Using Optimal Time Step Selection to Boost the Accuracy of FD Schemes for Variable-Coefficient PDEs

Kevin T. Chu* and James V. Lambers[†]

Abstract—**We extend the technique of optimal time step (OTS) selection for finite difference (FD) schemes of time dependent PDEs to PDEs where the leading-order spatial derivative term has a spatially varying coefficient. The basic approach involves identifying a transformation of the domain that eliminates the spatial dependence of the coefficient for the leading-order term. This change of variables is then used to define an optimal computational grid for the FD scheme on the *original* domain. By using both the optimal grid and OTS selection, we are able to boost the order of accuracy above what would be expected from a formal analysis of the FD scheme. We illustrate the utility of our method by applying it to variable-coefficient wave and diffusion equations. In addition, we demonstrate the viability of OTS selection for the two-step Kreiss-Petersson-Yström discretization of the wave equation.**

Keywords: optimal time step selection, optimal grid selection, finite difference schemes, time dependent PDEs, variable-coefficient PDEs

1 Introduction

Optimal time step (OTS) selection is a surprisingly simple and effective way to boost the order of accuracy of finite-difference (FD) schemes for time-dependent partial differential equations [1]. The basic principle underlying OTS selection is that a careful choice of time step (and the addition of a few correction terms) can boost the *order* of accuracy for formally low-order finite difference schemes. For instance, it is possible to obtain a fourth-order accurate solution of the 1D diffusion equation using only the standard second-order central difference approximation and forward Euler time integration. As demonstrated in [1], OTS selection works for linear and semilinear PDEs in any number of space dimensions on both regular and irregular domains.

Unfortunately, a limitation of the existing formulation of OTS selection is the requirement that the leading-order spatial derivative of the PDE have a constant coefficient. In this paper, we remove this limitation and extend OTS selection to general variable-coefficient semilinear PDEs. Our approach is to identify a transformation of the domain which eliminates the spatial dependence of the coefficient on the leading-order spatial derivative. Using this transformation, we define an optimal computational grid which can be used in conjunction with OTS selection to boost the order of accuracy of formally low-order FD schemes for the PDE. Optimal grid selection is an important extension of the philosophy that the accuracy of numerical methods can be boosted via optimization of the parameters used to compute the solution.

This paper is organized as follows. First, we briefly review OTS selection for PDEs with a constant-coefficient leading-order spatial derivative term. Next, we show how to combine optimal grid and optimal time step selection to boost the accuracy of finite difference schemes for variable-coefficient PDEs. We then demonstrate the use of variable-coefficient OTS selection on the variable-coefficient wave and diffusion equations. Our analysis of the wave is equation is particularly noteworthy because it is *not* based on a one-step time integration scheme. We conclude with a summary of our main results and thoughts on future directions for research.

2 Review of OTS Selection for Constant Coefficient PDEs

Optimal time step selection is not by itself a method for constructing finite-difference schemes. Rather, it is a technique for enhancing the performance of existing FD schemes by carefully choosing the time step to eliminate low-order numerical errors. There are two fundamental ideas underlying OTS selection. First, a judicious choice of time step can be used to eliminate the leading-order terms in the error. Second, the PDE provides valuable insight into the discretization errors for FD schemes. Combining these two simple ideas often yields an optimal time step which can be used to *boost* the order of accuracy of a given FD scheme above what would be expected from

a formal analysis of the scheme.

To illustrate the basic theory behind OTS selection, let us consider the constant-coefficient diffusion equation

$$u_t = Du_{xx} + f(x,t), \tag{1}$$

where D is the diffusion constant and $f(x,t)$ is a source term. Perhaps the simplest FD scheme for this equation uses forward Euler time integration and the standard second-order central difference approximation for the Laplacian:

$$u_j^{n+1} = u_j^n + \Delta t \left(D \left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} \right] + f_j^n \right). \tag{2}$$

This scheme is formally first-order in time and second-order in space. The stability constraint $\Delta t \leq \Delta x^2/2D$ implies that the scheme is $O(\Delta x^2)$ accurate overall.

OTS selection is based on a detailed analysis of the leading-order errors in FD schemes. We begin by deriving the truncation error for the scheme (2). Employing Taylor series expansions and the PDE (1), we find that the true solution satisfies

$$
\begin{aligned}
\tilde{u}_j^{n+1} &= \tilde{u}_j^n + \Delta t \left(D\tilde{u}_{xx} + f \right) \\
&+ \frac{\Delta t^2}{2} \left(D^2 \tilde{u}_{xxxx} + Df_{xx} + f_t \right) + O\left(\Delta t^3\right) \tag{3}
\end{aligned}
$$

and that the central difference approximation for the Laplacian satisfies

$$\frac{\tilde{u}_{j+1}^n - 2\tilde{u}_j^n + \tilde{u}_{j-1}^n}{\Delta x^2} = \tilde{u}_{xx} + \frac{\Delta x^2}{12} \tilde{u}_{xxxx} + O(\Delta x^4). \tag{4}$$

Therefore, the truncation error for (2) is given by

$$
\begin{aligned}
&\tilde{u}_{xxxx} \left[\frac{\Delta x^2}{12} - \frac{D\Delta t}{2} \right] (D\Delta t) - \frac{\Delta t^2}{2} \left(Df_{xx} + f_t \right) \\
&+ O(\Delta t \Delta x^4) + O(\Delta t^3). \tag{5}
\end{aligned}
$$

From this expression, we see that choosing the time step to be $\Delta t = \Delta x^2/6D$ and adding the correction term

$$\frac{\Delta t^2}{2} \left(Df_{xx} + f_t \right) \tag{6}$$

eliminates the leading-order truncation error. Using the heuristic argument that the global error is equal to the local error divided by Δt [2], we find that the numerical solution is $O(\Delta x^4) + O(\Delta t^2) = O(\Delta x^4)$ accurate – the FD scheme has been boosted from second- to fourth-order accuracy.

As shown in [1], this general procedure can be used to boost the accuracy of FD schemes for any semilinear PDE that has a constant coefficient leading-order spatial derivative. It is important to emphasize that variable coefficients and nonlinearities in the lower-order spatial derivative terms do not pose a problem for OTS selection.

3 OTS Selection for Variable-Coefficient PDEs

Transformation of the spatial domain is a natural way to extend OTS selection to semilinear PDEs that have variable-coefficient leading-order spatial derivatives. Consider a semilinear PDE of the form:

$$\frac{\partial u}{\partial t} = a^n(x) \frac{\partial^n u}{\partial x^n} + F\left(\frac{\partial^{n-1}u}{\partial x^{n-1}}, \dots, \frac{\partial u}{\partial x}, u \right) + f(x,t) \tag{7}$$

on the domain $0 < x < 1$. Using the change of variables[1]

$$y = \Phi(x) = \bar{a} \int_0^x \frac{1}{a(\xi)} d\xi \tag{8}$$

with

$$\bar{a} \equiv \left(\int_0^1 \frac{1}{a(\xi)} d\xi \right)^{-1}, \tag{9}$$

we can completely eliminate the spatial dependence of the coefficient on the leading-order spatial derivative (at the expense of adding lower-order variable-coefficient spatial derivative terms). The PDE (7) on the transformed domain has the form

$$\frac{\partial u}{\partial t} = \bar{a}^n \frac{\partial^n u}{\partial y^n} + \tilde{F}\left(\frac{\partial^{n-1}u}{\partial y^{n-1}}, \dots, \frac{\partial u}{\partial y}, u \right) + f(y,t), \tag{10}$$

where $\tilde{F}$ includes any lower-order terms introduced by the process of changing variables.

The change of variables (8) allows us to apply OTS selection in one of two ways. First, we could simply apply OTS selection to the transformed PDE on the transformed domain. An important alternative, however, is to solve the PDE on the *original* domain using a variable spaced grid generated by mapping a uniform grid from the transformed to the original domain. Amazingly, OTS selection can be used to boost the accuracy of natural choices of finite difference schemes defined on this *optimal computational grid*.

Mathematically, these two approaches are equivalent. The former approach is numerically simpler but requires the solution of a more complicated PDE. The latter approach places more complexity on the construction of the FD scheme but requires no modification to the PDE. When using OTS selection, the latter approach is generally superior because it dramatically simplifies the derivation of the correction terms.

3.1 Construction of FD Schemes for Optimal Grid

When constructing FD schemes for the optimal grid on the original domain, it is important to define them as divided differences that use grid points corresponding to the

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[1]This transformation is a generalization of the change of variables proposed in [3] for the wave equation.

ones used on the transformed domain. Doing so ensures that the FD scheme for the PDE on the original domain is compatible with the FD scheme for the transformed PDE on the transformed domain (*i.e.* the FD scheme on the variable spaced grid automatically encapsulates the required transformation of the PDE that result from the change of variables). This compatibility preserves the fortuitous cancellation of errors on the optimal grid even though it is not uniform.

For instance, the generalization of the second-order central difference operator for the 1D Laplacian on a variable spaced grid is

$$
\begin{aligned}
(u_{xx})_i &\approx \frac{1}{(x_{i+1}+x_i)/2 - (x_i+x_{i-1})/2} \\
&\times \left(\frac{u_{i+1}-u_i}{x_{i+1}-x_i} - \frac{u_i-u_{i-1}}{x_i-x_{i-1}} \right) \\
&= \frac{2}{x_{i+1}-x_{i-1}} \left(\frac{u_{i+1}-u_i}{x_{i+1}-x_i} - \frac{u_i-u_{i-1}}{x_i-x_{i-1}} \right), (11)
\end{aligned}
$$

which is essentially a difference of fluxes computed at $(x_{i+1}+x_i)/2$ and $(x_i+x_{i-1})/2$.

3.2 Derivation of OTS Selection and Correction Terms for Optimal Grid

To derive the optimal time step, we apply the procedure presented in [1] to the PDE in the transformed domain (10). However, rather than analyzing the full PDE, we focus only on the simplified PDE containing only the time derivative term and leading-order spatial derivative:

$$
\frac{\partial u}{\partial t} = \bar{a}^n \frac{\partial^n u}{\partial y^n}. \tag{12}
$$

When a uniform grid and standard finite difference schemes are used to solve this PDE on the transformed domain, we find that the optimal time step is given by $\Delta t_{opt} = \alpha(\Delta y/\bar{a})^n$, where α depends on the particular FD scheme used approximate (12). Because the FD schemes on the original and transformed domains are chosen to be compatible, Δt_{opt} is also the optimal time step to use when solving the PDE on the optimal grid.

A more formal way to arrive at the same conclusion is to observe that $\Delta y \approx \bar{a}/a\Delta x$, which follows from (8). Using this approximation to convert Δx's to Δy's in the FD scheme defined on the optimal grid yields an approximation to the leading-order truncation error for the spatial derivative of the form:

$$
\frac{\alpha \bar{a}^n \Delta t \Delta y^n}{2} \frac{\partial^{2n}\tilde{u}}{\partial y^{2n}} = \frac{\alpha a(x)^n \Delta t \Delta x^n}{2} \frac{\partial^{2n}\tilde{u}}{\partial x^{2n}} + \dots, \tag{13}
$$

where the factor of $1/2$ is included for convenience. This observation makes it possible to cancel out the leading-order temporal error

$$
\frac{\Delta t^2}{2} \frac{\partial^2 \tilde{u}}{\partial t^2} = \frac{a(x)^{2n} \Delta t^2}{2} \frac{\partial^{2n}\tilde{u}}{\partial x^{2n}}. \tag{14}
$$

by choosing $\Delta t = \alpha \Delta x^n / a(x)^n = \alpha(\Delta y/\bar{a})^n$.

To boost the accuracy, we also need to derive the appropriate correction terms. When working on the transformed domain, we simply follow the procedure described in [1]. However, when working on the original domain using the optimal mesh, the analysis is more complicated and generally depends on the details of the FD scheme and PDE. The main challenge is deciding which terms of the leading-order temporal error are not cancelled out by the choice of time step.

Fortunately, a simple heuristic can be used to derive the correction terms. When deriving u_{tt}, each spatial derivative term in the PDE (on the original domain) gives rise to several potential correction terms. We conjecture that of these candidates, we need only retain those terms involving spatial derivatives of u with order not exceeding the order the originating spatial derivative term in the PDE. As a concrete example, consider a term in the PDE involving u_x. The corresponding correction terms should only involve u_x and u but not u_{xx} or higher derivatives. While this assertion has yet to be proven, it seems to hold for the PDEs we have examined.

4 Application to Model Problems

4.1 Variable-Coefficient Wave Equation

In this section, we apply OTS and optimal grid selection to the variable-coefficient wave equation. Because we choose a FD scheme based on the Kreiss-Petersson-Yström discretization scheme for the wave equation [4], we begin by analyzing OTS selection for the constant-coefficient wave equation and demonstrate its applicability to this multistep method.

OTS Selection for the KPY Discretization of the Constant-Coefficient Wave Equation

In [4], Kreiss, Petersson, and Yström analyzed the following direct discretization of the second-order wave equation, $u_{tt} - c^2 u_{xx} = f$, without conversion to a first-order system of equations:

$$
\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2 \left(\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \right) + f. \tag{15}
$$

They showed that it is second-order accurate in space and time with a stability constraint of the form $\Delta t = O(\Delta x)$.

Since the stability constraint implies that Δt and Δx are not truly independent numerical parameters, it is beneficial to use OTS selection to optimally choose the time step as a function of the grid spacing[2].

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[2]We choose to optimize Δt as a function of Δx (as opposed to Δx as a function of Δt) because time stepping is the most commonly used approach for numerically solving time-dependent PDEs.

To compute the optimal time step and correction terms for this scheme, we follow the procedure outlined in [1] and Section 2. We begin by deriving the truncation error for the scheme. Employing Taylor series expansions, it is straightforward to show that the true solution satisfies

$$\frac{\tilde{u}_i^{n+1} - 2\tilde{u}_i^n + \tilde{u}_i^{n-1}}{\Delta t^2} - \frac{\Delta t^2}{12}\tilde{u}_{tttt} + O(\Delta t^4) =$$
$$c^2 \left(\frac{\tilde{u}_{i+1}^n - 2\tilde{u}_i^n + \tilde{u}_{i-1}^n}{\Delta x^2} - \frac{\Delta x^2}{12}\tilde{u}_{xxxx} + O(\Delta x^4) \right)$$
$$+ f. \tag{16}$$

Combining this result with the observation that

$$\tilde{u}_{tttt} = c^4 \tilde{u}_{xxxx} + c^2 f_{xx} + f_{tt}, \tag{17}$$

we find that the truncation error is given by

$$c^2 \frac{\Delta x^2}{12}\tilde{u}_{xxxx} - \frac{\Delta t^2}{12}\left(c^4\tilde{u}_{xxxx} + c^2 f_{xx} + f_{tt}\right)$$
$$+ O(\Delta x^4) + O(\Delta t^4). \tag{18}$$

Thus, we can eliminate the leading-order term in the discretization error by choosing $\Delta t = \Delta x / c$ and adding the correction term

$$\frac{\Delta t^2}{12}\left(c^2 f_{xx} + f_{tt}\right) \tag{19}$$

to the right-hand side of (15).

With this choice of time step and correction term, the local truncation error is $O(\Delta t^6) + O(\Delta x^4 \Delta t^2)$. Using the heuristic for two-step methods that the global error should be approximately $1/\Delta t^2$ times the local error leads to a global error of $O(\Delta x^4) = O(\Delta t^4)$. That is, using OTS selection boosts the order of accuracy of the KPY scheme from second- to fourth-order. Figure 1 demonstrates that the expected accuracy is indeed achieved by applying OTS to the KPY scheme.
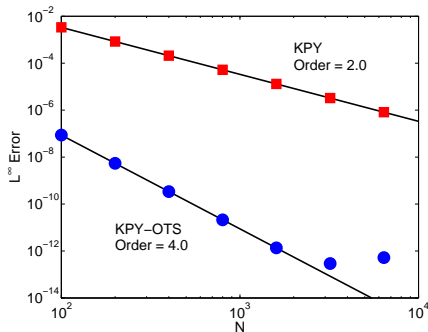

Figure 1: L^∞ error as a function of number of grid points for the KPY discretization of the second-order wave equation on with OTS selection (blue circles) and without OTS selection (red squares).

High Accuracy Required for First Time Step   For the KPY discretization of the wave equation, it is critical that a high-order accurate method is used to perform the first time step because the error introduced during this step affects the global error at all times. Specifically, for the error of the KPY scheme to be $O(\Delta x^p)$, the numerical solution at the first time step must be accurate to $O(\Delta x^{p+1})$. In other words, the error introduced by the first time step must be at least one order of accuracy higher than desired for the overall solution.

We can understand this need for higher-order accuracy of the first time step by solving the difference equation

$$\frac{\hat{e}^{n+1} - 2\hat{e}^n + \hat{e}^{n-1}}{\Delta t^2} = \Delta t^2 \lambda \hat{e}^n, \tag{20}$$

for the normal modes of the error, where $\hat{e}$ is the coefficient of an arbitrary normal mode of the spatial operator for the error $e \equiv u - \tilde{u}$. The solution of this equation is [5]

$$\hat{e}^n = \hat{e}^1 \frac{\kappa_+^n - \kappa_-^n}{\kappa_+ - \kappa_-} + \hat{e}^0 \kappa_+ \kappa_- \frac{\kappa_+^{n-1} - \kappa_-^{n-1}}{\kappa_+ - \kappa_-}, \tag{21}$$

where $\kappa_\pm$, the roots of the characteristic equation for (20), are given by [4]

$$\kappa_\pm = 1 + \frac{1}{2}\lambda\Delta t^2 \pm \Delta t\sqrt{\lambda + \frac{\lambda^2 \Delta t^2}{4}}. \tag{22}$$

Notice that the denominator of both terms in (21) is $O(\Delta t)$. As a result, the global error is always at least one temporal order of accuracy less than the error in the initial conditions. Therefore, the initial errors e^0 and e^1 must be $O(\Delta t^{p+1})$ in order to for the solution to be $O(\Delta t^p)$. For KPY without OTS selection, this observation indicates that the first time step should be at least third-order accurate, which is exactly the way that Kreiss *et. al.* chose to compute the first time step in [4]. Because the OTS selection transforms KPY into a fourth-order accurate scheme, we require that the first time step is at least fifth-order accurate.

It is straightforward to construct a fifth-order approximation for the first time step by using a fifth-order Taylor series expansion in time:

$$u^1 = u^0 + \Delta t u_t^0 + \frac{\Delta t^2}{2}u_{tt}^0 + \frac{\Delta t^3}{6}u_{ttt}^0 + \frac{\Delta t^4}{24}u_{tttt}^0$$
$$= u^0 + \Delta t u_t^0 + \frac{\Delta t^2}{2}\left(c^2 u_{xx}^0 + f\right)$$
$$+ \frac{\Delta t^3}{6}\left(c^2 \left(u_t\right)_{xx}^0 + f_t\right)$$
$$+ \frac{\Delta t^4}{24}\left(c^4 u_{xxxx}^0 + c^2 f_{xx} + f_{tt}\right). \tag{23}$$

Note that sufficiently high-order accurate finite difference stencils may be used to compute some of the higher order terms in this expression. However, when advancing the

solution using the optimal time step, special care must be exercised if finite differences are used to compute the derivatives in (23) because higher-order terms may be automatically (implicitly) included by lower-order terms in the expansion.

OTS Selection for Variable-Coefficient Wave Equation

We now consider the variable-coefficient second-order wave equation

$$u_{tt} - c(x)^2 u_{xx} = f, \qquad (24)$$

on the domain $0 < x < 1$. Using the change of variables defined in (8) and (9), we can transform (24) into the constant-coefficient wave equation

$$u_{tt} = \bar{c}^2 u_{yy} - \bar{c}c' u_y + f, \qquad (25)$$

where $c' = dc/dx$.

OTS Selection on Transformed Domain On the transformed domain, it is straightforward to apply OTS selection because the leading-order spatial derivative has a constant coefficient. If we use second-order central differences for both the Laplacian and gradient terms (on a uniform grid in the transformed domain), the optimal time step is $\Delta t_{opt} = \Delta x/\bar{c}$ and the correction term, which is calculated by identifying the terms in $(\Delta t^2 \tilde{u}_{tttt}/12)$ that are not eliminated by the use of Δt_{opt}, is given by

$$\frac{\Delta t^2}{12} \left(\begin{array}{c} -2\bar{c}^3(c')_y u_{yy} - \bar{c}^3(c')_{yy} u_y + \bar{c}^2(c')^2 u_{yy} \\ + \ \bar{c}^2 c'(c')_y u_y + \bar{c}^2 f_{yy} - \bar{c}c' f_y + f_{tt} \end{array} \right). \quad (26)$$

Using the optimal time step and the correction term, we obtain a fourth-order accurate KPY scheme for the variable-coefficient wave equation (see Figure 2). As mentioned earlier, a fifth-order accurate first time step is required to achieve this level of accuracy.

OTS Selection with Optimal Grid While applying OTS selection to the equation on the transformed domain yields the desired boost in order of accuracy, the lower-order spatial derivative and the correction term are tedious to deal with. It is more convenient to work on the original domain but optimally choose the grid so that use of an optimal time step still leads to fortuitous cancellation of the leading-order error.

Following the procedure outlined in Section 3, we define the location of the grid points in the optimal grid by mapping a uniform grid in the y-domain back to the x-domain and use the generalized finite difference approximation for the Laplacian (11). The optimal time step for the optimal grid is given by $\Delta t_{opt} = \Delta y/\bar{c}$, where Δy is the grid spacing in the y-domain.
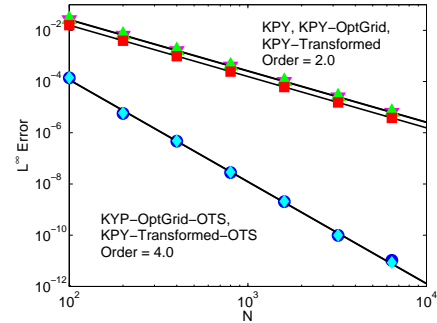

Figure 2: L^∞ error as a function of number of grid points for various KPY discretizations of the variable-coefficient second-order wave equation: KPY using a uniform grid on the original domain (red squares), KPY using a uniform grid on the transformed domain (green triangles), KPY using the optimal grid without OTS selection the original domain (magenta triangles), KPY using a uniform grid with OTS selection on the transformed domain (cyan diamonds), KPY using the optimal grid with OTS selection on the original domain (blue circles). Note that the green triangles overlap the magenta triangles and the cyan diamonds overlap the blue circles.

The required correction term can be derived by first computing u_{tttt} on the original domain

$$u_{tttt} = c^4 u_{xxxx} + 2c^2(c^2)_x u_{xxx} + c^2(c^2)_{xx} u_{xx} + c^2 f_{xx} + f_{tt}. \qquad (27)$$

Using the heuristic mentioned in Section 3.2, the terms involving u_{xxxx} and u_{xxx} are eliminated through the use of the optimal time step. Thus, the correction term is

$$\frac{\Delta t^2}{12} \left[c^2(c^2)_{xx} u_{xx} + c^2 f_{xx} + f_{tt} \right]. \qquad (28)$$

As shown in Figure 2, by using the optimal grid, optimal time step, and the correction terms, we are able to obtain a fourth-order accurate scheme for the variable-coefficient wave equation on the original domain. The error on the variable-spaced grid is almost identical to the error obtained when solving the equation on the transformed domain.

4.2 Application to Variable-Coefficient Diffusion Equation

In this section, we apply OTS and optimal grid selection to the variable-coefficient diffusion equation

$$u_t = (D(x)u)_{xx} + f(x, t), \qquad (29)$$

on the domain $0 < x < 1$. Note that we have expressed diffusion in a spatially inhomogeneous medium using the Fokker-Planck diffusivity law [6], which has been shown to often be more physically correct than Fick's law.
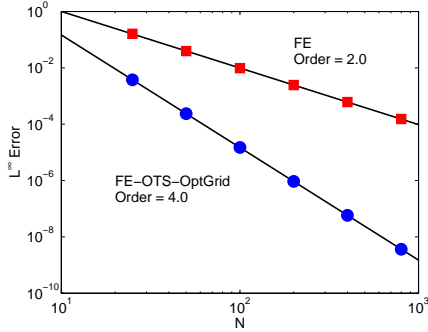
Figure 3: L^∞ error as a function of number of grid points with OTS/Optimal Grid selection (blue circles) and on a uniform grid without OTS selection (red squares).
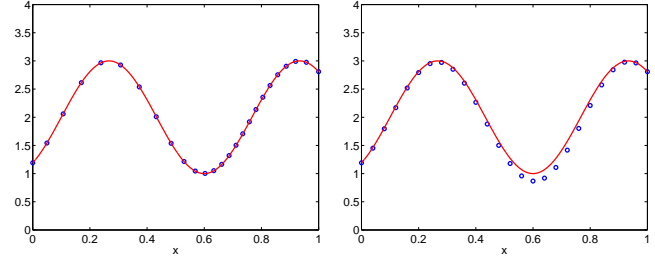

Figure 4: Comparison of numerical solutions for the variable-coefficient diffusion equation (29) computed using the optimal grid and OTS selection (left) and a uniform grid without OTS selection (right). Both figures compare the analytical solution (solid line) with the numerical solution (circles) computed using 25 grid points.

Following the procedure outlined in Section 3, the change of variables used to define the optimal grid is given by $y = \bar{d} \int_0^x D(\xi)^{-1/2} d\xi$ where $\bar{d} = \left(\int_0^1 D(\xi)^{-1/2} d\xi \right)^{-1}$. Since the optimal time step for the constant coefficient diffusion equation is given by $\Delta t_{opt} = \Delta x^2/6D$, the optimal time step for the variable-coefficient diffusion equation is given by $\Delta t_{opt} = \left(\Delta y/\bar{d} \right)^2/6$. The correction term for this scheme is

$$\frac{\Delta t^2}{2} \left[\begin{array}{c} 6DD_{xx}u_{xx} + 4DD_{xxx}u_x + DD_{xxxx}u + Df_{xx} \\ + 6D_x D_{xx} u_x + 2D_x D_{xxx} u + 2D_x f_x \\ + D_{xx}u_t + f_t \end{array} \right] \quad (30)$$

which is derived by computing u_{tt} and using the heuristic described in Section 3.2 to exclude the following terms:

$$D^2 u_{xxxx} \ , \ 4DD_x u_{xxx} \ , \ 2D_x D u_{xxx} \ , \ 6\left(D_x \right)^2 u_{xx}. \quad (31)$$

Combining the optimal grid, optimal time step, and the correction term, we are able to obtain fourth-order solutions for (29) using only a formally second-order FD scheme (see Figure 3). Figure 4 shows a comparison of solutions computed with and without the optimal grid and OTS selection.

5 Summary and Conclusions

In this paper, we have extended the philosophy of optimizing the parameters of FD schemes (*e.g.* the time step size) for accuracy to the selection of the computational grid. In particular, we have presented a method to boost the order of accuracy of FD schemes for PDEs where the leading-order spatial derivative has a variable coefficient by using an optimal time step and an optimal grid. We have described the basic procedure for constructing the optimal grid, computing the optimal time step, and deriving the required correction terms. To demonstrate the power of these techniques, we have applied them to the variable-coefficient wave equation and the Fokker-Planck form of the diffusion equation in an inhomogeneous medium. Our analysis of the KPY scheme (used

to solve the wave equation) also serves as an example of OTS selection applied to multistep time integration schemes.

5.1 Future Work

An important direction for future work is the generalization of the current work to PDEs in higher spatial dimensions. We believe that the use of a change of variables may still be viable. However, we may need to allow for a change in the shape of domain and the possibility that the optimal grid may no longer be orthogonal. Both of these issues complicate the construction of the finite difference scheme on the original domain.

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