Available online at www.sciencedirect.com
SCIENCE DIRECT®
Advances in Water Resources 27 (2004) 311–322
Advances in Water Resources
www.elsevier.com/locate/advwatres

Single collocation point methods for the advection–diffusion equation ☆

I. Herrera *, M. Díaz-Viera, R. Yates

Instituto de Geofísica, Universidad Nacional Autónoma de México (UNAM), Apartado Postal 22-582, 14000 México, DF, Mexico

Received 19 December 2003; accepted 4 February 2004

Abstract

This article is offered to honor Professor George F. Pinder. Its technical contents were motivated by an Eulerian–Lagrangian method that was recently proposed by him and his collaborators. Two one-node-collocation algorithms, which may be used to advance that method are presented. Although they are here discussed for 1-D problems only, one of them has already been generalized to problems in several space variables. Thus, this paper essentially generalizes the above mentioned Eulerian–Lagrangian method of Pinder et al. to problems in several dimensions. Also, the results presented in this paper have a wider interest in water resources studies because they apply to advection diffusive transport processes in general. The methodology used to develop the new algorithms is a unified theory of domain decomposition methods (DDM), recently introduced by the authors and which owes much to George F. Pinder. The results reported in the present paper illustrate, by the way, its application and power.
© 2004 Elsevier Ltd. All rights reserved.

Keywords: Collocation; Trefftz–Herrera method; Localized adjoint method (LAM); Eulerian–Lagrangian LAM (ELLAM); Domain decomposition method (DDM)

1. Introduction

The subject matter of the present paper is specially adequate for honoring Professor George F. Pinder. On the one hand, it contributes to the development of a methodology initiated recently by Pinder and his collaborators, and on the other hand, to this end it applies a numerical procedure, which owes much to him and which combines collocation with domain decomposition methods (DDM). As it is well known, Pinder has contributed extensively to the progress of collocation methods (see, for example, [1–3]). In addition, as mentioned in the Dedication, he initiated Herrera not only in collocation methods, but in DDM as well. The new method, of Pinder and his collaborators, published in a paper that has just appeared [4], is a novel Eulerian–Lagrangian approach to advection diffusive transport, which applies a non-conventional single point collocation discretization procedure. The present paper contributes to its further development by offering two single point collocation discretization procedures, which allows an improvement in numerical efficiency and generalizes it to several spatial dimensions.

As it is well known, advection–diffusion transport is a process of great interest in water studies. Furthermore, the basic advection–diffusion transport models are constituted by parabolic differential equations in time-dependent problems, and by second order elliptic equations in steady-state problems. In addition, time-dependent problems are dealt with, most frequently, by a semi-discretization approach, as it is done in the method of Pinder and his collaborators. Thus, the numerical solution of elliptic differential equations is a subject of extreme importance in water studies and that is the subject of the research reported in the present paper. In particular, novel collocation approaches are introduced in it.

Collocation methods are known to be very precise and easy to implement, but their application had been

☆ The authors acknowledge the valuable help given by Ernesto Rubio and Luis Ochoa in different aspects of the developments presented in this article and the financial support received from CONACYT and DGAPA (UNAM) through their Projects 32051-A and IN105998, respectively.
* Corresponding author.
E-mail address: iherrera@servidor.unam.mx (I. Herrera).
URL: http://ihrserver.igeofcu.unam.mx/iherrera.

0309-1708/$ - see front matter © 2004 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2004.02.003

restricted mainly because, in the past, in its formulation "splines" with a high degree of regularity had been needed [5–8]. Recently, however, a wide range of applications and new forms of applying collocation have been opened by a unified theory of collocation methods [9] introduced by the authors, whose origin is briefly explained in the Dedication of the present paper. In the setting of this unified theory, the regularity requirements of trial and test functions are very much relaxed and one can apply collocation to functions possessing not only discontinuous derivatives, but as well to functions which are themselves discontinuous. These are referred as "fully" discontinuous functions. For one-dimensional problems and second order differential equations, in the traditional approach, the lowest polynomial degree that is admissible is three, and at least two collocation points in each one of the subintervals are needed. This is due to the high degree of regularity required from the trial functions in that approach. On the other hand, when collocation is carried out in the framework of the unified theory, due to the relaxed regularity requirements, one can use quadratic polynomials and one collocation point, separately in each one of the subintervals, as was pointed out in [10]. This can be done not only in 1-D, but in several dimensions as well [11].

The unified theory classifies domain decomposition methods into two broad categories [12,13]: "direct" and "indirect" (or Trefftz–Herrera) methods. In the present article, two single collocation point methods for the second order differential equations of elliptic type are described: One is derived using the "direct" approach [14] and the other is derived using the "indirect" approach [10,11]. Each one of these algorithms yields tri-diagonal global matrices. Moreover, such matrices are positive definite when the differential operator is symmetric and positive (as for non-advective transport or the flow equations). In the case of the indirect approach, as mentioned before, the results have already been extended to several dimensions [11]. However, up to now, we cannot say the same about the direct approach, although we think it can be done in a similar manner because through our experience we have seen that there is a parallelism between both approaches. In addition, it is worth mentioning that we have found that the indirect approach—paradoxically—is more direct, clear and easy to apply. And this is corroborated in the present paper. In Section 5, only a single arithmetic division is needed for the construction of the special test functions, which the application of the indirect method requires, while the construction of the auxiliary functions of the direct method, in Section 6, requires solving a 2×2 system instead.

In view of what has been said in the first part of this Introduction, the bearing of these results in water resources studies is clear. Firstly, an important element of the Eulerian–Lagrangian method, introduced by Pinder and his collaborators [4], is a single collocation discretization procedure that yields, in one spatial dimension, a five-diagonal matrix. The schemes here presented, on the other hand, yield tri-diagonal matrices. This is a substantial reduction. Even more, the extension to several dimensions of the indirect approach has already been published [11]. It yields, when piecewise linear functions are applied for the interpolation at the internal boundary, systems with only one degree of freedom associated with each node, independently of the dimension [11]. It must be mentioned that this is an outstanding reduction with respect to the standard collocation method for which, using cubic Hermites, the number of degrees of freedom associated with each node grows exponentially with the dimension (2^D): 2 for 1-D, 4 for 2-D and 8 for 3-D.

Secondly, from a more general perspective, any improvements in the numerical treatment of elliptic equations are immediately reflected in progress for water resources studies. In particular, the implications that our results have for the Eulerian–Lagrangian method of Pinder and his collaborators illustrate well this point. In addition, similar remarks apply to the groundwater flow models, with the additional feature that in this latter case, for the steady-state, the differential operators are symmetric and our algorithms yield symmetric positive matrices. This is a significant property that is not enjoyed by the standard collocation methods and it is a very important one, because of many reasons, to mention just one: The application of parallel processing resources becomes much more effective when the matrices involved are symmetric and positive definite. And, we recall that the contributions of parallel processing methods to the growth of the computational capabilities, in recent times, have been extremely significant [15,16].

The paper is organized as follows: Section 2 is devoted to explain, in a rather brief manner, the main ideas of the unified theory of DDM. We think the inclusion of this section in the paper will help unfamiliar readers to get a general perspective of our methods, grasp their scope and be better oriented when applying them. The advective diffusion transport problem to be considered is introduced in Section 3. In Section 4, it is shown that single collocation discretization schemes cannot be more accurate than $O(h^2)$. Sections 5 and 6 are devoted to introduce the results of references [10] and [14] that will be needed for the application of the indirect and direct approaches, respectively. Finite difference procedures, such as those introduced in Sections 5 and 6, only yield information about the sought solution at the nodes and, in order to extend it beyond those points, it is necessary to resort to interpolation methods. The unified theory of DDM, itself, implies an interpolation procedure that is referred as *optimal interpolation*. This is explained in Section 7. It is applicable indistinctly

of the approach, direct or indirect, that is used. Section 8 is devoted to present numerical experiments, and Section 9 to discussion and conclusions.

2. Unified theory of domain decomposition methods

The general theory of collocation methods [9] stems from a unified theory of domain decomposition methods [12] and a brief explanation of its basic idea follows. Consider a boundary value problem—or initial boundary value problem—for a partial differential equation, or system of such equations, formulated in a domain Ω (Fig. 1). Then, given a partition $\Pi \equiv \{\Omega_1, \ldots, \Omega_E\}$ of such a domain, the general problem of domain decomposition methods consists in establishing procedures which permit solving the "global" problem defined in Ω, by solving exclusively "local" problems defined in each one of the subdomains of the partition Ω_i, $i = 1, \ldots, E$. The unified theory of domain decomposition methods considers DDM as procedures for gathering information—about the global solution of the problem—at the internal boundary of the partition Σ, i.e., that which separates the subdomains from each other. In the general method of the unified theory, a target of information on Σ—the *sought-information*—is defined beforehand, such that it is sufficient for defining well-posed local problems, which the global solution must satisfy in each one of the subdomains of the partition Ω_i, $i = 1, \ldots, E$. Then a search is directed to obtaining the *sought-information*. Two very broad categories of procedures for achieving this goal are identified by the theory: "direct" and "indirect" (or Trefftz–Herrera) methods.

In the usual interpretation of direct methods, they are seen as techniques for building the global solution by putting together, just as "bricks", the local solutions. In the unified theory, however, a slightly more sophisticated point of view is adopted, since the local solutions of the differential operator are used to establish compatibility relations that the *sought-information* must fulfill. These relations give rise to the global system of equations, from which the *sought-information* is obtained.

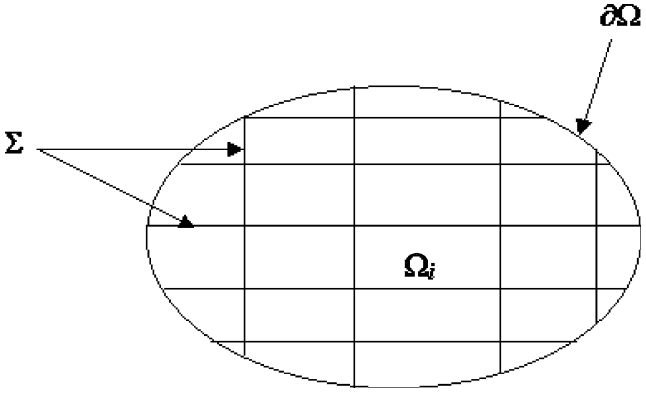

Fig. 1. A partition $\Pi \equiv \{\Omega_1, \ldots, \Omega_E\}$ of the domain Ω.

In Trefftz–Herrera methods, on the other hand, a system of weighting functions of a special kind, with the property of yielding the *sought-information* at the internal boundary, exclusively, is developed and applied. The idea of constructing such test functions stems from the observation that, in the method of weighted residuals, the information about the exact solution that the approximate one contains, depends on the system of weighting functions which is applied [17]. And, in order to fabricate the special test functions, it is necessary to have a procedure for analyzing such dependence. In the theory of indirect domain decomposition methods, the basic ingredient of such analysis are Green–Herrera formulas. These are formulas, which apply when both trial and test functions are fully discontinuous, something that cannot be done when the standard theory of distributions is used. They were originated by Herrera [18,19]. They have already played a fundamental role in establishing the theoretical foundations of a method that is very important in water resources studies; we refer to the Eulerian–Lagrangian Localized Adjoint Method (ELLAM) [20].

Using them, necessary and sufficient conditions that the test functions must fulfill, in order to yield the *sought-information* exclusively, are established. Also, a characterization of the *sought-information* in terms of a variational principle (or weak characterization) is supplied, which holds when test functions of the special kind described above, are applied. This principle constitutes a very general, although abstract, formulation of indirect methods [11]. In addition, techniques to fabricate the special kind of test functions are developed in the theory. Ref. [11] supplies an updated version of indirect domain decomposition methods, where the theory and its applications to problems in several dimensions are discussed with considerable detail. In addition, a plenary lecture of the 14th International Conference on Domain Decomposition Methods was devoted to the indirect method of domain decomposition [21] and further applications can be found in its proceedings [22]. In the applications that have been done thus far, many advantages of TH-Collocation with respect to standard collocation methods have been exhibited [11]. Among others, generally the structure of the global matrix is simpler and, if desired, a significant reduction of the number of degrees of freedom associated with each node can be achieved. A common feature of "direct", when formulated as in the unified theory, and "indirect" methods is that in both, the information about the solution is obtained at the internal boundary exclusively and, consequently, the interpolation functions used to approximate the sought solution are also applied at the internal boundary only. Such information

can be extended to the interior of the subdomains of the partition by a procedure, which is implied by the theory, referred as *optimal interpolation*. This is explained in Section 7.

3. The one-dimensional boundary problem with jumps (BVPJ)

The problem to be considered in this article is the two-point boundary value problem with jump conditions (BVPJ) of the general differential equation of second order in one space variable. It consists of the differential equation

$$\mathscr{L}u \equiv -\frac{\mathrm{d}}{\mathrm{d}x}\left(a\frac{\mathrm{d}u}{\mathrm{d}x}\right)+\frac{\mathrm{d}}{\mathrm{d}x}(bu)+cu = f_\Omega \text{ in } (x_{i-1},x_i), \quad i=1,\ldots,E \tag{1}$$

to be fulfilled in an interval $\Omega \equiv (0,\ell)$;

The boundary conditions, for simplicity, are assumed to be of Dirichlet type

$$u(0)=g_{\partial 0}, \quad u(\ell)=g_{\partial \ell}, \tag{2}$$

together with the jump conditions

$$[u]=j_i^{\,0}\equiv[u_\Sigma] \quad \text{and} \quad \left[\frac{\mathrm{d}u}{\mathrm{d}x}\right]=j_i^{\,1}\equiv\left[\frac{\mathrm{d}u_\Sigma}{\mathrm{d}x}\right], \quad i=1,\ldots,E-1, \tag{3}$$

where the square brackets stand for the "jump" of the function contained inside, i.e., $[u]\equiv u_+-u_-$, limit on the right (u_+) minus limit on the left (u_+).

These latter conditions have to be satisfied at the internal boundary, which for this simple one-dimensional problem, consists of the collection, $\{x_i\}_{i=1}^{E-1}$, of internal nodes of the partition $\Pi\equiv\{(0=x_0,x_1),(x_1,x_2),\ldots,(x_E-1,x_E=\ell)\}$. Observe that the differential equation is required to be satisfied at interior points of the subdomains, only, since the functions considered may be discontinuous at the internal boundary.

This BVPJ is the one-dimensional version of the BVPJ of second order and elliptic type in several dimensions, considered in [11]

$$\mathscr{L}u \equiv -\nabla\cdot(\underline{a}\cdot\nabla u)+\nabla\cdot(\underline{b}u)+cu = f_\Omega, \text{ in } \Omega_i, \quad i=1,\ldots,E-1, \tag{4}$$

$$u=u_\partial \quad \text{on } \partial\Omega, \tag{5}$$

$$[u]=j_\Sigma^0 \quad \text{and} \quad [\underline{a}_n\cdot\nabla u]=j_\Sigma^1 \quad \text{on } \Sigma. \tag{6}$$

It will be assumed that the Dirichlet problem is well-posed in the whole interval $\Omega\equiv(0,\ell)$, as well as is in each one of the subintervals of the partition Π. The notation, $u(x)$, is adopted for the unique solution of this BVPJ, in Ω. In the framework of the unified theory of collocation methods, whose basic ideas were presented in Section 2, throughout this article the *sought-information* is chosen to be, the average of the solution, $\dot{u}\equiv\frac{1}{2}(u_++u_-)$, across Σ. That is, the *sought-information* is the finite sequence $\{\dot{u}_1,\ldots,\dot{u}_{E-1}\}$. Observe that this information, when it is complemented with the data of the problem, is sufficient to define well-posed problems in each one of the subintervals (x_{i-1},x_i), $i=1,\ldots,E$. Indeed, using the relationships

$$u_+=\dot{u}+\frac{1}{2}[u]=\dot{u}+\frac{1}{2}j_i^0 \quad \text{and} \quad u_-=\dot{u}-\frac{1}{2}[u] = \dot{u}-\frac{1}{2}j_i^0 \tag{7}$$

together with the differential equation (1) and the boundary conditions of Eq. (2), when necessary, such problems can be formulated.

4. Remark on the order of approximation

In single collocation point methods, the order of approximation cannot be better than $\mathrm{O}(h^2)$. This can be seen using a standard argument [23]. Indeed, assume the differential equation (1) is fulfilled, exclusively, at the single Gaussian collocation point, x_i^*—this is the midpoint—of each subinterval (x_{i-1},x_i). Let $e(x)\equiv u(x)-\hat{u}(x)$ be the error, where $u(x)$ and $\hat{u}(x)$ are the exact and the approximate solutions, respectively. Then

$$\varepsilon(x)\equiv\mathscr{L}e(x)=\sum_{i=1}^{E}g_i(x)\Theta_{x_i^*}(x), \tag{8}$$

where $\Theta_{x_i^*}(x)\equiv x-x_i^*$ on the subinterval (x_{i-1},x_i) and vanishes identically outside of it. In terms of the Green's function, $G(x,\xi)$, one can write

$$e(x)=\int_0^\ell G(x,\xi)\varepsilon(\xi)\,\mathrm{d}\xi = \sum_{i=1}^{E}\int_{x_{i-1}}^{x_i}G(x,\xi)g_i(\xi)\Theta_{x_i^*}(\xi)\,\mathrm{d}\xi. \tag{9}$$

Expressing $g_i(\xi)$ by means of a Taylor expansion around the point $\xi=x_i^*$, one gets

$$e(x)=\sum_{i=1}^{E}\sum_{j=1}^{\infty}\int_{x_{i-1}}^{x_i}C_j(\xi-x_i^*)^{j+1}\,\mathrm{d}\xi=\sum_{i=1}^{E}\mathrm{O}(h^3) = \mathrm{O}(h^2), \tag{10}$$

where C_j are the coefficients of the Taylor series expansion. In addition, here the fact that

$$\int_{x_{i-1}}^{x_i}\Theta_{x_i^*}(\xi)\,\mathrm{d}\xi=\int_{x_{i-1}}^{x_i}(\xi-x_i^*)\,\mathrm{d}\xi=0 \tag{11}$$

when x_i^* is the midpoint of the interval (x_{i-1},x_i), has been used.

5. The algorithm of the indirect approach

In [11], the indirect method was applied to the BVPJ for the general second order elliptic equation, defined by Eqs. (7) to (6), in several dimensions. However, here the indirect method will only be applied to the 1-D case, corresponding to Eqs. (1)–(3). For the *sought-information*, several choices are possible; for example, if the average of the flux is chosen, a mixed method is obtained. However, as stated before, throughout this article the averages of the solution, $\{\dot{u}_1,\ldots,\dot{u}_{E-1}\}$, are chosen to be the *sought-information*. Then, the system of equations fulfilled by the *sought-information* is [10]

$$\rho_i^-\dot{u}_{i-1}+\rho_i\dot{u}_i+\rho_i^+\dot{u}_{i+1}=\langle f-j,w^i\rangle,\quad i=2,\ldots,E-2, \tag{12}$$

$$\rho_1\dot{u}_1+\rho_1^+\dot{u}_2=\langle f-g-j,w^i\rangle \tag{13}$$

and

$$\rho_{E-1}^-\dot{u}_{E-2}+\rho_{E-1}\dot{u}_{E-1}=\langle f-g-j,w^i\rangle. \tag{14}$$

Here

$$\rho_i^-=-\left(a\frac{\mathrm{d}w^i}{\mathrm{d}x}+bw^i\right)_{x=x_{i-1}}, \tag{15}$$

$$\rho_i=-\left[a\frac{\mathrm{d}w^i}{\mathrm{d}x}+bw^i\right]_i, \tag{16}$$

$$\rho_i^+=\left(a\frac{\mathrm{d}w^i}{\mathrm{d}x}+bw^i\right)_{x=x_{i+1}}, \tag{17}$$

$$\langle f,w^i\rangle\equiv\int_{x_{i-1}}^{x_{i+1}}w^i f_\Omega\,\mathrm{d}x,\quad i=1,\ldots,E-1, \tag{18}$$

$$\langle g,w^1\rangle\equiv-u_{\partial 0}\left(a\frac{\mathrm{d}w^1}{\mathrm{d}x}\right)_{x=0}\quad\text{and}$$
$$\langle g,w^{E-1}\rangle\equiv u_{\partial l}\left(a\frac{\mathrm{d}w^{E-1}}{\mathrm{d}x}\right)_{x=l}, \tag{19}$$

$$\langle j,w^i\rangle\equiv\sum_{k=i-1}^{k=i+1}\left\{w_k^i j_k^1-j_k^0\left(\overline{a\frac{\mathrm{d}w^i}{\mathrm{d}x}}+bw^i\right)_k\right\},\quad i=2,\ldots,E-2, \tag{20}$$

$$\langle j,w^1\rangle\equiv\sum_{k=1}^{k=2}\left\{w_k^1 j_k^1-j_k^0\left(\overline{a\frac{\mathrm{d}w^1}{\mathrm{d}x}}+bw^1\right)_k\right\}\quad\text{and}$$
$$\langle j,w^{E-1}\rangle\equiv\sum_{k=E-2}^{k=E-1}\left\{w_k^{E-1}j_k^1-j_k^0\left(\overline{a\frac{\mathrm{d}w^{E-1}}{\mathrm{d}x}}+bw^{E-1}\right)_k\right\}. \tag{21}$$

For each $i=1,\ldots,E-1$ the test function $w^i(x)$ (Fig. 2) is defined to be identically zero outside the interval (x_{i-1},x_{i+1}). In addition,

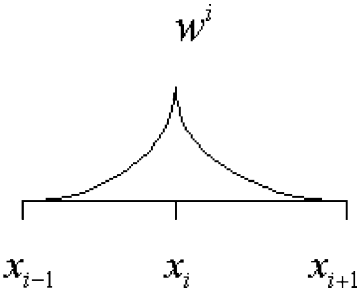

Fig. 2. Support of the weighting function $w^i(x)$.

$$\mathscr{L}^*w^i\equiv-\frac{\mathrm{d}}{\mathrm{d}x}\left(a\frac{\mathrm{d}w^i}{\mathrm{d}x}\right)-b\frac{\mathrm{d}w^i}{\mathrm{d}x}+cw^i=0,\quad i=1,\ldots,E-1 \tag{22}$$

in (x_{i-1},x_i) and (x_i,x_{i+1}), separately. Also, $w^i(x_{i-1})=0$, $w^i(x_i)=1$ and $w^i(x_{i+1})=0$. This set of conditions defines $w^i(x)$ uniquely, because they are sufficient to formulate two well-posed problems to be satisfied by $w^i(x)$: one of them in the interval (x_{i-1},x_i) and the other in the interval (x_i,x_{i+1}). When the differential equation (22) is satisfied exactly, the solution of the system of equations defined by Eqs. (12)–(14) yields the exact values of the *sought-information*. However, only in simple cases, such as that of constant coefficients, it is possible to obtain the exact solution of Eq. (22). For more general situations, it is necessary to resort to approximate numerical methods. If the numerical method applied to obtain the test functions is collocation, the resulting procedure for solving the global boundary value problem is a non-standard method of collocation. In this paper, one such collocation method is derived, which has the peculiarity of using only one collocation point at each one of the subintervals (x_{i-1},x_i) and (x_i,x_{i+1}), for the construction of each one of the test functions $w^i(x)$—recall that when cubic Hermites are applied, two collocation points are used in each subinterval. Then, three conditions have to be fulfilled by each $w^i(x)$, at the subinterval (x_{i-1},x_i): two boundary conditions and one collocation equation. If a polynomial of degree G is used for representing $w^i(x)$ in the interval (x_{i-1},x_i), it must have three free coefficients in order to be determined uniquely there by those three conditions. Thus, $G=2$. Of course the same reasoning applies at the interval (x_i,x_{i+1}). This argument shows that, when a single collocation point is applied at each subinterval, $w^i(x)$ must be taken as a piecewise continuous quadratic polynomial. At the only two subintervals, (x_{i-1},x_i) and (x_i,x_{i+1}), in which such polynomial does not vanish identically, it must fulfill the local boundary conditions mentioned before: $w^i(x_{i-1})=0$, $w^i(x_i)=1$ and $w^i(x_{i+1})=0$. Any piecewise quadratic polynomial satisfying these conditions can be expressed as

$$w^i(x)\equiv l_i(x)+\lambda_i^- l_i(x)l_{i-1}(x)\quad\text{for } x_{i-1}<x<x_i \tag{23}$$

and

$$w^i(x) \equiv l_i(x) + \lambda_i^+ l_i(x) l_{i+1}(x) \quad \text{for } x_i < x < x_{i+1}. \tag{24}$$

Here, for every $i = 1, \ldots, E-1$, $l_i(x)$ is the piecewise linear Lagrange polynomial, with the property that it vanishes at every node $x_j \neq x_i$ and $l_i(x_i) = 1$. In addition, λ_i^- and λ_i^+ are two real numbers. When orthogonal collocation is used in the construction of the special test function $w^i(x)$, these two numbers are determined by the condition that they must satisfy the adjoint differential equation (22) at the midpoints of the two subintervals, (x_{i-1}, x_i) and (x_i, x_{i+1}), respectively. Observe that this pair of equations is uncoupled, so a simple arithmetic division solves each one of them. In conclusion, the construction of each one of the test functions, $w^i(x)$, is rather simple: It is given by formulas (23) and (24), where each one of the coefficients, λ_i^- and λ_i^+, are obtained by a simple arithmetic division.

After the set of special test functions, $\{w^1, \ldots, w^{E-1}\}$, has been constructed, one can apply Eqs. (18)–(21), to evaluate all the terms occurring in the system of Eqs. (12)–(14). The solution of the tri-diagonal system of equations, obtained in this manner, yields the *sought-information*, $\{\dot{u}_1, \ldots, \dot{u}_{E-1}\}$. Of course, the value of the *sought-information* so obtained is no longer exact, because the special test functions that have been applied are not exact. A preliminary analysis of the error, which was presented in [10], indicates that the error is $O(h^2)$. This has been corroborated through numerical experiments that are reported in Section 8. It must be added that the solution, $\{\dot{u}_1, \ldots, \dot{u}_{E-1}\}$, of the tri-diagonal global system of equations, only gives information about the solution at the internal nodes of the partition. If one desires to obtain information in the interior of the subintervals of the partition, one can apply *optimal interpolation*, as it is explained in Section 7.

6. The direct approach algorithm

The method to be applied was derived in detail in [14]. Any number of collocation points per subinterval can be used, but here a procedure with only one such point is explained. According to [14], the averages at the internal nodes fulfill the following tri-diagonal system of equations:

$$-\rho_-^i \dot{u}_{i-1} + \dot{u}_i - \rho_+^i \dot{u}_{i+1} = \mu_i, \quad i = 2, \ldots, E-2, \tag{25}$$

$$\dot{u}_i - \rho_+^i \dot{u}_{i+1} = \mu_i, \quad i = 1 \tag{26}$$

and

$$-\rho_-^i \dot{u}_{i-1} + \dot{u}_i = \mu_i, \quad i = E-1, \tag{27}$$

where

$$\rho_-^i = \phi_-^i(x_i), \quad \rho_+^i = \phi_+^i(x_i), \qquad i = 1, \ldots, E-1, \tag{28}$$

$$\mu_i = \frac{\rho_-^i}{2} j_{i-1}^0 + \dot{u}_P^i(x_i) - \frac{\rho_+^i}{2} j_{i+1}^0, \quad i = 2, \ldots, E-2, \tag{29}$$

$$\mu_i = \rho_-^i g_{\partial 0} + \dot{u}_P^i(x_i) - \frac{\rho_+^i}{2} j_{i+1}^0, \quad i = 1 \tag{30}$$

and

$$\mu_i = \frac{\rho_-^i}{2} j_{i-1}^0 + \dot{u}_P^i(x_i) + \rho_+^i g_{\partial \ell}, \quad i = E-1. \tag{31}$$

Here, $\phi_-^i(x)$, $\phi_+^i(x)$ and $u_P^i(x)$ are auxiliary functions which vanish identically outside (x_{i-1}, x_{i+1}), and within, they are defined as the unique solutions of the following "local" boundary value problems:

For $i = 1, \ldots, E-1$,

$$\mathscr{L} u_P^i = f_\Omega, \quad \text{in } (x_{i-1}, x_i) \quad \text{and} \quad (x_i, x_{i+1}), \text{ separately}, \tag{32}$$

$$u_P^i(x_{i-1}+) = u_P^i(x_{i+1}-) = 0, \tag{33}$$

$$[u_P^i]_i = j_i^0 \quad \text{and} \quad \left[\frac{\mathrm{d}u_P^i}{\mathrm{d}x}\right]_i = j_i^1, \tag{34}$$

$$\mathscr{L}\phi_+^i = 0, \quad \phi_+^i(x_{i-1}) = 0, \quad \phi_+^i(x_{i+1}) = 1, \tag{35}$$

$$\mathscr{L}\phi_-^i = 0, \quad \phi_-^i(x_{i-1}) = 1, \quad \phi_-^i(x_{i+1}) = 0, \tag{36}$$

$$[\phi_+^i]_i = [\phi_-^i]_i = \left[\frac{\mathrm{d}\phi_+^i}{\mathrm{d}x}\right]_i = \left[\frac{\mathrm{d}\phi_-^i}{\mathrm{d}x}\right]_i = 0. \tag{37}$$

The above results are exact [14]. In particular, the solution of the system of equations (25) and (26), yields the exact values of the *sought-information*, $\{\dot{u}_1, \ldots, \dot{u}_{E-1}\}$. However, one can apply the system of equations (25)–(27), only if the functions $\phi_-^i(x)$, $\phi_+^i(x)$ and $u_P^i(x)$, are available. When such functions are known exactly (i.e., the analytical solutions are known), then the direct method yields exact results. However, more generally, it is necessary to compute them by approximate numerical methods. For the single collocation procedures presented here, each one of the local boundary value problems imposes six conditions: two boundary conditions, two jump conditions and two collocation conditions (one in each one of the subintervals neighboring the node x_i). These six conditions define a unique piecewise quadratic polynomial which vanishes identically outside (x_{i-1}, x_{i+1}). Working with functions that satisfy the jump and local boundary conditions from the start, this system can be reduced to a 2×2 system, as was done in [14]. Notice that even so, the final system is a little more complicated than that corresponding to the indirect method. The interested reader may see additional details in the reference just mentioned.

7. Optimal interpolation

If the solution of the problem is continuous, the values of $\dot{u}_i$ yield directly the values of the functions at the nodes. In standard finite difference procedures, this is all that such methods give, and if the values outside of the nodes are desired, one has to apply some kind of interpolation procedure. However, the interpretation of the indirect and direct approaches as domain decomposition methods provides a very efficient interpolation procedure; this is referred as *optimal interpolation* [24]. After obtaining the averages $\dot{u}_i$, $(i = 1, \ldots, E-1)$, by either one of the methods described in Sections 5 and 6, one applies the identities

$$u(x_i+) \equiv \dot{u}_i + \frac{1}{2}[u]_i = \dot{u}_i + \frac{1}{2} j_i^0 \tag{38}$$

and

$$u(x_i-) \equiv \dot{u}_i - \frac{1}{2}[u]_i = \dot{u}_i - \frac{1}{2} j_i^0. \tag{39}$$

When these values are complemented with the data of the BVPJ, Eqs. (1)–(3), enough information is available for defining well-posed boundary value problems in each one of the subintervals of the partition. Therefore, the information that has been obtained in the internal boundary exclusively, extends uniquely into the interior of the subdomains, as the solution of such local boundary value problems. Furthermore, that is the only extension that is compatible with the available information. All that is required to apply these ideas to reconstruct the solution of the BVPJ in the interior of the subintervals of the partition is solving such "local problems" by a numerical method that preserves the accuracy with which the information in the internal boundary is known. Of course, this can be done using only a single collocation point in each subinterval of the partition, in which case three conditions have to be satisfied by the approximate solution $u(x)$ at every subinterval (x_{i-1}, x_i), $i = 1, \ldots, E$: two boundary conditions and one collocation equation. Thus a quadratic polynomial approximation is suitable. This way of proceeding yields precisely the precision which is compatible with the precision with which the averages at the nodes have been obtained. Any additional effort, involving a more elaborate procedure for solving the local problems with greater precision, would be wasteful.

8. Numerical examples

To test the algorithms that were presented in previous sections, numerical results have been obtained for several examples, see [10,14]. They were treated by both the direct approach of Section 6 and the indirect approach of Section 5. The numerical experiments that were performed consist in solving Eq. (1), subject to Dirichlet boundary conditions for several choices of the coefficients, which are given in Table 1, and for each one of them the analytical solutions are known and are given in Table 2. In all cases, the domain of definition was the interval $[0, 1]$. The prescribed boundary values are those implied by the analytical solutions of Table 2 and, except for Example 6, the prescribed jumps are taken to be zero. The meshes were successively refined to test the asymptotic order of approximation. To this end, the number of elements was increased from 10 to 200.

The numerical results are summarized in Figs. 3–11. In each one of Figs. 3–11, the behavior of the error—measured in terms of the norm $\|.\|_\infty$—for indirect Trefftz–Herrera and direct collocation methods using one collocation point is shown.

The differential equation for Example 5 depends on the parameter α. This parameter was varied to take the values: 20 and 100, Figs. 7 and 8, respectively. Large α corresponds to steady-state advection dominated transport. The shape of the sharp-front solution is illustrated in Fig. 9.

The results of all these numerical experiments corroborate the theoretical order of approximation, of Section 4, for the two single point collocation procedures, here presented: $O(h^2)$. Observe that in some cases the results yielded by the two methods are remarkably similar.

Table 1
Definitions of the examples treated

Example	a	b	c	f_Ω
1	1	$2px/q$	$-\left\{\frac{4p(1+p)}{q^2} + \frac{2p^2}{q} + p^2\right\}$	0
2	1	0	$-40\pi^2$	0
3	$x^2 - 1$	0	30	0
4	$4x^2 + 3$	$3x - 1$	$3x(x+1)$	$-(x+1)^2 e^x$
5	-1	$-\alpha$	0	0
6	-1	0	-1	0
7	-1; $0 \leqslant x \leqslant 1$ -4; $1 < x \leqslant 2$	0	1	0

Table 2
Solution for each one of the examples

Example	Exact solution
1	$\sin(px) + x\cos(px)$, where $p = \sqrt{40}\pi$, $q = 1 + p(1 + x^2)$
2	$\sin(\sqrt{40}\pi x)$
3	$(63x^5 - 70x^3 + 15x)/8$
4	e^x
5	$\frac{e^{\alpha x} - e^{\alpha}}{1 - e^{\alpha}}$, $\alpha = 20, 100$ e^x, $0 \leqslant x < 1/2$ $\frac{1}{4} + e^{1/2}$, $x = 1/2$
6	$\left(1 - \frac{1}{2}\frac{e^{-1/2}}{e-1}\right)e^x + \frac{1}{2}\frac{e^{3/2}}{e-1}e^{-x}$, $1/2 < x \leqslant 1$, where the jump conditions are $j^0(0.5) = 0.5$, $j^1(0.5) = 0.5(\frac{1+e}{1-e})$,
7	$A\sin x$, $0 \leqslant x \leqslant 1$ $C\sin\frac{x}{2} + D\cos\frac{x}{2}$, $1 < x \leqslant 2$, where A, C and D are defined by $\begin{bmatrix} \sin(1) & -\sin(\frac{1}{2}) & -\cos(\frac{1}{2}) \\ \cos(1) & -2\cos(\frac{1}{2}) & 2\sin(\frac{1}{2}) \\ 0 & \sin(\frac{1}{2}) & \cos(1) \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$.

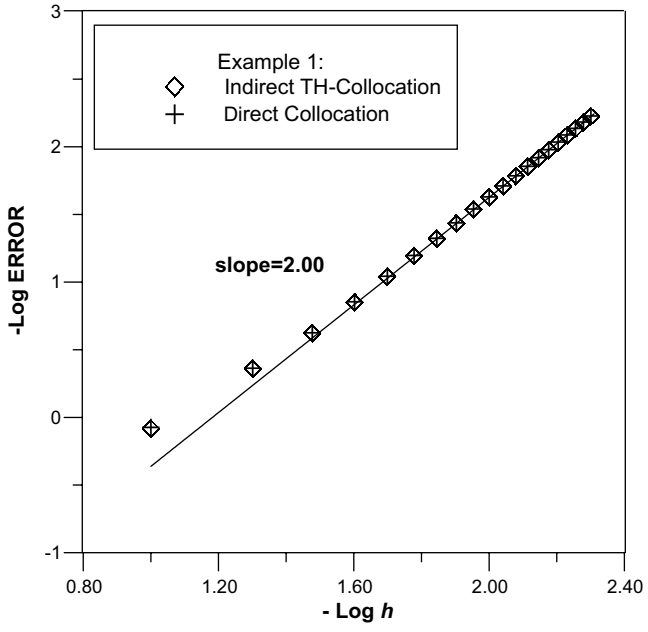

Fig. 3. Example 1: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

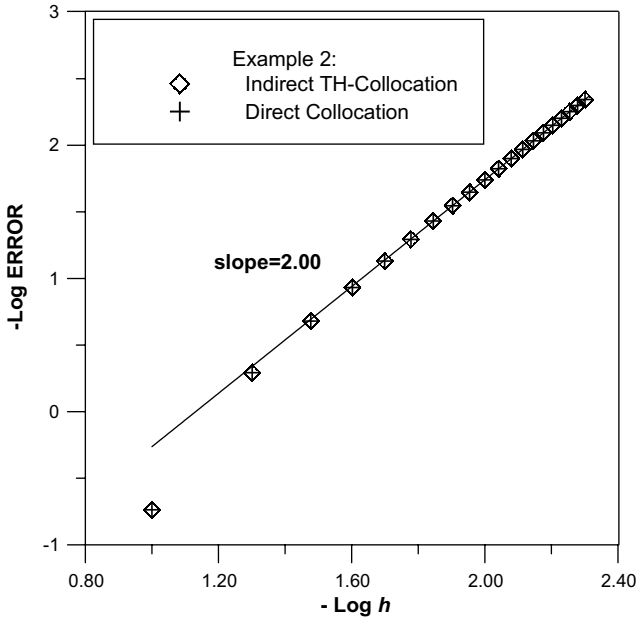

Fig. 4. Example 2: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

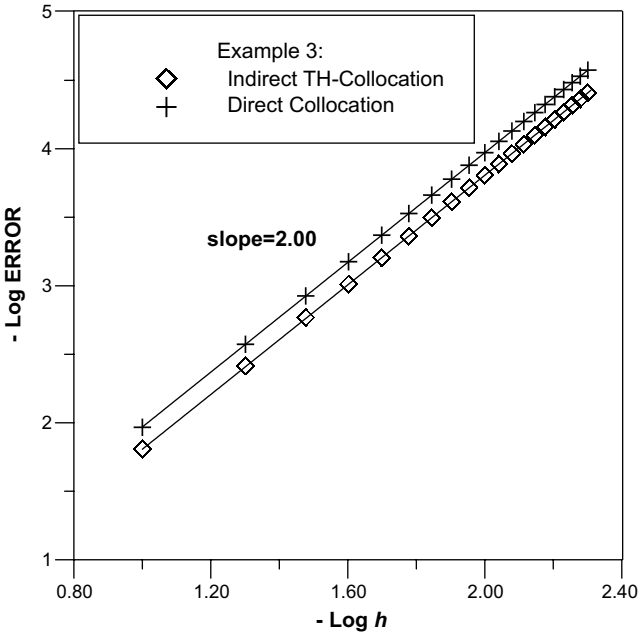

Fig. 5. Example 3: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

9. Discussion and conclusions

The present paper is devoted to honor Professor George F. Pinder. Its subject matter is quite adequate for such purpose because it has been motivated by some of his recent research and also, because it exhibits the power of a methodology that owes much to him, as it is explained in the Dedication and Introduction of this article. Pinder and his collaborators recently published [4] a novel Eulerian–Lagrangian approach to advection diffusive transport, which applies a non-conventional single collocation discretization procedure. The present paper contributes to its further development by offering

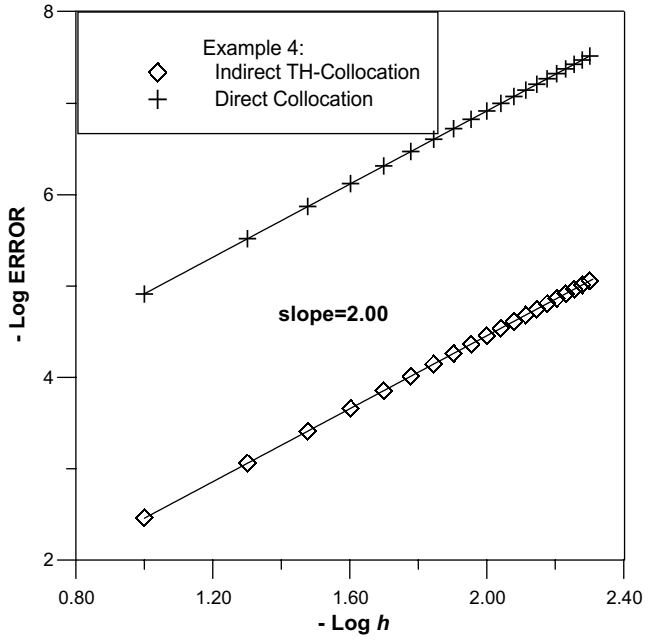

Fig. 6. Example 4: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

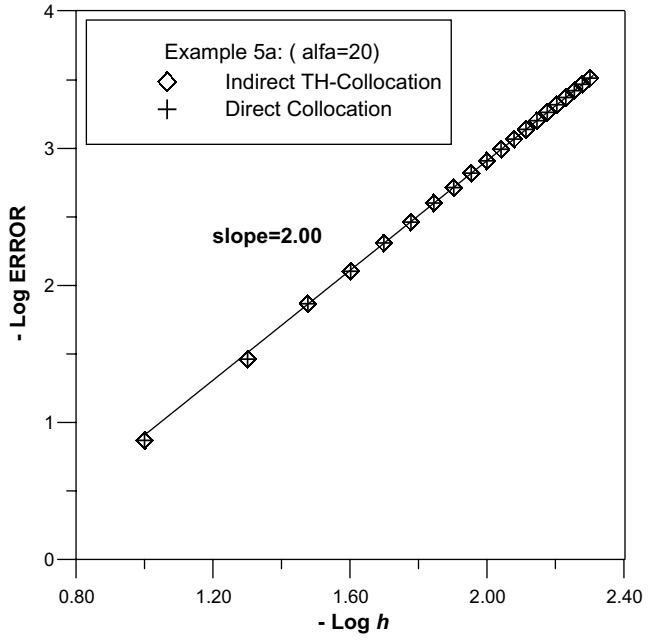

Fig. 7. Example 5: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions ($\alpha = 20$).

two single point collocation discretization procedures which may be used to improve its numerical efficiency and to generalize it to several spatial dimensions.

Domain decomposition methods have received much attention in recent years [25], mainly because they are

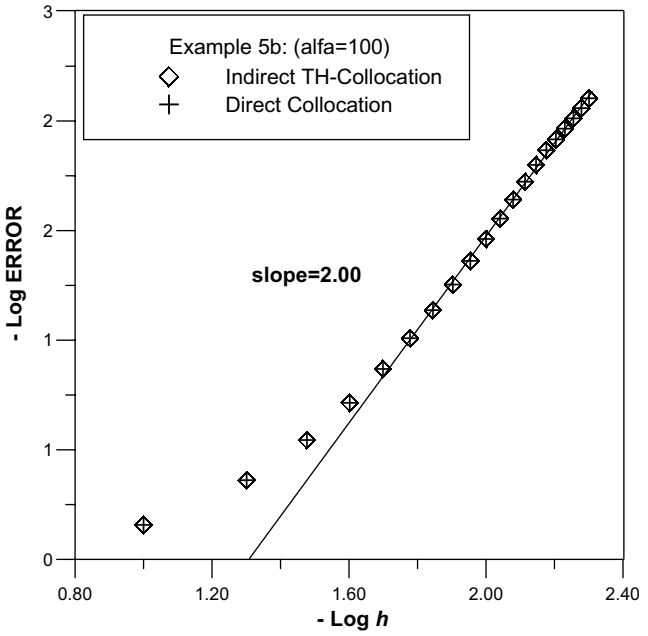

Fig. 8. Example 5: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions ($\alpha = 100$).

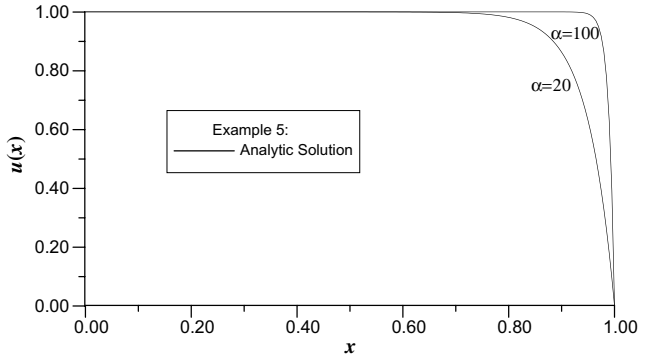

Fig. 9. Example 5: Graphic of analytical solution for $\alpha = 20$ and 100.

the most effective means for parallel processing mathematical models of continuous systems and the contribution of parallel processing to the growth of the computational capabilities has been extremely significant [15,16]. In addition, domain decomposition concepts are fundamental for many numerical methods of partial differential equations, since a first step, for most of such methods, consists in the introduction of a partition of the problem domain. Thus, research on DDM can also enlighten many aspects of numerical methods for partial differential equations, in general, and it is in this context that the authors, in a series of articles, have introduced and are developing a unified theory of domain decomposition methods [12]. This is briefly described in Section 2 of the present paper. According to it, there are two general classes of domain decomposi-

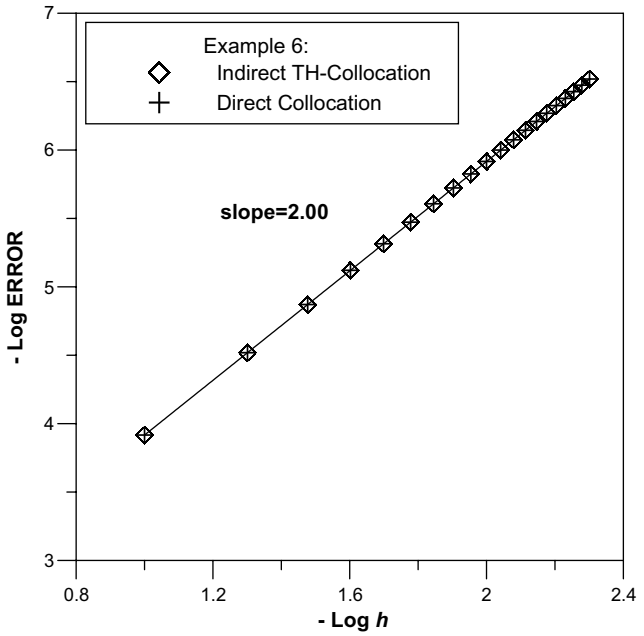

Fig. 10. Example 6: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

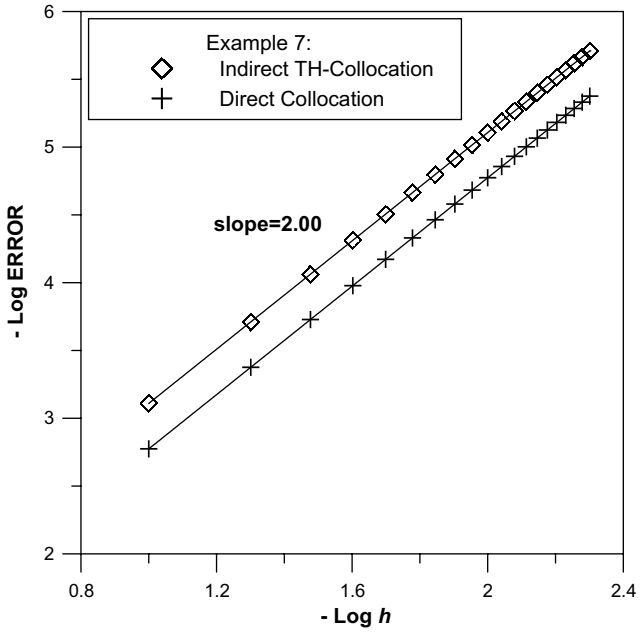

Fig. 11. Example 7: Convergence rate of direct and indirect Trefftz–Herrera collocation methods using one collocation point and quadratic weighting functions.

tion methods: direct and indirect (or Trefftz–Herrera) methods. Most formulations of domain decomposition methods that have been applied, up to now, fall in the category of direct methods. Indirect methods, on the other hand, were introduced by Herrera et al. [11], and stem from previous developments; in particular, Localized Adjoint Method [26] and Jirousek's version of Trefftz method [27].

The two discretization non-conventional algorithms that constitute the main technical objective of the present paper were derived by means of the domain decomposition methods of the unified theory; one corresponds to the direct approach and the other one to the indirect one. Through numerical experiments, they were both shown to be $O(h^2)$ and, in Section 4, a theoretical discussion shows that single-node collocation algorithms cannot be more accurate than that. Both of them yield tri-diagonal global matrices, a fact that is clearly advantageous when compared with the five-diagonal matrices of the original paper of Pinder and his collaborators. In this manner, they contribute to enhance the efficiency of their method. Also, the application of the algorithm yielded by the indirect approach is specially simple, as explained in Section 5 with considerable detail.

The algorithms discussed with detail in this paper refer to one-dimensional formulations exclusively, but our one-collocation point algorithm, derived using the indirect approach, readily extends to problems in several dimensions. Indeed, in [11], we presented collocation procedures that can be applied in any number of dimensions. When the indirect method of domain decomposition is applied, the functions approximating the sought solution are defined in the internal boundary only and, in [11], two algorithms were derived using piecewise cubic and piecewise linear interpolations on the internal boundary, respectively. The special test functions, on the other hand, were developed using, locally, cubic Hermites. For the 2-D case, four collocation points (2×2) per rectangular subdomain were used (more generally 2^D). Another manner in which the special test functions can be developed is by locally using quadratic polynomials, as it is done in the present paper, and only one collocation point, independently of the dimension. Notice the analogy: $1^D = 1$. The precision achieved when piecewise linear interpolations on the internal boundary are applied, is $O(h^2)$, which is consistent with the use of only one collocation point in each rectangular subdomain for the construction of the special test functions. Thus, our results establish a way in which the non-conventional Eulerian–Lagrangian single-node method of Pinder and his collaborators [4] can be extended to multi-dimensional problems. It remains, however, to test numerically the expected precision of the procedure, $O(h^2)$, for the multi-dimensional case. In any event, some attractive features of the algorithm so obtained can be anticipated. In [11], when the special test functions were constructed applying cubic-Hermites, locally, and the interpolation in the internal boundary was piecewise linear, the precision was shown to be $O(h^2)$ and only one degree of freedom was asso-

ciated with each internal node. This latter property is independent of the dimension. This is an outstanding reduction when compared with standard collocation methods. For them, that number grows exponentially with the dimension (2^D): 2 for 1-D, 4 for 2-D and 8 for 3-D. Finally, it is worth mentioning that for differential operators that are symmetric and positive, as for the flow equations, the matrices are symmetric and positive definite. This is a very important property that is not enjoyed by standard collocation. A more systematic comparison of the indirect method of collocation and conventional collocation, is available [11].

10. In summary

The contribution contained in this paper to the water resources literature is four-fold:

(1) It introduces two algorithms that can be used for improving a method recently proposed by Pinder and his collaborators. This was the main motivation for its writing.
(2) These two algorithms can be applied in some other instances of advection–diffusion transport problems of interest in water resources studies.
(3) The methodology used to obtain the results reported in the paper, which owes much to George Pinder, is very general and with many potential applications to water resources, but it is little known by the water resources community. Thus, exhibiting its power and usefulness in an article whose expected audience comes mainly from that community, is also significant.
(4) In addition, when the method of Pinder and his collaborators is incorporated in the framework of this general methodology, it immediately generalizes to several dimensions, since one of the algorithms that are introduced in the paper has already been so generalized.

Acknowledgements

The present article is offered to honor Professor George F. Pinder in his 60th anniversary in recognition of the international leadership he has held for more than 30 years in water resources research, as well as to celebrate his pioneering work on computational modeling of groundwater systems. At a more personal level, I wish to express my high regard for the important influence he has had in my research and academic carrier.

Applied Mathematics, when it is understood as knowledge of those branches of Mathematics which are important for applications in other Sciences and Engineering, have the potential of being used in a wide variety of human activities. This is a feature that, when properly developed, enriches the life of applied mathematicians. However, if an applied mathematician intends to develop applications in a specific field of Science or Engineering by himself, without the guidance of an expert of such field, he would be frustrated. To make contributions that are really relevant, it is essential to work in association with a leader, the higher his level the better, of the specific area of application. In this respect, for me, my collaboration and friendship with George Pinder has been very fortunate, because of many reasons; in particular, his undisputed leadership in water resources and his foresightedness has inspired much of my own research. In addition, his encouragement and support for my own academic activities has been an invaluable stimulus. My personal relationship with George started in September 1982, when I gave a talk, at Princeton, in which I explained a theory I had developed, which was later known as the Localized Adjoint Method (LAM). We almost immediately initiated an international exchange, known as MAXIMA, that was organized every year, once in the USA and once in Mexico. He also invited me to join the Advisory Council of the Princeton Department of Civil Engineering and Operations Research. In 1985, we organized and initiated the publication of the Journal "Numerical Methods for Partial Differential Equations", for John Wiley, of which we are still Editors, jointly with John Whiteman, and George has been Editor in Chief, since its foundation.

Regarding my research work, he proposed to me to apply LAM to transport problems, when we had just met. This led, a little after, to the development of the Eulerian–Lagrangian LAM (ELLAM), which was created, in alphabetical order, by Celia, Ewing, Herrera and Russell. The methodology to be applied in the present paper, offered for this special volume, the indirect (or Trefftz–Herrera) method of domain decomposition, also owes much to George Pinder. He suggested to me to apply collocation in combination with LAM in the summer of 1985, at Laramie, Wyoming, when we were preparing our book, with Myron Allen, which appeared in 1988. This greatly widened LAM's range of applicability and gave considerable impetus to its development. In addition, George initiated me in Domain Decomposition Methods (DDM). Indeed, in the summer of 1993, at Burlington Vermont, I collaborated with him in a project in which we applied DDM and my first papers on such methods, in which we reported the results of that project, were co-authored jointly with him and Guarnaccia [28,29]. Since then, much of my own research has been devoted to DDM: LAM has been interpreted as a domain decomposition method, which when combined with Trefftz Method, led to the development of Trefftz–Herrera domain decomposition method and to proposing a unified theory of DDM.

In this occasion, my co-authors join me in expressing him our recognition and wishing him that his very productive life continues for many years.

References

[1] Celia MA, Pinder GF. Generalized alternating-direction collocation methods for parabolic equations. I. Spatially varying coefficients. Numer Meth Partial Differen Equat 1990;6(3):193–214.

[2] Celia MA, Pinder GF. Generalized alternating-direction collocation methods for parabolic equations. II. Transport equations with application with application to seawater intrusion problems. Numer Meth Partial Differen Equat 1990;6(3):215–30.

[3] Celia MA, Pinder GF. Generalized alternating-direction collocation methods for parabolic equations. III. Nonrectangular domains. Numer Meth Partial Differen Equat 1990;6(3):231–43.

[4] Wu L, Wang H, Pinder G. A nonconventional Eulerian–Lagragian single-node collocation method with Hermite polynomials for unsteady-state advection–diffusion equations. Numer Meth Partial Differen Equat 2003;19(3):271–83.

[5] Russell RD, Shampine LG. A collocation method for boundary value problems. Numer Meth 1972;19:1–28.

[6] de Boor C, Swartz B. Collocation at Gaussian points. SIAM J Numer Anal 1973;10(4):582–606.

[7] Carey GF, Finlayson BA. Orthogonal collocation on finite elements. Chem Engrg Sci 1975;30:587–96.

[8] Bialecki B, Fairweather G. Orthogonal spline collocation methods for partial differential equations. J Comput Appl Math 2001;128:55–82.

[9] Herrera I. Collocation from a broad perspective. In: Bentley LR et al., editors. Computational methods in water, surface water systems and hydrology. Computational methods, vol. 2. Rotterdam: Balkema; 2000. p. 661–7.

[10] Herrera I, Díaz M. Indirect methods of collocation: Trefftz–Herrera collocation. Numer Meth Partial Differen Equat 1999;15(6):709–38.

[11] Herrera I, Yates R, Díaz M. General theory of domain decomposition: indirect methods. Numer Meth Partial Differen Equat 2002;18(3):296–322.

[12] Herrera I. Trefftz method: a general theory. Numer Meth Partial Differen Equat 2000;16(6):561–80.

[13] Herrera I. Unified theory of domain decomposition methods. In: Herrera I, Keyes DE, Widlund OB, Yates R, editors. 14th International Conference on Domain Decomposition Methods, 2003. p. 243–8.

[14] Herrera I, Yates R. General theory of domain decomposition: beyond Schwarz methods. Numer Meth Partial Differen Equat 2001;17(5):495–517.

[15] Keyes D. Domain decomposition in the mainstream of computational science. In: Herrera I, Keyes DE, Widlund OB, Yates R, editors. 14th International Conference on Domain Decomposition Methods, 2003. p. 79–94 [invited plenary lecture].

[16] Keyes D. Scalable solvers in Doe's SciDAC initiative. In: 7th US National Congress on Computational Mechanics, 2003 [plenary lecture].

[17] Oden TJ. Finite elements of non-linear continua. New York: McGraw-Hill; 1972.

[18] Herrera I. Unified approach to numerical methods. Part 1. Green's formulas for operators in discontinuous fields. Numer Meth Partial Differen Equat 1985;1(1):12–37.

[19] Herrera I, Chargoy L, Alduncin G. Unified approach to numerical methods. Part 3. Finite differences and ordinary differential equations. Numer Meth Partial Differen Equat 1985;1(4):241–58.

[20] Herrera I, Ewing RE, Celia MA, Russell TF. Eulerian–Lagrangian localized adjoint method: the theoretical framework. Numer Meth Partial Differen Equat 1993;9(4):431–57.

[21] Herrera I. The indirect approach to domain decomposition. In: Herrera I, Keyes DE, Widlund OB, Yates R, editors. 14th International Conference on Domain Decomposition Methods, 2003. p. 51–62 [plenary lecture].

[22] Herrera I, Keyes DE, Widlund OB, Yates R, editors. Proceedings of the 14th International Conference on Domain Decomposition Methods, 2003. Available from: www.ddm.org.

[23] Prenter PM. Splines and variational methods. New York: Wiley; 1975.

[24] Herrera I. Innovative discretization methodologies based on LAM. In: Morgan K et al., editors. Finite elements in fluids: new trends and applications, vol. 2. Swansea: Pineridge Press; 1993. p. 1437–47.

[25] International Scientific Committee for Domain Decomposition. In: 14 Proceedings of the International Conferences on Domain Decomposition Methods that took place in the period 1988–2002. Available from: www.ddm.org.

[26] Herrera I. Localized adjoint methods: a new discretization methodology. In: Fitzgibbon WE, Wheeler MF, editors. Computational methods in geosciences. Philadelphia: SIAM; 1992. p. 66–77 [chapter 6].

[27] Jirousek J, Wroblewski A. T-elements: state of the art and future trends. Arch Comput Meth Engrg 1996;3(4):323–434.

[28] Guarnaccia J, Herrera I, Pinder GF. Solution of flow and transport problems by a combination of collocation and domain decomposition procedures. In: Peters A et al., editors. International Conference on Computational Methods in Water Resources, Heidelberg. Computational methods in water resources X, vol. 1. Dordrecht: Kluwer Academic Publishers; 1994. p. 265–72.

[29] Herrera I, Guarnaccia J, Pinder GF. Domain decomposition method for collocation procedures. In: Peters A et al., editors. International Conference on Computational Methods in Water Resources, Heidelberg. Computational methods in water resources X, vol. 1. Dordrecht: Kluwer Academic Publishers; 1994. p. 273–80 [invited talk].