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On the characterization of finite differences "optimal" meshes *

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Abstract

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Regridding methods has become an important tool in the integration of PDE systems whose solutions exhibit sharp transitions in spatial derivatives. This paper improves the results presented in an earlier contribution of the author and F. Oliveira (1988). Theoretical justifications of finite differences regridding criteria for the transport and heat equations are presented. The nonuniform meshes in the physical space are generated by the use of coordinate transforms which map them into uniform meshes in the computational space. After the two mesh systems have been generated two approaches are used for solving the PDE: to construct the approximations on the uniform mesh in the computational space or to construct the finite-difference approximations on the nonuniform mesh in the physical space. In this paper we are concerned with the question of the relationship between the two approaches, namely the characterization of the mesh density (coordinate transform) which improves the spatial accuracy of the approximation in the physical (computational) space.

Keywords: Finite differences, computational space, physical space, truncation error.

1. Introduction

A large class of physical problems is described by time-dependent systems of partial differential equations (PDEs) whose solutions exhibit sharp transitions in spatial derivatives. Regridding methods has become an important tool in the integration of such systems. In fact, past experience proved that they give high accuracy, reliability and robustness per computational cost, essentially because they avoid the use of excessive numbers of mesh points. In the recent numerical analysis literature various principles of regridding methods have been proposed and tested. We can mention without being exhaustive [1–5,8,10,11]. However, there is an increasing gap between the practical use of these methods and its theoretical justification. In fact, in most works, the very convincing numerical results are only accompanied by empirical justifications of the proposed criteria.

The nonuniform spatial meshes, used by regridding techniques, in the physical space are commonly generated by the use of coordinate transforms which map them into uniform meshes

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in the transformed space. After the two mesh systems have been generated two approaches are used for solving the PDE: to construct the spatial approximations on the uniform mesh in the computational space, or to construct the finite-difference approximations on the nonuniform mesh in the physical space. In the first case centered finite-difference operators provide second-order approximations, but the transformed PDE to be solved is generally more complicated than the original one. In the second case, if finite-difference approximations are used on the nonuniform mesh of the physical space, the original PDE is solved but the finite-difference operators do not yield formal second-order approximations. In this paper we are concerned with the question of the relationship between the two approaches, namely the characterization of the mesh density (coordinate transform) which improves the accuracy of the approximation in the physical space (computational space). The approach considered here follows our earlier contributions [6,7], where we were concerned with a theoretical justification of adaptive regridding for spatial finite-difference approximations of PDE solutions. The main idea was to introduce a continuous description of the mesh via a C^∞-transformation. This transformation was then used to transport the initial PDE posed in a physical space with a nonuniform mesh, into a computational space where an equally spaced mesh of stepsize h is defined. When the problem was posed in the computational space we studied the dependence of the spatial truncation error on the coordinate transform. Namely for the transport and the convection-diffusion equations we gave a characterization [6,7] of the coordinate transform associated with an $O(h^4)$ spatial truncation error in the computational space. This was done by exhibiting a particular solution of the auxiliary PDE that describes the annulment of the h^2 truncation error coefficient.

However in these works only the spatial truncation error of the transported problem, in the computational space, was studied. The questions concerning the accuracy of the problem in the physical space like the order of accuracy and the spatial truncation error of the original problem, when solved in a nonuniform mesh defined by the coordinate transform, were not studied.

To answer such questions we follow the ideas in [6,7] and construct general solutions of both the auxiliary PDE which describe the annulment of the truncation error coefficients of order two, respectively in the physical and computational spaces. We observe that in order to clarify the exposition we limit ourselves to the study of the transport and heat equations. For other linear equations, as the convection-diffusion or the wave equation, the study would follow the same lines.

The paper is organized as follows. In Section 2 after recalling the study of the simple transport equation we present the characterization of an "optimal mesh" which yields a spatial fourth-order finite-difference algorithm. We also prove that this "optimal mesh" corresponds to a coordinate transform which annuls the spatial truncation error coefficient of order two in the computational space. In Section 3 we study the case of the heat equation and finally in Section 4 we present some conclusions.

2. The transport equation

In this section we study the simple transport equation

$$\begin{cases} \dfrac{\partial u}{\partial t} = -\alpha_1 \dfrac{\partial u}{\partial x}, & \text{in } \Omega \subset \mathbb{R}, \\ B(u) = 0, & \text{on } \partial\Omega, \end{cases} \tag{2.1}$$

with initial conditions $u(x, 0) = f(x)$, $\forall x \in \Omega$, and where $\alpha_1 > 0$ and B represents a boundary operator. We consider an auxiliary C^∞-function defined in $\Omega^* \subset \mathbb{R}$,

$$\begin{cases} g: \Omega^* \to \Omega, \\ x = g(\xi), \end{cases} \tag{2.2}$$

and we recall the following definition [7].

Definition 2.1. Let $g: \Omega^* \to \Omega$ be a function of $C^\infty(\Omega^*)$, such that $g'(\xi) \neq 0$ in Ω^*. Let G^* be an equally spaced mesh defined in Ω^* and $G = g(G^*)$. We define the *density* of the mesh G in a point $x = g(\xi)$ as $1/g'(\xi)$, represented by $d(\xi)$.

Remark 2.2. We observe that in fact for each t we define a coordinate transform g. This means that (2.2) could be viewed as a coordinate transform

$$g^t: \Omega^* \to \Omega$$

and that we are dealing with a family $\{g^t\}_{t \geq 0}$ of functions depending on a parameter t; this kind of coordinate transform is appropriate to the study of the spatial truncation error. To simplify the notations we have omitted the parameter t.

We associate problem (2.1) to the transported problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = -\alpha_1 \dfrac{\partial u}{\partial \xi} \dfrac{1}{g'(\xi)}, & \text{in } \Omega^*, \\ B^*(u) = 0, & \text{on } \partial\Omega^*, \end{cases} \tag{2.3}$$

where B^* is the boundary operator associated with B.

We begin by studying the spatial truncation error in the computational space where two cases will be treated. First we will assume that the coordinate transform g can be exactly computed and secondly we will work under the more realistic assumption that g is not exactly known. Finally we present the study of the spatial truncation error in the physical space.

2.1. Study of the spatial truncation error in the computational space

Let h be the steplength used in the discretization of the spatial derivative in (2.3). We represent the mesh G^* in Ω^* by $\{\xi_i\}_{i=1}^N$.

2.1.1. Computation of the spatial truncation error under the assumption that g can be exactly computed

We discretize the spatial derivative in (2.3) with central finite differences and define the spatial truncation error associated with (2.3) as

$$\tilde{T}_c = -\tfrac{1}{6} h^2 \frac{\alpha_1}{g'(\xi)} \left(\frac{\partial^3 u}{\partial \xi^3} \right) + \bar{T}, \tag{2.4}$$

provided that u is enough smooth and where $\bar{T} = O(h^4)$.

Equation (2.4) is easily established from the Taylor expansions

$$u(\xi_i + h, t) = u(\xi_i, t) + h\frac{\partial u}{\partial \xi}(\xi_i, t) + \frac{h^2}{2!}\frac{\partial^2 u}{\partial \xi^2}(\xi_i, t) + \frac{h^3}{3!}\frac{\partial^3 u}{\partial \xi^3}(\xi_i, t) + \mathrm{O}(h^4)$$

and

$$u(\xi_i - h, t) = u(\xi_i, t) - h\frac{\partial u}{\partial \xi}(\xi_i, t) + \frac{h^2}{2!}\frac{\partial^2 u}{\partial \xi^2}(\xi_i, t) - \frac{h^3}{3!}\frac{\partial^3 u}{\partial \xi^3}(\xi_i, t) + \mathrm{O}(h^4).$$

To characterize a coordinate transform such that

$$\tilde{T}_c = \mathrm{O}(h^4), \tag{2.5}$$

we conclude from (2.4) that we must solve

$$\frac{\partial^3 u}{\partial \xi^3} = 0. \tag{2.6}$$

As the general solution of (2.6) is

$$\frac{\partial u}{\partial \xi} = C(t)\xi + \bar{C}(t), \tag{2.7}$$

where $C(t)$ and $\bar{C}(t)$ are functions of the time, we proposed in [7] the coordinate transform to be defined by the particular solution associated with $C(t) = 0$, that is,

$$\frac{\partial u}{\partial x} = \bar{C}(t)d(\xi), \quad x = g(\xi), \tag{2.8}$$

where $d(\xi) = 1/g'(\xi)$.

However, we can characterize the coordinate transform (the mesh density) in a more realistic way such that it involves higher derivatives of the solution. In fact from (2.6) we have

$$\frac{\partial^2 u}{\partial \xi^2} = C(t), \tag{2.9}$$

where $C(t)$ represents a function of the time.

As

$$\frac{\partial^2 u}{\partial \xi^2} = \frac{\partial^2 u}{\partial x^2}(g'(\xi))^2 + \frac{\partial u}{\partial x}g''(\xi), \quad \text{for } x = g(\xi), \tag{2.10}$$

we conclude from (2.9), (2.10) and Definition 2.1 that (2.5) is equivalent to

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x}d'(\xi) = C(t)d^2(\xi), \quad \text{for } x = g(\xi). \tag{2.11}$$

We have from (2.11) and provided that $\partial u/\partial x \neq 0$,

$$d'(\xi) = \frac{\partial^2 u/\partial x^2}{\partial u/\partial x} - \frac{C(t)d^2(\xi)}{\partial u/\partial x}, \quad \text{for } x = g(\xi). \tag{2.12}$$

Regridding procedures are essentially "feedback procedures", i.e., the solution is computed in a certain mesh and after that the mesh is adjusted, following some criteria. In this sense we may consider in (2.10) that $\partial^2 u/\partial x^2$ and $\partial u/\partial x$ are known and then (2.12) can be viewed as an ordinary differential equation in d and ξ. Using Picard iterations we can give an approximation for the solution of (2.12) as follows:

$$d(\xi) \approx C_1(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/2} + C_2(t)\int_0^\xi \frac{\partial^2 u/\partial x^2}{\partial u/\partial x}, \tag{2.13}$$

where $C_i(t)$, $i = 1, 2$, are certain functions of the time. We observe that in order to establish (2.13) we considered as a first approximation

$$d_0(\xi) = C_1(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/2}, \tag{2.14}$$

which corresponds to $d'(\xi) = 0$ in (2.12).

The characterization (2.13) has been done under the assumption that g can be exactly computed. But from (2.13) we easily conclude that such an assumption is not realistic, because g' depends on the solution derivatives which are not exactly known.

In what follows we will study in an analogous way the spatial truncation error in the computational space but considering now that there is a truncation error associated with g'.

2.1.2. *Study of the spatial truncation error assuming that g is not exactly known*

Following [6] we introduce the function

$$B(h) = \frac{\text{Ap } u'}{\text{Ap } g'}, \tag{2.15}$$

where Ap u' and Ap g' stand for the central finite-difference approximation of $\partial u/\partial\xi$ and g', respectively. Expanding $B(h)$ in Taylor series, in the neighbourhood of $h = 0$ we have

$$\begin{aligned} B(h) &= \frac{\partial u/\partial\xi + h^2 T_{u'} + h^4 \overline{T}_{u'} + \cdots}{g' + h^2 T_{g'} + h^4 \overline{T}_{g'} + \cdots} \\ &= \frac{\partial u}{\partial\xi}\frac{1}{g'(\xi)} + hB'(0) + \frac{h^2}{2!}B''(0) + \frac{h^3}{3!}B'''(0) + \frac{h^4}{4!}B'''(\bar{h}), \end{aligned} \tag{2.16}$$

where $\bar{h} \in]0, h[$, $T_{u'}$, $T_{g'}$ represent the spatial truncation error coefficients, of order two, associated respectively with $\partial u/\partial\xi$ and g'. The notations $\overline{T}_{u'}$, $\overline{T}_{g'}$ represent the spatial truncation error coefficients of order four. In what follows we will drop the argument ξ from g and its derivatives. After some computations we can conclude that

$$\begin{cases} B'(0) = 0, \\ B''(0) = 2\alpha_1 \dfrac{T_{u'}g' - T_{g'}(\partial u/\partial\xi)}{(g')^2}, \\ B'''(0) = 0. \end{cases} \tag{2.17}$$

The spatial truncation error coefficient is now defined by

$$T_c = \alpha_1 h^2 \frac{T_{u'}g' - T_{g'}(\partial u/\partial\xi)}{(g')^2} + O(h^4).$$

Considering that

$$T_{u'} = -\frac{1}{6}\frac{\partial^3 u}{\partial \xi^3} \quad \text{and} \quad T_{g'} = -\tfrac{1}{6}g'''$$

and replacing in this last expression we obtain

$$T_c = -\tfrac{1}{2}\alpha_1 h^2 \frac{(\partial^3 u/\partial \xi^3)g' - g'''(\partial u/\partial \xi)}{(g')^2} + O(h^4). \tag{2.18}$$

As

$$\frac{\partial u}{\partial \xi} = \frac{\partial u}{\partial x} g'$$

and

$$\frac{\partial^3 u}{\partial \xi^3} = \frac{\partial^3 u}{\partial x^3}(g')^3 + 3\frac{\partial^2 u}{\partial x^2} g' g'' + \frac{\partial u}{\partial x} g''',$$

we finally have from (2.18)

$$T_c = -\tfrac{1}{6}\alpha_1 h^2 \frac{(\partial^3 u/\partial x^3)(g')^4 + 3(\partial^2 u/\partial x^2)(g')^2 g''}{(g')^2} + O(h^4). \tag{2.19}$$

In order to obtain an approximation of order four we must have

$$\frac{\partial^3 u}{\partial x^3}(g')^2 + 3\frac{\partial^2 u}{\partial x^2} g'' = 0 \tag{2.20}$$

and integrating we easily obtain

$$\frac{1}{g'} = C(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/3}, \tag{2.21}$$

where $C(t)$ represents a function of the time. We remark that we represent the functions of the time indistinctly by $C(t)$. The characterization (2.21), of the coordinate transform g', guarantees that the approximation in the computational space is of order four. The question now arises what happens to the spatial accuracy of problem (2.1) when the nodes of the nonuniform mesh are chosen so as to satisfy (2.21). What is the real accuracy of the approximation? Can we achieve an order four?

2.2. Study of the spatial truncation error in the physical space

Let us consider a grid $\{x_i\}_{i=1}^N$ defined in the physical space by the coordinate transform g, that is $x_i = g(\xi_i)$, $i = 1, \ldots, N$. Representing $x_{i+1} - x_i$ by Δx_i^+ and $x_i - x_{i-1}$ by Δx_i^- we have

$$x_{i\pm1} = x_i \pm g'(\xi_i)h + \tfrac{1}{2}g''(\xi_i)h^2 \pm \tfrac{1}{6}g'''(\xi_i)h^3 + O(h^4) \tag{2.22}$$

and consequently, dropping the indices i in Δx_i^+ and Δx_i^- and ξ_i, we have

$$\Delta x^+ = g'(\xi)h + \tfrac{1}{2}g''(\xi)h^2 + \tfrac{1}{6}g'''(\xi)h^3 + O(h^4), \tag{2.23}$$

$$\Delta x^- = g'(\xi)h - \tfrac{1}{2}g''(\xi)h^2 + \tfrac{1}{6}g'''(\xi)h^3 + O(h^4). \tag{2.24}$$

Considering that

$$\frac{(\Delta x^+)^3 + (\Delta x^-)^3}{\Delta x^+ + \Delta x^-} = (\Delta x^+)^2 + (\Delta x^-)^2 - \Delta x^+ \, \Delta x^-$$

and replacing (2.23), (2.24) in

$$\frac{u(x_i + \Delta x^+, t) - u(x_i - \Delta x^-, t)}{x_{i+1} - x_{i-1}} = \frac{\partial u}{\partial x}(x_i, t) + \tfrac{1}{2}(\Delta x^+ - \Delta x^-)\frac{\partial^2 u}{\partial x^2}(x_i, t) + \tfrac{1}{6}\left[(\Delta x^+)^2 + (\Delta x^-)^2 - \Delta x^+ \, \Delta x^-\right]\frac{\partial^3 u}{\partial x^3}(x_i, t) + \cdots, \tag{2.25}$$

we obtain

$$\frac{u(x_i + \Delta x^+, t) - u(x_i - \Delta x^-, t)}{x_{i+1} - x_{i-1}} = \frac{\partial u}{\partial x}(x_i, t) + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} g'' h^2 + \frac{1}{6}\frac{\partial^3 u}{\partial x^3}(g')^2 h^2 + O(h^4). \tag{2.26}$$

Observing (2.25) we deduce that the truncation error of problem (2.1) in the physical space is formally of the first order in Δx but second-order accurate in h and is defined by

$$T_{\mathrm{PH}} = -\tfrac{1}{2}\alpha_1 h^2 \left[\frac{\partial^2 u}{\partial x^2} g'' + \frac{1}{3}\frac{\partial^3 u}{\partial x^3}(g')^2\right] + O(h^4). \tag{2.27}$$

In order to obtain an $O(h^4)$ approximation in the physical space, we solve the auxiliary equation

$$3\frac{\partial^2 u}{\partial x^2} g'' + \frac{\partial^3 u}{\partial x^3}(g')^2 = 0. \tag{2.28}$$

Considering Definition 2.1, (2.28) is equivalent to

$$d'(\xi) = \frac{1}{3}\frac{\partial^3 u/\partial x^3}{\partial^2 u/\partial x^2}. \tag{2.29}$$

Finally integrating (2.29) as an ordinary differential equation in d and ξ we have

$$d(\xi) = C(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/3}. \tag{2.30}$$

From (2.21) and (2.30) we conclude that we can construct $O(h^4)$ spatial approximations both in the computational space and in the physical space. As the coordinate transform g, which annuls the h^2 truncation error coefficient in the computational space (2.19), defines a mesh density in the physical space which is a solution of (2.28), the two approximations can be simultaneously of order four.

We point out that if the truncation error coefficient (2.4) was considered for the transported problem, which corresponds to a transport function exactly known, we would conclude that the h^2 truncation error coefficients of the original and transported problem are equal if and only if $g''' = 0$. This conclusion agrees with [9].

We can summarize the results obtained in this section in the following theorem.

Theorem 2.3. *Let us consider the transport equation* (2.1) *and the associated equation* (2.3). *Then assuming that the solutions of both problems are enough smooth we can state the following assertions.*

(a) *Discretizing the spatial derivatives in* (2.3) *with centered finite-difference approximations, in a uniform mesh of steplength h defined in the computational space, we obtain an accuracy of* h^4 *iff the coordinate transform satisfies*

$$\frac{1}{g'} = C(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/3},$$

where $C(t)$ *is a function of the time.*

(b) *Discretizing the spatial derivatives in* (2.1) *with centered finite differences, in a nonuniform mesh defined in the physical space, the accuracy of the spatial discretization is* h^2. *We obtain an accuracy of* h^4 *iff the mesh density* $d(\xi)$ *satisfies*

$$d(\xi) = C(t)\left(\frac{\partial^2 u}{\partial x^2}\right)^{1/3},$$

where $C(t)$ *is a function of the time.*

3. The heat equation

Let us consider the heat equation

$$\begin{cases} \dfrac{\partial u}{\partial t} = \alpha_2 \dfrac{\partial^2 u}{\partial x^2}, & \text{in } \Omega \subset \mathbb{R}, \\ Bu = 0, & \text{on } \partial\Omega, \end{cases} \tag{3.1}$$

and $u(x, 0) = f(x)$, $\forall x \in \Omega$. In (3.1) α_2 is a positive constant, B is a boundary operator and $f(x)$ a known function.

Using the coordinate transform (2.2) previously defined we associate with problem (3.1) the transported problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = \alpha_2 \left[\dfrac{\partial^2 u}{\partial \xi^2}\left(\dfrac{1}{g'}\right)^2 - \dfrac{\partial u}{\partial \xi}\dfrac{g''}{(g')^3}\right], & \text{in } \Omega^*, \\ B^*(u) = 0, & \text{on } \partial\Omega^*, \end{cases} \tag{3.2}$$

with initial condition $u(\xi, 0) = f \circ g(\xi)$. In (3.2) B^* is the operator associated with B.

In this section we will proceed analogously to Section 2. We begin by proving that the centered finite-difference approximations of (3.2) can achieve order four when g' is judiciously selected.

We also prove that even if the centered difference approximation of the spatial derivative in (3.1), in a nonuniform mesh, in the physical space is formally of order one, it is in fact of second order in h. We present the characterization of the mesh density — in the physical space — which guarantees an accuracy of fourth order in h.

3.1. The spatial truncation error in the computational space

Let us consider problem (3.2) and discretize the spatial derivatives with centered finite-difference approximations of steplength h.

As we already commented in the previous section, the case where the coordinate transform is exactly known is of no practical interest. For this reason we will not consider it in the study of the heat equation.

In order to compute the spatial truncation error associated with a centered finite-difference discretization of (3.2) we define [6]

$$B(h) = \alpha_2 \left[\frac{\text{Ap } u''}{\text{Ap } (g')^2} - \frac{\text{Ap } g'' \text{ Ap } u'}{\text{Ap } (g')^3} \right], \tag{3.3}$$

where Ap u', Ap u'', Ap $(g')^j$, Ap g'' stand respectively for the central finite-difference approximations of $\partial u/\partial\xi$, $\partial^2 u/\partial\xi^2$, $(g')^j$ for $j = 2$, 3 and g''.

Using Taylor expansions we have

$$B(h) = \frac{\partial^2 u/\partial\xi^2 + h^2 T_{u''} + h^4 \overline{T}_{u''} + \cdots}{\left(g' + h^2 T_{g'} + h^4 \overline{T}_{g'} + \cdots\right)^2} - \frac{\left(g'' + h^2 T_{g''} + h^4 \overline{T}_{g''} + \cdots\right)\left(\partial u/\partial\xi + h^2 T_{u'} + h^4 \overline{T}_{u'} + \cdots\right)}{\left(g' + h^2 T_{g'} + h^4 \overline{T}_{g'} + \cdots\right)^3}, \tag{3.4}$$

where $T_{u'}$, $T_{u''}$, $T_{g'}$, $T_{g''}$ ($\overline{T}_{u'}$, $\overline{T}_{u''}$, $\overline{T}_{g'}$, $\overline{T}_{g''}$) represent the spatial truncation error coefficients of order two (four) associated respectively with $\partial u/\partial\xi$, $\partial^2 u/\partial\xi^2$, g' and g''.

After some computations we can establish that the spatial truncation error associated with the discretization is given by

$$T_c = \tfrac{1}{12}\alpha_2 \left(\frac{\partial}{\partial\xi} \left[\frac{\partial^3 u}{\partial\xi^3} \frac{1}{(g')^2} - \frac{\partial u}{\partial\xi} \frac{g'''}{(g')^3} \right] - 3\frac{\partial^2 u}{\partial\xi^2} \frac{g'''}{(g')^3} + 9\frac{\partial u}{\partial\xi} \frac{g'' g'''}{(g')^4} \right)^2 h^2 + O(h^4). \tag{3.5}$$

Returning to the initial configuration, and imposing to the approximation an order four we have

$$\frac{\partial^4 u}{\partial x^4} + 4\frac{\partial^3 u}{\partial x^3} \frac{g''}{(g')^2} - 3\frac{\partial^2 u}{\partial x^2} \frac{(g'')^2}{(g')^2} + 6\frac{\partial u}{\partial x} \frac{g'' g'''}{(g')^5} = 0. \tag{3.6}$$

Unfortunately it is not easy to obtain a characterization for a solution of (3.6). This means that we cannot always guarantee a fourth-order accuracy for the transformed problem in the computational space. This situation is in contrast with what happened with the transport equation where it was always possible to have fourth-order accuracy in the computational space.

We observe, however, that if we assume that g could be exactly computed we would obtain [7] for the spatial truncation error in the computational space

$$\tilde{T}_c = \tfrac{1}{12}\alpha_2 h^2 \frac{\partial}{\partial \xi}\left[\frac{\partial^3 u}{\partial \xi^3}\frac{1}{(g')^2}\right] + O(h^4). \tag{3.7}$$

The characterization of g which annuls the h^2-coefficient of (3.7) would be, also in this case, a difficult task.

3.2. The spatial truncation error in the physical space

Let us consider the same notations as in Section 2. Multiplying by Δx^- and Δx^+ respectively the Taylor expansions of $u(x_i + \Delta x^+, t)$ and $u(x_i - \Delta x^-, t)$ and subtracting them we obtain

$$\begin{aligned}\frac{\Delta x^- u_{i+1} + \Delta x^+ u_{i-1} - (\Delta x^+ + \Delta x^-)u_i}{\frac{1}{2}\Delta x^+\ \Delta x^-(\Delta x^+ + \Delta x^-)} &= \frac{\partial^2 u}{\partial x^2} + \frac{1}{3}\frac{\partial^3 u}{\partial x^3}(\Delta x^+ - \Delta x^-) \\ &\quad + \frac{1}{12}\frac{\partial^4 u}{\partial x^4}\left((\Delta x^+)^2 + (\Delta x^-)^2 - \Delta x^+\ \Delta x^-\right) \\ &\quad + O(\Delta x)^3,\end{aligned} \tag{3.8}$$

where u_{i-1}, u_i, u_{i+1} represent respectively $u(x_{i-1}, t)$, $u(x_i, t)$, $u(x_{i+1}, t)$.

As expected the central finite-difference approximation (3.8) is formally of the first order, when computed in a nonuniform mesh.

Substituting (2.23) and (2.24) in (3.8) we conclude that this approximation is in fact of order two in h, with a truncation error given by

$$T_{PH} = \alpha_2 h^2\left(\frac{1}{3}\frac{\partial^3 u}{\partial x^3}g'' + \frac{1}{12}\frac{\partial^4 u}{\partial x^4}(g')^2\right) + O(h^4). \tag{3.9}$$

We observe that the truncation error in the computational space is different from T_{PH}, the truncation error in the physical space. We investigate now the annulment of the h^2-coefficient in T_{PH} by solving

$$4\frac{\partial^3 u}{\partial x^3}g'' + \frac{\partial^4 u}{\partial x^4}(g')^2 = 0. \tag{3.10}$$

Representing $1/g'$ by $d(\xi)$ and proceeding as previously we easily establish that

$$d(\xi) = C(t)\left(\frac{\partial^3 u}{\partial x^3}\right)^{1/4} \tag{3.11}$$

is a solution of (3.10) where $C(t)$ is a function of the time. As already mentioned we can approximate the derivatives in the physical space or in the computational space. In the case of the heat equation we concluded that while we can easily characterize the mesh density which corresponds to an accuracy of h^4 in the physical space (3.11), the same does not happen in the computational space because (3.6) may have no solution.

We summarize the results of this section in the following theorem.

Theorem 3.1. *We consider the heat equation* (3.1) *and the associated transported equation* (3.2). *Let us assume that the solutions of both* (3.1) *and* (3.2) *are enough smooth.*

(a) *Discretizing the spatial derivatives in* (3.2) *with centered finite-difference approximations in a uniform mesh of steplength h defined in the computational space we obtain an accuracy of* h^4 *iff the coordinate transform verifies* (3.6).

(b) *Discretizing the spatial derivatives in* (3.1), *with centered finite differences* (3.8), *in a nonuniform mesh defined in the physical space the accuracy of the spatial discretization is* h^2. *We obtain an accuracy of* h^4 *iff the mesh density* $d(\xi)$ *is given by*

$$d(\xi) = C(t)\left(\frac{\partial^3 u}{\partial x^3}\right)^{1/4},$$

where $C(t)$ *is a function of the time.*

4. Conclusions

The objective of applying a coordinate transform is to generate a nonuniform mesh in the physical space. In this paper we make a theoretical study of the spatial truncation errors of both the original and the transported problems. For the transport equation the choice between writing finite-difference approximations in the physical space or in the computational space should be based on considerations of computational efficiency. In fact both approximations are second-order accurate in h and can give, under certain conditions, a fourth-order accuracy (Theorem 2.3).

We note that Hoffman [9] states that the h^2 computational and physical truncation error coefficients are the same only if $g''' = 0$. This is a consequence of the fact that this author considers that g is exactly known. In fact in this case the spatial truncation error in the computational space would be given by (2.4). Comparing with the spatial truncation error in the physical space given by (2.27) we would obtain

$$\tilde{T}_c - T_{PH} = \tfrac{1}{6}\alpha_1 h^2 \frac{\partial u}{\partial x}\frac{g'''}{g'} + O(h^4).$$

As far as the heat equation is concerned we can prove that the finite-difference approximation (3.8), in the physical space, while being formally of the first order in Δx is in fact second-order accurate in h. We can also characterize for the original problem the mesh density which gives an accuracy of the fourth order in h. In contrast with what happens in the case of the transport equation we do not know how to characterize explicitly the coordinate transform, if it exists, associated with a truncation error of fourth order, in the computational space.

Summarizing our results the truncation errors of the original and transported problem are second-order accurate in h. For the original problem — for the transport and heat equations — we know the characterization of the mesh density associated with an $O(h^4)$ accuracy. For this last reason, and also because the original problem is generally simpler than the transformed one, computational efficiency considerations would certainly indicate the solution of this last problem as the one to be preferred.

The approach followed here can be used for other PDEs. We note that for the convection-diffusion equation

$$\frac{\partial u}{\partial t} = -\alpha_1 \frac{\partial u}{\partial x} + \alpha_2 \frac{\partial^2 u}{\partial x^2}, \quad \alpha_1, \alpha_2 > 0;$$

if a coordinate transform of type

$$x = g(\xi) + \alpha_1 t \tag{4.1}$$

is used, then (4.1) is easily transformed into (3.2). The conclusions of Theorem 3.1, as far as the computational space is concerned, are true. For the characterization of the mesh density which annuls the h^2 coefficient of the spatial truncation error, in the physical space, some work still must be done.

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