, 0$ that we use to determine the new solution and discretization error at iteration $m+1, 0$ by solving (7) iteratively, after which a new inner grid iteration process is started. The outer grid iteration process begins at iteration $1, 0$ by solving (7) on a uniform grid.

Uniform and adaptive grid results for problem (5) using a grid of 50 finite volumes are shown in the Figs. 1 and 2. The values of the parameters in (7) and (8) were $c_\nu = 10$ and $c_E = 2$, respectively. For this particular problem the adaptive grid converges in about 8 outer iterations to engineering accuracy (maximum relative grid corrections $< 10\%$) and converges linearly to a grid convergence error of less than 10^{-9} in 35 outer iterations.

A comparison of the uniform grid result of Fig. 1 and the adaptive grid result of Fig. 2 shows that the smoothness of the numerical solution with respect to the grid is similar; in both cases discontinuities

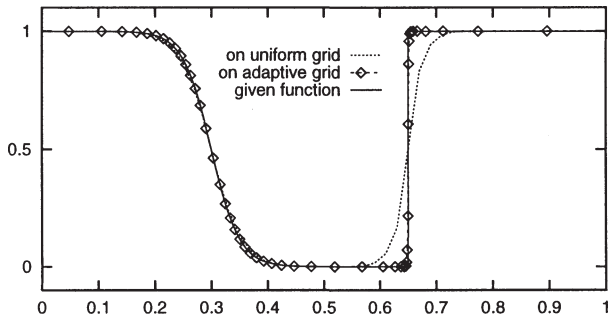


Fig. 1. Numerical solution of problem (5).

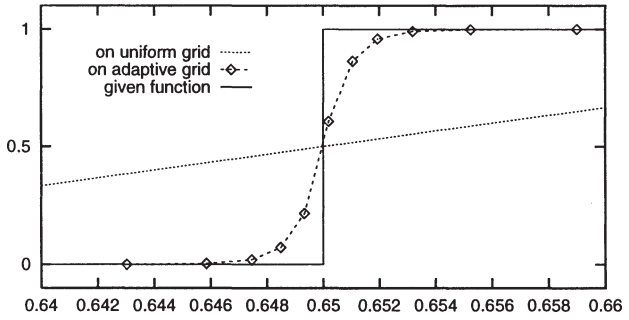


Fig. 2. Numerical solution of problem (5), detail.

are smeared out over about 6 to 7 grid cells. The results are reliable in the sense that the numerical modeling error due to discretization is much smaller than that caused by the known added smoothing. This allows easy modeling error inspection by, e.g., comparing the difference between u and $\overline{u}$ with the error bound of the given function u_{giv}.

In Fig. 3 we present the convergence of numerical solution error $\| u - \overline{u} \|_1$ as a function of the number of finite volumes. The results for uniform and adaptive grid were obtained with the described method, while the "best" fit on a uniform grid was obtained by taking $\nu^h = \frac{1}{8}\Delta x^2$, which results roughly in a nodally exact solution. Despite the added smoothing, the uniform grid result is about as accurate as the best fit. This is the result of the mass matrix in (7), which ensures that for smooth functions the accuracy of the compatible discretization is better (worse in the neighborhood of discontinuities, because of the added smoothing) than that of a nodally exact solution. More important is the difference in behavior of the solution error, which for the best fit is highly irregular and, therefore, not a suitable basis for grid adaptation. This demonstrates clearly the need for a smoothing step.

A considerable gain in accuracy is obtained by applying the error-minimizing adaptive grid algorithm. Fig. 3 shows that grid adaptation leads to a significant increase of the effective *order* of accuracy of the scheme; despite the presence of the discontinuity, the error behavior in the range of 50 to 100 volumes appears to be $\mathrm{O}(N^{-3.8})$, where N is the number of volumes. On a uniform grid it is only $\mathrm{O}(N^{-1})$. This is because moving adaptive grids are especially suited for the calculation of very steep gradients. On the other hand, the asymptotic order of accuracy for smooth solutions is, of course, limited by the order of accuracy of the discretization scheme. So, when more and more

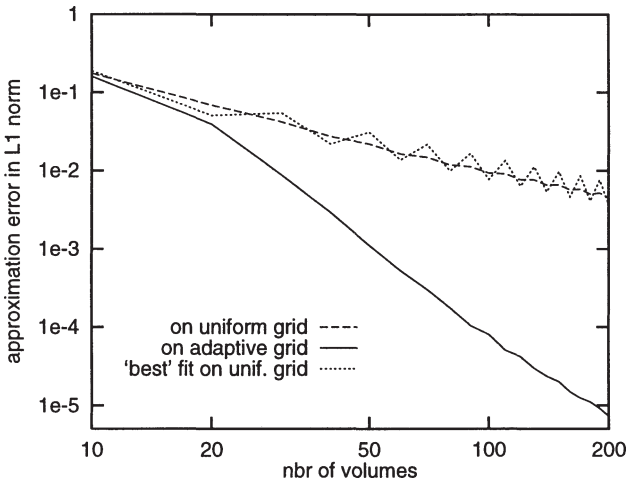


Fig. 3. Numerical solution error of problem (5).

volumes are used, it should slowly reduce to $O(N^{-2})$. This has been verified by solving problem (5) with 400 and 500 volumes, where we found the error behavior to be $O(N^{-2.6})$. However, with 500 volumes the L_1 approximation error is already as small as 5.8×10^{-7}, which is a factor 3.1×10^4 smaller than the error obtained from a uniform grid calculation.

5. Conclusions

Paraphrasing the title of a well-known article by Gresho and Lee, the approach presented in this paper can be summarized by: "suppress the wiggles, but such that they keep telling you something" [5]. The former can be realized by introducing a suitable smoothing for *all* variables to be approximated numerically, and the latter by applying a compatible discretization scheme that allows reformulation of the residual in terms of local modeling errors in the numerical solution and other numerically approximated variables. The stable error-minimizing adaptive grid results that we obtained for a simple test problem confirm the advantages of this two-step modeling approach. The methodology is, however, not easy to apply. Besides the extension to unsteady problems, systems of equations and several dimensions, one of the things to be studied in the future is how to compromise between a rigorous approach and a practical approach.

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