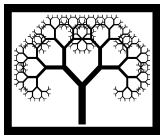
Paper 102



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A Frequency Domain Formulation of Kansa's Method to Simulate Transient Heat Conduction

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Abstract

In the last decade, a number of works have been published proposing the solution of heat diffusion problems by first transforming the relevant partial differential equation (PDE) to the frequency domain. Many of those works make use of the boundary element method, thus requiring the previous knowledge of fundamental solutions for the problem. These are, however, only known for the simplest cases, and thus more general strategies may be interesting for example when the domain is not homogeneous, exhibiting varying properties. In this paper, we present an implementation of Kansa's method for the solution of this type of problems, and test the accuracy of such implementation. Kansa's method is a general numerical technique in which the solution of a given PDE is reproduced within a specific sub-domain as a linear combination of RBFs, and thus does not require the prior knowledge of fundamental solutions. Here, the mathematical formulation of the method in the frequency domain will be presented and discussed; since the most commonly used RBFs (MQ) include a free parameter, we also focus on the choice of the correct value of this parameter for the specific physical problem type addressed here. The method is implemented and tested for a number of problems, and the results it provides are then compared with some reference solutions computed with other analysis strategies (namely direct time-domain analysis).

Keywords: heat conduction, frequency domain, meshless, Kansa's method, radial basis functions, shape parameter.

1 Introduction

The solution of transient heat conduction problems has been address using a large variety of method, ranging from simple analytical solutions known for simple cases, to complex numerical formulations, applicable to more general configurations. Two major groups of solution strategies have been developed over the years, the first

corresponding to a direct solution of the problem in the time domain [1-4], and the second to obtaining the solution first in a transformed domain (usually by means of a Laplace transform), and then performing an inverse transformation to synthesize the time response [5-7].
More recently, a different strategy has been devised for the solution of such problems, in which a Fourier transformation is applied to the governing differential equation, and then the solution is pursued in the frequency domain (see for example Simões et al [8] or Godinho et al [9]). After solving the problem for each individual frequency, an inverse Fourier transformation allows synthesizing the temperature field in the time domain. This approach has been efficiently applied together with Boundary Element Method and Method of Fundamental Solutions formulations; however, both the MFS and the BEM require the previous knowledge of fundamental solutions for the PDE, which are only known for specific situations. Very little exists in the literature concerning its application together with other numerical techniques, such as domain-based methods, which are usually of more general application.
In this work, the authors present an implementation of this methodology together with a domain-based meshless method, testing the accuracy of such implementation. Kansa's method, or radial basis functions (RBF) collocation method, is here used for this purpose. Kansa's Method is a general numerical technique which tries to reproduce the solution of a given partial differential equation (PDE) within a specific sub-domain as a linear combination of RBFs, and thus does not require the prior knowledge of Green's functions. Many types of RBFs may be used with Kansa's method, some of those including a free (shape) parameter, whose definition is non-trivial and that greatly influences the accuracy of the computed responses. This is still an open discussion in the scientific literature [10-14], since the parameter can be strongly problem dependent.
Here, the mathematical formulation of the method in the frequency domain will be presented and discussed, also focusing on the choice of the RBF and free-parameter for the specific physical problem type addressed here. The method is implemented and tested for a number of problems, and the results it provides are compared with some reference solutions computed with other analysis strategies (namely direct time-domain analysis). Since the chosen RBFs involve the introduction of a free (or shape) parameter, a numerical strategy is proposed for the estimation of its optimal value.

2 Mathematical formulation

2.1 Governing PDEs

To mathematically formulate the problem, we start by considering the standard time-dependent heat diffusion equation, which can be written as

$$\nabla^2 T(\mathbf{x}) = \frac{1}{K}\frac{\partial T(\mathbf{x})}{t} \tag{1}$$

where $T(\mathbf{x})$ is the temperature at domain point $\mathbf{x}$, $K = k/\rho c$ being the diffusivity, k, c and ρ being the thermal conductivity, specific heat and density, respectively. Following the works of Simões et al [15], and considering an initial temperature distribution defined by $T_0(\mathbf{x})$, by application of a Fourier transformation in the variable t, equation (1) may be written, in the frequency domain, in the form of

$$\nabla^2 \hat{T}(\mathbf{x}) + \lambda^2 \hat{T}(\mathbf{x}) = -\frac{T_0(\mathbf{x})}{K}, \text{ with } \lambda^2 = -\frac{\mathrm{i}\omega}{K} \tag{2}$$

which is a frequency dependent equation, where $\omega = 2\pi f$ is the angular frequency. After solution of this equation over a full range of frequency values, an inverse Fourier transformation may be applied in order to recover the response in the time domain (see also [9] for further details).

2.2 Formulation of Kansa's method in the frequency domain

To formulate Kansa's method (or RBF collocation method), we next consider a closed domain (Ω), bounded by a boundary (Γ). Within this domain, consider a set of N collocation points $\{\mathbf{x}_k\}_{k=1}^{N}$, of which $\{\mathbf{x}_k\}_{k=1}^{NI}$ are NI internal points and $\{\mathbf{x}_k\}_{k=NI+1}^{N}$ are boundary points, as illustrated in Figure 1. Next, we consider that an approximate solution ($\tilde{T}(\mathbf{x})$) of the relevant PDE in equation (2), can be written using a linear combination of radial basis functions (RBFs), expressed as

$$\tilde{T}(\mathbf{x}) = \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}) \tag{3}$$

where $\varphi_k(\mathbf{x})$ is the RBF and $(a_k)_{k=1}^{N}$ are N unknown coefficients to be determined. Substituting this approximation in equation (2), we may write

$$\nabla^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}) + \lambda^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}) = -\frac{T_0(\mathbf{x})}{K} \tag{4}$$

Based on this approximation of the relevant PDE, and also imposing the necessary boundary conditions at each boundary point, we may write a system of N equations on N unknowns, which allows calculation of the $(a_k)_{k=1}^{N}$ coefficients. After calculating these coefficients, the approximate solution at any given domain point can be computed using equation (3). It is worth noting that the intrinsic characteristics of the method make it very simple to ascribe varying physical properties (in this case varying values of conductivity) to each point, and thus the method is applicable to problems in non-homogeneous domains. One should also note that the solution of the PDE in equation (2) using Kansa's method requires no domain integration; thus,

implementation of the method becomes simple, and does not depend on the quality of possible domain integrations, as seen in other methods (such as the BEM).

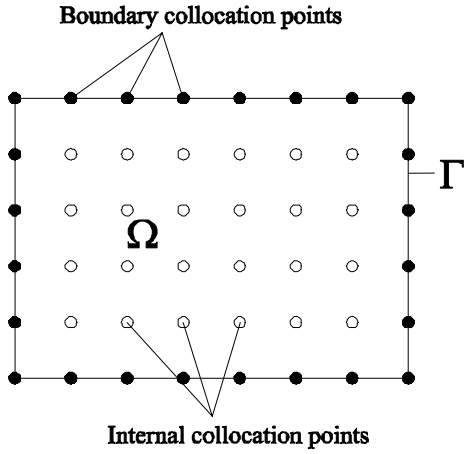


Figure 1: Illustration of the typical distribution of collocation points

Although several types of RBF can be used, multiquadric functions (MQ) are probably the most usual choice of researchers, since they usually provide more accurate results. These functions are defined as

$$\varphi_k(\mathbf{x}) = \sqrt{r_k^2 + c^2}\ , \tag{5}$$

with $r_k = \|\mathbf{x} - \mathbf{x}_k\|$, $\mathbf{x}_k$ being the center of the RBF, and c being a shape (or free) parameter of the RBF.

2.3 Optimization of the RBF free parameter

Several studies have pointed out that the correct choice of this parameter is crucial to allow accurate results to be obtained. Larger values of the parameter usually lead to smoother functions and can provide better solutions, although they may also lead to ill-conditioned equation systems, which can hinder the computation of accurate results. In different published works, such as those by Sarra and Sturgill [10], Kansa and Hon [11], Fasshauer and Zhang [12], or Cheng [13], this topic has been analyzed; however, the optimization of the *c* value is still an open question.
A recent work by Godinho et al [14] addressed this question for the specific case of acoustic problems, and considering a coupled approach between BEM and Kansa's method. According to that work, a good estimation of an adequate value of c can be obtained by progressively increasing its value and evaluating the residual of the PDE; the best approximation should correspond to the one that minimizes that residual. To extend the approach for the present case, one should take into account that the residual of the PDE treated in this study at a domain point $\mathbf{x}$ can be written as

$$\varepsilon(\mathbf{x}) = \nabla^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}) + \lambda^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}) + \frac{T_0(\mathbf{x})}{K} \tag{6}$$

If $\mathbf{x} \in \{\mathbf{x}_k\}_{k=1}^{NI}$, then a null value of $\varepsilon(\mathbf{x})$ occurs; if otherwise, then $\varepsilon(\mathbf{x})$ is not null, and represents an error in the enforcement of the PDE. Thus, considering a set of points $\{\mathbf{x}_i^R\}_{i=1}^{NPR}$ that do not coincide with the collocation points, one may compute an average residual as

$$\overline{\varepsilon} = \sum_{i=1}^{NPR} \varepsilon(\mathbf{x}_i^R) = \sum_{i=1}^{NPR} \left(\nabla^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}_i^R) + \lambda^2 \sum_{k=1}^{N} a_k \varphi_k(\mathbf{x}_i^R) + \frac{T_0(\mathbf{x}_i^R)}{K} \right) \tag{7}$$

This average residual can be used as a guideline for the evaluation of the error of the computed approximation, and consequently for the choice of the adequate shape parameter of the RBFs. The proposed approach can be further complemented and automated making use of optimization techniques, thus incorporating the parameter c as an unknown in the system of equations and trying to find the minimal value of the average residual as a function of c; thus, the goal is to find $\min(\overline{\varepsilon})$, while still satisfying the relevant boundary conditions. A nonlinear least squares minimization subroutine, based in the subroutine LMDIF1 from MINPACK, is used for that purpose.

3 Verification against frequency domain results

To verify the behavior of Kansa's method in frequency domain analysis of a heat conduction problem, we initially consider a simple square domain, subject to null temperatures along all boundaries. The medium has a density of 2500 kg/m3, a conductivity of 1.4 w/m/ºC and a specific heat of 840 J/kg/ºC. Within this medium, at x=0.25 m and y=0.35 m, a heat source is positioned. In the frequency domain, its effect can be accounted for assuming its contribution to be given by

$$Ts(\mathbf{x}, \mathbf{x}_s) = \frac{-\mathrm{i}}{4K} H_0^{(2)} \left(\lambda \left\| \mathbf{x} - \mathbf{x}_s \right\| \right) \tag{8}$$

This function corresponds to the fundamental solution of the homogeneous PDE obtained from equation (2) when $T_0(\mathbf{x}) = 0$ (see Simões et al [8]).

To analyse this problem, consider that a Kansa's model is used, with a grid of 10 x 10 points as defined in Figure 2, and that the response is calculated for frequencies of $f = 5 \times 10^{-8}$ Hz and $f = 1.5 \times 10^{-5}$ Hz. As reference solution, we consider the response calculated using a BEM model [9], discretizing each side using 20 elements. Figure 3a illustrates the computed reference responses for these two frequencies, clearly revealing the effect of the source, and exhibiting the prescribed null temperature boundary conditions.

In Figure 3b, the residual of the PDE obtained when using Kansa's method is plotted against the free parameter (c). In the results calculated for both frequencies, it can be seen that the residual progressively decreases as c increases, up to a point at which the residual curve starts oscillating significantly. Indeed, at this point the value of c becomes sufficiently large so as to originate instabilities in the equation system, which becomes ill-conditioned. Thus, for higher values of c, the response is no longer reliable.

To allow for a more convenient and automatized choice of c, the problem has also been solved making use of nonlinear least squares minimization, implemented so as to find the value of c that minimizes the average residual of the PDE. In the plots, a mark has been added corresponding to the value of the free parameter obtained using this solver; as can be seen, the chosen value always corresponds to a local minimum of the curve, and is always located in the smooth (non-oscillating) part of the curve.

To scrutinize in more detail the quality of the temperature distribution calculated using this "optimal" parameter, Figure 3c illustrates the error computed against the reference solution. As can be seen, for both frequencies the maximum error is below 10^{-4}.

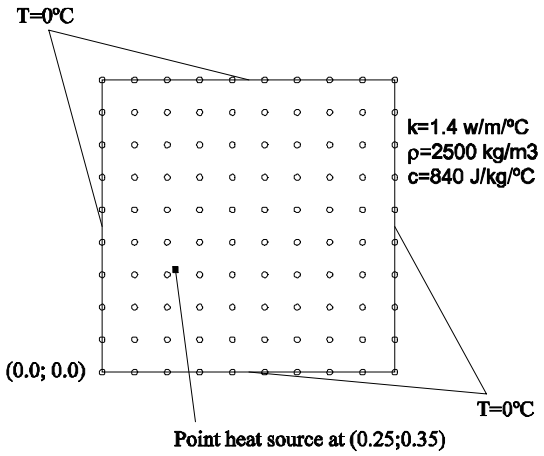


Figure 2: Test model for verification of the proposed formulation, consisting of a unit square domain with null boundary temperatures, and subject to a point heat source within the domain.

To further analyse the behaviour of the method, results were also computed for more refined descriptions of the domain. Figure 4 illustrates both the c-residual curve and the domain error when 12 x 12, 15 x 15 and 18 x 18 points are used to define the model based in Kansa's method. It becomes clear that the "optimal" c parameter tends to decrease when more points are adopted, and that progressively lower residuals are obtained when more refined models are used. Similarly, the domain error also tends to decrease with the refinement of the model, indicating a convergence to the correct solution.

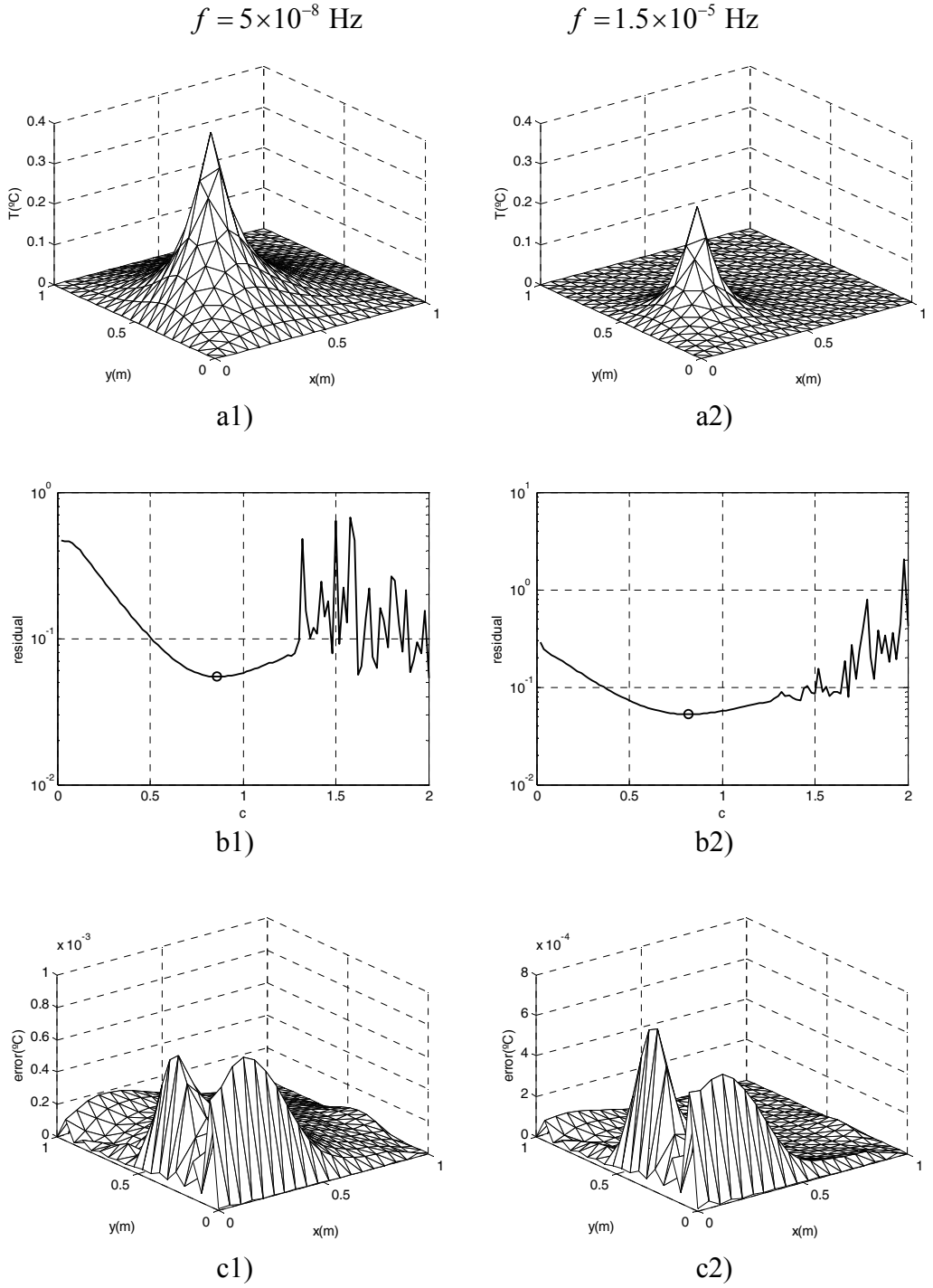


Figure 3: Results computed in the frequency domain for two different frequencies: a) reference absolute temperature response; b) residual of the PDE for Kansa's method computed through equation (7) as a function of c; c) error in the calculation of the temperature when using Kansa's method with the "optimal" c value.

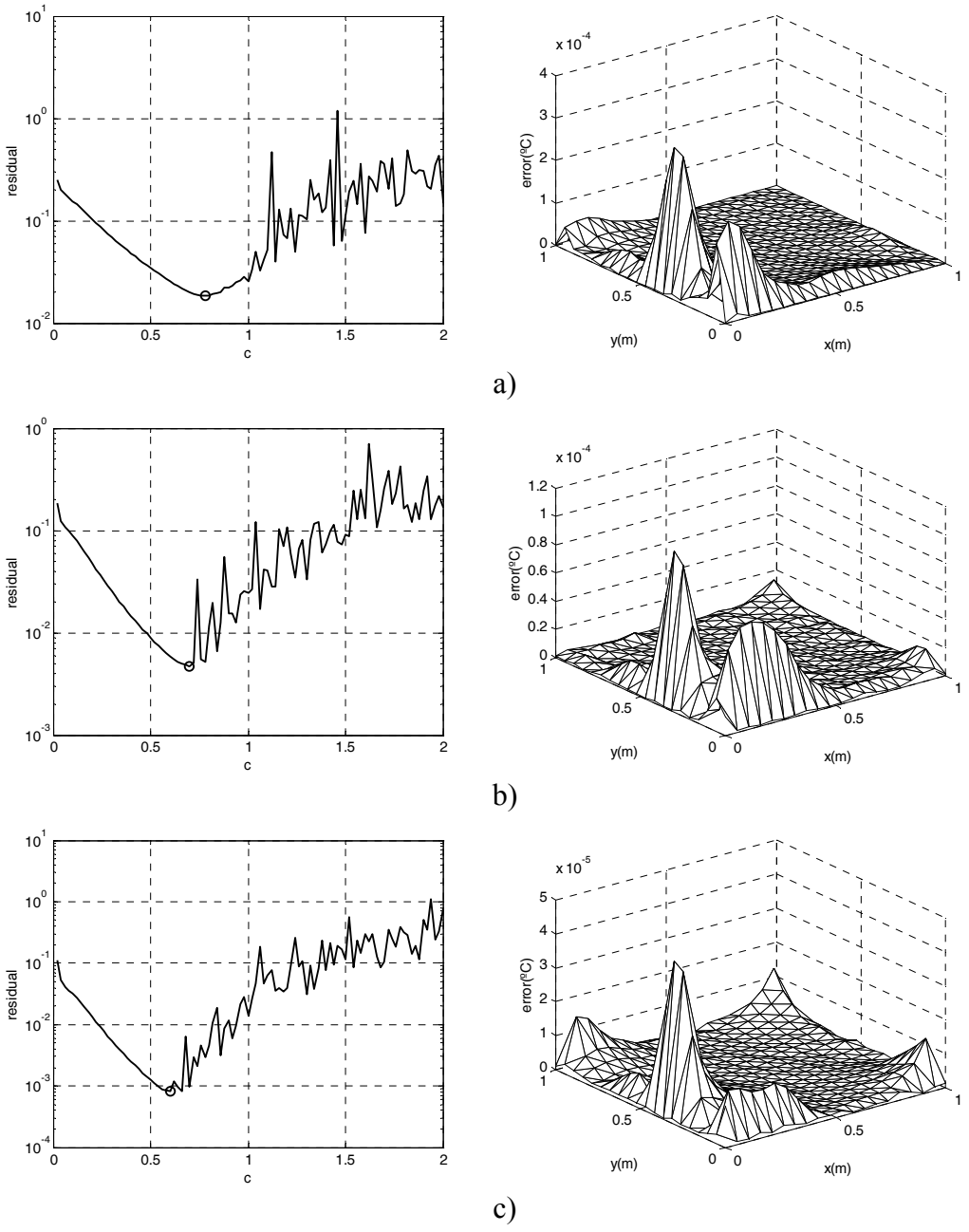
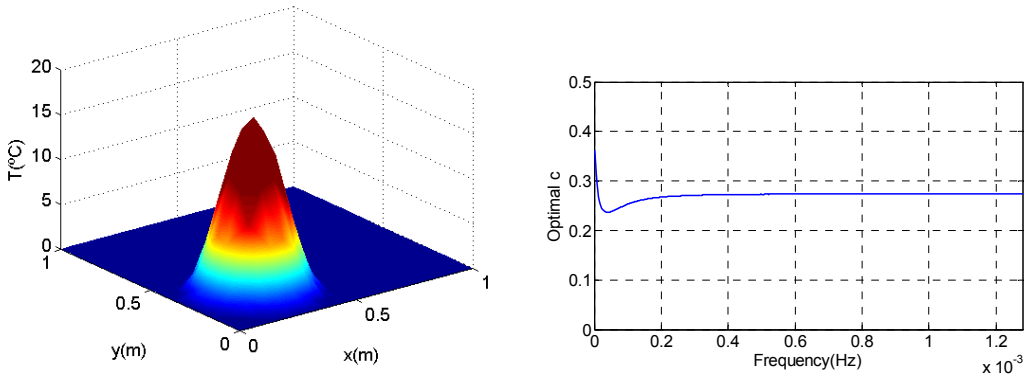


Figure 4: Behaviour of Kansa's method for progressively refined models: a) 12x12 points; b) 15x15 points; c) 18x18 points. Left column represent the variation of the PDE residual with c, while right column presents the domain error in the calculation of temperatures.

4 Comparison with time domain results

The proposed Kansa's method formulation was also applied to simulate problems in which an initial temperature distribution is given throughout the domain. For this

purpose, we consider the same geometry as depicted in Figure 2, but we now consider that the initial temperature distribution depicted in Figure 5a is prescribed. This distribution corresponds to a cosine shaped variation in the vicinity of the point with coordinates (0.25 m; 0.25 m), reaching a maximum of 20ºC at this point. Thus, for, for this case, the PDE must include the right-hand-side term as given in equation (2); additionally, in order to synthesize a time domain response, computations are first performed for a full frequency range, from 0 Hz to 1.28×10^{-3} Hz, with an increment of $.25\times10^{-5}$ Hz, and the corresponding results are then Fourier-transformed back to the time domain. One should note that for the null frequency the right-hand-side term cannot be computed, and thus a complex frequencies with a very small imaginary part are used (see [15] for details). Figure 5b illustrates the calculated "optimal" c values along the analyzed frequency domain, revealing that they exhibit some variation, although they tend to stabilize around c=0.28 for the higher frequencies.



a) b)

Figure 5: a) Initial temperature distribution (at t=0.0s) for the second example; b) Variation of the optimal values of the free parameter along the frequency domain.

To verify the correctness of the calculated responses, a time-domain model was used, based on an implicit Crank-Nicholson marching scheme; the time-domain model was first checked to ensure that adequate values were computed, and a final grid of 20 x 20 points, together with a time step of 200 s, was used in the calculation of reference responses. Figure 6 depicts both the results computed using the direct time-marching scheme and the frequency domain approach, for instants corresponding to 5000 s (25 time steps) and to 10000 s (50 time steps). As can be seen, the responses calculated using both methods are very similar, without any visible differences being observable within the analysis domain. As expected, the temperature progressively decreases around the region of maximum temperature, with the energy spreading to other points where the initial temperature was null. This effect is clear when observing the snapshot taken for the later time, where non-null temperatures are observable for x>0.5 m and beyond y>0.5 m.

To have a better picture of the quality of the solutions, the temperature variation was recorded at a point located at (0.158m; 0.316m), and its evolution is depicted in Figure 7. At that point, a progressive decrease of the temperature can be seen, and

the responses calculated by both the frequency domain and time domain approaches are identical.

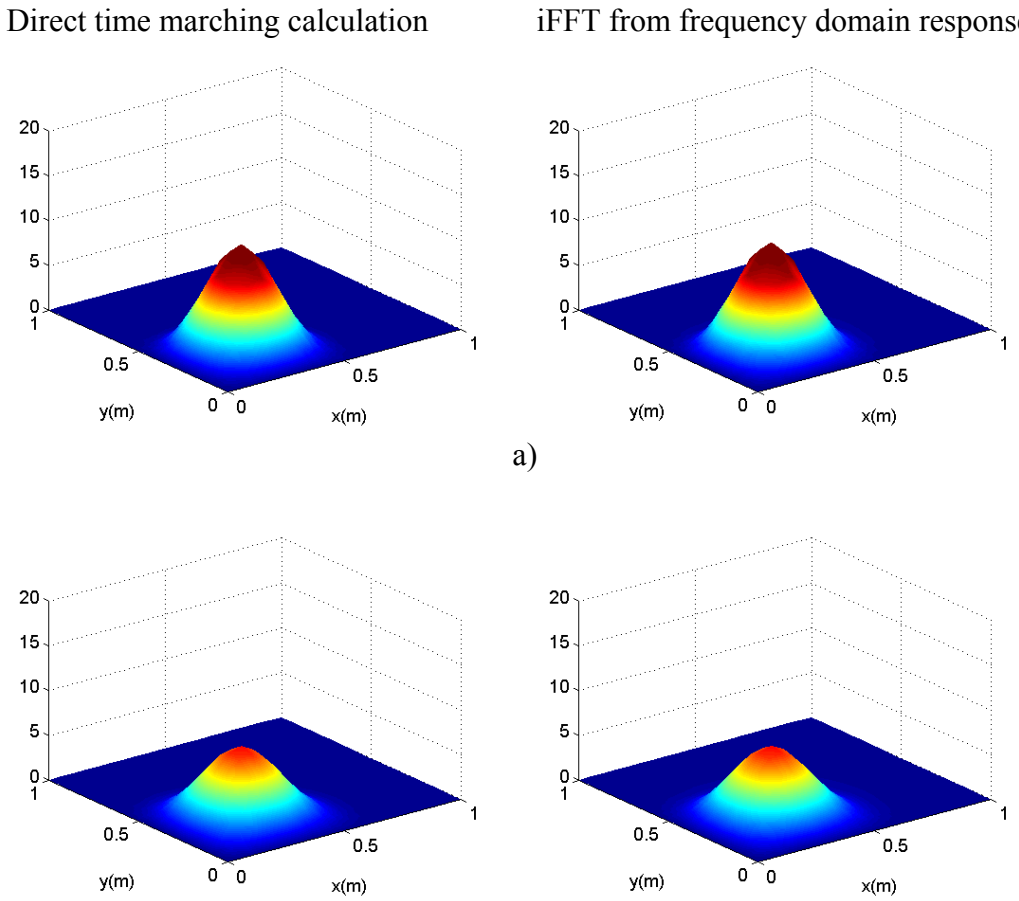


Figure 6: Temperature distribution at calculated with a classic time-marching algorithm and with the proposed method at: a) t=5000.0s ; b) t=10000.0 s.

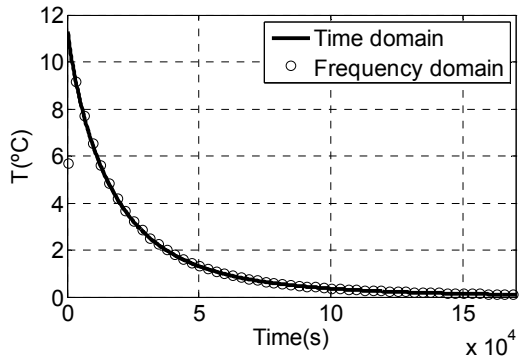


Figure 7: Temperature variation at a point located at (0.158m; 0.316m), calculated using the proposed formulation and a classic time-marching algorithm.

5 Final remarks

This paper presented and discussed an implementation of Kansa's method for calculation of transient heat diffusion problems, based on the solution of the problem in a transformed (frequency) domain. The implementation of the method made use of an optimization scheme for the calculation of the free parameter of the MQ RBFs, which was shown to compute different values of c as a function of the frequency and of the domain discretization. Comparison with reference results calculated using a BEM model revealed that good responses are computed by the proposed method.
The method was also applied to calculate the evolution of the temperature within a domain, considering an initial non-uniform distribution of temperatures. Comparison with a standard time-marching algorithm, based on an implicit Crank-Nicholson implementation, also revealed a good accuracy of the method. One should note that, for that case, the response is first calculated in the frequency domain and then transformed to time domain by means of an inverse FFT.

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References

[1] Y.P. Chang, C.S. Kang, D.J. Chen, "The use of fundamental Green functions for solution of problems of heat conduction in anisotropic media", Int. J. Heat and Mass Transfer, 16, 1905-1918, 1973.
[2] R.P. Shaw, "An integral equation approach to diffusion", Int. J. Heat and Mass Transfer, 17, 693-699, 1974.
[3] L.C. Wrobel, C.A. Brebbia, "A formulation of the boundary element method for axisymmetric transient heat conduction", Int. J. Heat and Mass Transfer, 24, 843-850, 1981.
[4] G.F. Dargush, P.K. Banerjee, "Application of the boundary element method to transient heat conduction", Int. J. Numerical Methods in Engineering, 31, 1231 1247, 1991.
[5] A.H.-D. Cheng, Y. Abousleiman, T. Badmus, "A Laplace transform BEM for axysymmetric diffusion utilizing pre-tabulated Green's function", Eng. Anal. Bound. Elmts., 9, 39-46, 1992.
[6] S.P. Zhu, P. Satravaha, X. Lu, "Solving the linear diffusion equations with the dual reciprocity methods in Laplace space", Eng. Anal. Bound. Elmts., 13, 1-10, 1994.
[7] S.P. Zhu, P. Satravaha, "An efficient computational method for nonlinear transient heat conduction problems", Appl. Mathematical Modeling, 20, 513-522, 1996.

[8] N. Simões, A. Tadeu, “Fundamental solutions for transient heat transfer by conduction and convection in an unbounded, half-space, slab and layered media in the frequency domain”, Eng. Anal. Bound. Elmts., 29(12), 1130-1142, 2005.

[9] L. Godinho, A. Tadeu, N. Simões, “Study of transient heat conduction in 2.5D domains using the Boundary Element Method”. Eng. Anal. Bound. Elmts., 28(6), 593-606, 2004.

[10] S.A. Sarra, D. Sturgill, “A random variable shape parameter strategy for radial basis function approximation methods”, Eng. Anal. Bound. Elmts., 33, 1239-1245, 2009.

[11] E. Kansa, Y.C. Hon, “Circumventing the ill-conditioning problem with multiquadric radial basis functions: applications to elliptic partial differential equations”, Comput. Math. Appl., 39, 123-137, 2000.

[12] G.E. Fasshauer, J.G. Zhang, “On choosing "optimal" shape parameters for RBF approximation”, Numerical Algorithms, 45(1-4), 345-368, 2007.

[13] A.H.-D. Cheng, “Multiquadric and its shape parameter – a numerical investigation of error estimate, condition number, and round-off error by arbitrary precision computation”, Eng. Anal. Bound. Elmts., 36(2), 220-239, 2012.

[14] L. Godinho, A. Tadeu, “Acoustic analysis of heterogeneous domains coupling the BEM with Kansa’s method”, Eng. Anal. Bound. Elmts., 36(6), 1014-1026, 2012.

[15] N. Simões, A. Tadeu, J. António, W. Mansur, “Transient heat conduction under nonzero initial conditions: a solution using the boundary element method in the frequency domain”, Eng. Anal. Bound. Elmts., 36(4), 562-567, 2012.