Computational Methods in Water Resources XI
Volume 1
Computational Methods in Subsurface Flow and Transport Problems

EDITORS:

A.A. Aldama
Mexican Institute of Water Technology, México

J. Aparicio
Mexican Institute of Water Technology, México

C.A. Brebbia
Wessex Institute of Technology, UK

W.G. Gray
University of Notre Dame, USA

I. Herrera
National Autonomous University of México, México

G.F. Pinder
University of Vermont, USA

Computational Mechanics Publications
Southampton Boston

COMPUTATIONAL METHODS IN WATER RESOURCES XI
COMPUTATIONAL MECHANICS PUBLICATIONS
SOUTHAMPTON BOSTON
Vol. 1, pp. 515-524, 1996.

Trefftz method, domain decomposition and TH-collocation

I. Herrera
Instituto de Geofisica, Universidad Nacional Autónoma de México, Apartado Postal 22-582, 14000 México, D.F., México

ABSTRACT

The author's Algebraic Theory of Boundary Value Problems has permitted systematizing Trefftz method and expanding its scope. The concept of TH-completeness has played a key role for such developments. A generalized version of Trefftz method, known as LAM (Localized Adjoint Method), has been quite successful in numerical applications. Here, the relations between these methods are discussed. Some implications on collocation procedures and domain decomposition methods, are analyzed. In particular, a non-standard collocation procedure -TH-collocation-, is described, whose interpolation properties are shown to be much superior to other numerical methods.

1 Introduction

There are two main approaches to formulating boundary methods; one is based on boundary integral equations and the other one, on the use of complete systems of solutions. The latter one is frequently associated with the name of Trefftz [1,2]. The author has studied extensevily a version of Trefftz method (Trefftz-Herrera, or simply TH-method), whose peculiarity is that the weighting functions that are applied, are solutions of the homogeneous differential equation, or more generally -for non-symmetric operators- of the adjoint differential equations [2-8]. When such weighting functions are used, all the information about the sought solution, contained in approximate solutions, is concentrated at the boundaries of the domain of the problem. For weighting functions that are only defined in a subdomain -as in finite elements, or domain decomposition procedures-, such information is concentrated at the internal boundaries that limit those subdomains [3-8].

Research by the author, especially his Algebraic Theory of Boundary Value Problems [3-8], has clarified the theoretical foundations of the TH-method and has expanded its versatility, making it applicable to any linear problem which is governed by partial differential equations or systems of such equations (in [9], a section was devoted to explain the application of the method to systems of partial differential equations).

Classical boundary methods deal with problems in which boundary conditions are prescribed at outer boundaries. However, in a more general version of boundary value problems, additional conditions are prescribed at interior boundaries. Trefftz method, in its original formulation, dealt with boundary value problems of the first class, exclusively [2,3]. However, the generalized version of Trefftz method -TH-method- has been formulated for boundary value problems in which jumps are prescribed at interior boundaries [4,6,8,9]. Generally, the region may be decomposed into many subdomains -or finite elements-, and in this manner the results of the theory are quite relevant for numerical methods [4,6,8-11]. Indeed, in this connection they have been applied to ordinary differential equations [6,10], and elliptic [11-13] and parabolic [9,14] partial differential equations. The numerical treatment of advection dominated transport, using this approach, has been very successful and has received much attention (see [15], for a brief review).

There is a class of applications for which analytical methods may be used successfully to develop weighting functions that satisfy the differential equation. Indeed, function theoretic methods supply general results for developing analitically complete systems of solutions. The work by Vekua [16], by Bergman [17] and by Gilbert [18], on this subject was followed by many others. In addition, the author's algebraic theory of boundary problems permitted applying the results of function theoretic methods to specific problems; in particular the concept of TH-completeness, first proposed by the author in [19], has been quite relevant. According to Begehr and Gilbert, in their recent survey of function theoretic methods ([20], p115):

> *The function theoretic approach which was pioneered by Bergman, and Vekua and then further developed by Colton, Gilbert, Kracht-Kreyszig [21], Lanckau [22] and others, may now be effectively applied because of results of the formulation by Herrera, as an effective means to solving boundary value problems.*

However, for more general applications, one must resort to numerical methods for developing such weighting functions (see, for example, [10]). When this is done, one is led to a kind of numerical discretizations or to domain decomposition procedures, depending on the point of view adopted. Using this approach, TH-domain decompositions were introduced in a previous paper that appeared in an anniversary volume of Trefftz method [11].

On the other hand, a class of non-standard numerical methods called TH-collocation was introduced in [11,13]. Standard collocation has been studied by many authors (for an extensive exposition, see [23]). TH-collocation differs from standard collocation in many respects and possesses many advantages over it; for example, standard collocation requires continuity of the function and its derivative, while TH-collocation only continuity of the function. Also, for symmetric operators, TH-collocation yields positive definite systems, while standard collocation does not enjoy this property. In addition to previous presentations [11,13], a more complete discussion of TH-collocation and TH-domain decomposition will appear soon [24]. In Section 3 of the present article, the general ideas of TH-Collocation are briefly explained and, as an example, an algorithm is introduced, that may thought as the simplest version of TH-collocation and which yields non-standard nine-point finite difference systems, positive definite, possessing very convenient interpolation properties, which other nine-point finite difference schemes do not possess. Numerical experiments and comparisons are carried out in Section 4.

2 TH-Domain Decomposition

To illustrate TH procedures, attention will be restricted to symmetric elliptic operators of second order:

$$\mathcal{L}u \equiv -\nabla\bullet(\underline{\underline{a}}\bullet\nabla u) + cu \qquad (2.1)$$

where $\underline{\underline{a}}$ is positive definite and $c \leq 0$. A domain Ω is considered, which will be decomposed into a system of subdomains Ω_i (i=1,...,E). The union of the common boundaries between the subdomains will be Σ.
The boundary value problem -with prescribed jumps- is defined by

$$\mathcal{L}u = f_\Omega \text{ in } \Omega \qquad (2.2)$$

subjected to Dirichlet boundary conditions:

$$u = u_\partial; \qquad \text{on } \partial\Omega \qquad (2.3)$$

On Σ, it will be required that u and its derivative be continuous -i.e., that the jumps be zero-: $[u] = [\partial u/\partial n] = 0$, on Σ. Here, the square brackets stand for the "jump" of the functions inside them. The spaces of trial and test functions will be D_1 and D_2, respectively. For simplicity, functions beloging to these spaces will be required to be continuous -with, possibly, discontinuous derivative. In addition, test functions $w \in D_2$, satisfy:

$$\mathcal{L}^* w \equiv \mathcal{L} w = 0, \text{ in } \Omega \qquad (2.4)$$

and vanish on the boundary.

Using the author's Algebraic Theory of Boundary Value Problems, it can be shown that the values on Σ, of any solution $u \in D_1$ of this problem, are characterized by the following variational principle [11,13]:

$$-\int_\Sigma u a_n [\partial w / \partial n] \bullet \underline{n} \, d\underline{x} = \int_\Omega w f_\Omega \, d\underline{x} - \int_{\partial\Omega} u_\partial a_n \partial w / \partial n \, d\underline{x} \quad \forall w \in W \qquad (2.5)$$

where $W \subset D_2$, is any TH-complete system [11,19]. More precisely:

Given a solution $u \in D_1$ of the boundary value problem -with prescribed jumps- and any function $\hat{u} \in D_2$, then $\hat{u} \equiv u$, on Σ, if and only if, the variational equation:

$$-\int_\Sigma \hat{u} a_n [\partial w / \partial n] \bullet \underline{n} \, d\underline{x} = \int_\Omega w f_\Omega \, d\underline{x} - \int_{\partial\Omega} u_\partial a_n \partial w / \partial n \, d\underline{x} \quad \forall w \in W \qquad (2.6)$$

is satisfied.

In addition, the bilinear form on the left-hand side of (2.5), is symmetric and positive definite on $D_2 \subset D_1$, because [11]

$$-\int_\Sigma v a_n [\partial w / \partial n] \bullet \underline{n} \, d\underline{x} = \int_\Omega (\nabla v \bullet \underline{\underline{a}} \bullet \nabla w + c v w) \, d\underline{x} \qquad (2.7)$$

whenever $v \in D_2$ and $w \in D_2$. Therefore, there is a minimum principle associated with the variational principle of Eq.(2.6). This was discussed in [11,13].

Observe that the left-hand side of Eq.(2.5) involves the values of u, on Σ, exclusively and can be applied using any trial function $\hat{u} \in D_1$; i.e., functions $\hat{u}$ that do not belong to D_2, can be used. In view of the identity (2.7), this variational principle can be modified, as follows:

Given a solution $u \in D_1$ of the boundary value problem, with prescribed jumps, and any function, $\hat{u} \in D_2$ then $\hat{u} \equiv u$, on Σ, if and only if:

$$\int_\Omega (\nabla \hat{u} \bullet \underline{\underline{a}} \bullet \nabla w + c \hat{u} w) \, d\underline{x} = \int_\Omega w f_\Omega d\underline{x} - \int_{\partial\Omega} u_\partial a_n \partial w / \partial n \, d\underline{x} \; \forall w \in W \qquad (2.8)$$

However, this last form of the variational principle requires $\hat{u} \in D_2$. Recalling the definiton of D_2, which only involves the homogeneous differential equation, an important observation is that when the variational principles of Eq.

(2.8) or (2.6), are applied, a particular solution of the inhomogeneous equation is not required in order to obtain the values of the solution on Σ.

3 TH-Collocation: a Nine-Points Finite Differences Scheme

General and sytematic procedures for developing TH-domain decompositions are presented in [11,13,24]. Also, TH-collocation in general. Here, to be specific, the region Ω will be the unit square [0,1]X[0,1] and the partition $\{\Omega_1,...\Omega_E\}$ of it, will be made of squares, with 'h' as side-length. In this case the total number of subregions is $E=1/h^2$ .Referring to Fig. 1a, with each interior node (x_i, y_j), we associate weighting functions $w_{ij} \in D_2$ -possibly many-, such that they satisfy $\mathcal{L}w_{ij}=0$, at the four elemental squares that

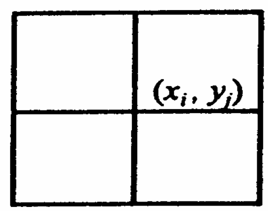

Fig 1a: Node (x_i, y_j), surrounded by four squares.

surround the node (x_i, y_j), and vanish identically outside of them. Since such functions are required to be continuous, they satisfy the condition of being zero at the outer boundary of the four squares. In addition, the internal boundaries associated with node (x_i, y_j), are numbered as indicated in Fig. 1b. Then five groups of weighting functions are constructed:

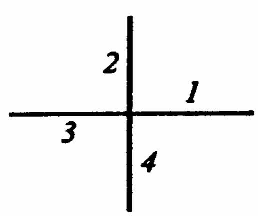

Fig 1b: Numbering of internal boundaries at each interior node.

Group 0).- This group is made of only one function, which is linear in each one of the four interior boundaries between the squares of Fig.1b, and such that $w_{ij}(x_i, y_j)=1$.

Group 1).- The restriction to interval "1", of Fig.1b, is a polynomial of degree "G", at most, which vanishes at the end points of interval "1".

Group 2).- The restriction to interval "2", of Fig.1b, is a polynomial of degree "G", at most, which vanishes at the end points of interval "2".

Group 3).- The restriction to interval "3", of Fig.1b, is a polynomial of degree "G", at most, which vanishes at the end points of interval "3".

Group 4).- The restriction to interval "4", of Fig.1b, is a polynomial of degree "G", at most, which vanishes at the end points of interval "4".

The support of functions of Group "0", is the whole square of Fig.1a, while those associated with Groups "1 to "4", have as support rectangles which can be obtained from each other by rotation [11,24].

In what follows we restrict attention to the simplest, but important, example for which the groups 1) to 4) are void. In this case a nine point, positive definite, finite difference scheme is obtained. Notice that only one weighting function is associated with each interior node. The approximation of the sought solution is written as

$$\hat{u}(x,y) = \sum_{K}^{E} \psi_K + \sum_{ij} U_{ij} w_{ij} \qquad (3.1)$$

where ψ_K is continuous, vanishes outside Ω_K satisfies the boundary condition (2.3), in $\Omega_K \cap \partial\Omega$, and $\mathcal{L}\psi_K = f_\Omega$, in Ω_K. Here, it is understood that the second summ ranges over pairs (i,j) corresponding to interior nodes. Then, when the variational principle of Eq. (2.8) is applied, the system of equations

$$M_{klij} U_{ij} = F_{kl} \qquad (3.2)$$

where the summation convention is understood -repeated indexes are summed over their ranges (interior nodes). The resulting matrix $\underline{\underline{M}}$ is nine-diagonal and symmetric, when the nodes are numbered using a natural ordering.

In the numerical applications, the weighting function have been approximated by polynomials, using Gaussian collocation [11,13,24]. For the particular case here considered, in which, only linear boundary values were prescribed on Σ, the approximate weighting function $\hat{w}_{ij}$ is taken as a linear combination of the functions $\xi\eta$, $\xi\eta xy$, $\xi\eta x^2 y$, $\xi\eta x y^2$, and $\xi\eta x^2 y^2$. Here, the function ξ is linear in x, and equals 1 at $x{=}x_i$, while η is linear in y, and equals 1, at $y{=}y_j$. The last four functions constitute a kernel -which is used to satisfy four collocation conditions, at the Gaussian points-, in the sense that all of them vanish on the internal boundaries Σ, while the first one is used to satisfy the internal boundary condition.

4 Numerical Experiments

The results of Section 3 were applied to Laplace equation; i.e., Eq.2.1 when $\underline{a}$ is the identity matrix and $c \equiv 0$. The discretized system of Eq.(3.2)

corresponds to a nine-point finite difference with weights 8/3 at the central node and -1/3 at the remaining eight nodes. This was compared with the performance of a 'standard'
9-point scheme, given by Collatz [25], with weights 1 at the central node, -1/20 at the corners, and -1/5 at the remaining nodes.

The boundary conditions on the unit square were taken so that the exact solution is $u=x^2-y^2$. The side-lengths for the squares of the partition, were taken successively as: .2, .1, .05, .025, .02, .01, .005, .0025, and .002. The resulting systems of equations were solved by iteration, using the same conjugate gradient algorithm for both discretization procedures.

It was found that the number of iterations required to achieve a given level of accuracy at the nodes, do not differ much for the 'standard' and the TH scheme (Fig. 2). However, the interpolation properties of the TH-nine-point finite differences, are clearly superior. For the TH-finite-difference scheme, the interpolation was carried out by means

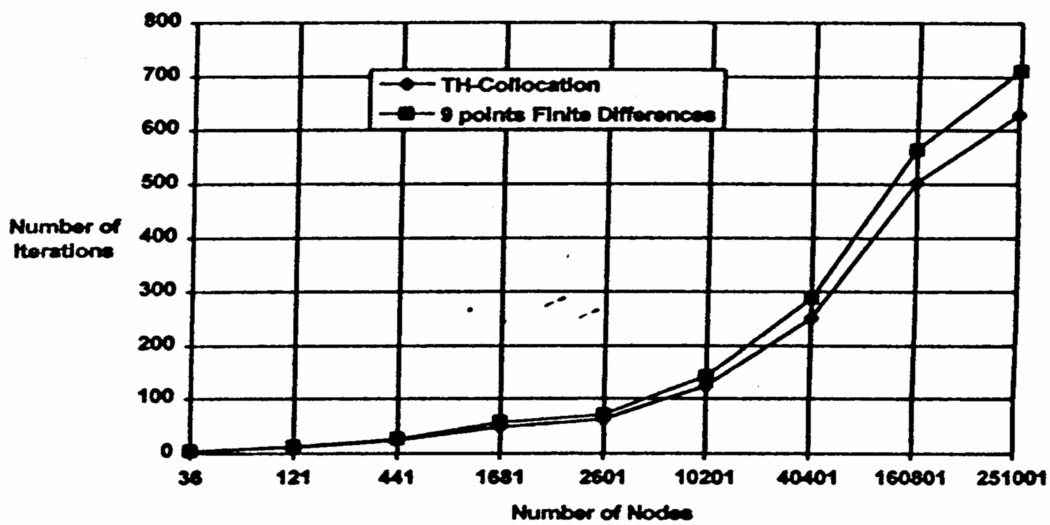

Fig. 2 Number of iterations to achieve a desired order of accuracy

of Eq.(3.1), while for the standard 9-point scheme, bi-cubic splines (SURFER FOR WINDOWS), were used. The results are compared in Fig.3. It is seen that the errors, for the standard procedure, are many orders of magnitude larger than those for TH-Collocation.

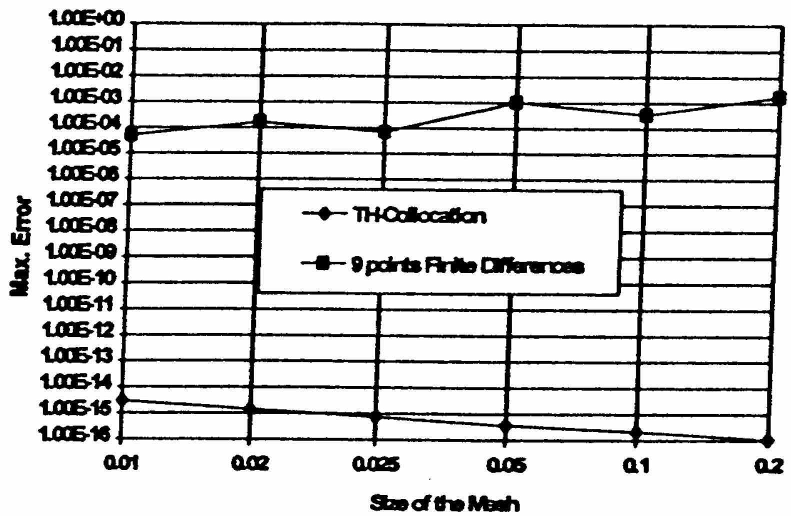

Fig. 3 Comparison of errors for different mesh sizes

Acknowledgements

The computations presented in the Section on numerical experiments were carried out by Martin Diaz Viera. The research reported in this article was supported by NSF-CONACYT, Primavera '94, "Solución de ecuaciones de flujo Subterráneo usando métodos de colocación y procesamiento en paralelo", DGAPA.-IN102695, UNAM-CRAY.-SC002695 & SC003495.

REFERENCES

1.- Trefftz, E., "Ein Gregensttck zum Ritz'schen Verfahren", Proc. Second Int. Congress Appl. Mech. Zurich, 1926.
2.- Herrera, I., "Trefftz Method" In Topics in Boundary Element Research, Vol.1: Basic Principles and Applications, C.A. Brebbia, Ed., Springer-Verlag, Chapter 10, pp 225-253, 1984.
3.- Herrera, I. "Boundary methods. An algebraic theory". Pitman Advanced Publishing Program, Boston, London, Melbourne, 1984.
4.- Herrera, I., "Unified approach to numerical methods. Part 1. Green's formulas for operators in discontinuous fields", Numerical Methods for Partial Differential Equations, 1(1), pp 12-37, 1985.
5.- Herrera, I., "Unified Approach to Numerical Methods. Part 2. Finite elements, boundary methods and its coupling", Numerical Methods for Partial Differential Equations, 1(3), pp 159-186, 1985.

6.- Herrera, I., L. Chargoy y G. Alduncin "Unified approach to numerical methods. Part 3. Finite differences and ordinary differential equations", Numerical Methods for Partial Differrential Equations, 1,241-258 (1985).

7.- Herrera, I.,"Some unifying concepts in applied mathematics", In The Merging of Disciplines: New Directions in Pure, Applied, and Computational Mathematics, Edited by R.E. Ewing, K.I. Gross and C.F. Martin. Springer Verlag, New York, 1986 (Ponencia Invitada).

8.- Herrera, I.,"Localized Adjoint Methods: A New Discretization Methodology", Chapter 6 of Computational Methods in Geosciences, Eds. W.E. Fitzgibbon and M.F. Wheeler, SIAM, Philadelphia, 1992.

9.- Herrera, I., Ewing, R.E., Celia, M.A., and T.F. Russell., "Eulerian-Lagrangian Localized Adjoint Method: The Theoretical Framework", Numerical Methods for Partial Differential Equations, 9, pp 431-457, 1993.

10.- "The algebraic theory approach to ordinary differential equations: Highly accurate finite differences", Numerical Methods for Partial Differential Equations, John Wiley, New York, 3(3), pp 199-218, 1987. Herrera, I

11.- "Trefftz-Herrera Domain Decomposition", Special Volume on Trefftz Method: 70 years anniversary; Advances in Engineering Software, 24, pp 43-56, 1995 (Invited Chapter).

12.- Celia, M.A., Herrera, I., and Bouloutas, E.T. "Adjoint Petrov-Galerkin Methods for Multi-Dimensional Flow Problems", Finite Element Analysis in Fluids, T.J. Chung and R. Karr, Eds. University of Alabama Press, pp 953-958, 1989.

13.- Herrera, I., Camacho A. and Hernsndez J., "TH-Collocation Method", Second UNAM-Cray Supercomputing Conference, Numerical Simulations in the Environmental and Earth Sciences, June 1995.

14.- Celia, M.A., Russell, T.F., Herrera, I., y Ewing, R., "An Eulerian-Lagrangian Localized Adjoint Method for the Advection-Diffusion Equation". Advances in Water Resources, 13(4), pp.187-206, 1990.

15.- Celia, M. A.,"Eulerian-Lagrangian localized adjoint methods for contaminant transport simulations", Computational Methods in Water Resources X, Vol 1, Eds. A. Peters., et.al., Kluwer Academic Publishers, Heidelberg, pp 207-216, 1994.

16.- Vekua, I.N., "New methods for solving elliptic equations", North Holland, Amsterdam etc. and John Wiley, New York, XII, 358 pp, 1967.

17.- Bergman, S.,"Integral operators in the theory of partial differential equations", Erbeg. Math. Grenzgeb 23, Spinger, Berlin etc., 1961; 2 rev. print., 1969.

18.- Gilbert, R.P., "Function theoretic methods in partial differential equations", Academic Press, New York, XVIII, 311 1969.

19.- Herrera, I., "Boundary methods: A criterion for completeness", Proc. National Academy of Sciences, USA, 77(8), pp 4395-4398, 1980.

20.- Begehr, H. and Gilbert, R.P.,"Transformations, transmutations, and kernel functions", Vol 1, Longman Scientific & Technical Essex, England, 399 pp, 1992.

21.- Kracht, M and Kreyszig, E., "Methods of complex analysis in partial differential equations with applications", Wiley & Sons, New York etc., XIV, 394 pp, 1988.

22.- Lanckau E., "Complex integral operators in mathematical physics", Akademie-Verlag Berlin, to appear.

23.- Celia, M.A. "Collocation on deformed finite elements and alternating direction collocation methods", Doctoral dissertation, Department of Civil Engineering, Princeton University. September 1983.

24.- Herrera, I., To be published. Num.Part.Diff.Eqs. 1996.

25.- Collatz, L., "Numerical Treatment of Different Equations", Third Edition, Springer-Verlag, 1960.