Journal of Physics: Conference Series

PAPER • OPEN ACCESS

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To cite this article: H Kunze and D La Torre 2018 *J. Phys.: Conf. Ser.* **1047** 012005

IOP Conf. Series: Journal of Physics: Conf. Series **1047** (2018) 012005 doi:10.1088/1742-6596/1047/1/012005

An inverse problem for a system of steady-state reaction-diffusion equations on a porous domain using a collage-based approach

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Abstract. We consider an inverse problem for a system of steady-state reaction-diffusions acting on a perforated domain. We establish several results that connect the parameter values for the problem on the perforated domain with the corresponding problem on the related unperforated of solid domain. This opens the possibility of estimating a solution to the inverse problem on the perforated domain by instead working with the easier-to-solve inverse problem on the solid domain. We illustrate the results with an example.

1. Introduction

In the context of the subject work, the "direct problem" involves determining the solution to a completely prescribed two-dimensional system of steady-state reaction-diffusion equations, including known boundary conditions. On the other hand, the "inverse problem" involves estimating the values of (perhaps only some of the) parameters of the system given some information about the solution, perhaps observational data values.

In the next section, we present a summary of the collage method for solving inverse inverse problems for variational equations [5] and related systems [4]. Although the frameworks for the single equation and system cases have significant theoretical differences, both settings lead to a minimization problem for a function of the parameters λ one desires to estimate. Letting u denote the observed solution, perhaps an interpolation of observational data values, we must solve

$$\min_{\lambda\in\Lambda} F(u,\lambda).$$

In fact, in the case that the parameters λ appear linearly in the variational equation/system, upon approximating the problem in an appropriate finite-dimensional subspace, the function F is a quadratic function of the parameters and once F is built its minimization is quite straightforward.

In this paper, we wish to consider inverse problems on perforated or porous domains. A porous medium or perforated domain is a material characterized by a partitioning of the total volume into a solid portion often called the "matrix" and a pore space usually referred to as "holes" that can be either materials different from that of the matrix or real physical holes. When formulating differential equations over porous media, the term "porous" implies that the state equation is written in the matrix only, while boundary conditions should be imposed on the whole boundary of the matrix, including the boundary of the holes. Porous media can be found in many areas of applied sciences and engineering including petroleum engineering, chemical engineering, civil engineering, aerospace engineering, soil science, geology, material science, and many more areas.

Since porosity in materials can take different forms and appear in varying degrees, solving differential equations over porous media is often a complicated task and the holes' size and their distribution play an important role in its characterization. Furthermore numerical simulations over perforated domains need a very fine discretization mesh which often requires a significant computational time. The mathematical theory of differential equations on perforated domains is usually based on the theory of "homogenization" in which heterogeneous material is replaced by a fictitious homogeneous one. Of course this implies the need of convergence results linking together the model on a perforated domain and on the associated homogeneous one. In the case of porous media, or heterogeneous media in general, characterizing the properties of the material is a tricky process and can be done on different levels, mainly the microscopic and macroscopic scales, where the microscopic scale describes the heterogeneities and the macroscopic scale describes the global behavior of the composite.

In [3], two related problems for a single steady-state reaction-diffusion, problem (P_ε) on a perforated domain Ω_ε and problem (P) on the related solid domain Ω are considered:

$$\begin{cases} \nabla \cdot (K^\lambda(x,y)\nabla u(x,y)) = f^\lambda(x,y), & \text{in } \Omega_\varepsilon, \\ u(x,y) = 0, & \text{on } \partial\Omega_\varepsilon, \end{cases} \tag{P_ε}$$

and

$$\begin{cases} \nabla \cdot (K^\lambda(x,y)\nabla u(x,y)) = f^\lambda(x,y), & \text{in } \Omega, \\ u(x,y) = 0, & \text{on } \partial\Omega. \end{cases} \tag{P}$$

The inverse problem of interest for (P_ε) is to estimate λ given observational data for a solution. The paper establishes that a relationship between parameter values λ in the two problems: one can use the data from the solution to (P_ε) in the inverse problem for (P) to estimate λ, with the connection strengthening as ε decreases.

In many applications to material science it happens that data are collected without a priori knowledge of the geometry of the domain: In these situations is much simpler to assume the hypothesis of solid domain and use it to determine an estimation of the unknown parameters of the model.

In the third section, we build on these preceding results in developing a solution approach for the inverse problem for a system of steady-state reaction-diffusion equations on a perforated domain. Following that, in the final section we present an example to illustrate the method.

2. The Collage Method for Variational Equations

Consider the variational equation associated with a single elliptic equation,

$$a(u,v) = \phi(v), \qquad v \in H, \tag{1}$$

where ϕ and a are linear and bilinear maps, respectively, both defined on a Hilbert space H. We denote by $\langle \cdot,\cdot \rangle$ the inner product in H, $\|u\|^2 = \langle u,u \rangle$ and $d(u,v) = \|u-v\|$, for all $u, v \in H$. Typically $H = H_0^1(\Omega)$, that is the space of all $L^2(\Omega)$ functions that possess a weak derivative in $L^2(\Omega)$. The existence and uniqueness of solutions to this kind of equation are provided by the classical Lax-Milgram representation theorem, which requires that the bilinear form satisfy coercivity and boundedness properties and the linear map be bounded.

The following theorem proves particularly useful for treating a related inverse problem of approximating a target element u by a solution of a family of operators a^λ and ϕ^λ, satisfying (1) for each $\lambda \in \Lambda$.

IOP Conf. Series: Journal of Physics: Conf. Series **1047** (2018) 012005 doi:10.1088/1742-6596/1047/1/012005

Theorem 1. *(Generalized Collage Theorem) [5] For all $\lambda \in \Lambda$, suppose that $a^\lambda : \Lambda \times H \times H \to \mathbb{R}$ is a family of bilinear forms and $\phi^\lambda : \Lambda \times H \to \mathbb{R}$ is a family of linear functionals, satisfying*

$$\begin{aligned} a^\lambda(u,u) &\geq m^\lambda \|u\|^2 \ \ \forall u \in H \quad (\textit{coercivity}) \\ a^\lambda(u,v) &\leq M^\lambda \|u\|\|v\| \ \ \forall u, v \in H \\ \phi^\lambda(u) &\leq \mu^\lambda \|u\| \ \ \forall u \in H, \end{aligned}$$

for some positive constants m^λ, M^λ, and μ^λ. Let u^λ denote the solution of the equation $a^\lambda(u,v) = \phi^\lambda(v)$ for all $v \in H$ as guaranteed by the Lax-Milgram theorem. Then, given a target element $u \in H$,

$$\|u - u^\lambda\| \leq \frac{1}{m^\lambda} F(u,\lambda), \tag{2}$$

where

$$F(u,\lambda) = \left\| a^\lambda(u,\cdot) - \left(\phi^\lambda\right)^* \right\|. \tag{3}$$

If $\inf_{\lambda\in\Lambda} m^\lambda \geq m > 0$ then the inverse problem can be reduced to the minimization of the function $F(u,\lambda)$ on Λ, that is,

$$\min_{\lambda\in\Lambda} F(u,\lambda), \tag{4}$$

and we refer to this minimization as a "generalized collage method." To finite dimensionalize the problem, let $V_n = \langle e_1, e_2, \ldots, e_n \rangle$ be the finite dimensional vector space generated by e_i, so that $V_n \subset H$. Given a target $u \in H$, let $P_n u$ be the projection of u on the space V_n. We approximate the true error by $\|P_n u - u^\lambda\|$, noting that u^λ in this expression is in general not the same as the u^λ in the infinite dimensional problem. We can establish that

$$\|P_n u - u^\lambda\| \leq \frac{R}{m} \sum_i \left| a^\lambda(u, e_i) - \phi(e_i) \right|^2,$$

where R is a constant, leading to the minimization problem

$$\inf_{\lambda\in\Lambda} F_n(u,\lambda), \ \text{where } F_n(u,\lambda) = \sum_{i=1}^n \left| a^\lambda(u,e_i) - \phi^\lambda(e_i) \right|^2. \tag{5}$$

This approach has been extended in [4] to the case of linear systems,

$$\begin{cases} a_1^\lambda(u, v_1) &= \phi_1(v_1) \\ &\vdots \\ a_N^\lambda(u, v_N) &= \phi_N(v_N) \end{cases}, \ \forall\, v_1, \ldots, v_N \in H,$$

where $u = (u_1, \ldots, u_N)$, to arrive at

$$F(u,\lambda) = \max_{1\leq k\leq N} \left\| a_k^\lambda(u,\cdot) - \left(\phi_k^\lambda\right)^* \right\| = \max_{1\leq k\leq N} \sup_{\|v\|=1, v\in H} \left| a_k^\lambda(u,v) - \phi_k^\lambda(v) \right|. \tag{6}$$

In this setting,

$$\|u - u^\lambda\| \leq \frac{1}{m^\lambda} F(u,\lambda),$$

where $m^\lambda = \min_k m_k^\lambda$.

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3. A System of Steady-State Reaction-Diffusion Equations on Perforated and Unperforated Domains

Given a compact and convex set Ω, we denote by Ω_B the collection of circular holes $\cup_{j=1}^{m} B(x_j, \varepsilon_j)$ where $x_j \in \Omega$, ε_j are strictly positive numbers, and the holes $B(x_j, \varepsilon_j)$ are nonoverlapping and lie strictly in the interior of Ω. We let $\varepsilon = \max_j \varepsilon_j$. We denote by Ω_ε the closure of the set $\Omega \backslash \Omega_B$. In this section, we will set $H = H_0^1(\Omega)$ and $H_\varepsilon = H_0^1(\Omega_\varepsilon)$. We consider the linear system

$$(P)\text{: Find } u = (u_1, ..., u_N) \in H^N \text{ that satisfies } \begin{cases} a_1^\lambda(u, \cdot) &= \left(\varphi_1^\lambda\right)^* \\ & ... \\ a_N^\lambda(u, \cdot) &= \left(\varphi_N^\lambda\right)^* \end{cases}$$

where $\lambda \in \Lambda$ denotes some parameters of the functionals, and, on the domain with holes, the corresponding system

$$(P_\varepsilon)\text{: Find } u = (u_1, ..., u_N) \in (H_\epsilon)^N \text{ that satisfies } \begin{cases} a_{1,\varepsilon}^\lambda(u, \cdot) &= \left(\varphi_{1,\varepsilon}^\lambda\right)^* \\ & ... \\ a_{N,\varepsilon}^\lambda(u, \cdot) &= \left(\varphi_{N,\varepsilon}^\lambda\right)^* \end{cases}$$

Our goal is to address the inverse problem: Given observational data for a solution to (P_ε), estimate λ. Our approach is to use the data in (P) to estimate λ by establishing connections between the parameters λ in (P) and (P_ε) for ε small.

As any function in $H_0^1(\Omega_\varepsilon)$ can be extended to be zero over the holes, it is trivial to prove that $H_0^1(\Omega_\varepsilon)$ can be embedded in $H_0^1(\Omega)$. Let $u = (u_1, ..., u_N)$ and $P_\varepsilon u_k$ be the projection of $u_k \in H_0^1(\Omega_\varepsilon)$ onto $H_0^1(\Omega)$, $k = 1, ..., N$. It is easy to prove that

$$||u_k - P_\varepsilon u_k||_{H_0^1(\Omega)} \to 0 \text{ whenever } \varepsilon \to 0.$$

When Neumann boundary conditions are considered, it is still possible to extend a function in $H_0^1(\Omega_\varepsilon)$ to a function of $H_0^1(\Omega)$: these extension conditions are well studied (see [7]) and they typically hold when the domain Ω has a particular structure. In any case, it holds for a wide class of disperse media, that is, media consisting of two media that do not mix.

We assume that there exist three strictly positive constants m, M, and μ such that

$$\begin{aligned} a_k^{\lambda,\epsilon}(u, u) &\geq m||u||^2 \;\; \forall u \in H_\varepsilon \\ a_k^{\lambda,\epsilon}(u, v) &\leq M||u||||v|| \;\; \forall u, v \in H_\varepsilon \\ \phi_k^{\lambda,\epsilon}(u) &\leq \mu||u|| \;\; \forall u \in H_\varepsilon, \end{aligned}$$

Then by the Lax-Milgram type theorem in [4], problem (P) has a unique solution u^λ for each $\lambda \in \Lambda$ and problem (P_ε) has a unique solution u_ε^λ and for each positive ε and each $\lambda \in \Lambda$.

In the following results, we establish relationships between (P) and (P_ε). For each $u \in (H_0^1(\Omega_\varepsilon))^N$, let us introduce the function

$$F_\varepsilon(u, \lambda) = \max_{1 \leq k \leq N} \left\| a_k^{\lambda,\varepsilon}(u, \cdot) - \left(y_k^{\lambda,\varepsilon}\right)^* \right\|. \tag{7}$$

associated with problem (P_ε).

Proposition 1. *The function $F(u, \lambda)$ is Lipschitz with Lipschitz constant equal to M.*

Proof. Computing, we have:

$$\begin{aligned} F(u,\lambda) &= \max\nolimits_{1\le k\le N} \left\| a_k^\lambda(u,\cdot) - (\varphi_k^\lambda)^* \right\| \\ &= \max\nolimits_{1\le k\le N} \sup\nolimits_{\|v\|=1} |a_k^\lambda(u,v) - \varphi_k^\lambda(v)| \\ &= \max\nolimits_{1\le k\le N} \sup\nolimits_{\|v\|=1} |a_k^\lambda(u,v) - a_k^\lambda(w,v) + a_k^\lambda(w,v) - \varphi_k^\lambda(v)| \\ &\le \max\nolimits_{1\le k\le N} \sup\nolimits_{\|v\|=1} |a_k^\lambda(u-w,v)| + |a_k^\lambda(w,v) - \varphi_k^\lambda(v)| \\ &\le M\|u-w\| + F(w,\lambda) \end{aligned}$$

which easily implies that

$$|F(u,\lambda) - F(w,\lambda)| \le M\|u-w\|.$$

□

In what follows, for each $u \in (H_0^1(\Omega_\varepsilon))^N$ let us $P_\varepsilon u = (P_\epsilon u_1, \dots, P_\varepsilon u_N)$.

Proposition 2. *The following inequality holds:*

$$\|P_\varepsilon u - u_\varepsilon^\lambda\| \le \frac{F(u,\lambda)}{m} + \frac{M}{m}\|P_\varepsilon u - u\|$$

Proof. Computing, we have:

$$\begin{aligned} \|P_\varepsilon u - u_\varepsilon^\lambda\| &\le \tfrac{1}{m} F_\varepsilon(P_\varepsilon u,\lambda) \\ &\le \tfrac{1}{m} F(P_\varepsilon u,\lambda) \\ &\le \tfrac{1}{m}[F(u,\lambda) + M\|P_\varepsilon u - u\|] \end{aligned}$$

□

Proposition 3. *The exists a constant $C(\varepsilon,u)$, which depends only on ε and u, such that the following inequality holds:*

$$F(P_\varepsilon u,\lambda) \le F_\varepsilon(P_\varepsilon u,\lambda) + C(\varepsilon,u)\sup_{\|v\|=1}\|P_\varepsilon v - v\|$$

Proof. Easy calculations imply that:

$$\begin{aligned} F(P_\varepsilon u,\lambda) &= \max\nolimits_{k=1\ldots N} \sup\nolimits_{\|v\|=1} |a_k^\lambda(P_\varepsilon u,v) - \phi_k^\lambda(v)| \\ &\le \max\nolimits_{k=1\ldots N} \sup\nolimits_{\|v\|=1} |a_k^\lambda(P_\varepsilon u,v) - a_k^\lambda(P_\varepsilon u,P_\varepsilon v)| \\ &+ \max\nolimits_{k=1\ldots N} \sup\nolimits_{\|v\|=1, v\in H_\varepsilon^N} |a_k^\lambda(P_\varepsilon u,v) - \phi_k^\lambda(v)| \\ &+ \max\nolimits_{k=1\ldots N} \sup\nolimits_{\|v\|=1} |\phi_k^\lambda(P_\varepsilon v) - \phi_k^\lambda(v)| \\ &\le \sup\nolimits_{\|v\|=1} M\|P_\varepsilon u\|\|P_\varepsilon v - v\| \\ &+ F_\varepsilon(P_\varepsilon u,\lambda) + \mu\sup\nolimits_{\|v\|=1}\|P_\varepsilon v - v\| \\ &\le (M\|P_\varepsilon u\| + \mu)\sup\nolimits_{\|v\|=1}\|P_\varepsilon v - v\| + F_\varepsilon(P_\varepsilon u,\lambda) \\ &= C(\varepsilon,u)\sup\nolimits_{\|v\|=1}\|v - P_\varepsilon v\| + F_\varepsilon(P_\varepsilon u,\lambda) \end{aligned}$$

□

Let us notice that the constant $C(\epsilon,u) = M\|P_\varepsilon u\| + \mu$ converges to $C(u) = M\|u\| + \mu$ whenever ε tends to zero. The following proposition states a convergence theorem for the sequence of minimizers.

Proposition 4. *Let us suppose that, for each fixed $u \in (H_0^1(\Omega_\varepsilon))^N$, F is lower continuous w.r.t. $\lambda \in \Lambda$. If $\lambda_{\varepsilon_n} = \arg\min_{\lambda\in\Lambda} F_{\varepsilon_n}(P_{\varepsilon_n}u, \lambda)$, and $\lambda_{\varepsilon_n} \to \lambda^* \in \Lambda$ then $\lambda^* = \arg\min_{\lambda\in\Lambda} F(u, \lambda)$.*

Proof. Computing, we have:

$$\begin{aligned}
F(u,\lambda^*) &\leq \liminf_{\varepsilon_n\to 0} F(u,\lambda_{\varepsilon_n})\\
&\leq \liminf_{\varepsilon_n\to 0} F(P_{\varepsilon_n}u,\lambda_{\varepsilon_n}) + M\|P_{\varepsilon_n}u - u\|\\
&\leq \liminf_{\varepsilon_n\to 0} F_{\varepsilon_n}(P_{\varepsilon_n}u,\lambda_{\varepsilon_n}) + C(\varepsilon_n,u)\sup_{\|v\|=1}\|P_{\varepsilon_n}v - v\| + M\|P_{\varepsilon_n}u - u\|\\
&\leq \liminf_{\varepsilon_n\to 0} F_{\varepsilon_n}(P_{\varepsilon_n}u,\lambda_{\varepsilon_n}) + \tilde{C}(\varepsilon_n,u)\varepsilon_n\\
&\leq \liminf_{\varepsilon_n\to 0} F_{\varepsilon_n}(P_{\varepsilon_n}u,\lambda) + \tilde{C}(\varepsilon_n,u)\varepsilon_n\\
&\leq \liminf_{\varepsilon_n\to 0} F(P_{\varepsilon_n}u,\lambda) + \tilde{C}(\varepsilon_n,u)\varepsilon_n\\
&\leq \liminf_{\varepsilon_n\to 0} F(u,\lambda) + \tilde{C}(\varepsilon_n,u)\varepsilon_n + M\|P_{\varepsilon_n}u - u\| = F(u,\lambda)
\end{aligned}$$

for all $\lambda \in \Lambda$, which implies that λ^* is a global minimizer. □

4. Examples

We consider the problem

$$\begin{aligned}
-\nabla\cdot(K_1(x,y)\nabla u_1) + b_1u_2 &= f_1(x,y) \qquad (8)\\
-\nabla\cdot(K_2(x,y)\nabla u_2) + b_2u_1 &= f_2(x,y) \qquad (9)
\end{aligned}$$

on Ω_ε, the perforated unit square, with N arbitrarily placed holes, and with $u_k = 0$ on the boundary of the square and $\frac{\partial u_k}{\partial n} = 0$ on the boundaries of the holes, $k = 1, 2$.

We consider the following inverse problem: given a target solution $u = (u_1, u_2)$, f_1, and f_2 on Ω_ε, estimate K_k and b_k, $k = 1, 2$.

Following Proposition 4, we solve the associated inverse problem on $\Omega = [0, 1]^2$, the unit square with no holes. We minimize the objective function $F(u, \lambda)$, where λ is the vector of parameters defining K_i and b_i. The functions a_k^λ and ϕ_k^λ in F are straightforward to construct: multiply (8) by $v_1 \in H_0^1(\Omega)$ and (8) by $v_2 \in H_0^1(\Omega)$ and integrate over Ω. Using Green's Identity on the left, we obtain

$$a_k^\lambda(u, v_k) = \phi_k^\lambda(v_k),\ k = 1, 2,$$

where

$$\begin{aligned}
a_k^\lambda(u,v_k) &= \int_\Omega K_k\nabla u_k\cdot\nabla v_k\,dA\\
\phi_k^\lambda(v_k) &= \int_\Omega f_kv_k\,dA.
\end{aligned}$$

To finite dimensionalize the problem, we introduce n^2 nodes, positioned at the points $(x_i, y_i) = \left(\frac{i}{n+1}, \frac{j}{n+1}\right)$, $i, j = 1, 2, \ldots, n$, and we define the triangles

$$D_n^{ij^+} = \left\{(x,y)\ :\ x_{i-1}\leq x\leq x_i,\ \frac{y_i - y_{i-1}}{x_i - x_{i-1}}x + y_{i-1}\leq y\leq y_i\right\},\ i,j = 1,\ldots,n+1,$$

and

$$D_n^{ij^-} = \left\{(x,y)\ :\ x_{i-1}\leq x\leq x_i,\ y_{i-1}\leq y\leq \frac{y_i - y_{i-1}}{x_i - x_{i-1}}x + y_{i-1}\right\},\ i,j = 1,\ldots,n+1.$$

We will work with functions v_k in

$$V_n^1 = \{v \in C(\Omega) \,:\, v \text{ is piecewise linear on } D_n^{ij^+} \text{ and } D_n^{ij^-},\ i,j = 1,\ldots,n+1, \text{ and } v = 0 \text{ on } \partial\Omega\}.$$

A basis for V_n^1 consists of the n^2 functions $e_{ij}(x,y)$ satisfying

$$e_{ij} \text{ is piecewise linear and } e_{ij}(x_k,y_l) = \begin{cases} 1 & \text{if } (k,l) = (i,j) \\ 0 & \text{if } (k,l) \neq (i,j) \end{cases},\ i,j = 1,\ldots,n.$$

Similar to [5] and [4], the problem we solve is

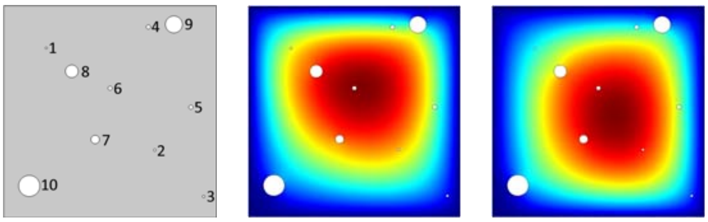
$$\min_{\lambda} \sum_{k=1}^{2} \sum_{i,j=1}^{n} \left(a_k^{\lambda}(u,e_{ij}) - \phi_k^{\lambda}(e_{ij})\right)^2. \tag{10}$$

In the examples that follow, we choose values for K_i, f_i, and b_i, $i = 1,2$, solve the problem on the perforated domain, and then sample the numerical solutions at the n^2 nodes to produce observational data. If a node lies inside one of the holes, we discard it. We produce a target solution $u = (u_1,u_2)$ by performing a least squares fit of the polynomial function (of degree $L+4$)

$$w(x,y) = xy(1-x)(1-y) \sum_{j=0}^{L} \sum_{i=0}^{k} a_{ij} x^i y^{j-i},$$

which satisfies the homogenous Dirichlet boundary conditions on $\partial\Omega$, to each component. We then solve the inverse problem, as outlined above, to obtain estimates of K_i and b_i.

Example 1: We set $K_1(x,y) = 1 + 2x + \frac{1}{2}y$, $K_2(x,y) = 1 + \frac{1}{4}x + 2y$, $b_1 = 2$, $b_2 = 1$, $f_1(x,y) = x^2 + y^2$, and $f_2(x,y) = x + 2y$. We arbitrarily distribute 10 holes of various sizes inside Ω. The domain Ω_ε and the level curves of the solution are presented in Figure 1. In the figure, the holes are numbered by increasing



(a) (b) (c)

Figure 1. (a) The unit square with 10 assorted holes. (b-c) Isotherms for numerical solutions u_1 and u_2, respectively.

radius. In solving the problem, we set $n = 9$, $L = 8$,

$$K_1(x,y) = \lambda_1 + \lambda_2 x + \lambda_3 y,\ K_1(x,y) = \lambda_4 + \lambda_5 x + \lambda_6 y,\ b_1 = \lambda_7, \text{ and } b_2 = \lambda_8.$$

Table 1 presents the results for 11 different choices of domain: we solve the problem with N holes, $N = 0,\ldots,10$, each time using the first N holes, as numbered in Figure 1(a). It is instructive to visualize the solutions as the number of holes changes; in Figure 2, we present the isotherms for several cases. When comparing rows, it is important to note that the numerical solutions, and hence the target solutions, change for each run. We see that most of the cases, the parameter values are recovered well. As the number of holes grows, which corresponds to the larger holes being part of the problem, the recovered values of the adsorption coefficients b_1 and b_2 become poorer.

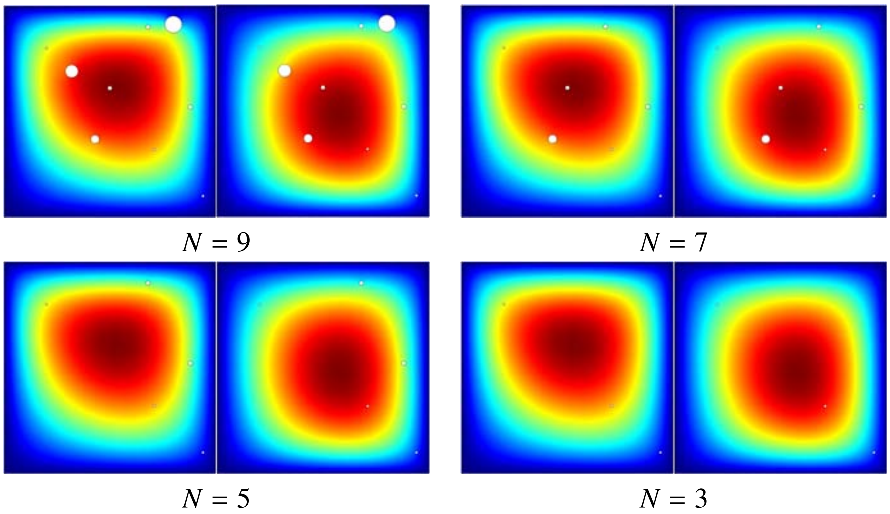


Figure 2. Isotherms for numerical solutions on the domain with N holes.

# holes	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
10	0.9816	1.9292	0.4962	0.8718	0.3178	1.8689	2.4295	5.1526
9	1.0600	1.8997	0.4332	0.9746	0.2316	1.8578	2.1646	3.8523
8	1.0064	1.9819	0.5075	0.9927	0.2374	1.9967	2.0416	1.6407
7	1.0044	1.9972	0.4968	1.0178	0.2305	2.0013	1.9665	0.7470
6	1.0035	1.9995	0.4979	1.0089	0.2400	2.0039	1.9366	0.7560
5	1.0071	2.0002	0.4946	1.0099	0.2407	2.0035	1.8871	0.6711
4	0.9953	1.9999	0.5040	1.0041	0.2439	2.0012	2.0069	0.8857
3	0.9882	2.0055	0.5111	1.0006	0.2472	2.0085	2.0375	0.8906
2	0.9958	2.0067	0.5040	1.0029	0.2477	2.0075	1.9835	0.8333
1	0.9951	2.0060	0.5052	1.0034	0.2465	2.0083	1.9861	0.8213
0	0.9907	2.0084	0.5065	0.9985	0.2508	2.0056	2.0176	0.9427
true values	1.0000	2.0000	0.5000	1.0000	0.2500	2.0000	2.0000	1.0000

Table 1. Recovered parameter values, to 4 decimal places, for Example 1.

Example 2: We use the same true parameter values and position 10 circular holes in Ω, as in Example 1. This time, however, all of the holes have the same radius. As in Example 1, we set $n = 9$, $L = 8$, and recover λ_i, $i = 1, \ldots, 8$. Table 2 presents the results for 4 different radius values. As the radius decreases, the accuracy of the recovery improves.

radius	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
0.02	1.0403	1.9089	0.5002	1.0571	0.1616	1.9873	1.9242	0.5144
0.01	1.0124	1.9832	0.4972	1.0198	0.2241	2.0028	1.9278	0.6748
0.005	0.9961	2.0024	0.5045	1.0049	0.2433	2.0061	1.9906	0.8389
0.001	0.9908	2.0079	0.5065	0.9987	0.2505	2.0055	2.0195	0.9435
true values	1.0000	2.0000	0.5000	1.0000	0.2500	2.0000	2.0000	1.0000

Table 2. Recovered parameter values, to 4 decimal places, for Example 2.

Figure 3 shows the numerical solutions' isotherms for the different cases.

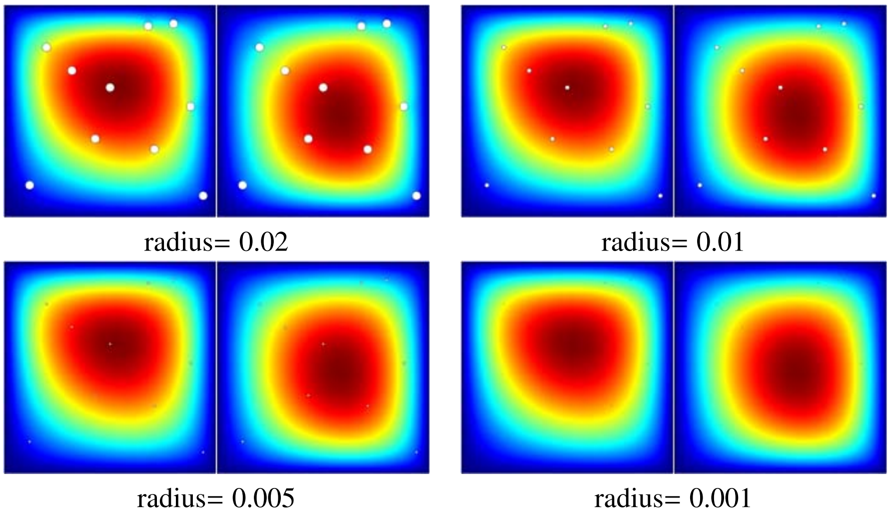


Figure 3. Isotherms for numerical solutions with different radius.

References

[1] Engl H W and Grever W 1994 Using the L-curve for determining optimal regularization parameters *Numer Math* **69** 1 pp 25-31

[2] Kunze H, Hicken J and Vrscay E R 2004 Inverse Problems for ODEs Using Contraction Maps: Suboptimality of the "Collage Method" *Inverse Problems* 20 pp 977-991

[3] Kunze K and La Torre D 2015 Collage-type approach to inverse problems for elliptic PDEs on perforated domains *Electronic Journal of Differential Equations* 48 pp 1-11

[4] Kunze H, La Torre D, Levere K, and Ruiz Gálan M 2015 Inverse problems via the "generalized collage theorem" for vector-valued Lax-Milgram-based variational problems *Mathematical Problems in Engineering* 764643

[5] Kunze H, La Torre D and Vrscay E R 2009 A generalized collage method based upon the Lax-Milgram functional for solving boundary value inverse problems *Nonlinear Analysis* **71** 12 pp 1337-1343

[6] Kunze H and Vrscay E R 1999 Solving inverse problems for ordinary differential equations using the Picard contraction mapping *Inverse Problems* 15 pp 745-770

[7] Marchenko V A and Khruslov E Y 2006 Homogenization of Partial Differential Equations (Boston: Birkhauser)