INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng (2009)
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nme.2697

Generalized finite differences using fundamental solutions

V. M. A. Leitão*, †

DECivil-ICIST, Instituto Superior Técnico, TULisbon, Av. Rovisco Pais 1049-001 Lisboa, Portugal

SUMMARY

It is well known that solutions for linear partial differential equations may be given in terms of fundamental solutions. The fundamental solutions solve the homogeneous equation exactly and are obtained from the solution of the inhomogeneous equation where the inhomogeneous term is described by a Dirac delta distribution. Fundamental solutions are the building blocks of the boundary element method and of the method of fundamental solutions and are traditionally used to build boundary-only global approximations in the domain of interest. In this work the same characteristic of the fundamental solutions, that of solving the homogeneous equation exactly, is used but not to build a global approximation. On the contrary, local approximations are built in such a manner that it is possible to construct finite difference operators that are free from any form of structured grid. Copyright © 2009 John Wiley & Sons, Ltd.

Received 26 March 2009; Revised 1 June 2009; Accepted 9 June 2009

KEY WORDS: solids; finite difference methods; mesh-free methods; fundamental solutions; collocation

1. INTRODUCTION

Approximate solutions for problems governed by systems of partial differential equations (PDEs) may be obtained by a variety of methods. Some of these methods, such as the boundary element method (BEM) (e.g. [1]), other boundary integral methods and the method of fundamental solutions (e.g. [2]) on one side, and the Trefftz method (be it the collocation, e.g. [3, 4], or the Galerkin approaches, e.g. [5–7]) on the other side, rely on the use of specific knowledge about the solution of the PDE being analysed. The Trefftz concept [8], as it is known, is the general framework when the extra information available is the actual solution of the homogeneous equation. The main characteristic of these methods that take advantage of this extra information is that only the boundary of the problem needs to be discretized. That is why they are usually referred to as being *boundary-only solution methods*. This is true at least for homogeneous problems and techniques

*Correspondence to: V. M. A. Leitão, DECivil-ICIST, Instituto Superior Técnico, TULisbon, Av. Rovisco Pais 1049-001 Lisboa, Portugal.
†E-mail: vitor@civil.ist.utl.pt

Contract/grant sponsor: Instituto de Engenharia de Estruturas Território e Construção do Instituto Superior Técnico (ICIST)
Contract/grant sponsor: Fundação para a Ciência e a Tecnologia (FCT)

are available that even for some inhomogeneous problems the domain needs not discretization. Another characteristic shared by these methods is the fact that global approximations are used, that is, the approximation is single valued at every point as the support of each function (be it the fundamental solution or not) contributing to the approximation is global.

The more popular numerical methods, such as the finite element method (FEM) and the finite difference method (FDM), follow different paths [9]: the domain is discretized into elements or grids, whereby local approximations using functions exhibiting only basic properties of continuity and differentiability are used in an explicit, as in the FEM, or an implicit manner, as in the FDM. These methods may be commonly referred to as being *domain methods*.

Every method has its own merits. The local character of the domain methods approximations is quite convenient: local effects may be captured in an efficient manner and undesirable characteristics (eventually leading to ill-conditioned matrices) are not numerically propagated to the whole domain. It also adds to the advantages of, in particular, the FEM that complex geometries may be accurately modelled and that complex characteristics of the governing equations themselves (geometrical and physical non-linearities, for example) are also properly simulated.

Some of the aspects referred above are, in fact, known disadvantages of the boundary solution methods: the difficulty to deal with non-linear problems (at least without resorting to domain discretization as well); and the possibility of ill-conditioning when the number of unknowns increases.

As for the FDM, the main disadvantage of the standard approach is the need to define a structured grid of points in order to define the difference operator. To overcome the need for a structured grid, some non-standard approaches have been proposed, which attempt to generalize the distribution of points by relaxing the grid requirements, thus allowing for difference operators to be obtained on non-structured distribution of points.

A possible way to achieve that is to rewrite the operators by using a convenient basis of functions. This is the approach followed in [10, 11] where radial basis functions (RBF) are used to construct local interpolations on localized sets of points. The interpolations are subsequently used to find the difference operators which are then used in a similar way to traditional finite differences (FDs). The same approach would also be possible with polynomials, but RBFs provide better rates of convergence and higher accuracy for unstructured grids.

One of the more successful of the non-standard approaches is the Generalized Finite Difference Method (GFDM) [12]. In this method a moving least-squares scheme is used to obtain the coefficients of the unknown function being approximated. The least-squares scheme minimizes the squares of the differences between the function and its approximation. However, it is a relatively complex procedure that requires, for a given set of neighbouring points, the definition of a polynomial basis, the definition of a weight function and the inversion of a matrix involving these functions for that particular neighbourhood.

In this work another approach is followed to build the difference operator. It is linked to the work of Mickens [13] on non-standard finite differences (NSFD), whereby the approximated difference operator takes into account properties of interest of the problem being modelled. If all the relevant properties are considered then, in this limiting case, the result is an exact difference scheme thus reducing the difficulties related to consistency, stability and convergence. But this is very difficult to achieve and there are not many applications of NSFD for problems other than the one-dimensional case.

This idea was further developed by Tsukerman [14], who proposed to resort to the Trefftz concept, that is, to use actual solutions of the homogeneous equation and to define the coefficients

DOI: 10.1002/nme

by taking advantage of that property. The NSFD schemes may be seen to share some of the properties of Tsukerman's class of difference schemes and may be considered to be particular cases of that broader class.

The novelty in the work now being proposed is that fundamental solutions are used instead of the sets of regular Trefftz functions used by Tsukerman. As referred above, the fundamental characteristic of the Trefftz functions and of the fundamental solutions is that they satisfy the underlying differential equation. As the Trefftz functions are more general (in the sense that these functions are valid on a given domain and also at its boundary, whereas the fundamental solutions are valid at the domain but not at the boundary where the sources are located), then there are reasons to consider fundamental solutions as a particular case of Trefftz functions. Historically, however, researchers (depending on their origin and in particular for those dealing with boundary integral equations) have tended to emphasize the distinguishing aspects as these lead to different numerical methods. At this point it is convenient to cite Zielinski [15] '*It is not easy to introduce a distinct border separating the modern Trefftz method from the other similar boundary methods of mathematical modelling. The most popular definition consists of the application of analytically derived trial functions*, *sometimes called T-functions*, *identically fulfilling certain governing differential equations inside a considered area* Ω (*including its boundary* Γ). *This definition would eliminate all singular boundary integral equation methods* (*e.g. various versions of the singular BEM*), *which apply functions fulfilling the differential equations everywhere except* Γ'.

When it comes to implementation, and in a general framework of application of the methods to PDEs not in the framework of local approximations, fundamental solutions have some slight advantages over regular Trefftz functions (*regular* as opposed to the *singular* character of fundamental solutions):

- for a given problem a unique fundamental solution is used, whereas the complete series of regular Trefftz functions has an infinite number of terms. Of course, the series is truncated but there are more functions to code than with a unique generic expression for the fundamental solution;
- the passage from two-dimensional to three-dimensional applications is much facilitated when fundamental solutions are used as these solutions do not vary greatly as compared with the different Trefftz functions required.

The first item above is just a minor one at least for the simplest cases: for the Laplace two-dimensional problem, for example, the elements of the Trefftz series, after the linear term, are defined in a unique manner depending only on the degree of that particular term being calculated. Going from two to three dimensions and for other types of problems there are more visible differences. Take, for example, the elasticity problem. While the fundamental solution is still represented by a single function, [16], the elements of the Trefftz series obtained from the Papkovitch–Neuber potentials by using, for example, Legendre and/or Chebyshev polynomials have to be derived in advance (meaning, prior to coding) as linear dependencies have to be removed and completeness, up to that degree, has to be guaranteed [17]. Of course, once these terms of the series are coded there are no more difficulties (than with fundamental solutions) except if one decides to increase the number of terms in the series.

Generally speaking, the main disadvantage of the fundamental solutions is the need to define the location of the sources on a fictitious boundary as this fictitious boundary cannot coincide with the actual boundary of the problem. This can pose some difficulties for standard applications of the method of fundamental solutions (in particular for complex geometries and high number

DOI: 10.1002/nme

of unknowns), but it hardly causes any problems in the approach proposed here. As it will be made clear later, the geometry of the local regions (where the approximations are defined) is very simple and the number of unknowns is very low; the combination of these two factors precludes the occurrence of numerical problems related to ill-conditioning or loss of accuracy that may normally be associated with a non-optimal definition of the fictitious boundary. A disadvantage of the Trefftz method (which, in a certain way, is equivalent to that of the fictitious boundary when fundamental solutions are used) is the need to conveniently choose the origin of the system of coordinates where to place the Trefftz functions and this includes choosing the proper axes and also normalizing the distances between the points of interest. Again, in the context of the local approximations that are of interest in Tsukerman's as well as in this work, the geometry of the local regions is so simple and the number of unknowns is so low that there are no reasons for concern in the choice of the origin and the direction of the axes and there is no need for normalizing the distances.

In this paper a new technique to define generalized difference operators for completely irregular distribution of points by means of fundamental solutions is proposed. The potential of this technique is, to say the least, appreciable. Points can be added to a given distribution without any special care except that the two points cannot be coincident. It is possible to think of adding patches of points in any shape or size or density on a given geometry if needed and still obtain a local difference operator of very high quality.

Applications of this technique to two-dimensional potential problems are considered here. Comparison to other results available in the literature show that the method is accurate, reliable and may be considered to be an alternative to other numerical methods. As for applications to other types of problems it is expected that generalized FD operators constructed in the form here described will work as efficiently as for the potential case. As long as fundamental solutions or regular Trefftz series solution exist for a given differential equation there is no reason why generalized FD schemes of the type described here cannot be obtained. In Tsukerman's work, [14, 18], flexible local schemes with regular Trefftz functions have been successfully applied to a variety of problems such as the Schrödinger equation, time-domain scalar wave equation, wave propagation, scattering from a dielectric cylinder among other electromagnetic applications. The same is to be expected by using fundamental solutions.

2. FUNDAMENTAL SOLUTIONS

Consider the boundary problem

$$\begin{aligned} \mathscr{L}_\Omega u(\mathbf{x}) &= 0 \in \Omega \\ \mathscr{L}_\Gamma u(\mathbf{x}) &= g(\mathbf{x}) \in \Gamma = \partial\Omega \end{aligned} \tag{1}$$

where $\mathscr{L}_\Omega$ stands for an elliptic differential operator valid in the domain of the problem and the boundary condition on Γ is given by the boundary operator $\mathscr{L}_\Gamma$. For simplicity only the homogeneous setting is considered here, extension to various classes of inhomogeneous problems is straightforward as will be seen later.

The fundamental solution Φ for the $\mathscr{L}_\Omega$ operator is such that its solution, when operated by $\mathscr{L}_\Omega$, is the Dirac delta distribution

$$\mathscr{L}_\Omega \Phi(\mathbf{x}, \mathbf{z}) = \delta(\mathbf{x}, \mathbf{z}) \quad \forall \mathbf{z} \in \Omega^d, \ \ \mathbf{z} \neq \mathbf{x} \tag{2}$$

DOI: 10.1002/nme

where $\mathbf{x}$ is any given point in the domain of the problem, also known as the *field* point, and $\mathbf{z}$ is the point where the Dirac distribution is centered, also known as the *source* point. At this point it should be mentioned that fundamental solutions may be seen (and are, in some fields, known in that way) as Greens functions for the inhomogeneous problem. Alternatively, Green's function may be seen as a fundamental solution of a linear differential equation satisfying homogeneous boundary conditions. Mathematicians tend to distinguish Green's functions from fundamental solutions in the sense that Green's functions are restricted to the space of solutions that satisfy at least part of the boundary conditions, whereas the space of fundamental solutions is not required to satisfy any of the boundary conditions [16].

For the particular case of the Laplace operator in a two-dimensional space

$$\mathscr{L}_{\Omega} u(x_1, x_2) = \frac{\partial^2 u(x_1, x_2)}{\partial x_1^2} + \frac{\partial^2 u(x_1, x_2)}{\partial x_2^2} \tag{3}$$

the fundamental solution is

$$\Phi(\mathbf{x}, \mathbf{z}) = -\frac{1}{2\pi} \log(r(\mathbf{x}, \mathbf{z})) \tag{4}$$

where $r(\mathbf{x}, \mathbf{z})$ is the distance between the field and the source points. As can be easily seen this function exactly solves the Laplace equation at all points except the exact place where the fundamental solution is located.

The fundamental solution may be interpreted as an influence function that represents at every field point the effect of a single unit Dirac-like distribution source:

$$u(\mathbf{x}) = \Phi(\mathbf{x}, \mathbf{z}), \quad \mathbf{x} \neq \mathbf{z} \tag{5}$$

Unit sources are considered in the definition of the fundamental solution only to ensure that the field function may be reproduced in the following form:

$$u(\mathbf{x}) = \int \mathscr{L}_{\Omega} \Phi(\mathbf{x}, \mathbf{z}) u(\mathbf{z}) \, \mathrm{d}\mathbf{z} \quad \forall \mathbf{z} \neq \mathbf{x} \tag{6}$$

To keep the formulation as general as possible it is convenient to introduce a scaling factor that amplifies the effect of each source by an unknown quantity σ and it is also convenient to allow for multiple sources instead of just a single one. The superposition of all these effects results in the following approximation:

$$u(\mathbf{x}) = \sum_i \Phi(\mathbf{x}, \mathbf{z}_i) \sigma_i \quad \forall \mathbf{z}_i \neq \mathbf{x} \tag{7}$$

This is the basis of the methods that rely on the use of fundamental solutions, namely the BEM and the method of fundamental solutions. The main difference between these methods is that the method of fundamental solutions, in its basic form as given in (7), uses discrete sources on a fictitious boundary ($\mathbf{z}_i \neq \mathbf{x}$) and the BEM uses distributed sources on the actual boundary of the problem after going through a limiting process that allows the sources to be placed on the boundary.

The method of fundamental solutions is no more than the simultaneous application of (7) on a set of suitably chosen boundary points and by considering a set of sources of unknown magnitudes. Notice that as the fundamental solution exactly satisfies the field equation at all domain points, all

DOI: 10.1002/nme

that remains to match are the boundary conditions. Notice also that Equation (7) is the condition that one needs to verify in the case of a pure Dirichlet problem, that is, when the boundary conditions are given in terms of the actual primary variable. When the conditions are also given in terms of the variable derivatives then it is necessary to find the corresponding approximation, for example:

$$\frac{\partial}{\partial x_1} u(\mathbf{x}) = \sum_i \frac{\partial}{\partial x_1} \Phi(\mathbf{x}, \mathbf{z}_i)\sigma_i \quad \forall \mathbf{z}_i \neq \mathbf{x} \tag{8}$$

The solution of the system is the set of actual scaling factors that affect each source. Once those are known it is straightforward to calculate the field variable (or any of its derivatives) anywhere in the domain of the problem by superposition.

3. T-COMPLETE SERIES

Fundamental solutions are not the only strategy for solving exactly the homogeneous field equation. Solutions exist, e.g. [19, 20], in the form of infinite and complete series where each term of the series is a non-singular function (as opposed to the singular fundamental solution). For the two-dimensional Laplace problem the T-complete (T- as in Trefftz) series is as follows (in polar coordinates, for convenience):

$$\sum_{n=0}^{\infty} (a_n r_i^n \cos n\theta_i + b_n r_i^n \sin n\theta_i) \tag{9}$$

where a_n and b_n are the unknowns to be found after matching the boundary conditions as seen for the method of fundamental solutions. This approach is known as the collocation approach. It should be mentioned that Galerkin-based approaches exist that use the T-complete series to build high-order macro finite elements, e.g. [5, 6].

4. LOCAL APPROXIMATIONS

The approximation that is obtained in the form described above is a global approximation, i.e. it is valid in the whole domain and it resulted from the superposition of the whole set of sources. Although it is possible to partition the domain of interest and build different approximations that are then made to match at the interfaces, the truth is that global approximations are still being built for each of the subdomains in which the original domain was decomposed. Global approximations are, by nature, single-valued functions and this is what is obtained with the method of fundamental solutions and other methods.

The main problem with global approximations is that they are inherently prone to ill-conditioning, the higher the number of unknowns (be it the number of sources or the number of terms taken in the T-series) the worse the numerical conditioning. It is a fact that the very high quality of the solutions allows for accurately solving many problems with a much lower number of unknowns than with the traditional local approximation methods such as FEM and FDM, but it is also true that the range of problems that can be solved with global approximations is not as complete as with the FEM and the FDM. For example, if the geometry is too complex then the number of unknowns grows fast and with that the potential for ill-conditioning.

DOI: 10.1002/nme

Local approximations based on fundamental solutions could naturally circumvent the ill-conditioning problems (as the number of unknowns is kept small) but only if they do not require a fixed domain decomposition, that is, if no interface matching is necessary. And this leads us to local approximations in overlapping regions without interfaces.

This seems a difficult task as even the FEM approximations are built on non-overlapping domain decompositions, the elements. An alternative way to build local approximations on overlapping domains could be one of the meshless methods based on the moving least-squares concept. This is an interesting approach that has, recently, been the subject of the attention of a number of researchers, e.g. [21]. These methods will not be addressed here as our focus is the use of fundamental solutions which do not seem to have a place in the framework of the moving least-square-based methods.

Looking now at FDs it is possible to see that multiple values are expected for a given point depending on how the approximated differential operator is constructed or, by using an alternative argument, the value at a given field point (which is not one of the grid points) depends on the neighbouring grid points and on any basis of functions used to reconstruct the approximation and this, of course, may vary.

5. STANDARD FD APPROXIMATION OF THE DIFFERENTIAL OPERATOR

The approach followed by the FDM is not that of building an approximation for the variable itself but rather for the differential operator that operates on the variables. And this is what allows for that overlapping local approximations. For the sake of clarity of the remainder of the work, a brief description of the FD concept will now be given.

Let us consider the Laplace equation and the primary variable $u(\mathbf{x})$, which is assumed to be known at a set of points distributed on a regularly spaced grid. It is well known that by writing Taylor expansions for points around the central point in each direction the following expression is obtained:

$$\left(\frac{\partial^2 u(\mathbf{x})}{\partial x_1^2}+\frac{\partial^2 u(\mathbf{x})}{\partial x_2^2}\right)_{x_1^i,x_2^j}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}+\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{h^2} \tag{10}$$

where h is the spacing between the points. This expression accurately (second-order accurate) represents the Laplace operator at the central point of a set of five symmetrically distributed points. The main problem with this scheme is that a fixed grid is necessary as the Taylor expansion is defined for fixed distances between points.

6. GENERALIZED FD APPROXIMATION

Generalized FD schemes (generalized in the sense of allowing for irregular distribution of points) have been obtained by resorting to the least-squares concept, [12]. Basically what the method does is to construct an overdetermined system of linear equations where each of them corresponds to the Taylor expansion at a given point but written relative to each of the points of a given local set. The system is solved by a least-squares algorithm in which each of the equations is weighted in a

DOI: 10.1002/nme

way which is inversely proportional to the distance between the given point and the point where the Taylor expansion is being written. It is not an easy procedure, but the end result is that FD operators are obtained for irregularly distributed points.

7. GENERALIZED LOCAL APPROXIMATION WITH FUNDAMENTAL SOLUTIONS

The method to build local approximations by means of the fundamental solutions, which is now being proposed is the fundamental solutions counterpart to the method proposed by Tsukerman [14] using Trefftz functions, a method that Tsukerman includes in a 'new class of flexible local approximation methods (FLAME)'. This also includes non-Trefftz (non-collocation, meaning variational) schemes that are not going to be considered in the sequence. Further details of the Trefftz and the non-Trefftz FLAME schemes may be found in the cited work [14]. In the following, attention will be focused on the application of fundamental solutions to the FLAME methodology for the Laplace equation in two dimensions (1).

Let us consider a set of n points distributed in the domain Ω. Assume also that the domain is decomposed into a set of n overlapping subdomains $\Omega^{(i)}$ that completely cover Ω:

$$\Omega = \bigcup \Omega^{(i)}, \quad i = 1, 2, \ldots, n \tag{11}$$

Each subdomain is centered on a particular point and includes a given number of other points. These subdomains are the supports of local approximations involving all the points within the support (see Figure 1). As the supports overlap there is no single value for $u(\mathbf{x})$, the value the function takes at a particular location $\mathbf{x}$ depends on which local approximation is being considered.

By using fundamental solutions the following approximation for $u(\mathbf{x})$ in Ω is obtained:

$$u_h^{(i)}(\mathbf{x}) = \sum_{j=1}^{m^{(i)}} \Phi^{(i)}(\mathbf{x}, \mathbf{z}_j^{(i)}) \alpha_j^{(i)} \quad \forall \mathbf{z}_j^{(i)} \neq \mathbf{x} \tag{12}$$

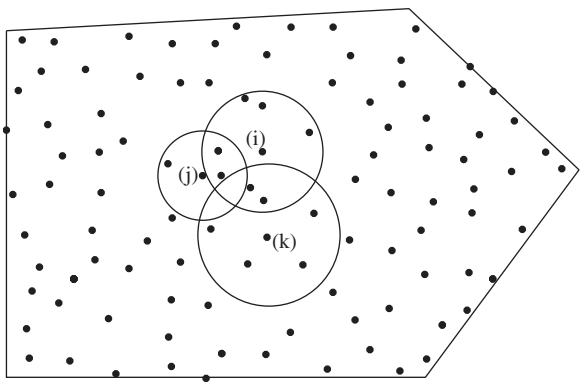

Figure 1. Distribution of points in Ω and local supports (i), (j) and (k).

DOI: 10.1002/nme

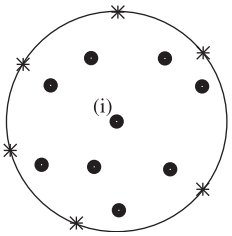

Figure 2. Generic local support, distribution of discrete points • and location of the fundamental solution sources ∗.

where $\Phi^{(i)}(\mathbf{x}, \mathbf{z}_j^{(i)})$ is given by (4) and the $\alpha_j^{(i)}$ coefficients represent the scaling factors of the fundamental solution. Extending the approximation to all points within the subdomain the following matrix form may be written as:

$$\mathbf{u}_h^{(i)} = \mathbf{\Phi}^{(i)} \boldsymbol{\alpha}^{(i)} \tag{13}$$

Owing to the singular behaviour of the fundamental solution the location of the sources cannot coincide with that of the discrete points within each subdomain. Figure 2 shows a schematic representation of the sources for a generic subdomain.

Notice now that (12) is written in terms of the $\alpha_j^{(i)}$ and not in terms of the actual values of $u(\mathbf{x})$ at the discrete points as needed in any FD scheme. Another difference is that if we were dealing with a standard application of the method of fundamental solutions, Equation (12) would be written for the boundary points only as the fundamental solution exactly satisfies the Laplace equation in the domain.

The FD approach requires the application of the field equations in the domain and at the boundary. For each point and each governing equation it is necessary to write an FD scheme at that point that only involves the function values at the neighbouring points. For example, for the central difference and the Laplace operator one has

$$0 = -4u_{i,j} + u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} \tag{14}$$

where unit spacing is considered for simplicity.

Therefore, the enforcement of each domain (or boundary) equation is, in the FD approach, written in the form

$$\mathbf{s}^{(i)\mathrm{T}} \mathbf{u}^{(i)} = 0 \tag{15}$$

where $\mathbf{s}^{(i)}$ is the vector of coefficients of the difference equation involving the $\mathbf{u}^{(i)}$ values.

Recalling (13) one may write:

$$\mathbf{s}^{(i)\mathrm{T}} \mathbf{\Phi}^{(i)} \boldsymbol{\alpha}^{(i)} = 0 \tag{16}$$

This condition has to be satisfied for all $\boldsymbol{\alpha}^{(i)}$ and this is only possible if $\mathbf{s}^{(i)}$ is orthogonal to $\mathbf{\Phi}^{(i)}$

$$\mathbf{\Phi}^{(i)\mathrm{T}} \mathbf{s}^{(i)} = 0 \tag{17}$$

DOI: 10.1002/nme

This may also be interpreted as $\mathbf{s}^{(i)}$ being in the null space of $\mathbf{\Phi}^{(i)\mathrm{T}}$:

$$\mathbf{s}^{(i)} \in \mathrm{Null}(\mathbf{\Phi}^{(i)\mathrm{T}}) \tag{18}$$

This expression is the central one in Trefftz FLAME's approach and leads to the following result: if the null space of the approximating matrix is of dimension one (if it is a vector), then $\mathbf{s}^{(i)}$ defines the sought FD scheme.

As fundamental solutions are being used, not only the differential equation is satisfied (for the chosen linear combination of fundamental solutions) but also the approximated difference equation defined by $\mathbf{s}^{(i)}$. The use of solutions of the actual governing equation, be it Trefftz functions or fundamental solutions as in this work, maximizes the possibilities of obtaining the best set of difference coefficients for a given local neighbourhood of points.

Consistency and convergence are important aspects of any formulation. In the framework of Trefftz flexible local approximation schemes it was shown, in [14], that the consistency error is bounded by the approximation error. As the Trefftz bases exhibit very good approximation properties the end result is that consistency and convergence are guaranteed. And the same may be expected when fundamental solutions are used instead of Trefftz functions. As a matter of fact Trefftz series and fundamental solutions are, despite its differences, intimately linked at the mathematical level, [22], and this allows to apply the same reasoning when addressing convergence and consistency issues.

8. IMPLEMENTATION ISSUES

Once the coefficients affecting all the grid points within each neighbourhood are known, it is necessary to construct the system of equations representing all the conditions to be enforced. This is done in a classical FD manner. For a Dirichlet boundary point this is quite trivial: a unit value is allocated to the diagonal term of the global matrix, all the other matrix terms in that row are zero and the right-hand side vector takes the corresponding value of the prescribed boundary condition.

Enforcing Neumann boundary conditions requires the approximation of normal derivatives along the boundary. This is not a trivial issue in traditional FD schemes. A number of techniques have been proposed, see [23, 24] among many others, which usually rely on, basically, two techniques: by using fictitious or ghost points; by using some elaborate Taylor schemes involving a number of interior points.

The generalized approach proposed in this work may use any of the existing FD schemes but other alternatives are possible. One of the more interesting approaches (by its generality and flexibility) is to define a local approximation for the normal derivative by using a set of RBFs based on each of the local grid points in the neighbourhood of a Neumann boundary point. The same technique, local approximation by RBFs, is used to obtain the necessary values for creating the plots of the variables of interest in a given neighbourhood. Details on the use of RBFs for building approximations may be found in, e.g. [25].

The equations representing the domain governing equation are also very simple to define. In the homogeneous case it is simply necessary to allocate the coefficients in the corresponding columns of the row being written in the system matrix and to allocate the zero value to the right-hand side vector.

For the inhomogeneous case, when there is a non-null right-hand side $b(\mathbf{x})$,

$$\mathscr{L}_{\Omega} u^{(i)}(\mathbf{x}) = b^{(i)}(\mathbf{x}) \tag{19}$$

DOI: 10.1002/nme

the general solution is decomposed into the homogeneous and a particular solution:

$$u^{(i)}(\mathbf{x}) = u_0^{(i)}(\mathbf{x}) + u_p^{(i)}(\mathbf{x}), \quad \mathbf{x} \in \Omega^{(i)} \tag{20}$$

Two options are now possible: one may consider a transformation of variables such that the homogeneous equation is solved for transformed boundary conditions, or one may use the particular solution to construct the right-hand side term by taking into account the actual difference coefficients for the neighbourhood of interest. The first option requires that, after obtaining the solution for the homogeneous problem, the particular solution is added to find the general solution.

The second approach is the result of the straightforward application of (15) to the decomposition:

$$\begin{aligned} \mathbf{s}^{(i)\mathrm{T}}\mathbf{u}^{(i)} &= b^{(i)} \\ \mathbf{s}^{(i)\mathrm{T}}(\mathbf{u_0}^{(i)} + \mathbf{u_p}^{(i)}) &= b^{(i)} \\ b^{(i)} &= \mathbf{s}^{(i)\mathrm{T}}\mathbf{u_p}^{(i)} \end{aligned} \tag{21}$$

The right-hand side term $b^{(i)}$ now includes the effect of the particular solution over all the grid points within local support $\Omega^{(i)}$.

9. APPLICATION TO POTENTIAL PROBLEMS

The proposed approach is now applied to a set of two-dimensional potential problems. The first application refers to the Laplace equation (no right-hand side term in the governing equation) under Dirichlet boundary conditions on a unit square region. It is a heat conduction problem for which there is an analytic solution in the form of an infinite series. Regular and irregular distribution of points are analysed.

The second application is that of a Poisson equation. The right-hand side term is a simple product of sin functions. It is a very simple case for which there is an exact solution.

The remaining applications concern torsion analysis of prismatic bars (again, Poisson). The first of these applications is on a rectangular region (the prismatic bar has a rectangular cross-section) of which only a quarter is modelled by taking advantage of symmetry. Neumann boundary conditions are enforced on the symmetry axes and Dirichlet are imposed on the other two sides.

Then, to emphasize the ease in the creation of distributions of points, a prismatic bar with an elliptical cross-section is analysed.

In all cases tested, and with reference to Figure 1, the fictitious sources are placed on a circumference centered at the point of interest (i). The radius of the circumference is 100 times the maximum distance between the points in the local neighbourhood.

For comparison purposes the Trefftz FLAME methodology was also coded. Comparison of the results obtained with fundamental solutions and harmonic polynomials is presented for the first two problems. As expected, and due to the above referred equivalence of fundamental solutions and harmonic polynomials for Laplace and biharmonic equations [22], there are virtually no differences.

DOI: 10.1002/nme

9.1. *Laplace equation*

Consider the case of a potential function, $u(x, y)$, on a unit square region. The potential has to satisfy the Laplace equation

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0$$

and the following Dirichlet boundary conditions:

$$u|_{x,y=1} = 1$$

$$u|_{x,y=0} = 0$$

$$u|_{x=0,y} = 0$$

$$u|_{x=1,y} = 0$$

The analytic solution, [26], for a rectangular region $a \times b$ in the form of a convergent series is

$$u_N(x,y) = \frac{2}{\pi} \sum_{n=1}^{N} \frac{(-1)^{n+1}+1}{n} \sin\left(\frac{n\pi x}{a}\right) \frac{\sinh(n\pi y/a)}{\sinh(n\pi b/a)}$$

where, for the case being analysed, $a = b = 1$.

The comparison of the results obtained with the proposed method was carried out by calculating a very good analytic solution where a total of 220 terms of the series were used ($N = 220$). This is about the numerical precision limit of the programming environment used, Matlab. In this example regular and irregular grids were considered. Irregular grids are obtained from the regular ones by adding or subtracting a random quantity to each point both in the x and y coordinates. An example of a regular and an irregular grid with a total of 225 points is shown in Figure 3.

A number of different grid distributions, with a total number of grid points varying between 25 and 2500, were considered.

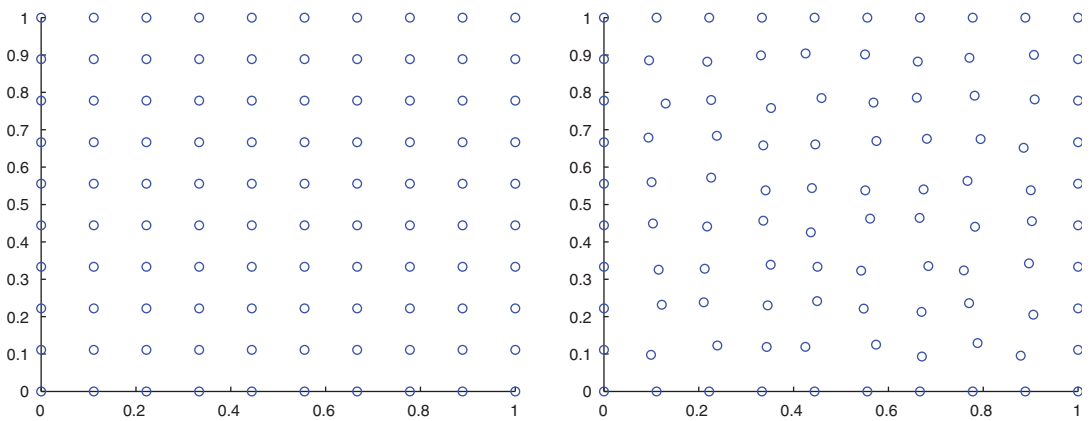

Figure 3. Example of regular and irregular grids.

DOI: 10.1002/nme

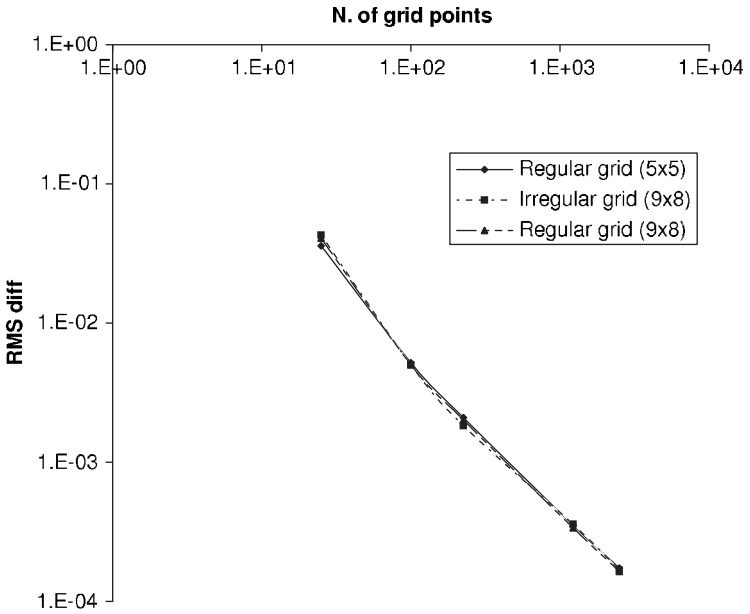

Figure 4. Difference to the series solution for a range of regular and irregular grids.

Comparison is made in terms of the difference to the analytic solution with 220 terms (L^2 norm or, more precisely, a normalized root mean square) as follows:

$$e_{220} = \sqrt{\frac{\int_\Gamma (u_h - u_{220})^2 \, \mathrm{d}y}{\int_\Gamma (u_{220})^2 \, \mathrm{d}y}}$$

where Γ is the middle section of the square region. Results are shown in Figure 4.

The curve denoted by (5×5) means that the local neighbourhood includes 5 points, whereas the (9×8) curves indicate that a total of 9 local neighbours are considered. The second number, 5 and 8, respectively, indicates the number of fundamental solutions used to construct the local approximation.

The (5×5) scheme leads, on a regular grid, to the central difference scheme. Each assembled equation is of the form given in (14), the resulting matrix is just a typical FD matrix, sparse and banded. The (9×8) scheme is the typical fourth-order scheme, other schemes are possible. The irregular grids are still banded and sparse, the only change is that the coefficients of the matrix vary from point to point depending on the distance between the point where the equation is being written to each of its neighbours.

This case was also tested with harmonic polynomials (the Trefftz approach). As the plots are virtually undistinguishable, the results (the e_{220} differences to the series solution) are shown in tabular form instead, see Table I. Only results for regular distributions are shown, but the same behaviour is observed for irregular distributions as well. The first column indicates the total number of grid points for each case tested. The remaining columns are, respectively, the difference to the series solution when fundamental solutions are used and when harmonic polynomials are used.

DOI: 10.1002/nme

Table I. Differences to the series solution.

n points	Fundamental solutions	Harmonic polynomials
25	0.03216941	0.03216941
100	0.00453156	0.00453158
225	0.00204721	0.00204724
1225	0.00035496	0.00035502
2500	0.00017155	0.00017164

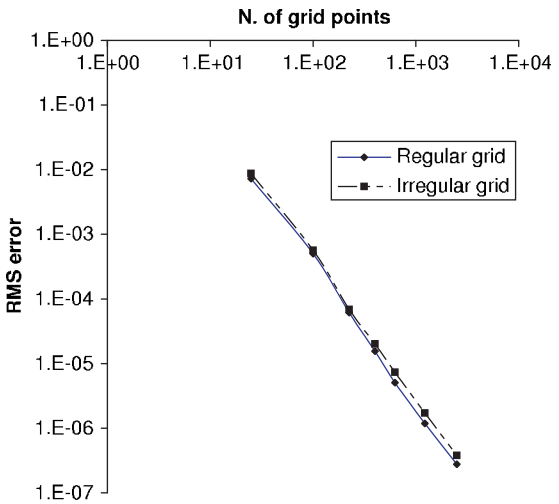

Figure 5. Root mean square error for a range of regular and irregular grids.

9.2. *Poisson equation*

Consider the case of a potential function, $u(x, y)$, on a unit square region. The potential has to satisfy the Poisson equation

$$\frac{\partial^2 u(x,y)}{\partial x^2}+\frac{\partial^2 u(x,y)}{\partial y^2}=-2\pi^2 \sin \pi x \sin \pi y$$

and homogeneous Dirichlet boundary conditions on all sides. The exact solution is:

$$u_{\text{ex}}(x, y)=\sin \pi x \sin \pi y$$

This case has been analysed in [10] by using RBFs in a 'FD mode'.

Results, in terms of the norm defined below, are shown in Figure 5.

$$\varepsilon=\sqrt{\frac{\int_\Gamma (u_h-u_{\text{ex}})^2\,\mathrm{d}y}{\int_\Gamma (u_{\text{ex}})^2\,\mathrm{d}y}}$$

This case was also tested with harmonic polynomials. Results, again virtually the same, are shown in Table II.

DOI: 10.1002/nme

Table II. Root mean square error.

n points	Fundamental solutions	Harmonic polynomials
25	7.24874E−3	7.24874E−3
100	5.00538E−4	5.00538E−4
225	6.126201E−5	6.12621E−5
1225	1.181149E−6	1.181149E−6
2500	2.762146E−7	2.762147E−7

9.3. Torsion of prismatic bars

The Saint–Venant-type torsion of prismatic bars when written in terms of Prandtl's stress function may be reduced for solving the Poisson equation, see [27],

$$\nabla^2\phi=-2G\theta \quad \text{in } \Omega \quad \text{subjected to } \phi=0 \text{ on all the boundary } \Gamma \tag{22}$$

where ϕ is Prandtl's stress function, G is the shear modulus and θ is the rate of twist (the torsion angle per unit length).

9.3.1. Elliptic cross-section. For an elliptic cross-section, defined by the equation

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1$$

the exact stress function is [27],

$$\phi=\frac{a^2b^2(-2G\theta)}{2(a^2+b^2)}\left(\frac{x^2}{a^2}+\frac{y^2}{b^2}-1\right) \tag{23}$$

and the stress components are

$$\tau_{xz}=\frac{\partial\phi}{\partial y} \quad \text{and} \quad \tau_{yz}=-\frac{\partial\phi}{\partial x} \tag{24}$$

The exact solution, for the case $a=2$, $b=1$ and assuming that both the shear modulus and θ are taken as unity for simplicity, is, after Equations (25) and (24), given by:

$$\phi=-0.8\left(\frac{x^2}{4}+y^2-1\right)$$

$$\tau_{xz}=-1.6y$$

and

$$\tau_{yz}=0.4x$$

The comparison of the results obtained with the proposed formulation and the exact ones is shown in Figure 6. Two types of irregular grids, one more irregular (A) than the other (B), were considered.

DOI: 10.1002/nme

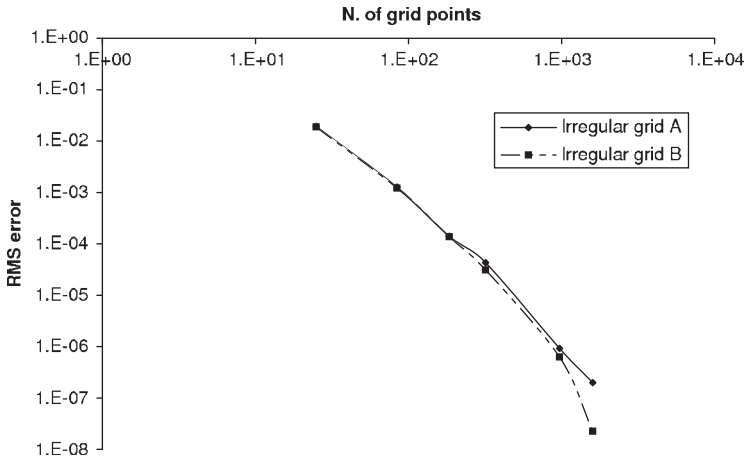

Figure 6. Torsion of an elliptical cross-section, root mean square error for a range of irregular grids.

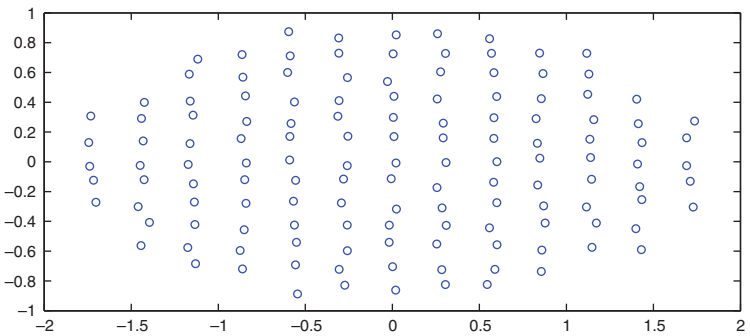

Figure 7. Domain grid.

This example clearly shows the potential of this generalized local approximation technique for dealing with more complex geometries and irregular distribution of points. The mesh of points was initially defined on a regular mesh in a domain that fully enclosed the ellipse. An irregular mesh was built by simply adding to each coordinate a random quantity. Then a simple test was carried out to reject all the points that did not belong to the ellipse, see Figure 7. The remaining points were then added to the boundary points previously defined (Figure 8). The irregular grid thus created, Figure 9, was then used to build the difference operators without any difficulty.

In the theoretical setup the distributions of points may be as irregular as needed. As long as the points are not coincident (or distributed along a line), good or, at least, reasonable solutions are obtained. The way in which the irregularities are created in this work, by perturbing a regular grid, is simply the easiest way to create an irregular grid. Other distributions may be used (and were used during the course of this work), the quasi-random Halton sequence, for example, or the Distmesh mesh generator (http://www-math.mit.edu/ persson/mesh/) [28], which is based on the Delaunay triangulation. This last method finds out a distribution that tends to cover uniformly

DOI: 10.1002/nme

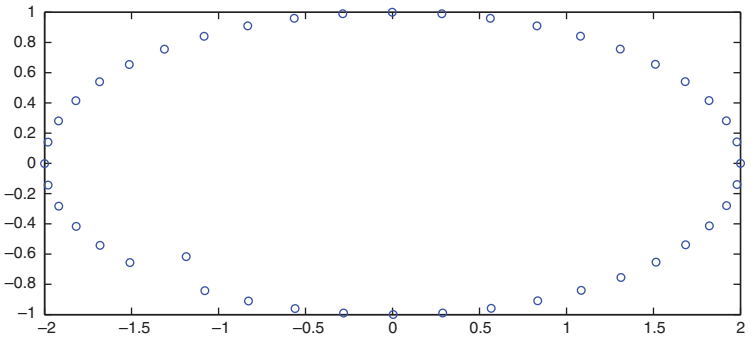

Figure 8. Boundary grid.

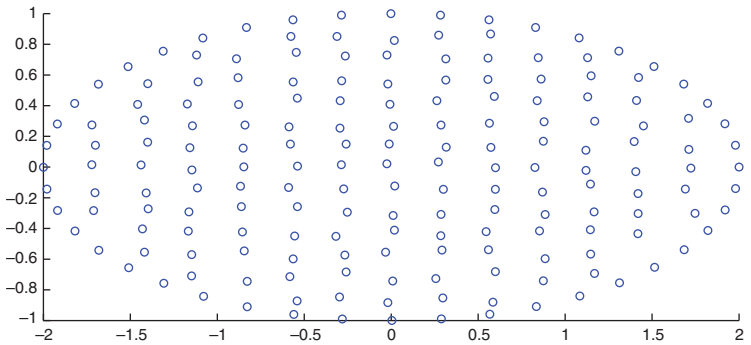

Figure 9. Combined boundary and domain grids.

(at least in parts of the domain) a given region and (although having been developed for finite element type meshes) is particularly suited for generalized FD schemes.

9.3.2. Rectangular cross-section. The stress function for a rectangular cross-section, $-a \leqslant x \leqslant a$, $-b \leqslant y \leqslant b$, exists only in the form of an infinite series. This analytic solution for the case $a=2$, $b=1$, and assuming that both the shear modulus and θ are taken as unity for simplicity, is given by [29]

$$\phi = (a^2 - x^2) + \sum_{i=1}^{\infty} C_i \cos((2i-1)\pi x/2a) \cosh((2i-1)\pi y/2a) \tag{25}$$

where

$$C_i = \frac{32(-1)^i a^2}{\pi^3 (2i-1)^3} \frac{1}{\cosh((2i-1)\pi b/2a)}$$

The comparison of the results obtained with the proposed formulation and the analytic ones (considering 200 terms) is shown in Figure 10. Only a quarter of the rectangular cross-section was considered, thus requiring the enforcement of Neumann-type boundary conditions. In all of the previously shown cases only Dirichlet-type boundary conditions have been considered.

DOI: 10.1002/nme

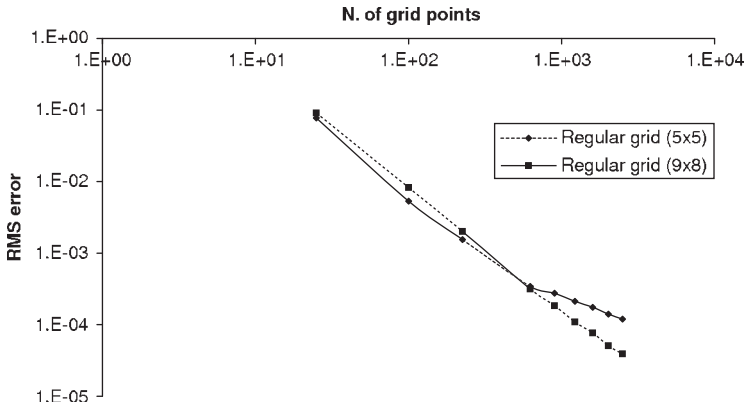

Figure 10. Torsion of a rectangular cross-section, root mean square difference for a range of regular grids.

As mentioned earlier, and besides the local approximation with RBFs proposed here, there are basically two traditional possibilities for enforcing Neumann conditions: ghost points or Taylor schemes based on interior points. For this particular case, as the normal vector is $\mathbf{n}(-1,0)$ when $x=0$ and $\mathbf{n}(0,-1)$ when $y=0$, the ghost point method would have been very simple to apply. For other geometries though, this scheme would not be appropriate and other more evolved schemes would have to been used. The local approximation with RBFs is completely general and is, therefore, the approach of choice.

10. CONCLUSIONS

The main disadvantage of traditional FDs is the need to use a structured grid in order to define the approximated difference operator. By removing this limitation the scope of applications that may be analysed by FDs (and the ease in which that analysis may be done) is significantly increased. If this generalization of the grids may be done without any noticeable loss of accuracy then it is even better.

In this paper a new technique to define generalized difference operators for completely irregular distribution of points by means of fundamental solutions is proposed. This work is based on that of Tsukerman [14] on Trefftz functions. The use of fundamental solutions (or sets of Trefftz functions as these are also solutions of the governing differential equation), as a basis to obtain the set of difference coefficients for a given grid, guarantees that there are no better sets of coefficients for that given grid.

Applications of this technique to two-dimensional potential problems (both Laplace and Poisson) are considered. Comparison with other results available in the literature shows that the method is accurate, reliable and may be considered to be an alternative to other numerical methods.

The use of fundamental solutions in the framework of FDMs guarantees accuracy while simultaneously eliminating (or strongly reducing) potential problems due to numerical ill-conditioning that are normally present in boundary-only solution methods.

The generalization of the grids allows for changing the grid in a quite effective manner: adding patches of grid points in any shape or size or density on different domains is now very easy.

DOI: 10.1002/nme

This is a strong indication of the capabilities of the method for dealing with complex geometries especially when coupled with domain decomposition techniques. Further work is being carried out in this respect.

ACKNOWLEDGEMENTS

The support of Instituto de Engenharia de Estruturas, Território e Construção do Instituto Superior Técnico (ICIST) and of Fundação para a Ciência e a Tecnologia (FCT) basic funding is acknowledged.

REFERENCES

1. Brebbia CA, Telles JCF, Wrobel LC. *Boundary Element Techniques*. Springer: Berlin, 1984.
2. Karageorghis A, Fairweather G. The method of fundamental solutions for axisymmetric potential problems. *International Journal for Numerical Methods in Engineering* 1999; **44**:1653–1669.
3. Zielinski AP, Herrera I. Trefftz method: fitting boundary conditions. *International Journal for Numerical Methods in Engineering* 1987; **24**:871–891.
4. Leitão VMA. On the implementation of a multi-region Trefftz-collocation formulation for 2-D potential problems. *Engineering Analysis with Boundary Elements* 1997; **20**:51–61.
5. Jirousek J, Zielinski AP. Survey of Trefftz-type element formulations. *Computers and Structures* 1997; **63**(2): 225–242.
6. Freitas JAT. Formulation of elastostatic hybrid—Trefftz stress elements. *Computer Methods in Applied Mechanics and Engineering* 1998; **153**:127–151.
7. Gyimesi M, Tsukerman I, Lavers D. Hybrid finite element—Trefftz method for open boundary analysis. *IEEE Transactions on Magnetics* 1996; **32**(3):671–674.
8. Trefftz E. Ein Gegenstuck zum Ritzschen Verfharen. *Proceedings of the 2nd International Congress on Applied Mechanics*, Zurich, 1926; 131–137.
9. Zienkiewicz OC, Taylor RL. *The Finite Element Method*. McGraw-Hill: London, 1989.
10. Tolstykh AI, Shirobokov DA. On using radial basis functions in a 'finite difference mode' with applications to elasticity problems. *Computational Mechanics* 2003; **33**:68–79.
11. Šarler B, Vertnik R. Mesh-free local radial basis function collocation method for diffusion problems. *Computers and Mathematics with Applications* 2006; **51**:1269–1282.
12. Liszka T, Orkisz J. The finite difference method at arbitrary irregular grids and its application in applied mechanics. *Computers and Structures* 1980; **11**:83–95.
13. Mickens RE. *Nonstandard Finite Difference Models of Differential Equations*. World Scientific: Singapore, 1994.
14. Tsukerman I. A class of difference schemes with flexible local approximation. *Journal of Computational Physics* 2006; **211**:659–699.
15. Zielinski AP. On trial functions applied in the generalized Trefftz method. *Advances in Engineering Software* 1995; **24**:147–155.
16. Hartmann F. *Introduction to Boundary Elements*. Springer: Berlin, 1989.
17. Freitas JAT, Bussamra FLS. Three-dimensional hybrid—Trefftz stress elements. *International Journal for Numerical Methods in Engineering* 2000; **47**:927–950.
18. Tsukerman I. Electromagnetic applications of a new finite difference calculus. *IEEE Transactions on Magnetics* 2005; **41**(7):2206–2225.
19. Herrera I. Trefftz method. In *Topics in Boundary Element Research—Basic Principles and Applications*, Brebbia CA (ed.). Springer: New York, 1984.
20. Piltner R. On the representation of three-dimensional elasticity solutions with the aid of complex valued functions. *Journal of Elasticity* 1989; **22**:45–55.
21. Belytschko T, Lu YY, Gu L. Element-free Galerkin methods. *International Journal for Numerical Methods in Engineering* 1994; **37**:229–256.
22. Chen JT, Wu CS, Lee YT, Chen KH. On the equivalence of the Trefftz method and method of fundamental solutions for Laplace and biharmonic equations. *Computers and Mathematics with Applications* 2007; **53**(6):851–879.
23. Hunt B. Finite difference approximation of boundary conditions along irregular boundaries. *International Journal for Numerical Methods in Engineering* 1978; **12**:229–235.

DOI: 10.1002/nme

24. Johnston H, Liu JG. Finite difference schemes for incompressible flow based on local pressure boundary conditions. *Journal of Computational Physics* 2002; **180**:120–154.
25. Leitão VMA. A meshless method for Kirchhoff plate bending problems. *International Journal for Numerical Methods in Engineering* 2001; **52**:1107–1130.
26. Incropera FP, De Witt DP. *Introduction to Heat Transfer*. Wiley: New York, 1985.
27. Timoshenko SP, Goodier JN. *Theory of Elasticity* (3rd edn). McGraw-Hill: New York, 1982.
28. Persson PO, Strang G. A simple mesh generator in MATLAB. *SIAM Review* 2004; **46**(2):329–345.
29. Barber JR. *Elasticity* (2nd edn). Kluwer Academic Publishers: Dordrecht, 2004.

DOI: 10.1002/nme