Variational imbedding approach to coefficient identification in an elliptic partial differential equation

C.I. Christov* and T.T. Marinov

Department of Mathematics,
University of Louisiana at Lafayette,
Lafayette, LA 70504-1010, USA
E-mail: christov@louisiana.edu E-mail: marinov@louisiana.edu
*Corresponding author

R.S. Marinova

Department of Mathematical and Computing Sciences,
Concordia University College of Alberta,
Edmonton, AB, Canada T5B 4E4
E-mail: rossitza.marinova@concordia.ab.ca

Abstract: We consider the inverse problem for identification of the coefficient in an elliptic partial differential equation inside the unit square *D*, with overposed boundary data. This problem is not investigated enough in the literature due to the lack of results about the uniqueness of the inverse problem. Following the main idea of the so-called Method of Variational Imbedding, we imbed the solution of the inverse problem into the elliptic Boundary Value Problem (BVP) stemming from the necessary conditions for minimisation of the quadratic functional of the original equation. The system contains a well-posed fourth-order BVP for the sought function and an explicit equation for the unknown coefficient. We solve imbedding BVP numerically by making use of operator-splitting for the fourth-order BVP. The convergence and stability of the numerical method are established. We introduce an effective way for finding the best approximation for the coefficient. Featuring examples are elaborated numerically.

Keywords: coefficient identification; inverse problems; operator splitting.

Reference to this paper should be made as follows: Christov, C.I., Marinov, T.T. and Marinova, R.S. (2007) 'Variational imbedding approach to coefficient identification in an elliptic partial differential equation', *Int. J. Computational Science and Engineering*, Vol. 3, No. 4, pp.277–286.

Biographical notes: Christo I. Christov is a Professor in the Department of Mathematics at the University of Louisiana, Lafayette, USA.

Tchavdar T. Marinov is a PhD student in the Department of Mathematics at the University of Louisiana, Lafayette, USA.

Rossitza S. Marinova is an Assistant Professor in the Department of Mathematical and Computing Sciences at the Concordia University College of Alberta, Edmonton, Canada.

1 Introduction

Many practically important problems involving elliptic Partial Differential Equations (PDEs) are classified as inverse in the sense that the way they are posed is not the standard initial, boundary, or initial-boundary value for which the correctness and well-posedness of the problem have been proved. Clearly, the incorrect problems are inverse in this sense. The first example for an incorrect problem was shown by Hadamard (1932) for the Initial Value Problem (IVP) for Laplace equation (the so-called 'analytical continuation'). If the equation is hyperbolic, IVP is a direct problem, since it is correct. For elliptic PDEs, IVP is inverse, and the direct problem is the Boundary Value Problem (BVP) since the Dirichlet, Neumann, or mixed problems are correct in the sense of Hadamard (1932), respectively, a BVP for the hyperbolic PDE will appear as inverse, because IVP is the correct one.

To list the whole variety of 'non-standard' problems that can be classified as inverse, requires on to go well beyond the Hadamard's definition of incorrect problem. According to Hadamard (1932), a problem is well-posed if three requirements are met: a solution exists, it is unique, and depends continuously on the data. Otherwise, the problem is ill-posed. The clear intention of Hadamard (1932) was that 'ill-posed' means 'of no physical interest'. Today, we know

that such problems arise in a fundamental way in modelling of complex physical systems. His definition does not cover all of them, and is pertinent only to the stability of a solution. For this reason, when we speak of 'inverse problems', we mean the whole set of problems which are unusually or inconveniently posed. To distinguish these 'from the problems for which Hadamard's definition applies', we shall call the latter 'incorrect in the sense of Hadamard'. Another famous problem of the latter type is the backward in time parabolic equation. The first regularisation procedure was proposed for this problem in Lattés and Lions (1967) and Tikhonov and Arsenin (1974).

The work of Hadamard (1932) spurred significant activity, aiming at the creation of regularising procedures (Tikhonov and Arsenin, 1974; Engl, Hanke and Neubauer, 1996; Isakov, 1998; Engl and Zou, 2000) for problems that are incorrect in the sense of Hadamard (1932), e.g. for smoothing the data in order to avoid the instability due to pollution of the data. Such an approach has an important implication for the practice. At the same time, the very notion of replacing the ill-formulated (e.g. ill-specified and inverse) or ill-posed problem by a well-formulated one, is of no lesser importance. Indeed, if one succeeds in doing so, one arrives at a problem that is also correct in the sense of Hadamard (1932) and then it is not susceptible to pollution of the data. For an elucidating exposition of the inverse problems, the reader is referred to the monograph of Bellomo and Preziosi (1995).

The class of inverse problems is wider than the class of incorrect problems since the former contains also the problems involving an unknown coefficient which has to be estimated from additional (overposed) data at the boundary or at some internal points (lines, surfaces) in the domain. In this case, the problem is inverse in the sense that no explicit equation is available to evaluate the unknown coefficient. Intuitively speaking, one should adjust the coefficient in order to make solution to meet the overposed data at the boundaries. The coefficient identification may or may not be correct depending on existence and uniqueness of the solution. In most of the situations, these questions are hard to answer and any kind of approach capable to shed some light on the problem is welcome. Even if an abstract theorem of uniqueness is available, the actual computation of the unknown coefficient still remains a formidable difficulty and the quest for effective algorithms is still on. At the same time, the estimation of an unknown coefficient from overposed boundary data is of significant practical importance when creating non-invasive methods to identify the material properties of a continuum. To this class of problems belongs also the brain tomography.

The existence and the uniqueness of the solution is one of the main questions for the problem of a coefficient identification. A review on uniqueness and stability of identification of coefficients and right sides of PDEs from overdetermined boundary data is given in Isakov (1993), where a significant part is dedicated to many boundary measurements. For more information on the existing methods for solving inverse problems, we refer the reader to Engl, Hanke and Neubauer (1996), Isakov (1998), Tikhonov, Leonov and Yagola (1998), and references therein.

A method for transforming an inverse problem into a correct direct problem, but for a higher-order equation was proposed in Christov (1985) for identification of homoclinic trajectories of Lorentz system, and was called the Method of Variational Imbedding (MVI). MVI was also applied to homoclinic problems of Kuramoto-Sivashinsky equation (Christov and Velarde, 1993) and Boussinesq and Korteweg de Vries equations (Marinov, Christov and Marinova, 2005). The way of applying MVI to the classical inverse problems was sketched in Christov (1986) and Christov (1987) for analytical continuation and coefficient identification, respectively. The identification of coefficient of heat conductivity leads us to an elliptic problem of higher-order (second in time and fourth in space) (Christov, 1987; Christov and Marinov, 1998). In the same fashion, the boundary-layer thickness was identified using MVI in Christov and Marinov (1997).

In the present paper, we extend the application of MVI to the inverse problem of coefficient identification in elliptic equation from overposed boundary data.

2 Mathematical formulation

Consider the elliptic PDE

$$\Delta u(x,y) + n(x,y)u(x,y) = 0, \tag{1}$$

inside the unit square

$$D = \{(x,y) : 0 < x < 1; 0 < y < 1\}.$$

Equation (1) has a unique solution under the boundary condition

$$u\big|_{\partial D} = \varphi, \tag{2}$$

provided that the coefficient $n(x, y)$ is a known negative function (Colton and Kress, 1983).

Suppose that the coefficient n is unknown. In order to identify it, we need more information. There can be different sources of such information: the solution and/or its derivatives at additional lines, e.g. the boundary itself. Clearly, a function of two variables will require additional data on a 2D region but in some cases, posing the additional data on 1D sets that can also lead to unique solution. A general theory is lacking and some of these questions can only be answered *a posteriori* during the computations. Despite of lack of rigorousness, the research in coefficient identification is intensive because of the importance of the applications.

Let us consider the case when over-posed boundary data are available:

$$\left.\frac{\partial u}{\partial v}\right|_{\partial D} = \psi\,. \tag{3}$$

If the coefficient $n(x, y)$ is given, then the problem (Equations (1)–(3)) for $u(x, y)$ is over-determined, i.e. for arbitrary φ and ψ, there may not be a solution for $u(x, y)$

satisfying all of the conditions (Equations (2) and (3)). We assume that the boundary conditions (Equation (2) and (3)) are self-consistent and the solution of the problem (Equations (1)–(3)) does exist for certain, *a priori* unknown, $n(x, y)$.

On the other hand, when $n(x, y)$ is *a priori* not known, then under certain conditions, it may be possible to find a coefficient $n(x, y)$ such that Equation (1) has a solution $u(x, y)$ that satisfies Equations (2) and (3). Most probably, there will be more than one function $n(x, y)$ that will make possible to find a solution. Since the overposed data are given by a function of a single variable, one can hope that a coefficient that is a function of a single variable may be identified in a unique fashion. Of course, this is a heuristic argument, and the uniqueness must be proved for each particular case.

When it is possible to select n that makes u satisfy the overposed boundary conditions, we say that the functions u and n constitute a solution to the problem (Equations (1)–(3)).

We focus our attention only on problems that are clearly overposed, leaving aside the possible cases when the original problem may be undetermined, due to different reasons, including eigen-function solutions, etc. To this end, we consider the following two cases:

Case 1. The coefficient $n(x, y)$ is a piecewise constant function in D, i.e.

$$n(x, y) = c_y = \text{const},$$

for $(x, y) \in D_\gamma$, where D is divided into Γ disjoint regions D_γ and $D = \cup D_\gamma$.

Case 2. The coefficient is a function of a single variable,

$$n(x, y) = n(\omega),$$

where $\omega = \omega(x, y)$ is given. For example, $\omega = x$, or $\omega = x^2 + y^2$, etc.

3 Variational imbedding

We replace the original problem by the problem of minimisation of the following functional

$$J(u,n) = \iint_D [L(u,n)]^2 \mathrm{d}x\mathrm{d}y, \tag{4}$$

where

$$L(u,n) \overset{\text{def}}{=} \Delta u + nu,$$

and u must satisfy the conditions (Equations (2) and (3)).

Functional J is a quadratic and homogeneous function of $L(u, n)$ and hence, it attains its minimum if

$$L(u,n) = \Delta u + nu \equiv 0.$$

For a given $n(x, y)$, there is a one-to-one correspondence between the original equation (1) and the minimisation problem (Equation (4)), provided that there exists a solution to the original problem. Generally speaking, the functional J may have more than one local minimum, and some of its minimums are not being equal to zero.

3.1 The imbedding BVP for u(x, y)

The necessary conditions for the minimisation of the functional J from Equation (4) are the Euler–Lagrange equations for the functions $u(x, y)$ and $n(x, y)$. The equation for u reads

$$\Delta\Delta u + \Delta[n(x,y)u] + n(x,y)\Delta u + n^2(x,y)u = 0. \tag{5}$$

This equation is of the fourth-order and its solution can satisfy the two boundary conditions (Equations (2) and (3)). As a result, the problem (Equations (2), (3) and (5)) is well-posed if the function $n(x, y)$ is considered as known. Hence, using MVI, the inverse problem is imbedded into a higher-order but well-posed elliptic BVP. Note that if the coefficient $n(x, y)$ is not consistent with the boundary data, the solution of the imbedding BVP might not bring a trivial value to the functional J. The latter can be achieved only if the minimisation with respect to the function n is also considered.

3.2 Equation for coefficient n(x, y)

The Euler–Lagrange equation for the unknown coefficient $n(x, y)$ provides an explicit equation of the following form

$$n(x,y) = -\frac{A_1(x,y)}{A_2(x,y)}. \tag{6}$$

Functions $A_1(x, y)$ and $A_2(x, y)$ are different for the two cases discussed in Section 2. In Case 1, the functional $J(u, n)$ can be rewritten as a sum

$$J(u,n) = \iint_D (\Delta u + nu)^2 \mathrm{d}x\mathrm{d}y = \sum_{\gamma=1}^{\Gamma} \iint_{D_\gamma} (\Delta u + nu)^2 \mathrm{d}x\mathrm{d}y, \tag{7}$$

and, taking into account that $n(x, y) = c_\gamma = \text{const}$, if $(x, y) \in D_\gamma$, we get

$$A_1 = \iint_{D_\gamma} u\Delta u \mathrm{d}x\mathrm{d}y, \quad A_2 = \iint_{D_\gamma} u^2 \mathrm{d}x\mathrm{d}y, \tag{8}$$

which gives explicit equations for estimating the unknown constants c_γ, namely

$$c_\gamma = \iint_{D_\gamma} u\Delta u \mathrm{d}x\mathrm{d}y \Big/ \iint_{D_\gamma} u^2 \mathrm{d}x\mathrm{d}y.$$

To treat the problem in Case 2, we introduce a change of variables

$$\omega = \omega(x,y) \quad \text{and} \quad \eta = \eta(x,y), \quad \left|\frac{\partial(x,y)}{\partial(\omega,\eta)}\right| \neq 0,$$

where $\omega(x, y)$ is the specified dependence of n on (x, y). The functional $J(u, n)$ can be rewritten as

$$J(u,n) = \iint_{D^*} [\Delta u(\omega,\eta) + n(\omega)u(\omega,\eta)]^2 \left|\frac{\partial(x,y)}{\partial(\omega,\eta)}\right| \mathrm{d}\omega\mathrm{d}\eta.$$

Taking into account that $n(x, y) = n(\omega)$, the functions $A_1(x, y)$ and $A_2(x, y)$ adopt the form

$$A_1 = \int_{\Omega_c} u\Delta u \left|\frac{\partial(x,y)}{\partial(\omega,\eta)}\right| \mathrm{d}\eta, \quad A_2 = \int_{\Omega_c} u^2 \left|\frac{\partial(x,y)}{\partial(\omega,\eta)}\right| \mathrm{d}\eta \tag{9}$$

where $\Omega_c := \{(x, y) \in D; \omega(x, y) = c\}$.

3.3 MVI vs. regularisation methods

Common approach to the solution of inverse problems is based on regularisation methods (Tikhonov and Arsenin, 1974), which requires finding the minimum with respect to a parameter (called a regularisation parameter) of a properly constructed functional. However, in general, the numerical solution of the regularisation algorithm does not always approach the exact solution when the regularisation parameter becomes very small.

A comparison between the regularisation with respect to a small parameter and MVI, applied to the same problem, shows the advantages of the latter. Both methods come up with a numerical procedure for solving higher-order equations. MVI gives a solution of the original problem that coincides with the solution of the variational problem, while the solution of the regularisation methods is the limit with respect to an artificially introduced parameter. The numerical solution of the regularisation methods is often deteriorated because of instability as the parameter becomes very small. Another undesired effect is the appearance of a disagreement between the exact and numerical solutions in regions close to the boundary, (see, among many others, Lattés and Lions, 1967; Lesnic, Elliott and Ingham, 1999).

4 Existence and uniqueness

It is important to investigate the different components of MVI for existence and uniqueness of the solutions. Of course, the uniqueness of these sub-problems will not bring automatically the uniqueness of the full MVI problem, but they are of crucial importance for constructing algorithms for approximate solutions to them.

4.1 Correctness of the fourth-order BVP

Let us consider now the space $H(D)$ comprised by the functions α, defined in the domain D, and satisfying the following boundary conditions

$$\alpha|_{\partial D} = \left.\frac{\partial\alpha}{\partial\nu}\right|_{\partial D} = 0, \tag{10}$$

where ν is the outward unit normal. We expect that the functions under consideration are as many time differentiable as necessary. The following scalar product is introduced in $H(D)$

$$[\alpha, \beta] = \iint_D (\Delta\alpha + n\alpha)(\Delta\beta + n\beta)\mathrm{d}x\mathrm{d}y. \tag{11}$$

where $n(x, y) < 0$ is a function defined in D. Equation (11) is a scalar product since for $n(x, y) < 0$, the equation

$$\Delta\alpha + n\alpha = 0 \tag{12}$$

with the homogeneous boundary conditions, Equation (10) has only a trivial solution, i.e. $[\alpha, \alpha] = 0$ is true only when $\alpha(x, y) \equiv 0$ in D. The space $H(D)$ with the scalar product (Equation (11)) is a Hilbert space.

Let us introduce a sufficiently differentiable function $\chi(x, y)$, defined in D, and satisfying the respective boundary conditions (Equations (2) and (3)). Let us now define the function

$$F(\Phi) \overset{\text{def}}{=} -[\chi, \Phi] = -\iint_D (\Delta\chi + n\chi)(\Delta\Phi + n\Phi)\mathrm{d}x\mathrm{d}y,$$

where $\Phi \in H(D)$. Following the Riesz representation theorem, for the continuous linear functional F on the Hilbert space H, there is a unique $v \in H$ such that

$$F(\Phi) = [v, \Phi], \tag{13}$$

for all $\Phi \in H(D)$. Then, a generalised (weak) solution of Equations (2), (3) and (5), is defined as the function $u := v + \chi$. Therefore, for the weak solution u, the following expression holds true

$$[u, \Phi] = [v, \Phi] + [\chi, \Phi] = [v, \Phi] - F(\Phi) = [v, \Phi] - [v, \Phi] = 0, \tag{14}$$

for all $\Phi \in H(D)$. It is obvious that the classical solution of Equations (2), (3) and (5) is also a generalised solution. In order to prove the existence, we multiply Equation (5) by Φ, and integrate over the domain D to obtain

$$0 = \iint_D \Phi\left[\Delta\Delta u + \Delta(nu) + n\Delta u + n^2 u\right]\mathrm{d}x\mathrm{d}y = \iint_D \Phi\Delta\Delta u\mathrm{d}x\mathrm{d}y + \iint_D \Phi\Delta(nu)\mathrm{d}x\mathrm{d}y + \iint_D \Phi n\Delta u\mathrm{d}x\mathrm{d}y + \iint_D \Phi n^2 u\mathrm{d}x\mathrm{d}y.$$

Using Green's formula, this becomes

$$0 = \iint_D \Delta\Phi\Delta u\mathrm{d}x\mathrm{d}y + \iint_D \Delta\Phi(nu)\mathrm{d}x\mathrm{d}y + \iint_D \Phi n\Delta u\mathrm{d}x\mathrm{d}y + \iint_D \Phi n^2 u\mathrm{d}x\mathrm{d}y - \int_{\partial D} \Phi\nu\nabla\Delta u\mathrm{d}s + \int_{\partial D} \nu\nabla\Phi\Delta u\mathrm{d}s - \int_{\partial D} \Phi\nu\nabla(nu)\mathrm{d}s + \int_{\partial D} \nu\nabla\Phi(nu)\mathrm{d}s. \tag{15}$$

All the boundary integrals in Equation (15) vanish because $\Phi \in H(D)$. After some obvious manipulations we obtain

$$0 = \iint_D [\Delta u + nu][\Delta\Phi + n\Phi]\mathrm{d}x\mathrm{d}y = [u, \Phi]. \tag{16}$$

In order to prove the uniqueness, we consider the difference $\hat{u} = u_1 - u_2$ between two supposed solutions u_1 and u_2. It is obvious that $\hat{u} \in H(D)$. On the other hand, Equation (14) also holds for $\hat{u}$. Then, simply taking $\Phi = \hat{u}$, we have $[\hat{u}, \hat{u}] = 0$ and then $\hat{u} \equiv 0$.

Thus, we have shown that the Euler–Lagrange equation (Equation (5)) possesses a unique solution under the boundary conditions (Equations (2) and (3)), provided that the coefficient $n(x, y) < 0$ is given.

4.2 Correctness of the problem for coefficient

Since Equation (6) is an explicit expression for the coefficient, it provides a unique solution for $n(x, y)$, when the function $u(x, y)$ is thought of as known.

4.3 Existence of a solution to the full MVI problem

Up to this point, we have shown that the two Euler–Lagrange equations (Equations (5) and (6)), for $u(x, y)$ and $n(x, y)$, possess unique solutions, provided that in each of them the other function is thought of as known. This allows one to construct a procedure for finding a solution to the full non-linear problem by means of iterations replacing $n(x, y)$ (when calculating u), or $u(x, y)$ (when calculating n) with their values calculated at the previous iteration.

If the iterations converge, then they will give one of the possible solutions of the problem. Thus, the existence of the solution to the identification problem can be established *a posteriori*. In the light of what has been shown earlier in this section, one can conclude that divergence of the global iteration will necessarily mean that there exists no solution to the identification problem. In other words, for the specified data, there is no function $n(x, y)$ of the selected type (case 1 or 2) for which the overposed data stem from a second-order elliptic equation of type of Equation (1).

The convergence of the iterations, however, secure only the existence of the solution. It may not be unique, and the iterations can converge to different solutions depending on the initial guess for the functions $u(x, y)$ and $n(x, y)$. This reflects the physical nature of the problem since one cannot expect to recover the exact shape of an object behind a translucent screen using the shapes seen on the screen. There can exist objects that differ from each other in constitution, but throw similar shadows on the screen. Regardless to this limitation, the approach based on MVI is a very useful tool that allows one to find at least one possible coefficient that is consistent with the overposed data. In order to limit the uncertainty of the coefficient estimation, it is possible to incorporate additional restrictions on $n(x, y)$ based on additional physical information, but they go beyond the framework of the present paper.

5 Difference scheme

5.1 Grid pattern and approximations

Consider a model problem in the unit square

$$D = \{(x, y) : 0 < x < 1; 0 < y < 1\}.$$

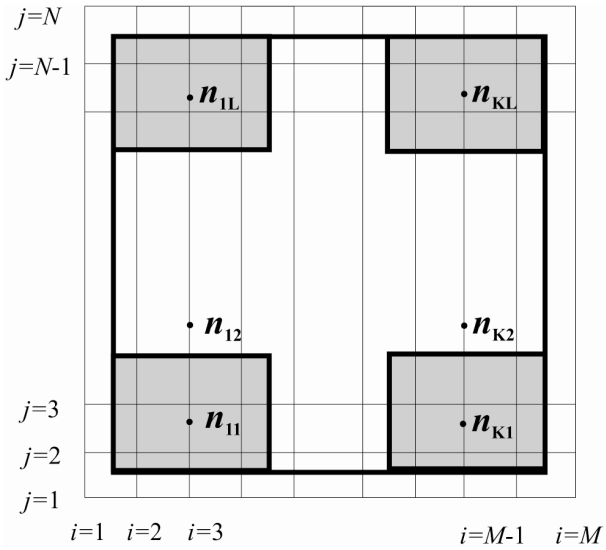
Introduce an orthogonal grid with a total number of grid lines equal to M and N in the x- and y-directions, respectively. In order to obtain second-order approximation of the derivatives that enter the boundary conditions, we use staggered grids in both directions which overflows the boundaries by half spacing (Figure 1). Then the spacings are related to the number of points as

$$h_x \equiv 1/(M-2) \quad \text{and} \quad h_y \equiv 1/(N-2),$$

and the grid lines are defined by

$$x_i = (i-1.5)h_x \quad \text{for} \quad i = 1, ..., M$$
$$y_j = (j-1.5)h_y \quad \text{for} \quad j = 1, ..., N.$$

Figure 1 Grid pattern



5.2 Grid pattern for coefficient $n(x, y)$

For Case 2, when the coefficient is a function of one of the variables, one can use the same grid lines for n. If the single variable in Case 2 is a combination of x and y, then the construction of the grid has to acknowledge the relationship between the number of unknown grid values of n and the number of available overposed data points. The same holds true for Case 1, when the coefficient is a piecewise constant function of the independent variables.

A straightforward approximation of Equation (1) with boundary condition (Equation (2)) gives the correct number of equations for identifying the discrete function $u(x, y)$. The number of additional equations obtained from the boundary condition (Equation (3)) is $2(M + N - 1)$. The goal of this paper is to show a way to transfer the information from additional boundary conditions to the unknown function. The number of unknown values of the function $n(x, y)$ must be equal to the number of equations we have available for this function, i.e. $2(M + N - 1)$. This means that it is not possible to use the same mesh for the coefficient: the number of grid nodes for the function $n(x, y)$ must be less or equal to $2(M + N - 1)$. For this reason, we construct a special numerical scheme.

The grid for the coefficient $n(x, y)$ is not staggered. The total number of grid lines in the x-direction is equal to K,

and the total number of grid lines in the y-direction is equal to L. The grid for $n(x, y)$ is given by

$$X_l = (l-1)H_x, \quad H_x \equiv \frac{1}{K-1}, \quad l = 1,...,L,$$
$$Y_k = (j-1)H_y, \quad H_y \equiv \frac{1}{L-1}, \quad k = 1,...,K. \tag{17}$$

and the grid lines are shown in Figure 1.

For the respective grid functions, we use the notations

$$u_{ij} = u(x_i, y_j) \quad \text{for} \quad i = 1,...,M, j = 1,...,N,$$
$$n_{kl} = n(x_k, y_l) \quad \text{for} \quad k = 1,...,K, l = 1,...,L. \tag{18}$$

It is convenient to use an additional piecewise constant grid function, $\tilde{n}_{ij}$, defined as

$$\tilde{n}_{ij} = n_{kl} \quad \text{for} \quad \begin{matrix} X_k - H_x/2 \le x_i \le X_k + H_x/2; \\ Y_l - H_y/2 \le y_j \le Y_l + H_y/2. \end{matrix} \tag{19}$$

Note that there are relationships between the grid spacings for the functions u and n as $H_x = ph_x$ and $H_y = qh_y$, where p and q are integers.

5.3 Scheme for the fourth-order elliptic equation

To solve the fourth-order problem, we introduce an artificial time and a scheme based on splitting the operators. The splitting schemes proved very efficient when first applied to classical parabolic equations. They allow obtaining a solution using less memory space and less computational time. The first splitting scheme for biharmonic operators was proposed in Conte and Dames (1960). It was also used for Navier–Stokes equations in Christov and Ridha (1994), and to non-linear problems with biharmonic operators in Christov and Pontes (2002). Recently, the acceleration of convergence of the Alternating-Direction Implicit (ADI) scheme for biharmonic equations was discussed in Tang and Christov (2006) but it goes beyond the scope of the present work to discuss it. Following the cited works, we design a splitting algorithm for solving efficiently the imbedded problem of the present work.

Let us introduce the notations Λ_{xx} and Λ_{yy} for the central difference approximation of the operators ∂_{xx} and ∂_{yy}, respectively. The straightforward scheme for the elliptic imbedding fourth-order problem would be

$$\left(\Lambda_{xx} + \Lambda_{yy}\right)\left[(\Lambda_{xx} + \Lambda_{yy}) + \tilde{n}_{i,j}\right]u_{i,j} + \tilde{n}_{i,j}(\Lambda_{xx} + \Lambda_{yy})u_{i,j} + \tilde{n}_{i,j}^2 u_{i,j} = 0 \tag{20}$$

for $i = 3, \ldots, M-2$ and $j = 3, \ldots, N-2$, respectively. We render Equation (20) into a parabolic difference equation after introducing a fictitious time. An implicit scheme to solve this parabolic equation, would have the form

$$\frac{u_{i,j}^{k+1} - u_{i,j}^{k}}{\sigma} = -(\Lambda_{xx}\Lambda_{xx} + \Lambda_{yy}\Lambda_{yy})u_{i,j}^{k+1} - 2\Lambda_{xx}\Lambda_{yy}u_{i,j}^{k} - \tilde{n}_{i,j}(\Lambda_{xx} + \Lambda_{yy})u_{i,j}^{k+1} - (\Lambda_{xx} + \Lambda_{yy})\tilde{n}_{i,j}u_{i,j}^{k+1} - \tilde{n}_{i,j}^2 u_{i,j}^{k+1}, \tag{21}$$

but the inversion of very large block diagonal matrices would require lots of resources, despite the fact that the matrices are relatively sparse. Instead of solving directly Equation (21), we use the following splitting scheme

$$\frac{\tilde{u}_{i,j} - u_{i,j}^{k}}{\sigma} = -\Lambda_{xx}\Lambda_{xx}\tilde{u}_{i,j} - (\Lambda_{yy}\Lambda_{yy} + 2\Lambda_{xx}\Lambda_{yy})u_{i,j}^{k} - \tilde{n}_{i,j}\Lambda_{xx}\tilde{u}_{i,j} - \tilde{n}_{i,j}\Lambda_{yy}u_{i,j}^{k} - (\Lambda_{xx} + \Lambda_{yy})(\tilde{n}_{i,j}u_{i,j}^{k}) - \tilde{n}_{i,j}^2\tilde{u}_{i,j} \tag{22}$$

$$\frac{u_{i,j}^{k+1} - \tilde{u}_{i,j}}{\sigma} = \left(-\Lambda_{yy}\Lambda_{yy} - \tilde{n}_{i,j}\Lambda_{yy}\right)\left(u_{i,j}^{k+1} - u_{i,j}^{k}\right), \tag{23}$$

where $\tilde{u}_{i,j}$ is a half-time-step (intermediate) variable, and $u^{k}_{i,j}$ is the solution at the full-time step. The fractional-step scheme (Equations (22) and (23)) approximates the full-time step scheme for Equation (21) within the same order of approximation $O(\tau + H^2)$. Here, we do not need the second-order of approximation in time, because the goal is the convergence in time, and the $O(\tau)$ scheme has a faster convergence than the $O(\tau^2)$ scheme because of the larger scheme viscosity.

Note, that the second-order of approximation in space is obtained easily on the grid that is staggered in both directions allowing one to use central differences with the second-order of approximation on two-point stencils for the boundary conditions.

5.4 Scheme for the coefficient

In Case 1, taking into account that the coefficient is piecewise, the Euler–Lagrange equation (Equation (6)) for the piecewise function $\tilde{n}(x, y)$ is approximated by the following second-order difference scheme:

$$n_{k,l} = -\frac{\sum_{\substack{X_{k-1/2} \le x_i \le X_{k+1/2} \\ Y_{l-1/2} \le y_j \le Y_{l+1/2}}}^{N} u_{i,j}(\Lambda_{xx} + \Lambda_{yy})u_{i,j}}{\sum_{\substack{X_{k-1/2} \le x_i \le X_{k+1/2} \\ Y_{l-1/2} \le y_j \le Y_{l+1/2}}}^{N} u_{i,j}^2}, \tag{24}$$

for $k = 1, \ldots K$ and $l = 1, \ldots L$. In Case 2, the idea is similar, although the calculations are more complicated.

5.5 Scheme for the direct problem

In order to gather 'experimental' data for the derivatives at the boundaries (Equation (3)), we solve numerically the 'direct' initial-BVP (Equations (1) and (2)). To this end, we use a similar iterative procedure based on the coordinate–splitting method with the second-order of approximation.

After the difference problem is solved, the 'experimental' values of the derivatives are calculated as follows

$$\psi(0,y_j)\overset{\text{def}}{=}\frac{u_{2,j}-u_{1,j}}{h_x},$$
$$\psi(1,y_j)\overset{\text{def}}{=}\frac{u_{N,j}-u_{N-1,j}}{h_x},$$
$$\psi(x_i,0)\overset{\text{def}}{=}\frac{u_{i,2}-u_{i,1}}{h_y},$$
$$\psi(x_i,1)\overset{\text{def}}{=}\frac{u_{i,M}-u_{i,M-1}}{h_y}, \tag{25}$$

with second-order of approximation on the staggered grid.

5.6 Algorithm

1 With a given initial guess for $n_{k,l}^{old}<0$, the fourth-order BVP (Equations (2), (3) and (4)) is solved for function $u_{i,j}$.

2 With the newly computed values of $u_{i,j}$, the function $n_{k,l}^{\text{new}}$ is evaluated. If the difference between the new and the old field for n is less than ε, i.e. $\max_{k,l}|n_{k,l}^{\text{new}}-n_{k,l}^{\text{old}}|<\varepsilon$, then the calculations are terminated, otherwise step I is repeated.

6 Validation of algorithm

6.1 Fourth-order imbedding problem

First, we check the accuracy of the difference scheme for the fourth-order problem using mandatory tests involving different grid spacing h_x, h_y. We use this test to verify that the solution of the linear imbedding problem for the unknown function does coincide with the solution of the 'direct' problem for a given coefficient. We use different expressions for the coefficient, including the constant. The findings are essentially the same. Here, we present the results with a coefficient that is a function of x only. The solution and the coefficient in this case are as follows

$$u_{\text{direct}}(x,y)=e^{(x^2+y)},$$
$$n_{\text{direct}}(x,y)=-(4x^2+3). \tag{26}$$

With this coefficient, we solve the direct problem, Equations (1) and (2), and then use the normal derivative of the obtained solution as the second boundary condition for the fourth-order problem.

This test consists of two steps. First, we solve the direct problem for the Helmholtz equation with a given coefficient, and from this solution, we apply difference approximation of the normal derivatives to serve as the overposed data. Second, we use the created data on the normal derivatives and solve the fourth-order imbedding problem.

We terminate the iterations in the splitting scheme, Equations (22) and (23), when the difference between two iterations satisfies

$$\|u^{n+1}-u^n\|<10^{-10}.$$

As a result, we get the solution of Equation (20) for the selected resolution. In the actual calculations, we used four different mesh resolutions, each of them being twice larger than the previous. The rate of convergence for the difference solution for function u, called r_u, is defined by

$$e_{N_g}=\|u_{i,j}-u_{\text{direct}}\|,\quad r_u=\log_2\frac{e_{N_g}}{e_{N_g/2}}, \tag{27}$$

where $N_g=N\times M$. The results for the norms of the differences between the solutions with four different resolutions are presented in Table 1, these results confirm unequivocally that the scheme is second-order accurate within the round-off error of double precision arithmetics. Thus, the practical convergence and consistency of the difference scheme for the fourth-order equation are established.

Table 1 Difference between the numerical solution of the fourth-order problem and the analytical solution

$N\times M$	*Error* e_{N_g}	r_u	J
16 × 16	1.2436867×10^{-4}	–	2.4418×10^{-3}
32 × 32	2.9918940×10^{-5}	2.0555	1.3607×10^{-4}
64 × 64	7.2486797×10^{-5}	2.0453	2.2190×10^{-5}
128 × 128	1.8572742×10^{-6}	1.9645	1.1847×10^{-4}

6.2 The imbedding functional

The actual value of the imbedding functional is very important when judging the success in identification of the solution. For this reason, we pay a special attention to the accuracy with which we compute it in the cases when it is supposed to be zero. When comparing to the analytical solution this functional must be of order of the truncation error. Indeed, it is seen from Table 1 that the imbedding functional is of order of $O(h^3)$, which is better than the truncation error. The only exception is the finest resolution, but it can be explained with the round-off error, because five-point finite differences enter in the calculation of the functional and they are subjected to large round-off error.

The above described model case is one of those experiments, for which we are sure that the identification procedure gives a unique solution and hence the functional must be equal to zero, not merely to a small value of order of truncation error. Naturally, this can be achieved numerically only within the round-off error. For calculations with double precision, the round-off error is of the order of 10^{-15}. Being reminded that in calculating the integrand of the imbedding functional we lose accuracy as h^{-2}, we established the criterion for terminating the convergence at 10^{-10}. This criterion is used for obtaining the values of the imbedding functional, which are presented in Table 1.

6.3 Scheme for coefficient

The last validation is of how well we are able to obtain the coefficient. We consider a test problem with a constant coefficient that has the following exact solution

$$u_{\text{direct}}(x,y) = e^{x+y}, \quad n_{\text{direct}}(x,y) = -2 \tag{28}$$

with five different sizes of the mesh-steps $h_x = h_y = h$.

We perform calculations with different grid parameters for the full cycle of MVI. This means that for the overposed data consistent with the direct problem, we solve the fourth-order problem with initial coefficient $n = 0$. Then, we compute for the coefficient according to the formula

$$\tilde{n} = -\left[\sum_{i=2}^{M-1}\sum_{j=2}^{N-1}(\Lambda_{xx}+\Lambda_{yy})u_{i,j}\right]\left[\sum_{i=2}^{M-1}\sum_{j=2}^{N-1}u_{i,j}^2\right]^{-1},$$

which stems from the general formula for piecewise constant coefficient (Equation (24)) for $K = L = 1$ and $H_x = H_y = 1$. With the newly computed coefficient, we repeat the calculation of the fourth-order problem completing thus a full iteration. We repeat these steps until convergence. The results for the identified coefficient are presented in Table 2.

Table 2 Obtained values of the coefficient n = const and the rate of convergence for five different mesh sizes

$N \times M$	n	r_n
8 × 8	–2.00260552	–
16 × 16	–2.00065112	2.000576511
32 × 32	–2.00016278	2.000192715
64 × 64	–2.00004070	2.000242553
128 × 128	–2.000010164	2.000838435
Exact	–2.0	–

The rate of convergence of the coefficient, r_n, is calculated in a similar fashion as the rate r_u for the function, namely

$$r_n = \log_2\left|\frac{n_{2h} - n_{\text{direct}}}{n_h - n_{\text{direct}}}\right|. \tag{29}$$

The results presented in Table 2 clearly demonstrate that the convergence for the coefficient is of the second-order. What is more important here is that the variational functional is of the order of magnitude smaller than the truncation error. It is typically of order of 7.710×10^{-9}, which is consistent with the criterion for termination of iterations. This means that taking computed coefficient in lieu of the analytical expression effects the computations of u in a manner that the two round-off errors, coming from u and n cancel each other, and for the difference version of MVI we can say that we have the functional strictly equal to zero (within the round-off error). This is very important when assessing the practical implementation of the method.

7 Results and discussion

After the algorithm was thoroughly validated in the previous section, we show the performance of the method for two generic cases: a coefficient that depends on one variable only, and a piecewise constant coefficient.

7.1 Coefficient is a function of a single variable

As a test example for Case 2 from Section 2 we consider the following problem with a known exact solution, as presented in Equation (26). In this case the coefficient is calculated according to the 1D version of Equation (24) in which $K = M = N$ and $L = 1$, i.e. $H_x = h_x$ and $H_y = 1$. Under these assumptions, the set of equations for identification of the difference approximation of the coefficient, read

$$\tilde{n}_{i,j} = n_i = -\left[\sum_{j=2}^{N-1}(\Lambda_{xx}+\Lambda_{yy})u_{i,j}\right]\left[\sum_{j=2}^{N-1}u_{i,j}^2\right]^{-1}, \tag{30}$$

for $i = 2, \ldots M-1$ and $j = 2, \ldots N-1$, since $H_y = 1$.

As already mentioned in the previous section, such a case was considered when the verification of the fourth-order equation had been done. Here, we add that the computations described in Equation (30) are held to the same values of the grid parameters. Thus, the convergence and the approximation of the difference scheme for the coefficient are verified. This allows us to assess the accuracy with which the coefficient is identified from the overposed data. We define the discretisation error for the coefficient as

$$E_n = (n_{\text{inverse}} - n_{\text{direct}})/n_{\text{direct}}, \quad n_{\text{direct}} = -(4x^2+3).$$

Figure 2 presents the profile of this error for three different grid spacings $h = h_x = h_y = H_x = h$ (note that $H_y = 1$). The error is function of x, but the ratio between the errors with the relevant resolution is approximately equal to four, which demonstrate clearly that the numerical solution approximates the analytical one with $O(h^2)$.

The most important point here is that in this case we found that the identification of the coefficient is unique in the sense that we started the iterative process from rather different initial conditions and in all cases, we ended up with the same numerical solution, whose error is depicted in Figure 2. This success can be attributed to the fact that the flexibility in the overposed data corresponds to a function of single variable and the flexibility for the sought coefficient is also restricted to a function of single variable.

7.2 Piecewise 2D coefficient

Now, if we allow the sought coefficient to belong to the class of functions of two spatial variables, the uniqueness cannot be established, as pointed out in the section on uniqueness of solution. Clearly, there are infinitely many 2D functions for the coefficient that can lead in the direct problem to the same computed data for the normal derivatives. The only thing one can hope in this case is to find a coarse-grain approximation to the coefficient as

described in the section on algorithm. Following this idea, we select K, L accordingly and compute the piecewise constant coefficient function from Equation (24). We choose a rather hard test case for which the coefficient to be identified is a discontinuous function, namely

$$n_{\text{direct}}(x,y)=\begin{cases}-1.1 & \begin{bmatrix}0.25<x<0.75\\0.25<y<0.75\end{bmatrix}\\ -1 & \text{otherwise.}\end{cases} \tag{31}$$

This test example illustrates the case 1 from the Section 2. Once again, we gather the 'experimental data' (Equation (3)) by solving the direct problem with the coefficient given in Equation (31). With thus created overposed data we conduct the iterations in the MVI algorithm until convergence is reached. The obtained result is in very good agreement with the 'direct' variables.

The surface and the level curves of the discretisation error for the identified solution $u_{i,\,j}$ for $h_x = h_y = 1/64$, $H_x = H_y = 1/8$ and $\varepsilon = 5.10^{-8}$ is shown in Figure 3. Naturally, the error is a function of the spatial variable, but its overall magnitude is consistent with the second-order truncation error.

Figure 2 Discretisation error for three different spacings

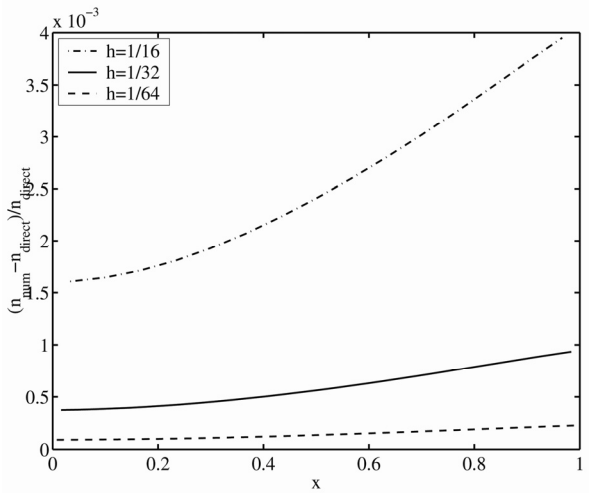
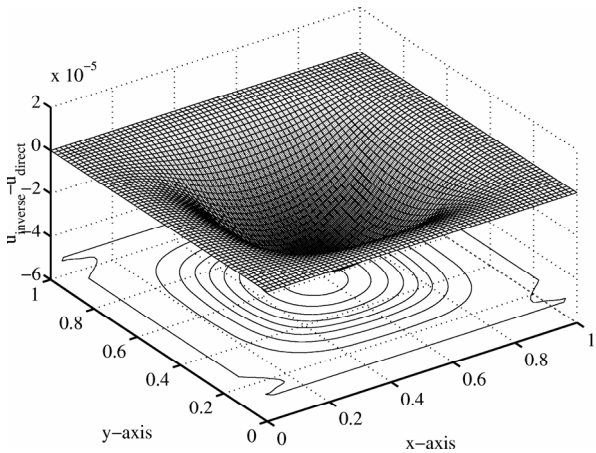
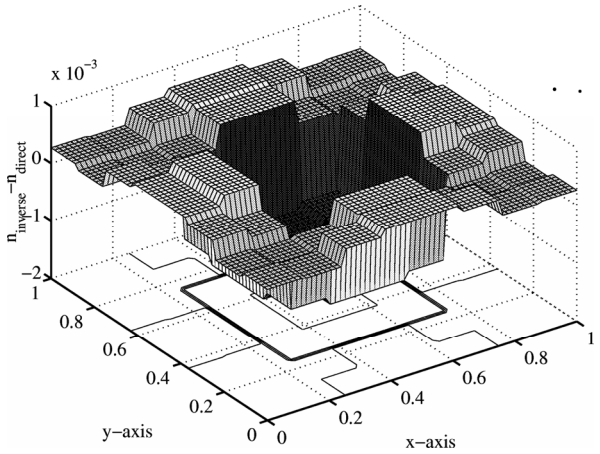


Figure 3 Discretisation error $u_{\text{inverse}} - u_{\text{direct}}$



The shape and the level curves of the discretisation error for the numerical obtained coefficient $n_{i,\,j}$ are shown in Figure 4. One can see that once again the error is compatible with the truncation error and it is bit larger only around the lines of discontinuity of the original coefficient.

Figure 4 Discretisation error $n_{\text{inverse}} - n_{\text{direct}}$



8 Conclusion

In the present paper, we demonstrated the performance of a technique called MVI for identification of a coefficient in an elliptic equation from overposed boundary data. The original inverse problem is replaced in this work by the minimisation problem for the quadratic functional of the original equation. The Euler–Lagrange equations for minimisation comprise a fourth-order elliptic equation for the function, $u = u(x, y)$, and an explicit equation for the unknown coefficient, $n = n(x, y)$. For this system, the boundary data are no longer over-posed. Thus, the original inverse problem is imbedded into a higher-order but well-posed problem. Two generic examples for the coefficient are considered: coefficient that depends upon a single variable only, and a piecewise constant coefficient. The numerical results show the efficiency of MVI for solving the inverse problem under consideration.

Acknowledgments

The work of R.S. Marinova was supported by the Natural Sciences and Engineering Research Council of Canada under an Industrial Research Fellowship PIN No. 243045.

References

Bellomo, N. and Preziosi, L. (1995) *Modeling, Mathematical Methods and Scientific Computation*. Boca Raton: CRC Press.

Christov, C.I. (1985) 'A method for identification of homoclinic trajectories', Paper presented in the Proceedings of the *14th Spring Conf, Sunny Beach* (pp.571–577). Sofia, Bulgaria, Union of Bulg. Mathematicians.

Christov, C.I. (1986) 'Method of variational imbedding for elliptic incorrect problems', *Comptes Rendus Academie des Sciences Bulgare*, Vol. 39, pp.23–26.

Christov, C.I. (1987) 'The method of variational imbedding for parabolic incorrect problems of coefficient identification', *Comptes Rendus Academie des Sciences Bulgare*, Vol. 40, pp.21–24.

Christov, C.I. and Marinov, T.T. (1997) 'Method of variational imbedding for the inverse problem of boundary-layer-thickness identification', *Mathematical Models & Methods in Applied Sciences (M^3AS)*, Vol. 7, pp.1005–1022.

Christov, C.I. and Marinov, T.T. (1998) 'Identification of heat-conduction coefficient via method of variational imbedding', *Mathematical and Computer Modelling*, Vol. 27, pp.109–116.

Christov, C.I. and Pontes, J. (2002) 'Numerical scheme for Swift-Hohenberg equation with strict implementation of lyapunov functional', *Mathematical and Computer Modelling*, Vol. 35, pp.87–99.

Christov, C.I. and Ridha, A. (1994) 'Splitting scheme for iterative solution of bi-harmonic equation. Application to 2D Navier–Stokes problems', in I. Dimov, Bl. Sendov and P. Vasilevskii (Eds), *Advances in Numerical Methods & Applications $O(h^3)$* (pp.341–352). Singapore: World Scientific.

Christov, C.I. and Velarde, M.G. (1993) 'On localized solutions of a model equation governing Beńard-Marangoni convection', *Applied Mathematical Modelling*, Vol. 17, pp.311–320.

Colton, D. and Kress, R. (1983) *Integral Equation Methods in Scattering Theory*. New York: Wiley-Interscience.

Conte, S.D. and Dames, R.T. (1960) 'On an alternating direction method for solving the plate problem with mixed boundary conditions', *Journal of the Association for Computing Machinery,* Vol. 7, pp.264–273.

Engl, H.W. and Zou, J. (2000) 'A new approach to convergence rate analysis of Tikhonov regularization for parameter identification in heat conduction', *Inverse Problems*, Vol. 16, pp.1907–1923.

Engl, H.W., Hanke, M. and Neubauer, A. (1996) *Regularization of Inverse Problems*. Dordrecht: Kluwer.

Hadamard, J. (1932) *Le Probleme de Cauchy et les Equations aux Derivatives Partielles Lineares Hyperboliques*. Paris: Hermann.

Isakov, V. (1993) 'Uniqueness and stability in multi-dimensional inverse problems', *Inverse Problems*, Vol. 9, pp.579–621.

Isakov, V. (1998) *Inverse Problems for Partial Differential Equations*. New York, NY: Springer.

Knowles, I. (1999) 'Uniqueness for an elliptic inverse problem', *SIAM Journal of Applied Mathematics*, Vol. 59, pp.1356–1370.

Lattés, R. and Lions, J-L. (1967) *Méthode de quasi-reversibilite at applications*. Dunod, Paris.

Lesnic, D., Elliott, L. and Ingham, D.B. (1999) 'Analysis of coefficient identification problems associated to the inverse Euler-Bernoulli beam theory', *IMA Journal of Applied Mathematics*, Vol. 62, pp.101–116.

Marinov, T.T., Christov, C.I. and Marinova, R.S. (2005) 'Novel numerical approach to solitary-wave solutions identification of Boussinesq and Korteweg-de Vries equations', *Int. J. Bifurcations and Chaos*, Vol. 15, pp.557–565.

Tang, X-H. and Christov, C.I. (2006) 'An operator splitting scheme for biharmonic equation with accelerated convergence', *Springer Lecture Notes in Computer Science (LNCS)*, Vol. 3743, pp.380–387. Springer Verlag.

Tikhonov, A.N. and Arsenin, V.Y. (1974) *Methods for Solving Incorrect Problems*. Moscow: Nauka.

Tikhonov, A.N., Leonov, A.S. and Yagola, A.G. (1998) *Non-Linear III – Posed Problems* (Vols. 1 and 2). London: Champmanand Hall.