Collocation methods: More efficient procedures for applying collocation

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Abstract

In recent years, new and more effective procedures for applying collocation have been published. This article is devoted to present a revision of this subject and complement its developments. From the general theory two broad approaches are derived, which yield the direct and the indirect TH-collocation methods. The former approach had not been published before, and it is a dual of the indirect approach. In particular, second order differential equations of elliptic type are considered and several orthogonal collocation algorithms are developed for them. In TH-collocation, the approximations on the internal boundary and in the subdomain interiors are completely independent. This yields clear computational advantages that are illustrated through the construction of such algorithms. In the implementations presented, three dimensional problems are included. In passing, single-point-collocation methods that have been the subject of several recent publications are revised.

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1. Introduction

Collocation is known as an efficient and highly accurate numerical solution procedure for partial differential equations; furthermore, its formulation is very simple. However, in its standard form, referred to as orthogonal spline collocation (OSC) [1,2], which consists in applying orthogonal collocation on cubic splines, such discretization method suffers from several drawbacks. Among them, it yields ill-structured matrices, which are non-positive and non-symmetric even when the differential operators are symmetric and positive. This produces difficulties for combining efficiently OSC with domain decomposition procedures (see also [3,4]). However, in previous papers [5–8] the TH-collocation method was introduced and it was shown to possess clear and important advantages over OSC, such as:

1. Better structured matrices. They are symmetric and positive when the differential operators have these properties [6];
2. Greater flexibility in selecting the approximating polynomial spaces. This property stems from the fact that in TH-collocation, the polynomials used on the internal boundary and in the interior of the partition subdomains may be different;
3. The number of collocation points to be applied may be reduced. This is due to the fact that the degree of the approximating polynomials required for its implementation, in the interior of each one of the partition subdomains, can be so reduced;
4. It is easily parallelized. Indeed, when dealing with positive and symmetric differential operators, or systems of such operators such as those of elasticity, the positive definiteness of the matrices derived by TH-collocation permits a direct application of the conjugate gradient method (CGM) when combining TH-collocation with domain decomposition methods (DDM) [7];
5. Greater generality. The new TH-collocation method can be applied to practically any linear partial...
differential equation or system of such equations, occurring in science and engineering. It has already been applied to elliptic and parabolic equations, including the most general second order elliptic equation [6] and the biharmonic equation [8], among the higher order equations.

All these results show that orthogonal collocation in its new form constitutes a versatile and powerful methodology capable of being effectively applied to a wide variety of engineering problems, and this paper is devoted to further its development.

The variety of such engineering applications is indeed broad, including steady state and time dependent problems of fluid and solid mechanics (such as elastostatics and dynamical elasticity); transport by fluids (when they move freely in the physical space or when they are restricted to move in a porous medium) of energy and dissolved matter; groundwater exploitation; petroleum engineering; and many more. This is because the basic methodology is applicable to any linear partial differential equation, or system of such equations, independently of its type. However, to be specific here the details of their implementation will be presented exclusively for the most general second-order elliptic equation that is linear and several algorithms will be so derived. Anyway, the range of its applicability remains wide even when attention is restricted in such a manner because the steady states of many engineering systems are modeled by second-order elliptic equations. Indeed, for example, Poisson equations govern the steady states of: the electric potential; the piezometric head in an aquifer; the temperature in thermal equilibrium; the distribution of a pollutant in the atmosphere; etc. Furthermore, the equations of elastostatics can be reduced to Poisson equations when, for instance, the Boussinesq–Papkovitch–Neuber representation [9], see also [10]) is used. Similar representations, in terms of Poisson equation solutions, exist for the solutions of the biharmonic equation [11], which is fundamental in plate theory, and for the solutions of Stokes equations [12], on which the treatment of a large variety of fluid engineering problems is based.

If the fluid is in motion, the governing equations of the steady states of heat and matter transport systems are not Poisson equations any longer; however, they are (generally, non-symmetric) second order elliptic equations anyway. Furthermore, although in most cases elliptic equations are not associated directly with the models of non-steady states, nevertheless, when a step-by-step solution procedure is adopted, elliptic equations have to be solved at each time step. Of special interest is the case of advection-dominated transport, a difficult problem for which the methods here presented are especially effective and in previous stages of their development, in which they were known as Localized Adjoint Methods (LAM), motivated the well-known Eulerian–Lagrangian Localized Adjoint Method (ELLAM) [14].

Later developments of the theory have further increased its flexibility and more fully clarified its foundations. The basic theory of TH-collocation stems from Herrera’s unified theory of DDM [15,16]. Such a unified theory classifies DDM approaches into two broad categories [15]; namely, ‘direct’ – or Steklov–Poincare – and ‘indirect’ approaches, which correspondingly induces two classes of TH-collocation methods. Furthermore, there exists a parallelism – or duality – between the direct and the indirect approaches, which was announced in [13] and by now it is fully developed. This led to the unifying concept of ‘finite element methods with optimal functions (FEM-OF)’ and in such a framework a third approach, the Petrov–Galerkin approach, is incorporated. The indirect collocation methods were already discussed in [5,6], where TH-collocation methods were introduced, but the implementation of direct collocation methods including 3D problems is here presented for the first time. A more thorough discussion of the Petrov–Galerkin version of TH-collocation, together with its implementation, is left for future publications.

In the present paper also a significant step forward is made in the theoretical analysis of the error associated with the algorithms derived from the TH-methodology. For this purpose some basic formulas that are useful for the error analysis, whose range of applicability is as broad as that of Herrera’s theory, were established and were applied to the six TH-collocation algorithms that are developed in this article, having obtained very satisfactory agreement between the theoretical predictions and the numerical experiments results, which also corroborate the advantages of TH-collocation over standard collocation procedures (OSC). It is also concluded that from a FEM perspective, TH-collocation supplies an effective tool for matrix condensation since it can be efficiently used to reduce the number of degrees freedom involved in the problems equations systems (reductions of 67% and 74% are obtained in the problems treated in this article).

On the other hand, recently there has been a significant interest and expectations about the so called ‘single-collocation-point methods’ [17,18], in which only one collocation point is used in each partition subdomain. For second order elliptic problems in dimensions n-dimensions, due to the high degree of spline smoothness that is required by OSC, the lowest degree of the approximating polynomials that can be used is 3 and, consequently, at least 2n collocation points are required. Thus, single-collocation-point methods cannot be constructed when OSC is applied in its standard form; however, in our approach this can indeed be done, as was pointed out in [6] and more thoroughly discussed in [13]. Since, Herrera’s theory supplies a very suitable framework for single-collocation-point methods in the present paper this topic is briefly revised. Although single-collocation-point methods possess several attractive features [17,18], our conclusions are not as positive in this respect; indeed, in the numerical experiments that were carried out single-collocation-point methods did not offer clear advantages over FEM.

Section 2 is devoted to a purely verbal description of the basic ideas of Herrera’s method, while the notation to be
used is explained in Section 3. A brief presentation, supported wherever possible by suitable references to previous work, of the required mathematical formalisms is made in Sections 4 and 5, and their application to general second-order elliptic-equations is made in Section 6. The concepts finite element methods with optimal functions (FEM-OF) are introduced in Section 7 and details of the numerical implementation are given in Section 8, while the error analysis is done in Section 9. Section 10 is devoted to explain the numerical experiments and the discussion of single-point-collocation methods is made in Section 11. Finally, the conclusions are presented in Section 12 and the basic formulas used for the error analysis are contained in Appendix.

2. An overview of TH-collocation

As discussed in the previous section the advantages of TH-collocation methods over the standard OSC can provide benefits for the numerical treatment of a large class of engineering problems (see also [19]). This is due to the broad scope of Herrera’s theory [5,6,14–16,20–23], on which TH-collocation is based.

Consider a partition \( \Pi = \{\Omega_1, \ldots, \Omega_E\} \) of a domain \( \Omega \) (Fig. 1), where a boundary-value problem is formulated. A first step that is made is to ‘localize’ the problem. To this end, a procedure is established which permits constructing the ‘global’ solution, defined in the entire domain, by solving exclusively ‘local’ problems in each one of the subdomains. The general strategy to achieve this goal consists in gathering information on the internal boundary \( \Sigma \) of the partition, sufficient for defining well-posed problems that are fulfilled by the exact solution in each one of the partition subdomains, separately. Thus, a target of information on \( \Sigma \) – the ‘sought-information’ – possessing this property, is chosen and defined beforehand. Then a search is conducted to obtain this sought-information.

There are two very broad categories of procedures for carrying out such a search: ‘direct’ and ‘indirect’ localization procedures. In the ‘direct localization method’, the local solutions of the original differential operator are used to establish compatibility conditions that the sought-information must fulfill. These are derived from a very general form of the Poincaré–Steklov conditions [15,24]. For this purpose, special kinds of trial, or base functions, are used, referred to as ‘optimal base functions’; they are in fact local solutions of the homogeneous equation associated with the original differential operator. The global system of equations, derived in this manner allows the sought-information to be obtained.

In the ‘indirect localization method’, on the other hand, a system of weighting, or test functions of a special kind, referred to as ‘optimal test functions’, with the property of yielding the sought-information in the internal boundary, exclusively, is developed and applied. These optimal test functions are in fact local solutions of the homogeneous equation associated with the adjoint differential operator. The idea of constructing such optimal 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 [21,22,25]. In order to design, so to speak, such optimal test functions, it is necessary to have a procedure for analyzing this dependence.

In the indirect localization method, the basic ingredients of such analysis are Green–Herrera formulas, which were originated by Herrera in 1985 [21,22] and can be applied even when both trial and test functions are fully discontinuous [23]. These optimal test functions are then applied to derive, as in the direct method, compatibility conditions from which the sought information is obtained.

Once the sought information is known, on \( \Sigma \), the local boundary value problems can be individually solved to obtain the solution in the interior of all the partition subdomains. This latter process, referred to as ‘optimal interpolation’, permits constructing the global solution everywhere in the domain \( \Omega \). If each one of the steps that have been described could be performed exactly, the function so obtained would be the exact solution of the original problem. However, in general, this is not possible. TH-collocation is the numerical method that results when the local approximations, in the subdomains of the partition, are carried out by means of orthogonal collocation, as it is explained in what follows.

3. Notations

A detailed explanation of the notation to be used is contained in [23]. In this paper trial and test functions will be taken from the same linear space of function, denoted by \( D \). The notation \( \langle Pu, w \rangle \) will be used when, for every \((u, w) \in D \times D\), when \( \langle Pu, w \rangle \) depends linearly on \( u \in D \) and on \( w \in D \) separately (i.e., \( \langle Pu, w \rangle \) is a ‘bilinear functional’ on \( D \times D \)). In such case we write \( \langle P^*u, w \rangle \equiv \langle Pw, u \rangle \) for the ‘transposed bilinear functional’. Also, \( Pu \) is the linear functional whose values \( Pu(V) \equiv \langle Pu, V \rangle \), and \( P:D \to D^* \) the operator defined in \( D \) whose values are \( Pu \) for every \( u \in D \). The null subspace of the operator \( P:D \to D^* \) will be denoted by \( N_P \).

The notations \( \Omega \subset \mathbb{R}^n \) \((n = 2 \text{ or } 3)\) and \( \partial \Omega \) will be used for a domain [26] of the Euclidean space \( n \) and its boundary, respectively. \( \Pi = \{\Omega_1, \ldots, \Omega_E\} \) will be a partition of \( \Omega \).
where \( \Omega_i, i = 1, \ldots, E \), are subdomains (Fig. 1). Given such a partition, the boundaries of the subdomains are \( \partial \Omega_i, i = 1, \ldots, E \). Clearly, \( \partial \Omega \subset \bigcup_{i=1}^{E} \partial \Omega_i \) and the ‘internal boundary’, \( \Sigma \), is defined to be the closed complement of \( \partial \Omega \) relative to \( \bigcup_{i=1}^{E} \partial \Omega_i \). Furthermore, it is assumed that \( \Sigma \) has been ‘oriented’, i.e., a positive and a negative side have been defined at every point of \( \Sigma \), except at corners. Then, a unique unit normal vector \( n \) is taken pointing towards the positive side, a.e. on \( \Sigma \).

Trial and test functions will be taken from a linear space \( D \) of functions, whose members are ‘piecewise-defined-functions’ [23]; i.e., they are defined separately in each one of the partition subdomains. Thus, any such a function is a finite sequence of functions \( u \equiv (u_i, \ldots, u_E) \), where each \( u_i, i = 1, \ldots, E \), is taken from a linear space of functions \( D(\Omega_i) \) defined in \( \Omega_i \). In particular, Sobolev spaces of discontinuous piecewise-defined-functions, denoted by \( \dot{H}^S(\Omega) \), with \( S \) is a nonnegative integer, were defined in [23] for them \( D(\Omega_i) \equiv \dot{H}^S(\Omega_i) \). For any function \( u \in \dot{H}^S(\Omega) \), the notation \( u_+ \) and \( u_- \) will be used for the traces on the positive and the negative sides respectively. Generally \( u_+ \neq u_- \) because functions of \( \dot{H}^S(\Omega) \) are usually discontinuous. Thus, the ‘jump’ and the ‘average’ of any function \( u \in D \) are defined, respectively, to be

\[
[u] = u_+ - u_- \quad \text{and} \quad \hat{u} = (u_+ + u_-)/2
\]

Then

\[
u_+ = \hat{u} + \frac{1}{2} [u] \quad \text{and} \quad u_- = \hat{u} - \frac{1}{2} [u]
\]

Let \( \mathcal{L} \) and \( \mathcal{L}^* \) be a differential operator and its formal adjoint, respectively. Then, there is a vector-valued bilinear form \( \mathcal{L}(u, w) \), such that

\[
w \mathcal{L} u - u \mathcal{L}^* w = \nabla \cdot \mathcal{D}(u, w), \quad \forall x \in \Omega
\]

Then it has been shown that (see for example [16])

\[
\sum_{i=1}^{E} \int_{\Omega_i} (w \mathcal{L} u - u \mathcal{L}^* w) \, dx = \sum_{i=1}^{E} \int_{\partial \Omega_i} \mathcal{D} \cdot n \, dx
\]

This relation is valid under very general conditions, including the case when the operator coefficients have jump discontinuities across \( \Sigma \).

Later on, the most general elliptic operator of second order

\[
\mathcal{L} u \equiv -\nabla \cdot (a \cdot \nabla u) + \nabla \cdot (bu) + cu
\]

will be considered, where \( a \) is a positive and symmetric tensor. When dealing with elliptic equations of second order trial and test functions will be taken from \( \dot{H}^2(\Omega) \); i.e., \( D \equiv \dot{H}^2(\Omega) \). For simplicity, we will write \( \mathcal{L} u = f_\Omega \), in \( \Omega \), to mean

\[
\mathcal{L} u = f_\Omega, \quad \text{at each} \, \Omega_i, \, i = 1, \ldots, E
\]

Similarly, we will write \( \int_\Omega w \mathcal{L} u \, dx \) instead of \( \sum_{i=1}^{E} \int_{\Omega_i} w \mathcal{L} u \, dx \). Furthermore, we adhere to the notation \( a_n = a \cdot n \).

It can be shown that

\[
\sum_{i=1}^{E} \int_{\partial \Omega_i} w a_n \cdot \nabla u \, dx = \int_{\partial \Omega} w a_n \cdot \nabla u \, dx - \int_{\Sigma} [w a_n \cdot \nabla u] \, dx
\]

(3.7)

This relation is valid under very general conditions, including the case when the coefficient \( a_n \) has jump discontinuities across \( \Sigma \).

4. Green–Herrera formulas and the BVPJ

These kind of formulas are extensions to the case of discontinuous functions of the standard Green’s formulas of the theory of partial differential equations (see, for example, Lions and Magenes [27]).

They are obtained when each one of the functions \( \mathcal{D}(u, w) \cdot g \) and \( \mathcal{L}(u, w) \cdot \tilde{n} \), occurring in Eq. (3.4), is written as the sum of two bilinear functionals:

\[
\mathcal{D}(u, w) \cdot \tilde{n} = \mathcal{B}(u, w) - \mathcal{G}(w, u), \quad \text{on} \, \partial \Omega \}
\]

(4.1)

For differential operators with continuous coefficients, one possible definition is

\[
\mathcal{J}(u, w) \equiv -\mathcal{D}(u, w) \cdot \tilde{n} \quad \text{and} \quad \mathcal{K}(w, u) \equiv \mathcal{D}(\hat{u}, [w] \cdot \tilde{n}
\]

(4.2)

For every \( u, w \in D \times D \), the following six bilinear functionals are defined by:

\[
\langle Pu, w \rangle \equiv \int_{\Omega} w \mathcal{L} u \, dx; \quad \langle Qw, u \rangle \equiv \int_{\Omega} u \mathcal{L}^* w \, dx
\]

(4.3)

\[
\langle Bu, w \rangle \equiv \int_{\partial \Omega} \mathcal{B}(u, w) \, dx; \quad \langle Cw, u \rangle \equiv \int_{\partial \Omega} \mathcal{G}(w, u) \, dx
\]

(4.3)

\[
\langle Ju, w \rangle \equiv \int_{\Sigma} \mathcal{J}(u, w) \, dx; \quad \langle Kw, u \rangle \equiv \int_{\Sigma} \mathcal{K}(w, u) \, dx
\]

and Eq. (3.4) implies the following identity between such bilinear functionals

\[
P - B = J = Q^* - C^* - K^*
\]

(4.4)

When discontinuous piecewise-defined-functions are used, to obtain well-posed boundary value problems it is necessary to complement the usual differential equation and boundary conditions with suitable jump conditions that have to be fulfilled across the internal boundary \( \Sigma [23] \). Such problems are referred to as ‘boundary value problem with prescribed jumps (BVPJ)’. Let \( u_\Omega, u_\Sigma, u_E \in D \) be any three functions which satisfy the differential equation, the boundary conditions and the jump conditions respectively, and define \( f \equiv Pu_\Omega, g \equiv Bu_\Sigma \) and \( j \equiv Ju_\Sigma \). Then the BVPJ can be formulated weakly as

\[
(P - B - J)u = f - g - j
\]

(4.5)

or, equivalently, by virtue of Green–Herrera formula,

\[
(Q^* - C^* - K^*)u = f - g - j
\]

(4.6)
We are only interested in problems that possess a solution at least, in which case the boundary and jump conditions are compatible. By this we mean that there exists a function \(u_{\Omega^2} \in D\) such that \(Bu_{\Omega^2} = g\) and \(Ju_{\Omega^2} = j\). When the boundary and jump conditions are compatible, the \(\text{BVPJ}\) possesses a solution if and only if the standard \(\text{BVP}\) has a solution, as it has been shown in [23]. For simplicity, it will be assumed that such a solution is unique and the notation \(u \in D\) will be reserved for it.

5. **FEM with optimal test functions (FEM-OF)**

Eqs. (4.5) and (4.6) are referred to as the weak formulation, of the \(\text{BVPJ}\), in terms of the data and the weak formulation in terms of the complementary information, respectively. The direct approach stems from the first one, while the indirect approach stems from the second one, and the concept of ‘finite element methods with optimal test functions (FEM-OF)’, next explained, allows a unified presentation of them.

To explain the FEM-OF method we introduce a ‘dual decomposition’; i.e., we write

\[
\mathcal{J}(u, w) = \mathcal{J}_\delta(u, w) + \mathcal{J}_\delta(u, w) \quad \text{on } \Sigma
\]

Then, we define:

\[
\langle S_j u, w \rangle \equiv \int_{\Sigma} \mathcal{J}_\delta(u, w) \, dx; \quad \langle S_k w, u \rangle \equiv \int_{\Sigma} \mathcal{J}_\delta(w, u) \, dx \\
\langle R_j u, w \rangle \equiv \int_{\Sigma} \mathcal{J}_\delta(u, w) \, dx; \quad \langle R_k w, u \rangle \equiv \int_{\Sigma} \mathcal{J}_\delta(w, u) \, dx
\]

In both the direct and indirect approaches ‘optimal functions’ are applied, as it is explained next. To this end the linear subspaces:

\[
O_B \equiv N_\Omega \cap N_B \cap N_{R_j} \quad \text{and} \quad O_T \equiv N_{\Omega} \cap N_C \cap N_{R_k}
\]

are defined. Members of \(O_B\) and \(O_T\) will be referred to as ‘optimal base and test functions’, respectively.

The general class of methods referred to as FEM-OF considers three approaches for deriving the sought information. Here, they are given only for the case when \(Bu \equiv g \equiv 0\), since the more general situation of non-vanishing boundary conditions can easily be reduced to this case.

1. **Direct (or Steklov–Poincaré) approach.** Assume \(O_B \subset D_1 \cap D_2\) and \(O_B\) is TH-complete for \(S_j : D_1 \to D_2\). Then, an optimal base function, \(\hat{u} \in O_B\), contains the sought information, if and only if,

\[
\langle (P - B - J)\hat{u}, w \rangle = \langle f - Pu_{\Omega^2}, w \rangle + \langle (P - B - J)(u_{\Omega^2} - u_p), w \rangle, \quad \forall w \in O_B
\]

2. **Indirect (or TH) approach.** Assume \(O_T\) is TH-complete for \(S_j : D_1 \to D_2\). A function \(\hat{u} \in D_1\) contains the sought information, if and only if,

\[
\langle (P - B - J)\hat{u}, w \rangle = \langle f - Pu_{\Omega^2}, w \rangle + \langle (P - B - J)u_{\Omega^2}, w \rangle, \quad \forall w \in O_T
\]

3. **Petrov–Galerkin approach.** Assume \(O_T\) is TH-complete for \(S_k : D_1 \to D_2\). Then, an optimal base function \(\hat{u} \in O_B\) contains the sought information, if and only if,

\[
\langle (P - B - J)\hat{u}, w \rangle = \langle f - Pu_{\Omega^2}, w \rangle + \langle (P - B - J)u_{\Omega^2}, w \rangle, \quad \forall w \in O_T \quad (5.6)
\]

We recall the identity

\[
P - B - J \equiv Q' - C' - K^*
\]

which implies alternative expressions of the equations given above. As for \(u_p \in D\), it is defined as a solution of the system equations

\[
(P - B - R_j)u_p = f - g - j_r \quad \text{and} \quad S_k u_p = 0 \quad (5.8)
\]

where

\[
j_r \equiv R_j u_{\Omega^2}
\]

By assumption, \(u_p\) as well as the optimal functions can be constructed by solving local problems exclusively. For a definition TH-completeness see [23]; it is:

‘A subset \(\mathcal{E} \subset D\) is said to TH-complete for an operator \(S\), when

\[
\hat{u} \in D \quad \text{and} \quad \langle S\hat{u}, w \rangle = 0, \quad \forall w \in \mathcal{E} \Rightarrow S\hat{u} = 0 \quad (5.10)
\]

A final comment is in order. The manner of expressing the variational Eqs. (5.4)-(5.6) has been elaborated in such a manner that in applications such equations can be expressed by means of linear and bilinear forms that involve integrals over the domain interiors exclusively (see, for example, Eqs. (6.11)-(6.15)). Then, the procedures derived in this manner become a special class of Finite Element Methods (FEM), which will be referred to as Finite Element Methods with Optimal Functions (FEM-OF). Of the three FEM-OF methods described above, only the direct and indirect methods will be implemented in this paper, leaving for the future the detailed study of the Petrov–Galerkin approach.

6. **Second order elliptic equations**

For this kind of problems trial and test functions will be taken from the space \(D \equiv H^2(\Omega)\). The most general elliptic operator of second order and its formal adjoint are

\[
L' u \equiv -\nabla \cdot (a \cdot \nabla u) + \nabla \cdot (b u) + cu \quad \text{and} \quad L^* w \equiv -\nabla \cdot (a \cdot \nabla w) - h \cdot \nabla w + cw
\]

where \(a\) is a positive and symmetric tensor. Then, Eq. (3.3) is fulfilled with

\[
L(u, w) = a \cdot (u \nabla w - w \nabla u) + bw
\]
The BVPJ to be considered is

$$\mathcal{L}u = -\nabla \cdot (a_1 \nabla u) + \nabla \cdot (a_2 u) + cu = f$$  \hspace{1cm} (6.3)$$

subjected to the boundary conditions

$$u = u_0 = 0, \text{ on } \partial \Omega$$  \hspace{1cm} (6.4)$$

and jump conditions

$$[u] = [u_x] \equiv j_x$$ \hspace{1cm} and \hspace{1cm} $$[a_1 \cdot \nabla u] = [a_2 \cdot u_x] \equiv j_x$$, on $$\Sigma$$  \hspace{1cm} (6.5)$$

Suitable definitions for treating this problem are:

$$\mathcal{B}(u, w) \equiv u(a_g \cdot \nabla w + b_n w);$$

$$\mathcal{C}^*(u, w) \equiv -\mathcal{B}(u, w) \cdot n = [u]a_1 \cdot \nabla w + [u]a_2 \cdot w$$

$$\mathcal{K}(u, w) \equiv \mathcal{B}(u, [w]) \cdot n = [a_1 \cdot \nabla w + b_n w]u$$

$$- [w]a_2 \nabla u$$  \hspace{1cm} (6.7)$$

Taking the sought information to be the average of the solution at the internal boundary, we define

$$\mathcal{B}_j(u, w) \equiv [a_1 \cdot \nabla u]$$ and \hspace{1cm} $$\mathcal{B}_j(u, w) \equiv -[u]a_1 \cdot \nabla w + b_n w$$

$$\mathcal{K}_j(w, u) \equiv [a_1 \cdot \nabla w + b_n w]u$$ and \hspace{1cm} $$\mathcal{B}_j(w, u) \equiv -[w]a_2 \nabla u$$  \hspace{1cm} (6.8)$$

As indicated in Section 4, we define $$f \equiv Pu_0, g \equiv Bu_0$$ and \hspace{1cm} $$j \equiv Ju_0$$.

The optimal functions spaces $$O_B \equiv \mathcal{N}_f \cap \mathcal{N}_R \cap \mathcal{N}_C$$ and \hspace{1cm} $$O_T \equiv \mathcal{N}_f \cap \mathcal{N}_C \cap \mathcal{N}_R$$ are characterized as follows:

1. A function $$v \in D$$ is an optimal base function, if and only if,

$$\mathcal{L}v = 0, \text{ in } \Omega, \quad \alpha = 1, \ldots, E$$

$$V = 0, \text{ on } \partial \Omega$$

$$[V] = 0, \text{ on } \Sigma$$  \hspace{1cm} (6.9)$$

2. A function $$w \in D$$ is an optimal test function, if and only if,

$$\mathcal{L}^*w = 0, \text{ in } \Omega, \quad \alpha = 1, \ldots, E$$

$$w = 0, \text{ on } \partial \Omega$$

$$[w] = 0, \text{ on } \Sigma$$  \hspace{1cm} (6.10)$$

3. The auxiliary function $$u_p \in D$$ is characterized by

$$\mathcal{L}u_p = f, \text{ in } \Omega, \quad \alpha = 1, \ldots, E$$

$$u_p = 0, \text{ on } \partial \Omega$$

$$[u_p] = \pm 1, [u_x]$$, on $$\Sigma$$  \hspace{1cm} (6.11)$$

Furthermore, if $$v \in O \equiv O_B \cup O_T$$ and $$w \in O \equiv O_B \cup O_T$$, then

$$\langle (P - B - J)u, w \rangle = \int_B \{ \nabla u \cdot a_1 \cdot \nabla w + w \nabla \cdot (b_u + cu) \} dx$$

$$= \int_B \{ \nabla u \cdot a_1 \cdot \nabla w - b_w \cdot \nabla w + cuw \} dx$$

$$= \langle (Q^* - C^* - K^*)u, w \rangle$$  \hspace{1cm} (6.12)$$

while

$$\langle (P - B - J)u_x, w \rangle = \int_B \{ \nabla u_x \cdot a_1 \cdot \nabla w + w \nabla \cdot (b_u) + cuw \} dx$$  \hspace{1cm} (6.13)$$

and

$$\langle f - Pu_x, w \rangle = \int_B w(f - \mathcal{L}u_x) dx$$  \hspace{1cm} (6.14)$$

In particular, for the positive-symmetric case ($$b = 0, c \geq 0$$), the bilinear form

$$\langle (P - B - J)u, w \rangle = \int_B \{ \nabla u \cdot a_1 \cdot \nabla w + cuw \} dx$$

$$= \langle (Q^* - C^* - K^*)u, w \rangle$$  \hspace{1cm} (6.15)$$

is positive definite and symmetric.

7. Optimal trial and test functions

**TH-complete** systems, in more than one dimension, are infinite families. A first step towards the construction of a discretization procedure consists in replacing such a family by a finite system of optimal functions. Exact optimal functions are uniquely determined by their traces on $$\Sigma$$. In this article, using the direct and indirect approaches, several algorithms will be explained in detail for the case when the whole domain and the partition subdomains are rectangles (Figs. 2 and 3). For each one of them, independently of the approach followed, two kinds of optimal functions families will be developed, to be referred as Classes 1 and 2, respectively. Class 1 of optimal functions is made of those whose traces on the internal boundary, $$\Sigma$$, span the linear subspace of piecewise linear polynomials that vanish on $$\partial \Omega$$ and belong to $$C^0(\Sigma)$$; while Class 2 of optimal functions is made of those whose traces on the internal bound-

![Fig. 2. Partition of the domain $$\Omega \equiv [x_{min}, x_{max}] \times [y_{min}, y_{max}]$$ in rectangular $$E_i \times E_j$$ elements, where $$h_i = x_i - x_{i-1}; i = 1, \ldots, E_x$$ and $$h_j = y_j - y_{j-1}; j = 1, \ldots, E_y.$$](image-url)
Only the case of a partition with rectangular elements will be considered (see Fig. 2). For the numerical algorithms to be presented the function families of exact optimal functions will be replaced by approximations to them and, for greater clarity, in what follows the exact optimal function families will be denoted by \( \mathcal{E} \) and \( \mathcal{F} \), while the linear subspaces spanned by them will be \( \mathcal{O}_B \) and \( \mathcal{O}_T \), respectively. Correspondingly, the approximate optimal function families will be denoted by \( \mathcal{E}_a \) and \( \mathcal{F}_a \), and the linear subspaces spanned by them will be \( \mathcal{O}_B \) and \( \mathcal{O}_T \), respectively. Furthermore, the conditions \( \tilde{V} = V \) and \( \tilde{w} = w \), on \( \Sigma \), will be imposed; then, this establishes a one-to-one correspondence between the families of optimal and approximate optimal functions. The approximate solution \( \tilde{u} \in H^2(\Omega) \) is taken to be

\[
\tilde{u} \equiv \tilde{u}_n + \sum_{s=1}^n C_s V^s
\]

where \( n \) is the common dimension of both \( \mathcal{O}_B \) and \( \mathcal{O}_T \).

As mentioned in the Section 1, our approach permits thoroughly separating the process of approximating the differential equation in the interior of the partition subdomains from that of approximating the solution on the internal boundary, \( \Sigma \). Due to this fact, the approximate optimal functions will be constructed by orthogonal collocation using in each direction of the subdomain interiors, 1 or 2 Gaussian points; then, in each one of such subdomain interiors the functions are taken to be bi-quadratic and bi-cubic polynomials, respectively. Observe that the total number of collocation points in each subdomain partition is 1, in the first case, and 2\( d \) in the second one. Here, \( d \) is the space dimension. When \( \tilde{V} \in \mathcal{O}_B \) and \( \tilde{w} \in \mathcal{O}_T \), recall that \( \mathcal{L}_V \tilde{V} = 0 \) and \( \mathcal{L}_w \tilde{w} = 0 \) at the Gaussian points of each one of the partition subdomains.

The algorithms obtained by the procedures here explained, are characterized by the kind of approach that is applied (D or ID), since in this paper only the Direct (or Steklov-Poincaré approach) and the Indirect (or TH-approach) will be used; the class of optimal functions (1 or 2); and the number of Gaussian collocation points in each direction 1 or 2. The notation adopted to identify each one of these algorithms is such that, for example, the algorithm derived using the indirect approach, \( C^0 \) linear polynomials on \( \Sigma \) (Class 1), and two collocation points in each direction of the subdomain interiors, will be designated as Algorithm ID12.

### 8. Construction details

Only 2D applications are explained in detail. Given any node \( n = (x_n, y_n) \), one or more optimal functions will be associated to it; the exact optimal functions are \( V_n^o \in \mathcal{O}_B \) and \( \tilde{w}_n^o \in \mathcal{O}_T \), while the corresponding approximate optimal functions are \( V_n \in \mathcal{O}_B \) and \( \tilde{w}_n \in \mathcal{O}_T \). Then the systems of optimal functions are obtained when \( n \) and \( \gamma \) range over the sets that are indicated next. When \( n = (x_n, y_n) \) is an interior node the support of each one of the optimal functions is the union of the four neighboring rectangular subdomains (see Fig. 3). Their construction by collocation is only explained for the subdomain located upright of the node \( n \), which is denoted by \( \Omega_n \).

**Algorithms ID11 and D11.** In this case \( \gamma \) takes only one value and will be deleted. With each interior node \( n \in \Omega \), we associate:

\[
\begin{align*}
\tilde{V}_n(x, y) &= l_n(x, y) + \lambda_n q_n(x, y) \\
\tilde{w}_n(x, y) &= l_n(x, y) + \mu_n q_n(x, y)
\end{align*}
\]

in \( \Omega_n \) (8.1)

Here, \( l_n(x, y) \) is the \( C^0(\Omega) \) piecewise bilinear polynomial which vanishes at every node, except at \( n = (x_n, y_n) \), where it takes the value 1; and \( q_n(x, y) \) is the unique continuous piecewise bi-quadratic function, which vanishes on \( \partial \Omega_n \) and takes on the value 1 at the Gauss point (the center) \( x_n^e \) of \( \Omega_n \). Clearly, \( q_n(x, y) \) is an affined translation of the function \( 16x(1-x)y(1-y) \). In Eq. (8.1) the parameters \( \lambda_n \) and \( \mu_n \) are determined by collocating the differential equations \( \mathcal{L}_V \tilde{V}_n = 0 \) and \( \mathcal{L}_w \tilde{w}_n = 0 \), at the Gauss point of \( \Omega_n \).

**Algorithms ID12 and D12.** First, we define a family of four linearly independent cubic polynomials, denoted by \( \{ q_i(x, y) \} \), where \( i \equiv (v, \tau), \tau = 0, 1 \) and \( v = 0, 1 \), in a manner that such a system of functions spans the space of bi-cubic polynomials with the property of vanishing on \( \partial \Omega_n \). It can be seen that the system \( \{ q^{00}_n(x, y), q^{01}_n(x, y), q^{10}_n(x, y), q^{11}_n(x, y) \} \) is obtained by suitable affine translates of the system of bi-cubic Hermite polynomials \( \{ H^3_0(x) H^1_0(y), H^1_0(x) H^3_0(y), H^3_0(x) H^1_0(y), H^1_0(x) H^3_0(y) \} \). Then, the optimal functions are defined by

\[
\begin{align*}
\tilde{V}_n(x, y) &= l_n(x, y) + \sum_{i} \lambda_i q_i(x, y) \\
\tilde{w}_n(x, y) &= l_n(x, y) + \sum_{i} \mu_i q_i(x, y)
\end{align*}
\]

\( \forall (x, y) \in \Omega_n \) (8.2)

For each \( n = (x_n, y_n) \), the four numerical coefficients \( \lambda_i^\gamma \) are determined by collocation at the four Gaussian points of the rectangle \( \Omega_n \).
Algorithms ID22 and D22. In this case, for each node \( n \in \mathcal{N} \) (interior or on the boundary), we write \( \{ h_n^0(x, y), h_n^1(x, y), h_n^2(x, y) \} \) for the system of bi-cubic polynomials that are affine translations of the system of bi-cubic Hermite polynomials \( \{ H_n^0(x)H_n^0(y), H_n^1(x)H_n^0(y), H_n^0(x)H_n^1(y) \} \). Then for each \( \kappa = 1, 2, 3 \), one has

\[
\hat{V}_n^\kappa = h_n^\kappa(x, y) + \sum \lambda_{n\ell} q_{n\ell}^\kappa \quad \forall (x, y) \in \Omega_n
\]

(8.3)

Again, as in the case of Eq. (8.2), for each \( n = (x_n, y_n) \) and each \( \kappa \), the four numerical coefficients \( \lambda_{n\ell}^{\kappa} \) are determined by collocation at the four Gaussian points of the rectangle \( \Omega_n \).

The construction of the auxiliary function \( u_p \in D \) is quite similar, except for the fact that the differential equation is not homogeneous, and will not be explained. For Algorithms D11, D12, ID11 and ID12, one optimal function is associated with each internal node. In the case of Algorithms D22 and ID22 three of them are associated with each internal node, one with each boundary node and zero optimal functions are associated with corner nodes. Notice also that the bases for the optimal functions spaces here presented are of local support (the support of each one of them is contained in the union of four partition rectangles, at most). Finally, the extension of these constructions to three dimensions offers no difficulty.

9. Error analysis

In this section, the following notation will be used:

\[
e \equiv u - \tilde{u}; \quad e_p \equiv u_p - \tilde{u}_p; \quad \eta \equiv \tilde{w} - \bar{w}; \quad e^\kappa \equiv \nabla^\kappa \tilde{V}^\kappa
\]

(9.1)

Furthermore, \( \| \cdot \|_\Sigma \) is the \( L^2(\Sigma) \)-norm while \( | \cdot | \) stands for the absolute value and “r” will be a number of collocation points, in each direction, used for the construction of the approximate optimal functions; thus, the possible values of r are 1 or 2.

For the direct approach, by construction and in view of Eq. (7.1), one has

\[
|\mathcal{L} e_p| = O(h^{3r}) \quad \text{and} \quad |\mathcal{L} e^\kappa| = O(h^{2r})
\]

By construction, for the indirect approach one has

\[
|\eta| = O(h^{2r})
\]

(9.2)

(9.3)

On the other hand, Eq. (A.6) of Appendix, for the elliptic equation under study, reads:

\[
- \int_{\Sigma} e^\kappa [\bar{g}_\kappa : \nabla \bar{w}] \, dx = \int_{\Sigma} \eta \mathcal{L} e, \quad \forall \tilde{w} \in \mathcal{O}_T
\]

(9.4)

When either of the Eqs. (9.2) or (9.3) holds, one has

\[
- \int_{\Sigma} e^\kappa [\bar{g}_\kappa : \nabla \bar{w}] \, dx = O(h^{3r}), \quad \forall \tilde{w} \in \mathcal{O}_T
\]

(9.5)

To complete the proof of this result, the following ansatz will be used: when the traces on \( \Sigma \) of the members of the linear space \( \mathcal{O}_T \) span the piecewise polynomials of degree “p”, then

\[
- \int_{\Sigma} e^\kappa [\bar{g}_\kappa : \nabla \bar{w}] \, dx = 0, \quad \forall \tilde{w} \in \mathcal{O}_T \Rightarrow \| e \|_\Sigma = O(h^{p+1})
\]

(9.6)

Furthermore, when

\[
- \int_{\Sigma} e^\kappa [\bar{g}_\kappa : \nabla \bar{w}] \, dx = O(h^s), \quad \forall \tilde{w} \in \mathcal{O}_T \Rightarrow \| e \|_\Sigma = O(h^s)
\]

(9.7)

where \( s \) is the smallest number of the set \( \{ p + 1, q \} \).

The proof of this ansatz is being developed, but as it will be seen next, its applications yield very satisfactory results. To apply it, we notice that for functions of Class 1, \( p = 1 \), while \( p = 3 \) for functions of Class 2. Then, in view of Eq. (9.5), one has that Algorithms ID11, ID12, D11 and D12, are \( O(h^4) \), while Algorithms ID22 and D22 are \( O(h^4) \). This has been corroborated in the numerical experiments that were performed with the new algorithms.

For Algorithm ID11, the number of Gaussian points is one, independently of the dimension of the problem. Thus, this is a single-point-collocation method. Another observation worth of mention is that for Algorithms ID12 and D12, are \( O(h^5) \) in spite of using two collocation points in each direction. This exhibits the fact that profiting of the increased accuracy in the subdomain interiors requires increasing the degree of the polynomials used on \( \Sigma \). The error estimate \( \| e \|_\Sigma \) can be further reduced if the Petrov–Galerkin approach, which was not implemented in this paper, is used. However, in order to profit from this increased accuracy piecewise cubic polynomials have to be used on \( \Sigma \).

10. Numerical experiments

The algorithms described before were implemented and applied to the set of examples that follows:

10.1. 2D problems

\[
\text{Problem (1)}
\]

\[
- u_{xx} - u_{yy} + u = (1 - x^2 - y^2)e^y, \quad \text{on} \quad \Omega = (0, 1) \times (0, 1)
\]

\[
u(x, y) = e^y, \quad \text{on} \quad \partial \Omega
\]

Solution: \( u(x, y) = e^y, \quad \text{on} \quad \Omega \)
Problem (2)
\[-e^{x} u_{xx} - e^{y} u_{yy} + u_{x} + u_{y} + 2u = -e^{-x} - e^{-y},\]
on $\Omega \equiv (0, 1) \times (0, 1)$
\[u(x, y) = e^{-x-y}, \quad \text{on } \partial \Omega\]
Solution: $u(x, y) = e^{-x-y}, \quad \text{on } \Omega$

10.2. 3D problems

Problem (3)
\[-u_{xx} - u_{yy} - u_{zz} + u = (1 + 3x^2) \sin \pi x \cdot \sin \pi y \cdot \sin \pi z,\]
on $\Omega \equiv (0, 1) \times (0, 1) \times (0, 1)$
\[u(x, y, z) = 0, \quad \text{on } \partial \Omega\]
Solution: $u(x, y, z) = \sin \pi x \cdot \sin \pi y \cdot \sin \pi z, \quad \text{on } \Omega$

The symmetric operators of Problems (1) and (3) yielded positive definite global-matrices for the Dirichlet-type boundary conditions, here considered. The differential operator of Problem (2), on the other hand, is non-symmetric.

As for the error, the results of the numerical experiments, summarized in Figs. 4–6, agree well with the theoretical predictions of Section 9, in the 2D and 3D examples here treated: the single collocation point methods are $O(h^2)$, while the algorithms that use two collocation points in each direction are $O(h^4)$. The nodes of the mesh were taken as control points for the definition of the error. Observe that for the symmetric Problems (1) and (3) the
numerical behaviors of the algorithms derived from the direct and indirect approaches are very similar (Figs. 4 and 6). However, in the non-symmetric problem the error behavior of the direct method is better (Fig. 5).

In Figs. 4 and 5 TH-collocation was also compared with standard FEM, using linear elements. Clearly, the behavior of TH-collocation with cubic interpolators on $\Sigma$ (Algorithms D22 and ID22) is much better. However, a similar error behavior can be expected if FEM is applied with bicubic functions, in which case the number of degrees of freedom increases to be approximately $9h^{-2}$, in 2D problems, and $27h^{-3}$, in 3D problems. On the other hand, for Algorithms D22 and ID22 this number is only $3h^{-2}$, in 2D problems, and $7h^{-3}$, in 3D problems. Thus, the use of TH-collocation produces a FEM algorithm with only $33\%$ and $26\%$, for 2D and 3D problems respectively, of the number of degrees of freedom of standard FEM; i.e., a reduction of $67\%$ and $74\%$, respectively. These are very important reductions whose significances increase as $h$ decreases. In conclusion: “TH-collocation supplies an effective tool for carrying out matrix condensation”.

As for single-collocation-point methods, according to Figs. 4 and 5 they do not offer any real advantage over FEM.

11. Single-collocation-point methods

This kind of methods cannot be developed in the framework of the standard OSC. However, in 1999 [5] it was thereby mentioned that as a result of the relaxed smoothness conditions required by the TH-collocation methodology it was possible to develop single-collocation-point methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point in each partition sub-domain, in spite of using an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework. A few years after the first implementation of orthogonal-collocation with a single collocation point appeared [17,18], which were done by means of an ingenious scheme that allows applying only one collocation point appeared [17,18], which were done by means of methods in its framework.

In previous papers the TH-collocation method was introduced and it was shown to possess clear advantages over the standard orthogonal collocation (OSC) [5–8]. This paper has been devoted to further develop and analyze such methodology; its conclusions can be summarized as follows:

1. TH-collocation has been incorporated in the class of Enhanced Finite Element Methods, nowadays under study by many authors [28], and in particular it belongs to a broad kind of methods known as Finite Element Methods with Optimal Functions (FEM–OF);
2. Formulating orthogonal collocation as a special class of Finite Elements has many computational advantages since in this manner collocation can profit from software and procedures that are available for FEM;
3. In this framework three versions of TH-collocation can be distinguished:
   (a) Direct (or Steklov–Poincaré) approach;
   (b) Indirect (or Herrera’s) approach; and
   (c) Petrov–Galerkin approach;
4. Such TH-collocation formulations can be used to treat a very broad variety of engineering problems, since they can be applied to any partial differential equation, or system of such equations (e.g., the equations of elasticity or Stokes Problem [14]), which is linear, including the case of equations with discontinuous coefficients;
5. Some basic formulas that are useful for the error analysis were established;
6. Six algorithms based on the Direct and Indirect TH-collocation formulations were implemented (the Petrov–Galerkin version of TH-collocation was not, since it is the subject of current research) for the most general second order elliptic equation;
7. By application of the basic formulas mentioned above, theoretical error estimates were derived that were verified experimentally;
8. In the numerical experiments, the advantages of TH-collocation over standard collocation procedures (OSC) were corroborated by the Algorithms D22 and ID22.
9. The single-point-collocation procedures of Algorithms D11, D12 and ID11 and ID12 did not offer a real advantage with respect to standard FEM; and
10. From a FEM perspective, TH-collocation supplies an effective tool for matrix condensation since it reduces efficiently the number of degrees freedom involved in the equations systems. Furthermore, this procedure can be equally used in the very broad variety of engineering problems to which TH-collocation formulations, in the manner explained in this paper, are applicable.
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Appendix A. Auxiliary results for error analysis

Notation
\[ e = u - \hat{u} = \check{e} + \hat{e}, \quad \check{e} = \bar{u} - \hat{u}, \quad \eta = \bar{w} - \hat{w} \]  \hspace{1cm} (A.1)

Our constructions are such that
\[ e, \check{e}, \hat{e} \in N_h \cap N_{\delta_2}, \quad \eta \in N_C \cap N_{\delta_2} \quad \text{and} \quad S_j \check{w} = S_j \hat{w} \]  \hspace{1cm} (A.2)

Observe
\[ -\langle S_j e, \check{w} \rangle = \langle Pe, \check{w} \rangle - \langle S_j e, \hat{w} \rangle \]  \hspace{1cm} (A.3)

Now
\[ \langle (P - B - J)u, \check{w} \rangle = \langle (P - B - J)e, \check{w} \rangle \quad \text{or} \quad \langle (P - B - J)u, \hat{w} \rangle = 0, \quad \forall \check{w} \in \hat{O}_T \]  \hspace{1cm} (A.4)

In view of Eq. (A.2), this equation implies
\[ \langle S_j e, \check{w} \rangle = \langle Pe, \check{w} \rangle \]  \hspace{1cm} (A.5)

which in turn, by virtue of Eq. (A.3), implies
\[ -\langle S_j e, \hat{w} \rangle = -\langle S_j e, \check{w} \rangle = \langle Pe, \eta \rangle \]  \hspace{1cm} (A.6)

References