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Abstract

The R-Function Method (RFM) solution structure is a functional expression that satisfies all given boundary conditions exactly and contains some undetermined functional components. It is complete if there exists a choice of undetermined component that transform the solution structure into an exact solution. Such a structure was used by Kantorovich (Kantorovich and Krylov, 1958) and his students to solve boundary value problems with homogeneous boundary conditions on geometrically simple domains. RFM is based on the theory of R-functions (Rvachev, 1982) that allows construction of a set of functions vanishing on the boundary and can be applied to problems with arbitrarily complex domains and boundary conditions. The resulting solution method is essentially meshfree, in the sense that the spatial discretization no longer needs to conform to the geometry of the domain, and can be completely automated. This paper summarizes the main principles of RFM, proves its completeness, and presents numerical results for several simple test problems.

1 Introduction

One of the main challenges for meshfree methods lies in constructing solutions to boundary value problems that satisfy the prescribed boundary conditions. The classical methods such as FEM and BEIM rely on spatial discretization of the domain and/or its boundary in order to enforce or approximate the imposed boundary conditions at discrete locations. By contrast, the meshfree methods discretize not the geometric domain but the underlying functional space. A number of techniques with basis functions that do not have to conform the geometry of the domain have been developed: smooth particle hydrodynamics (SPH) (Lucy, 1977; Randles and Libersky, 1996), the diffuse element method (DEM) (Nayroles et al., 1992), the reproducing kernel particle method (RKPM) (Liu et al., 1995; Chen et al., 1998), the HP cloud method (Duarte and Oden, 1996), and the partition of unity method (PUM) (Melenk and Babuska, 1996), and others. But geometric non-conformance of all such meshfree methods makes treatment of boundary conditions more problematic. Proposed remedies include the combination of Element Free Galerkin Method (EFG) (Belytschko et al., 1994) with finite element shape functions near the boundary (Krongauz and Belytschko, 1996), the use of modified variational principle (Lu et al., 1994), window or correction functions that vanish on the boundary (Duarte and Oden, 1996), and Lagrange multipliers. Although these techniques appear promising, they often contradict the meshfree nature of the approximation near the boundary, introduce additional constraints on solutions, or lead to systems with an increased number of unknowns (Gunter and Liu, 1998). Several promising transformation-based approaches to satisfying essential boundary conditions at desired nodal locations have been recently proposed and compared by J.-S. Chen (Chen and Wang, 1999).

In this paper we discuss the *R-functions method* (RFM) that allows *all* prescribed boundary conditions to be satisfied exactly on *all* boundary points. The original idea underlying RFM is due to Kantorovich (Kantorovich and Krylov, 1958). He proposed that the homogeneous Dirichlet conditions may be satisfied exactly by representing the solution as the product of two functions: (1) an real-valued function that takes on zero values on the boundary points;

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and (2) an unknown function that allows to satisfy (exactly or approximately) the differential equation of the problem. The idea appeared to have a limited use, because it was not clear how such functions may be constructed for complex shapes and because the method did not seem to generalize to other types of boundary value problems.

In (Rvachev, 1963) Rvachev suggested that both of these obstacles may be overcome using R-functions — the real valued functions that behave as continuous analogs of logical Boolean functions. With R-functions, it became possible to construct functions with prescribed values and derivatives at specified locations. Furthermore, the constructed functions possess desired differential properties and may be assembled into a solution structure that is guaranteed to contain solutions to the posed boundary value problems.

Over the last several decades, the theory of R-functions and RFM have matured and have been applied to numerous scientific and engineering problems by Rvachev and his students. Their work is published extensively in Russian (Rvachev, 1974; Rvachev, 1982), but English literature is also beginning to appear (Rvachev et al., 1986; Shapiro, 1991; Shapiro, 1994; Rvachev and Sheiko, 1995; Rvachev et al., 1997). The RFM has been applied to problems of thermoconduction, elasticity, magneto-hydrodynamics, various problems in inhomogeneous media, and many other areas. The success of RFM was fueled by development of software systems called POLYE (which means "field" in Russian) for scientific programming (Rvachev and Shevchenko, 1988; Rvachev et al., 1986; Rvachev and Manko, 1983). In POLYE, the geometric domain, boundary conditions, and solution structure are described in a symbolic programming language called RL. The RL programs specify how the constructed structures should be differentiated and integrated by POLYE in order to solve the boundary value problem.

Acceptance of RFM has been slow largely for two reasons: (1) completeness of the method has been formally established only for problems with homogeneous boundary conditions; and (2) creating solution structures manually is a difficult and tedious process that requires mastery of the R-functions theory and other analytical skills. The main contribution of this paper is the proof of completeness of RFM for general boundary value problems. It now appears that the second problem can be resolved as well.

Symbolic methods for construction of solution structures have been explored in (Kucwaj and Orkisz, 1986), but the main problem of automatically constructing functions that satisfy prescribed boundary conditions has not been addressed until recently. Briefly, construction of such functions relies on automatic construction of set-theoretic expressions for domains and their boundaries and interpolation techniques. Both of these problems have been solved for several large classes of geometric domains, and these solutions are being implemented in a SAGE (Semi-Analytic Geometry Engine) computational environment at the University of Wisconsin (Shapiro and Tsukanov, 1999). These results are outside the scope of this paper and will be described elsewhere.

1.1 Outline

The rest of the paper is organized as follows. Section 2 is devoted to boundary value problems with homogeneous Dirichlet boundary conditions. We explain the basic idea behind the RFM, introduce R-functions, and describe a fully implemented example of the RFM applied to a torsion problem. Completeness of the method follows from results in (Kharrik, 1963) which we recite.

Section 3 explains generalization of RFM to arbitrary boundary value problems. We derive solution structures for inhomogeneous Dirichlet and Neumann boundary conditions, and then explain the general methodology of RFM. The main result of the paper is Theorem 4 showing that a general solution structure can approximate the solution of boundary value problem with arbitrary precision. The proof relies on the theory of R-functions and the completeness result for problems with homogeneous boundary conditions. Brief discussion of a fully implemented RFM procedure for non-steady heat transfer problems with mixed boundary conditions is followed by summary and conclusions in Section 4.

2 The R-functions Method (RFM) for homogeneous problems

2.1 Basic principle

In its early form, RFM was an extension of the approach proposed by Kantorovich (Kantorovich and Krylov, 1958) to solving two-dimensional homogeneous boundary value problems with Dirichlet boundary conditions. The idea of the

method is based on the observation that the solution of a differential equation with boundary conditions

$$u_{|\partial\Omega} = 0 \tag{1}$$

can be represented in the form

$$u = \omega\Phi, \tag{2}$$

where $\omega : R^n \to R$ is a known function that takes on zero values on the boundary of the domain $\partial\Omega$ and is positive in the interior of Ω, and Φ is some unknown function. Let us consider the advantages of representing the solution u in this form.

- The expression (2) includes two independent types of information: (1) the function ω completely describes all the geometric information of this particular boundary value problem, and (2) the function Φ whose sole purpose is to satisfy the analytical constraints of the boundary value problem — exactly or approximately.
- Since ω is identically zero on the boundary $\partial\Omega$ of the domain, any function u of the form (2) will satisfy the boundary conditions (1) exactly — independently of the properties of the unknown function Φ or the type of differential equation.
- Expression (2) contains no information about the differential equation of the boundary value problem. Rather, it represents the *structure* of any solution to a boundary value problem satisfying the given geometric constraints.
- For any given boundary value problem, determination of the unknown Φ immediately translates into solution to the boundary value problem. Since we cannot expect to determine such Φ exactly, we can approximate it by a finite linearly-independent series

  $$\Phi = \sum_{i=1}^{n} C_i\chi_i, \tag{3}$$

  where C_i are scalar coefficients and χ_i are some basis functions.
- The structure (2) does not place any constraints on the choice of the functions $\{\chi_i\}$ that approximate the function Φ. And in particular, the choice of the coordinate functions does not depend on any particular spatial discretization of the geometric domains or its boundary.
- For any given boundary value problem and a choice of the coordinate basis $\{\chi_i\}$, the approximate solution is obtained as

  $$u = \omega \sum_{i=1}^{n} C_i\chi_i, \tag{4}$$

  using variational, projection, or variety of other numerical methods to solve for the numerical values of the coefficients C_i.

From a computational point of view, the intrinsic advantage of the above procedure is in the clean and modular separation of the geometric information represented by function ω from the differential equation and the numerical method used to determine the unknown function Φ.

2.2 Theory of R-functions

The applicability of RFM to homogeneous boundary value problems stems from the recognition that the solution u can be written in the form of expression (2), and therefore depends on the ability to construct a function w that vanishes precisely on the boundary of the domain and nowhere else. Equation $\omega = 0$ defines the geometry of the domain *implicitly*, and such functions ω are sometimes are called *implicit functions* for the specified geometric domain. Construction of implicit functions has been largely solved using the theory of R-functions and can now be completely automated (Shapiro, 1994; Shapiro and Tsukanov, 1999).

The theory of R-functions was developed in Ukraine by Rvachev and his students (Rvachev, 1982). A complete list of references through 1987 can be found in (Shidlovsky, 1988). A brief English summary of the theory of R-functions is available as a technical report (Shapiro, 1991). Numerous applications of the theory are beginning to appear in English literature (Waberski, 1978; Rimon and Koditschek, 1990; Sourin and Pasko, 1995; Pasko et al., 1995; Rvachev and Sheiko, 1995; Rvachev et al., 1997; Bloomenthal, 1997; Shapiro and Tsukanov, 1998).

An R-function is a real-valued function whose sign is completely determined by the signs of its arguments. For example, the function xyz can be negative only when the number of its negative arguments is odd. A similar property is possessed by functions $x+y+\sqrt{xy+x^2+y^2}$ and $xy+z+|z-yx|$, and so on. Such functions 'encode' Boolean logic functions and are called R-**functions**. Every Boolean function is a companion to infinitely many R-functions, which form a *branch* of the set of R-functions. For example, it is well known that $\min(x_1, x_2)$ is an R-function whose companion Boolean function is logical "and" ($\wedge$), and $\max(x_1, x_2)$ is an R-function whose companion Boolean function is logical "or" ($\vee$). But the same branches of R-functions contain many other functions, e.g.

$$\begin{aligned} x_1 \wedge_\alpha x_2 &\equiv \tfrac{1}{1+\alpha}\left(x_1+x_2-\sqrt{x_1^2+x_2^2-2\alpha x_1 x_2}\right); \\ x_1 \vee_\alpha x_2 &\equiv \tfrac{1}{1+\alpha}\left(x_1+x_2+\sqrt{x_1^2+x_2^2-2\alpha x_1 x_2}\right), \end{aligned} \tag{5}$$

where $\alpha(x_1, x_2)$ is an arbitrary function such that $-1 < \alpha(x_1, x_2) \leq 1$. The precise value of α may or may not matter, and often it can be set to a constant. For example, setting $\alpha = 1$ yields the functions $\min$ and $\max$ respectively, but setting $\alpha = 0$ results in much nicer functions $\vee_0$ and $\wedge_0$ that are *analytic* everywhere except when $x_1 = x_2 = 0$. Similarly, R-functions

$$x_1 \wedge_\alpha^m x_2 \equiv (x_1 \wedge_\alpha x_2)(x_1^2+x_2^2)^{\frac{m}{2}}; \qquad x_1 \vee_\alpha^m x_2 \equiv (x_1 \vee_\alpha x_2)(x_1^2+x_2^2)^{\frac{m}{2}} \tag{6}$$

are analytic everywhere except the origin ($x_1 = x_2 = 0$), where they are m times differentiable. Many other systems of R-functions are studied in (Rvachev, 1982). The choice of an appropriate system of R-functions is dictated by many considerations, including simplicity, continuity, differential properties, and computational convenience.

Just as Boolean functions, R-functions are closed under composition. Using R-functions, any object defined by a predicate on "primitive" geometric regions (e.g. regions defined by a system of inequalities) can now also be represented by a *single* function ω. The latter can be evaluated, differentiated, and possesses many other useful properties. In particular:

- the function ω can be constructed in a 'logical' fashion and can be controlled through intuitive user-defined parameters;
- ω can be normalized, in which case it behaves as the distance function near the boundary of the object and can be differentiated everywhere. To be more precise, function ω is called *normalized up to m-th order* when the following conditions are satisfied:

$$\omega_{|\partial\Omega} = 0; \qquad \frac{\partial\omega}{\partial\nu}_{|\partial\Omega} = 1; \qquad \frac{\partial^k\omega}{\partial\nu^k}_{|\partial\Omega} = 0; \qquad k = 2, 3, ..., m, \tag{7}$$

  where ν is the inner normal to the boundary $\partial\Omega$;
- the functions can be used to define time-varying geometry and for modeling various complex physical phenomena.

The theory of R-functions provides the connection between logical and set operations in geometric modeling and analytic constructions. For *every* logical or set-theoretic construction, there is a corresponding implicit real-valued function with the above properties. Furthermore, the translation from logical and set-theoretic description is a matter of simple syntactic substitution that does not require expensive symbolic computations. For example, the geometric domain in Figure 1(a) can be defined as a Boolean set combination of three primitives:

$$\Omega = \omega_1 \cap (\overline{\omega_2 \cap \omega_3}),$$

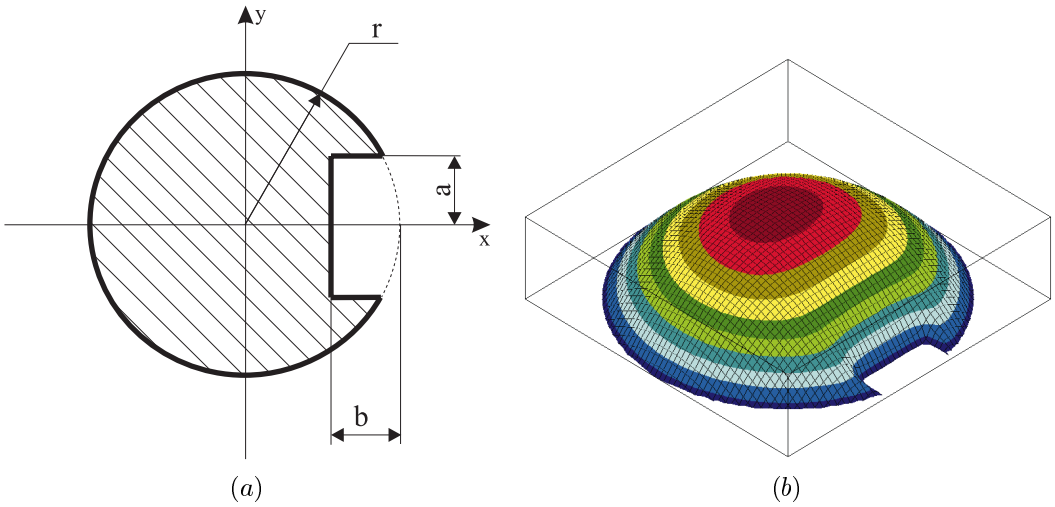


Figure 1: Two dimensional domain and function vanishes on the boundary of the domain

where $\overline{x}$ denotes the regularized complement of x, and individual primitives ω_1 through ω_3 are defined by the following inequalities:

$$\omega_1 = \frac{1}{2r}\left(r^2 - x^2 - y^2\right) \geq 0; \qquad \omega_2 = x - r + b \geq 0; \qquad \omega_3 = \frac{a^2 - y^2}{2a} \geq 0;$$

This set-theoretic representation can be translated into the function shown in Figure 1(b) using R-functions:

$$\omega = \omega_1 \wedge_0 \left(-\left(\omega_2 \wedge_0 \omega_3\right)\right), \tag{8}$$

which is also parameterized in terms of the shown parameters r, b, and a. This function is analytic everywhere except the corner points and is normalized on all regular points of the boundary. This example suggests how any Constructive Solid Geometry (CSG) representation of a geometric domain may be translated into the corresponding implicit function. Similarly, boundary representation of a solid is a union of solid's faces, each face is a subset of some surface bounded by edges, and so on. This logical description can also be directly translated into a real function such that it is zero for every point on the boundary and positive elsewhere. Analogous arguments hold for general cell complexes and other logical geometric constructions. For additional discussion and examples see (Shapiro and Tsukanov, 1999).

2.3 Example of homogeneous Dirichlet problem: torsion problem

We now apply RFM to the classical torsion problem for a rod with the cross section shown in Figure 1(a). This is a textbook problem (Timoshenko and Goodier, 1970) with many good approximations already known. For example, an approximate analytic expression for torque in terms of parameters r, b, and a has been derived for the same domain in (Pilkey, 1994) and will be used here for comparison.

It is well known that the torsion problem may be reduced to the boundary value problem with Poisson equation and homogeneous Dirichlet boundary conditions:

$$-\nabla^2 u = 2; \qquad u_{|\partial\Omega} = 0, \tag{9}$$

where $u(x, y)$ is the stress function. We will represent the solution in the form (2), with function ω defined by (8). For the undetermined function Φ we choose a linear combination $\sum_{i=1}^{n} C_i \chi_i$ of bicubic B-splines on a uniform 40×40 grid that covers the given two-dimensional domain but does not conform to it. An approximate solution to (9) will be found using Ritz's method that requires minimization of functional

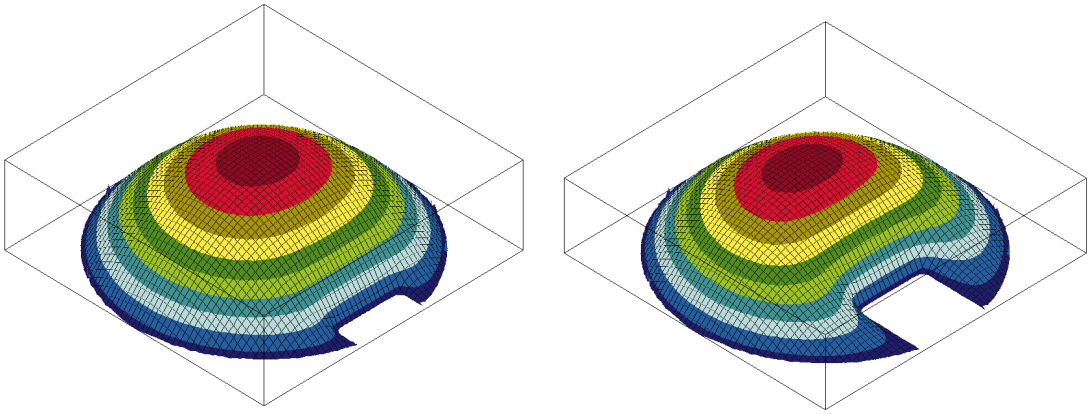
$$F = \iint_\Omega \left(\nabla\left(\omega \sum_{i=1}^{n} C_i \chi_i\right)\right)^2 d\Omega - 4 \iint_\Omega \left(\omega \sum_{i=1}^{n} C_i \chi_i\right) d\Omega. \tag{10}$$

Differentiating the functional (10) with respect to the unknown coefficients C_i we get a system of linear algebraic equations:

$$\mathbf{AC} = \mathbf{G}, \tag{11}$$

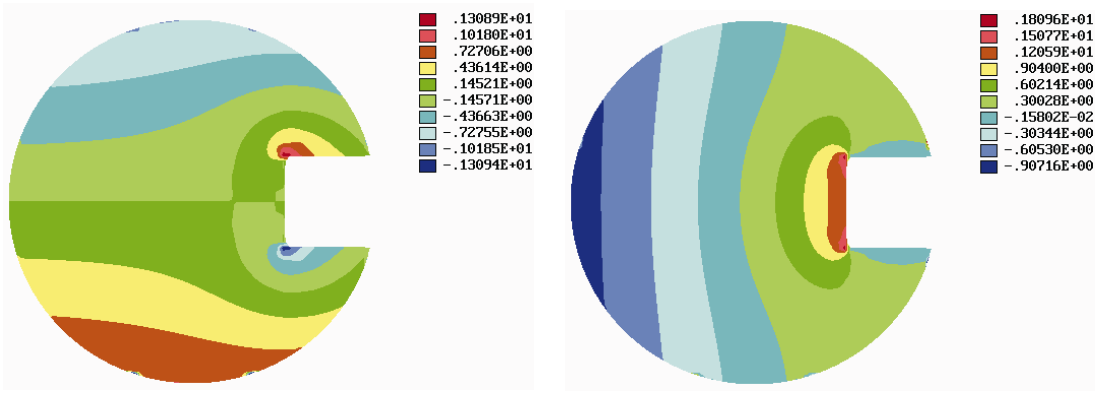
with elements of matrices $\mathbf{A}$ and vector $\mathbf{G}$ evaluated as:

$$a_{ij} = \iint_{\Omega} \left(\nabla\left(\omega\chi_i\right) \cdot \nabla\left(\omega\chi_j\right)\right) d\Omega; \qquad g_i = 2\iint_{\Omega} \omega\chi_i d\Omega.$$



(a) (b)

Figure 2: Stress function computed by RFM for $b = 0.2$ (a); $b = 0.5$ (b)



(a) (b)

Figure 3: Stresses τ_{xz} (a) and τ_{yz} (b) predicted by RFM with structure (2)

The solution procedure requires automatic differentiation of the constructed functions (Rall and Corliss, 1996; Shevchenko and Rokityanskaya, 1996; Rvachev and Shevchenko, 1988), integration over the domain (Piessens et al., 1983; Notaris, 1995), and solving the system of equations (11). While non-trivial, none of these steps require meshing of the geometric domain. Once numerical values of the coefficients C_i are known, the same tools may be used to compute the other integral and differential characteristics of interest. Specifically, torque (12) can be computed as

$$J = 2\iint_{\Omega} u \, d\Omega, \tag{12}$$

and the shearing stresses are given by

$$\tau_{xz} = \frac{\partial u}{\partial y}; \quad \tau_{yz} = -\frac{\partial u}{\partial x}. \tag{13}$$

Notice that any parametric changes in the domain are automatically translated into the parametric changes of the

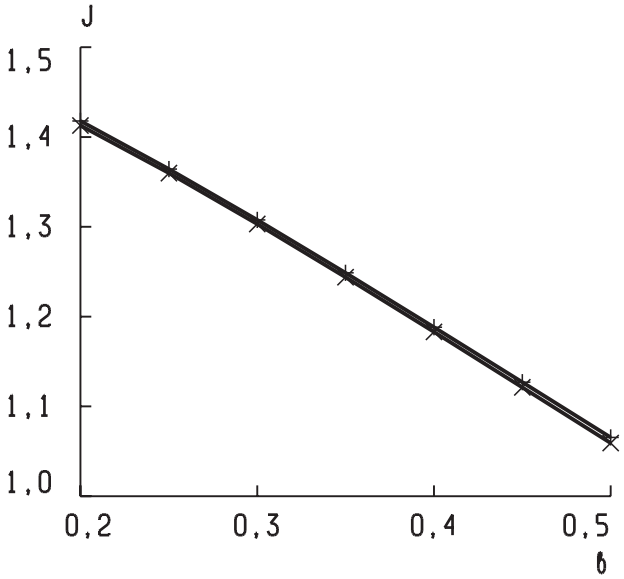


Figure 4: Comparison of torques: "+" torque predicted by closed-form approximation in (Pilkey, 1994); "×" torque computed by RFM

function ω and require no changes in the solution procedure. In our example, we fixed $r = 1$, $a = 0.25$ and varied b from 0.2 up to 0.5. The computed stress functions for $b = 0.2$ (a), and $b = 0.5$ (b) are shown in Figures 2. Figures 3 (a) and (b) show the computed shearing stresses τ_{xz} and τ_{yz} for geometric domain with $b = 0.5$. Finally, Figure 4 shows that the computed torque for multiple values of b are virtually identical to those predicted by the closed-form expression in (Pilkey, 1994).

2.4 Completeness of RFM for homogeneous Dirichlet problems

Completeness of the above RFM procedure follows from the proof in (Kantorovich and Krylov, 1958) that applies to boundary value problems formulated as second-order differential equations with homogeneous Dirichlet boundary conditions. This result was extended in (Kharrik, 1963) to higher-order problems and included estimates on the rate of convergence. We conclude this section by restating the main theorem from (Kharrik, 1963); it is also going to be the basis for our proof of completeness of RFM with more general boundary conditions.

Theorem 1 *(Kharrik, 1963) Suppose that Ω is a bounded region of m-dimensional space with boundary $\partial\Omega$. Let k and r be positive integers ($k > r$) and $\omega(\mathbf{x}) = \omega(x_1, x_2, ..., x_m)$ be a function defined in open region that contains Ω and satisfying the following conditions:*

1. $\omega(\mathbf{x})_{|\mathbf{x}\in\Omega} = 0, \quad \omega(\mathbf{x})_{|\mathbf{x}\notin\Omega} \neq 0;$
2. *function $\omega(\mathbf{x})$ is k times continuously differentiable function, and its derivatives of order k satisfy the Lipschitz condition;*
3. $\nabla\omega(\mathbf{x})_{|\mathbf{x}\in\partial\Omega} \neq 0.$

If function $\gamma(\mathbf{x}) = \gamma(x_1, x_2, ..., x_m)$ is k times continuously differentiable in the region Ω and vanishes on the boundary $\partial\Omega$ together with its derivatives up to order $(r-1)$, then for any positive ε it is possible to construct a sequence of polynomials $P_n(\mathbf{x})$ such that:

$$\|\gamma - \omega^r P_n\|_{C^p(\Omega)} < \varepsilon, \tag{14}$$

where $p = 1, 2, ..., k$.

In the context of RFM, ω is the function satisfying the homogeneous boundary conditions, γ is the sought solution of the differential equation, and the sequence of polynomials P_n plays the role of the undetermined functional component Φ. In other words, the theorem implies that the homogeneous solution structure $\omega^r\Phi$ is sufficiently complete for approximation of the functions γ and all its derivatives through order k. For additional details and estimates of ε the reader is referred to (Kharrik, 1963). It is worth noting that estimate (14) of the norm in Banach space $C^p(\Omega)$ also holds in the Hilbert space, i.e. $\|\gamma - \omega^r P_n\|_{H^p(\Omega)} < \varepsilon$. We will use this fact in the next section to prove completeness of the general RFM solution structure.

3 General Solution Structures

3.1 Inhomogeneous Dirichlet boundary conditions

Once we constructed the solution structure (2) for the boundary value problems with homogeneous Dirichlet boundary conditions, it is easy to obtain the solution structure for inhomogeneous conditions given by

$$u_{|\partial\Omega} = \varphi_0. \tag{15}$$

The function φ_0 may be defined only at the boundary points of Ω, so let φ be the extension of the φ_0 inside the domain Ω. Then the solution structure

$$u = \omega\,\Phi + \varphi \tag{16}$$

satisfies the prescribed boundary conditions exactly. In practice, the function φ_0 may be specified in a piecewise fashion, with a different value φ_i prescribed on each portion of the boundary $\partial\Omega_i$. Such individual boundary conditions may be combined into a single global function φ using the transfinite Lagrangian interpolation described in (Rvachev, 1982; Rvachev and Sheiko, 1995). Each set $\partial\Omega_i$ may be described by a single implicit equation $\omega_i = 0$, where ω_i is constructed using R-functions and is positive at all points not in $\partial\Omega_i$. Then

$$\varphi = \frac{\sum\limits_{i=1}^{m} \varphi_i \prod\limits_{j=1, j\neq i}^{m} \omega_j}{\sum\limits_{i=1}^{m} \prod\limits_{j=1, j\neq i}^{m} \omega_j}. \tag{17}$$

is a generalization of the classical Lagrangian interpolation functions ω_i playing the role of terms $(x - x_i)$. The resulting function φ interpolates the individual values φ_i on each set defined by $\omega_i = 0$. Notice that expression (17) places no restrictions on form, shape, or dimension of the sets $\omega_i = 0$. Another form of transfinite interpolation (Rvachev, 1982; Rvachev and Sheiko, 1995) is sometimes more convenient:

$$\varphi = \frac{\sum\limits_{i=1}^{m} \varphi_i \omega_i^{-1}}{\sum\limits_{i=1}^{m} \omega_i^{-1}} \tag{18}$$

The two functions defined by the expressions (17) and (18) are very similar, but have different types of singularities at the corner points where more than one ω_i vanish.

Solution structures for more general boundary conditions cannot be derived simply by inspection or *ad hoc* modification of the Dirichlet solution structure (16). Further generalization, even for Neumann boundary conditions, requires additional insight into the role of the function ω vanishing on the boundary $\partial\Omega$. This insight comes from the generalized Taylor series expansion.

3.2 Generalized Taylor series

The classical Taylor formula approximates a function in the neighborhood of the given point x_0. The neighborhood itself is described by a term $x - x_0$ which can be thought of as a function that vanishes at the point x_0. The generalized Taylor series expansion represents a function in the neighborhood of the boundary $\partial\Omega$, which is described by some implicit function ω that vanishes on $\partial\Omega$. The generalized expansion requires introducing a concept of the *function normalizer* (Rvachev, 1982).

Definition 1 *Let $\omega(\mathbf{x})$ be a normalized function that vanishes on the boundary $\partial\Omega$ of domain Ω. Then function*

$$f^*(\mathbf{x}) = f(\mathbf{x} - \omega\nabla\omega) \tag{19}$$

is called the normalizer *of function $f(\mathbf{x})$ with respect to $\omega(\mathbf{x})$ (Rvachev, 1982; Rvachev and Sheiko, 1995).*

If $\omega(\mathbf{x})$ is normalized up to m-th order then the normalizer $f^*(\mathbf{x})$ of $f(\mathbf{x})$ with respect to $\omega(\mathbf{x})$ satisfies the conditions (Rvachev, 1982):

$$f^*(\mathbf{x})_{|\partial\Omega} = f(\mathbf{x})_{|\partial\Omega}; \quad \frac{\partial^k f^*}{\partial\nu^k}_{|\partial\Omega} = 0; \quad (k = 1, 2, ..., m). \tag{20}$$

These properties of the normalizer imply that the function f^* behaves as a constant in the direction normal to the boundary. This in turn allows to use normalizers as coefficients in the generalized Taylor series expansion.

Theorem 2 *(Rvachev, 1982) If function $\omega(\mathbf{x})$ is normalized up to m-th order and function $u(\mathbf{x})$ satisfies conditions*

$$u(\mathbf{x})_{|\partial\Omega} = f_0(\mathbf{x}), \quad \frac{\partial^k u}{\partial\nu^k}_{|\partial\Omega} = f_k(\mathbf{x}), \quad (k = 1, 2, ..., m), \tag{21}$$

then u can be represented in neighborhood of the boundary $\partial\Omega$ in the form:

$$u = f_0^* + \sum_{k=1}^{m} \frac{1}{k!} f_k^* \omega^k + \omega^{m+1}\Phi \tag{22}$$

where $f_k^*(\mathbf{x}), k = 0, 1, ..., m$ are normalizers of functions $f_k(\mathbf{x}), k = 0, 1, ..., m$ with respect to $\omega(\mathbf{x})$.

The generalized Taylor polynomial (22) approximates function f near the boundary $\partial\Omega$ described by $\omega(\mathbf{x}) = 0$. The powers of $\omega(\mathbf{x})$ play the same role as the powers of the term $(x - x_0)$ in the classical Taylor formula, and the constant Taylor coefficients are replaced by the normalizers of functions f_k.

In the context of boundary value problems, functions f_k represent the prescribed values and derivatives of order k on the boundary $\partial\Omega$, while their normalizers f_k^* have the same values on the boundary $\partial\Omega$ but also behave as constants in the direction normal to the boundary. These properties of the generalized Taylor series expansion suggest a systematic way for deriving sufficiently complete solution structures for any and all boundary value problems.

3.3 General solution structures

Detailed and systematic derivations of solution structures can be found elsewhere (for example, see references (Rvachev, 1982; Rvachev and Sheiko, 1995)). Here we are mostly concerned with the general form of such structures that arises based on the generalized Taylor series expansion. For example, if the Neumann boundary conditions have the general form of

$$\frac{\partial u}{\partial\nu}_{|\partial\Omega} = \varphi_0, \tag{23}$$

then from (22) the implied solution structure can be written as:

$$u = \Phi^* + \varphi^*\omega + \omega^2\Phi, \tag{24}$$

where Φ^*, φ^* are normalizers of functions Φ and φ. Because condition (23) puts no restrictions on the function's value, we use the unknown function Φ^* instead of f_0^* in (22) to approximate the value of the function u. It should be intuitively clear that the remainder term $\omega^2\Phi$ assures completeness of this solution structure. In (Rvachev and Sheiko, 1995) it is shown that (24) can be further simplified to

$$u = \Phi - \omega D_1^{\omega}(\Phi) + \omega\varphi + \omega^2\Phi, \tag{25}$$

where $D_1^{\omega}(f) = \nabla\omega \cdot \nabla(f)$ is a differential operator in the direction of the internal normal to the boundary $\partial\Omega$.

Similar procedures can be used for virtually any boundary conditions. Derivations for most common boundary conditions arising in higher-order differential equations can be found in (Rvachev, 1982; Rvachev and Kurpa, 1987; Rvachev and Sinekop, 1990; Rvachev and Sheiko, 1995). The individual boundary conditions of the same type and the corresponding solution structures may be combined into a single global solution structure using further generalization of the transfinite interpolation expression (18). If P_i are generalized Taylor polynomials in form (22) satisfying boundary conditions of order $m_i - 1$ on the boundary $\partial\Omega_i$, then they can be interpolated into single solution structure by

$$u = \frac{\sum_{i=1}^{n} P_i \omega_i^{-m_i}}{\sum_{i=1}^{n} \omega_i^{-m_i}} + \Phi \prod_{j=1}^{n} \omega_j^{m_j}. \tag{26}$$

The first term in the expression satisfies all boundary conditions exactly, while the second term is simply a product of the remainder terms for each individual boundary condition. The power m_j of ω_j indicates that derivatives up to order $m_j - 1$ have been specified on $\partial\Omega_j$.

The above procedure for constructing solution structures can be fully automated, but the resulting expressions may often be optimized using special case analysis. For example, an efficient general solution structure for the second-order boundary value problem with mixed boundary conditions

$$u_{|\partial\Omega_1} = \varphi_0; \qquad \left(\frac{\partial u}{\partial \nu} + h_0 u\right)_{|\partial\Omega_2} = \psi_0 \tag{27}$$

can be written in the form that interpolates boundary conditions on $\partial\Omega_1 = (\omega_1 = 0)$ and $\partial\Omega_2 = (\omega_2 = 0)$ as(Rvachev, 1982):

$$u = \omega_1\Phi + \frac{\omega_1\omega_2}{\omega_1 + \omega_2}\left(\psi - h\omega_1\Phi - h\varphi - D_1^{\omega_2}(\omega_1\Phi) - D_1^{\omega_2}(\varphi)\right) + \varphi + \omega_1\omega_2^2\Phi \tag{28}$$

3.4 Proof of Completeness

Based on the above discussion, any *one* type of boundary conditions prescribed on $\partial\Omega$ leads to a solution structure that can be split into two parts:

$$u = u_0 + \omega^{m+1}\Phi, \tag{29}$$

where u_0 satisfies exactly the boundary conditions prescribed on $\partial\Omega$. It is easy to show that the second (remainder) term assures that the solution structure is complete by reduction to the statement of Theorem 1. Let $f(\mathbf{x})$ be the solution of the boundary value problem; and let (29) be the solution structure of the same problem that satisfies exactly given boundary conditions of order m. Then the function

$$\gamma = f - u_0 \tag{30}$$

vanishes on the boundary $\partial\Omega$ together with its derivatives up to order m. Completeness of (29) follows, since the function γ satisfies the conditions of the Theorem 1.

The general solution structure (26) may be also written as

$$u = u_0 + R, \tag{31}$$

where u_0 interpolates the exact boundary conditions on *all* portions $\partial\Omega_i$ and R is the remainder term. To show that this structure is complete we need to show that the difference between f and u can be made arbitrarily small. Unfortunately, we cannot apply the above argument in this case, because different order of derivatives may be prescribed on different portions of the boundary. We now give a different proof of completeness by showing that there is another function γ^* that does satisfy the conditions of Theorem 1 and that $\|\gamma - \gamma^*\|$ can be made arbitrarily small. First we prove a lemma indicating how to construct such functions in the neighborhood of each individual portion of boundary $\partial\Omega_i$

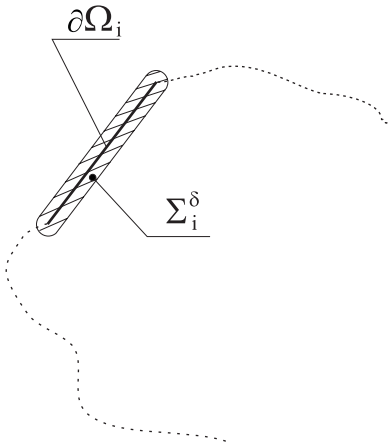


Figure 5: Illustration for Lemma 3

Lemma 3 *Let $\partial\Omega_i$ be defined by $(\omega_i = 0)$ where ω_i is a normalized function, and define region: $\Sigma_i^\delta \equiv (|\omega_i| \leq \delta)$. Then for any function $q \in C^{m-1}(\Sigma_i^\delta)$, and for any $\varepsilon_i > 0$ there exists a positive δ such that $\|\omega_i^m q\|_{H^{m-1}(\Sigma_i^\delta)} < \varepsilon_i$.*

Proof As illustrated in Figure 5, the region Σ_i^δ is a neighborhood of $\partial\Omega$. Since function ω_i is normalized, $\omega_i = O(\delta)$ in that neighborhood. It should be clear that $D_j(\omega_i^m q) = \omega_i^{m-j}\eta_{ij}$, $(j = 0, 1, 2, ..., m-1)$, where η_{ij} are continuous finite functions. Then

$$\|\omega_i^m q\|_{H^{m-1}(\Sigma_i^\delta)} = \sum_{j=0}^{m-1} \|\omega_i^{m-j}\eta_{ij}\|_{L_2(\Sigma_i^\delta)} \leq \delta \sum_{j=0}^{m-1} \delta^{m-j-1}\|\eta_{ij}\|_{L_2(\Sigma_i^\delta)} = \delta\zeta,$$

where ζ has finite value. □

The lemma shows that the remainder term on the boundary portion $\partial\Omega_i$ can be made arbitrarily small in the neighborhood of $\partial\Omega_i$. We now can apply the lemma in neighborhood of each Ω_i in order to prove the completeness of the structure (26).

Theorem 4 *Let Ω be a closed region; $f \in C^s(\Omega)$ be of $s > k$ times continuously differentiable function defined in the interior of Ω. Values of function f and its partial derivatives up to order k_i are prescribed on boundaries $\partial\Omega_i \subset \partial\Omega$. Then for any small ε there exists a polynomial P_r such that inequality*

$$\|\gamma - \mu P_r\|_{H^s(\Omega)} < \varepsilon \tag{32}$$

is satisfied, where $\gamma = f - u_0$ is a function that vanishes on $\partial\Omega_i$ together with its partial derivatives up to order k_i, and $\mu = \prod_{i=1}^N \omega_i^{k_i+1}$.

Proof From the given conditions, $\partial\Omega = \bigcup_{i=0}^{N} \partial\Omega_i$ and boundary conditions on $\partial\Omega_i$ specify derivatives up to order k_i. Let us construct regions Σ_i^δ for each $\partial\Omega_i$ as described in the conditions of Lemma 3. Let γ^* be another function that vanishes on $\partial\Omega$ together with its partial derivatives up to order $k = max\{k_i\}$, $(i = 0, 1, 2, ..., N)$ and coincides together with its partial derivatives up to order $k+1$ with function γ in the boundary region of domain $\Sigma^\delta = \bigcup_{i=0}^{N} \Sigma_i^{\delta_i}$. Then we can transform the expression (32):

$$\begin{aligned} \|\gamma - \mu P_r\|_{H^k(\Omega)} =& \|\gamma - \gamma^* + \gamma^* - \omega^{k+1} P_{r_1}^* + \omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Omega)} \\ \leq& \|\gamma - \gamma^*\|_{H^k(\Omega)} + \|\gamma^* - \omega^{k+1} P_{r_1}^*\|_{H^k(\Omega)} + \|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Omega)}, \end{aligned} \tag{33}$$

where $P_{r_1}^*$ is a polynomial of degree r_1. According to Lemma 3, $\|\gamma - \gamma^*\|_{H^k(\Omega)} = \|\gamma - \gamma^*\|_{H^k(\Sigma^\delta)} \leq \delta \sum_{i=0}^{N} \zeta_i$, where ζ_i are finite values. Therefore, for any $\varepsilon_1 > 0$, it is possible to choose a value of δ that the inequality

$$\|\gamma - \gamma^*\|_{H^k(\Omega)} \leq \varepsilon_1$$

is satisfied. The second term in expression (33) can be estimated by Theorem 1:

$$\|\gamma^* - \omega^{k+1} P_{r_1}^*\|_{H^k(\Omega)} \leq \varepsilon_2$$

Finally, we consider the last term in expression (33) separately in two regions — inside the domain $\Omega_\delta = \Omega - \Sigma^\delta$ and in the boundary region Σ^δ:

$$\|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Omega)} \leq \|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Omega_\delta)} + \|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Sigma^\delta)} \tag{34}$$

The first term in inequality (34) can be estimated by

$$\|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Omega_\delta)} \leq \|\mu\|_{H^k(\Omega_\delta)} \left\| \frac{\omega^{k+1}}{\mu} P_{r_1}^* - P_r \right\|_{H^k(\Omega_\delta)} \tag{35}$$

Because ω^{k+1} has the same order of magnitude that μ has, the quotient $\frac{\omega^{k+1}}{\mu}$ has a finite value and therefore according to the Weierstrass theorem there exists a polynomial P_r such that

$$\left\| \frac{\omega^{k+1}}{\mu} P_{r_1}^* - P_r \right\|_{H^k(\Omega_\delta)} \leq \varepsilon_3$$

is satisfied. The term $\|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Sigma^\delta)}$ can be made arbitrary small by choosing sufficiently small value of δ. More precisely,

$$\|\omega^{k+1} P_{r_1}^* - \mu P_r\|_{H^k(\Sigma^\delta)} \leq \|\omega^{k+1} P_{r_1}^*\|_{H^k(\Sigma^\delta)} + \|\mu P_r\|_{H^k(\Sigma^\delta)}.$$

Both terms on the right side of this inequality satisfy the conditions of the Lemma 3 and consequently can be made arbitrary small by appropriate choice of δ. □

3.5 Example: non-steady heat transfer problem with non-homogeneous mixed boundary conditions

As an illustration of how RFM solution structures perform in practice, we consider the non-steady heat transfer problem with non-homogeneous mixed boundary conditions solved in (Liu and Reitz, 1998) and (Shapiro and Tsukanov, 1998). A simple one-dimensional problem served as a benchmark (Figure 6): a 3 mm thick slab with thermal conductivity $\lambda = 53.1 W m^{-1} K^{-1}$, density $\rho = 7870 kg \cdot m^{-3}$ and specific heat $c_\rho = 447 J \cdot kg^{-1} K^{-1}$. The slab is initially at uniform temperature of $T = 300K$ which is maintained at the right end of the slab ($x = x_1$). A steady heat flux of $q = 2MW \cdot m^{-2}$ is applied at the left side ($x = 0$) beginning at $t = 0$. We need to compute temperature distributions from beginning until moment when heat transfer becomes steady.

The problem is formulated as the boundary value problem:

$$\frac{\partial^2 T}{\partial x^2} = c_\rho \rho \frac{\partial T}{\partial t} \tag{36}$$

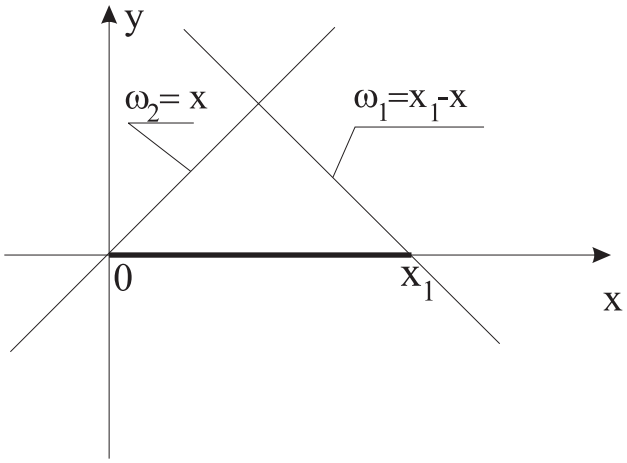


Figure 6: One dimensional slab

with mixed boundary conditions

$$-\lambda \frac{\partial T}{\partial \nu}_{|x=0} = \psi_0 = 2 \cdot 10^6 \frac{W}{m^2}; \quad T_{|x=x_1} = \varphi_0 = 300K, \tag{37}$$

where $x_1 = 0.003$ m and ν is the interior normal to the boundary, and with the initial condition of

$$T\left(x\right)_{|t=0} = 300K. \tag{38}$$

We discretize equation (36) by time and rewrite it in the form:

$$\frac{\partial^2 T_i}{\partial x^2} - c_\rho \rho \frac{T_i}{\Delta t} = -c_\rho \rho \frac{T_{i-1}}{\Delta t}, \tag{39}$$

where Δt is time step, and T_i and T_{i-1} are temperature distributions at the current and the previous time step respectively. Then at each time step we need to solve the quasi-steady problem (39, 37) starting with the initial temperature distribution (38).

The RFM formulation requires constructing implicit functions to describe the region's boundaries and an appropriate solution structure. The boundaries of the one-dimensional slab are described by two functions $\omega_1 = x_1 - x \geq 0$; $\omega_2 = x \geq 0$ that are substituted into solution structure (28) with $T = u$. The remaining problems may be solved using any variational technique. Note that the solution structure remains the same on all time intervals. Figures 7(a) and (b) show temperature distribution predicted by the least squares method for two different time steps: 0.01 s in Figure 7(a) and 0.1 s in Figure 7(b). The results are essentially identical to those computed in (Liu and Reitz, 1998) using an order of magnitude smaller time steps. Another indication of the convergent solution is given in Figure 8 which compares the solution at time $t = 0.8$ s with respect to the number nx of the basis functions in Φ and the time step Δt.

Additional details may be found in (Shapiro and Tsukanov, 1998), where the same solution structure was applied to a two-dimensional problem with moving boundary conditions. Figure 9 shows temperature distributions in a (moving) engine combustion chamber, all computed in a meshfree manner with the same solution structure (28).

4 Conclusions

4.1 Properties of RFM

We described the basic principle of RFM and have shown that properly constructed RFM solution structures are complete in the sense that they converge to the exact solution of a problem. Some estimates on the rate of convergence

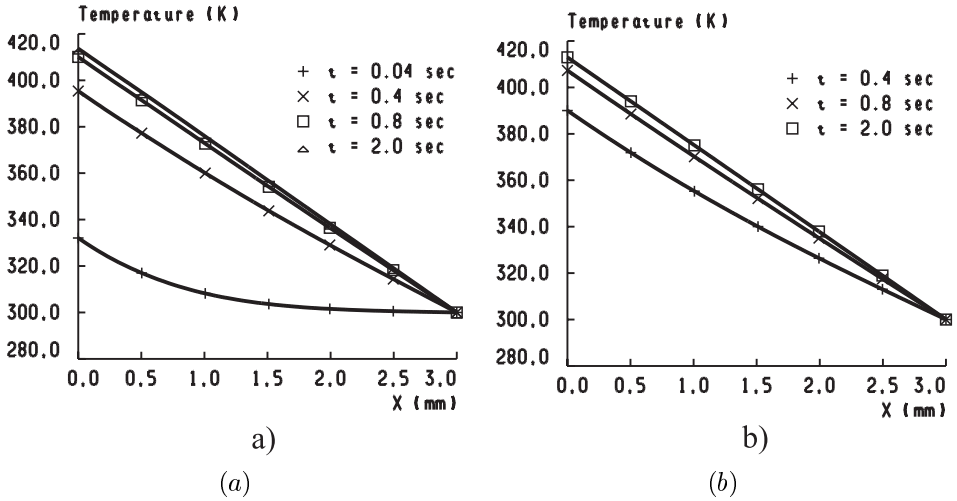


Figure 7: Temperature distributions computed using different time step

in the homogeneous case can be found in (Kantorovich and Krylov, 1958; Kharrik, 1963). RFM is unique amongst meshfree methods because RFM solution structures can be constructed to satisfy all boundary conditions exactly. This property of RFM has a number of important consequences:

- the solution procedure does not require geometric representation conversion and approximation via grid generation or meshing;
- RFM can be used in conjunction with most basis functions and numerical procedures, including other meshfree methods, for example those surveyed in (Belytschko et al., 1996);
- we conjecture (based on our experience) that exact satisfaction of the boundary conditions leads to higher precision with fewer degrees of freedom, though this remains to be verified;
- parameterized solution structures provide computational support for problems with changing geometry and boundary conditions.

The last point deserves some clarification. In general terms, the solution structure can be written in the form

$$u = B[\Phi], \tag{40}$$

where $B = B(\omega, \{\omega_i\}, \{\varphi_i\})$ is an operator that depends on geometry of the domain $\omega \geq 0$ and boundary conditions φ_i prescribed on boundary portions defined by $\omega_i = 0$. If the functions ω_i are parameterized in terms of the motion parameters, so is the resulting solution structure. This makes meshfree RFM a natural choice for problems where changes in geometry occur over time, including moving boundary conditions and shape optimization. See (Shapiro and Tsukanov, 1998) for additional discussion.

A number of further RFM generalizations are already known. Our examples involved boundary value problems with a single scalar function. Theory of R-functions, RFM, and the completeness of solution structures generalize to vector or tensor-valued functions in a straightforward manner (Rvachev, 1982; Rvachev and Sheiko, 1995). Furthermore, the theory of R-functions allows the construction of implicit equations $\omega = 0$ for pointsets with heterogeneous geometric and topological properties. This immediately extends RFM and our results to problems where values and derivative information are prescribed throughout regions or isolated points. For example, Figure 10(b) shows a function φ constructed as transfinite Lagrangian interpolation of functions $\varphi_0 = 0$, $\varphi_1 = -3x + y + 6$, $\varphi_2 = -5$, $\varphi_3 = 5$ prescribed on one and two dimensional geometrical loci $\omega_i = 0$, $i = 0, \ldots, 3$ indicated in Figure 10(a). Figure 10(c) shows a global normalized function ω that takes zero value on the same geometry. Combining functions φ and ω with undetermined function Φ into a single functional expression for solution u according to (16), we obtain the Dirichlet

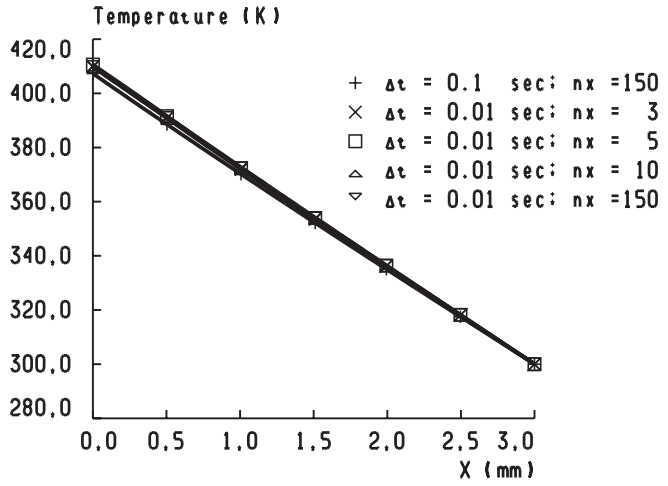


Figure 8: Temperature distributions computed at the same time point using different time step and degrees of freedom

solution structure that exactly satisfies all prescribed conditions. Figure 10(d) shows the function u that approximates Laplace equation $\nabla^2 u = 0$ by choosing Φ to minimize the Ritz's functional:

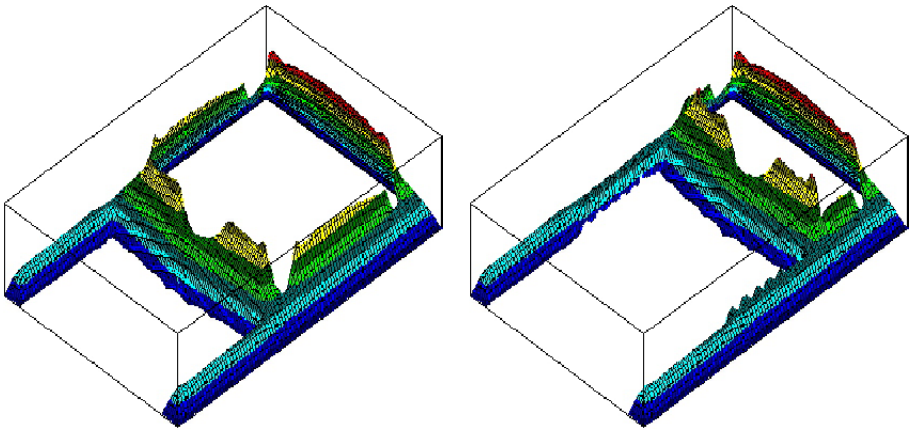
$$F = \iint_\Omega \left(\nabla\left(\omega\Phi\right)\right)^2 \, d\Omega + 2 \iint_\Omega \nabla\left(\omega\Phi\right) \cdot \nabla\varphi \, d\Omega$$

4.2 Automation issues

RFM has one significant disadvantage when compared to the usual spatial discretization and other meshfree methods: the solution structure is constructed, differentiated, and integrated at runtime. The resulting computational overhead is the price of satisfying the boundary conditions and achieving the "meshfreedom". Thus, a fully automatic implementation of RFM requires four main ingredients:

- Automatic construction of implicit functions and structures, given a geometric model and prescribed boundary conditions;
- Automatic differentiation of the constructed functions and structures at various points of the domain;
- Integration of the structures and their derivatives over the geometric model of the domain in the absence of finite element or grid approximation of the domain;
- Constructing and solving the resulting linear system for values of the coefficients C_i in the undetermined functional component Φ.

All these tasks are feasible today with existing technology, but their detailed discussion is outside the scope of this paper. Additional information on construction of implicit functions may be found in (Shapiro, 1994; Shapiro, 1997; Shapiro and Tsukanov, 1998). Automatic differentiation techniques are well understood (Rall and Corliss, 1996; Shevchenko and Rokityanskaya, 1996; Rvachev and Shevchenko, 1988) and have been used in system POLYE; a more recent implementation is available from the authors at the University of Wisconsin. Adaptive integration methods can be easily implemented in most geometric modeling systems. And the properties of the resulting linear system are determined by the computational properties of the basis functions. For example, when Φ is a uniform grid of B-splines such as used in our examples, the resulting sparse banded system can be solved in linear time using standard techniques. All of these ingredients are currently being implemented in the SAGE computational environment at the University of Wisconsin.



(a) (b)

Figure 9: Temperature distributions in a engine combustion chamber

Acknowledgments

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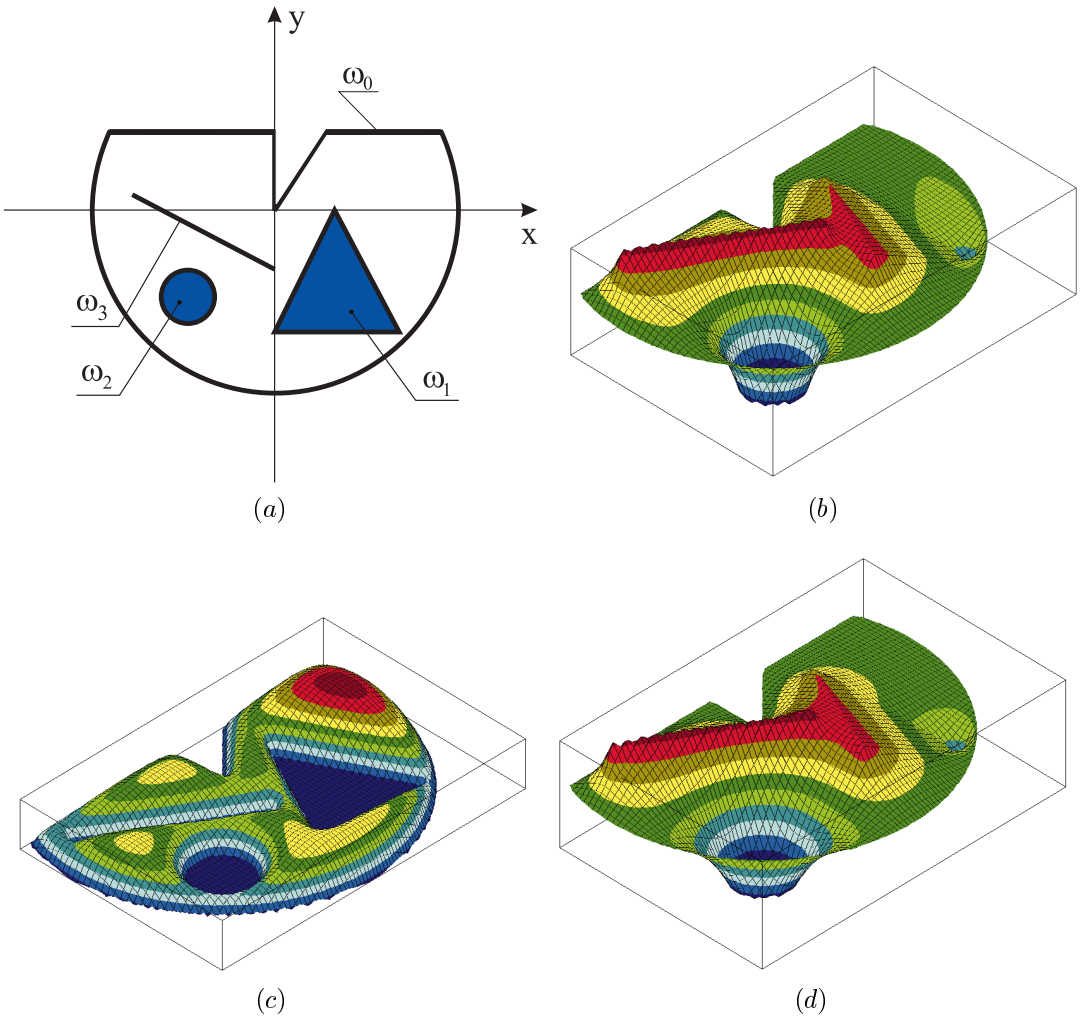

Figure 10: (a) Domain with functional values prescribed on heterogeneous loci ω_i; (b) function that interpolates the values prescribed on the loci; (c) function that vanishes on the indicated loci; (d) solution of boundary value problem for Laplace equation with prescribed boundary conditions

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