Nonlinear Reduced Order Source Identification

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***Abstract*—In this paper we propose a novel approach to the problem of model-based source identification in steady-state transport phenomena given a set of noisy measurements. We formulate the problem as an optimization problem in function space and utilize the adjoint method to calculate the gradient. To obtain a finite dimensional representation of this problem we employ proper orthogonal decomposition, which provides a small number of basis functions that best approximate the function space in which the concentration function lives. Similarly, we parametrize the source function by nonlinear tower functions, which allow us to reduce the size of the problem from thousands of unknowns to a handful of variables. The above approximations give rise to a low dimensional nonlinear optimization problem, for which we provide explicit expressions for the gradient and Hessian that can be used with available optimization techniques to solve for the desired source function. We provide simulation results that demonstrate a drastic reduction in computation time. At the same time we are able to solve complex advection-diffusion problems in non-convex environments.**

I. Introduction

The problem of Source Identification (SI) refers to the estimation of the location, intensity, and shape of a source using a set of measurements of a quantity, such as concentration, that is generated under the action of that source. The SI problem has various applications spanning from environmental protection [1] to human safety [2]. In addition, the SI problem can be an important part in higher level tasks like search and rescue missions and crowd evacuation [3].

The available literature on SI problems can be classified depending on, e.g., the state of the transport phenomenon, the number of sources, and their shape. Generally, SI problems that involve transport phenomena in transient-state are more challenging than situations where transport is in steady-state. Similarly, sources can be formulated as points of zero-measure, or areas of nonzero-measure in the domain. While the former assumption yields closed form solutions for the forward model, the latter is more general as it provides information about the area and shape of sources as well.

The problem of localizing a single point source in transient state is considered in [4]–[6]. The solution in [4] relies on the premise that *a priori* knowledge of the plausible source locations is available. In a different track the authors of [5], [6] utilize statistical signal processing techniques along with a closed form solution of the mathematical model to attack the SI problem. For problems with multiple point sources, closed form solutions are not available and consequently optimization-based methods are used. One such method is [7] in which the emphasis is on minimizing the number of required measurements to localize a set of point heat sources. On the other hand, the work in [8] presents an approach based on sparse recovery techniques to localize multiple instantaneous point sources in a transient heat transfer system.

More general problems that involve sources of arbitrary shapes in arbitrary domains are typically solved numerically using, e.g., the Finite Element Method (FEM). For example, in [9] the FEM along with total variation regularization is used to solve the SI problem. Similarly, in our previous work [10], we proposed the RWDL1 algorithm which is an iterative sparse recovery approach to the SI problem. Nevertheless, numerical methods involving FEM are computationally very demanding.

In the current work, we propose a computationally efficient method to solve SI problems that involve sources of arbitrary shapes and intensities in generally non-convex environments. Assuming the transport phenomenon is modeled by an elliptic PDE in steady-state and given a set of noisy point measurements, we formulate the SI problem as an infinite dimensional optimization problem in function space. In order to numerically solve this problem, we approximate the function spaces by finite dimensional subspaces. Specifically, we use proper orthogonal decomposition to construct a set of optimal basis functions for the concentration. Moreover, we use nonlinear tower functions to model the source term. These approximations lower the dimension of the problem considerably at the expense of introducing nonlinearities. To address this challenge, we provide a simple way to initialize the nonlinear optimization problem that facilitates the identification of the true sources. We also provide explicit expressions for the gradient and Hessian that can be used with available nonlinear optimization methods. Specifically, we employ the adjoint method to obtain the gradient and a Lagrangian-based procedure to obtain the second order information. Numerical simulations demonstrate a significant improvement in computational cost while maintaining the ability of the method to efficiently localize the sources. The main contribution of this work is the proposed nonlinear formulation of the SI problem and our ability to efficiently solve this problem for arbitrary sources and non-convex environments.

The remaining parts of this paper are organized as follows. In Section II, we define the SI problem and formulate it as an optimization problem. Section III addresses the derivation of the gradient in function spaces using the adjoint method. In Section IV we determine finite dimensional basis functions to approximate the concentration and source terms. In Section V, we combine our previous developments to derive the explicit first and second order information of the optimization problem. Section VI contains the numerical simulations and finally Section VII concludes the paper.

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II. Source Identification Problem

A. Advection-Diffusion Partial Differential Equation

Let $\Omega \subset \mathbb{R}^l$ be the domain of interest ($1 \leq l \leq 3$), and assume the presence of sources is modeled by a nonnegative function, $s : \Omega \to \mathbb{R}_+$, which is the sum of a finite number of compactly supported functions.[1] Let $c : \Omega \to \mathbb{R}_+$ be the measurable quantity, such as concentration, generated by this source function. Moreover, let the velocity at which this quantity is transported via advection be $\mathbf{q} \in \mathbb{R}^l$ and $D \in \mathbb{R}_+$ denote the diffusivity of the medium. Under a steady-state assumption and applying a zero-valued Dirichlet condition to the boundaries Γ of domain, we arrive at the following Boundary Value Problem (BVP)

$$-D\nabla^2 c + \mathbf{q} \cdot \nabla c - s = 0 \quad \text{in} \quad \Omega, \tag{1a}$$

$$c = 0 \quad \text{on} \quad \Gamma. \tag{1b}$$

In order for the BVP (1) to have a solution we assume that $s \in L^2(\Omega)$, i.e., s is twice integrable over Ω, and we define the feasible set for the source term as $S = \{s \in L^2(\Omega) \mid s \geq 0\}$.

Consider the set $V \subset H_0^1(\Omega)$, i.e., the set of functions that themselves and their first weak derivatives are twice integrable and have compact supports. Thus, every $v \in V$ satisfies the boundary condition (1b). Then, the BVP (1) can be equivalently represented in variational form as

$$\mathcal{M}(c; s) = a(c, v) - \ell(v; s) = 0, \ \forall v \in V, \tag{2}$$

where $a(\cdot, \cdot) : V \times V \to \mathbb{R}$ is a non-symmetric continuous V-elliptic bilinear form and $\ell : V \to \mathbb{R}$ is a continuous functional defined as $a(c, v) \triangleq \int_\Omega D\nabla c \cdot \nabla v \ d\Omega + \int_\Omega v\, \mathbf{q} \cdot \nabla c \ d\Omega$ and $\ell(v; s) \triangleq \langle \ell(s), v \rangle \triangleq \int_\Omega sv \ d\Omega$, respectively. Note that we have included the source term s in the definition of the model, i.e., we write $\mathcal{M}(c; s) = 0$, to emphasize that to any given source term s corresponds a unique solution c. For theoretical details, see e.g., [11, ch. 8,9]. In the next section, we formulate the SI problem as a constrained optimization problem subject to the advection-diffusion (AD) model introduced here.

B. Problem Definition

Consider m sensors deployed in the domain Ω that make measurements of the concentration c, and let $E \subset \Omega$ be the set of m compactly supported measurement areas enclosing the sensor locations.[2] Define, further, the indicator function for the set E as $\chi_E(\mathbf{x}) = 1$ if $\mathbf{x} \in E$ and zero otherwise, and let $c^m : \Omega \to \mathbb{R}_+$ be a function that assigns to each point $\mathbf{x} \in \Omega$ the noisy concentration measured by the sensor that is deployed at that location, i.e., $c^m(\mathbf{x}) = \chi_E(\mathbf{x})(c(\mathbf{x}) + \epsilon(\mathbf{x}))$, where the measurement noise $\epsilon(\mathbf{x}) \sim \mathcal{N}(0, \ \sigma^2)$ is spatially independent and identically distributed. Then, the Source Identification (SI) problem that we consider in this paper can be defined as follows.

[1]For the problem considered here, we assume that the sources are strictly positive functions. In general, sources can also be negative in the case of sinks. Sinks can appear, e.g., in the presence of chemical reactions that consume a contaminant. The treatment of the problem in the case of sinks is similar.

[2]Note that the compact measurement area around any given sensor can be made arbitrarily small so that this sensing model approximates point measurements.

Problem 2.1 (Source Identification): Given a set E of m noisy measurements in the domain Ω, determine an estimate s of the source term $\bar{s}$ so that the AD model $\mathcal{M}(c; s) = 0$ defined in (2) predicts the measurements c^m as close as possible in the least squares sense.

Problem 2.1 can be formulated as a constrained optimization problem as follows. Let $\|c - c^m\|_{\chi_E}^2 \triangleq \int_\Omega (c - c^m)^2 \ \chi_E \ d\Omega$, denote a measure of the distance between the predicted and measured concentrations at the sensor locations and define the cost functional $\mathcal{J}(c, s) : V \times S \to \mathbb{R}_+$ to be optimized by $\mathcal{J}(c, s) \triangleq \frac{1}{2} \|c - c^m\|_{\chi_E}^2 + \tau \mathcal{R}(s)$. Here, τ is a regularization parameter and $\mathcal{R}(s)$ is the regularization functional. In this work, we select $\mathcal{R}(s) \triangleq \|s\|_{L^1} = \int_\Omega |s| \ d\Omega = \int_\Omega s \ d\Omega$. This choice of regularization penalizes the size of the source term. Optimization of the cost functional $\mathcal{J}(c, s)$ subject to the model $\mathcal{M}(c, s) = 0$ gives rise to the following problem

$$\min_{(c,s) \in V \times S} \mathcal{J}(c, s) \text{ s.t. } \mathcal{M}(c, s) = 0; \tag{3}$$

$$\mathcal{J}(c, s) = \frac{1}{2} \int_\Omega (c - c^m)^2 \ \chi_E \ d\Omega + \tau \int_\Omega s \ d\Omega. \tag{4}$$

In the following section we discuss how to obtain the gradient of the cost functional $\mathcal{J}(c, s)$ that is necessary to solve the optimization problem (3). This is done via the so called Adjoint Method.

III. Adjoint Method

The Adjoint Method allows us to solve problem (3) directly in the reduced space S of source functions rather than in the full space $V \times S$ of concentration and source functions. This is possible by using the model $\mathcal{M}(c, s) = 0$ to represent the concentration c as a function of the source term s, i.e., $c = \mathcal{F}(s)$, [3] and then moving along the gradient with respect to s of the cost functional $\mathcal{J}(\mathcal{F}(s), s)$ to determine the desired source function that minimizes this cost functional.

Specifically, consider the Lagrangian of the constrained optimization problem (3), defined by

$$\mathcal{L}(c, s, w) = \mathcal{J}(c, s) + a(c, w) - \ell(w; s), \tag{5}$$

where $w \in V$ is the Lagrange multiplier. In what follows, we use the notion of a Gateaux derivative to differentiate the Lagrangian (5); see e.g., [11, sec. 9.4].

The Adjoint Method consists of the following three steps that yield an organized procedure for the calculation of the desired gradient; see e.g., [12, sec. 4]. First, the Gateaux derivative of the Lagrangian (5) with respect to the multiplier w in an arbitrary direction v is set to zero. The two terms containing w in the Lagrangian are the bilinear form $a(c, w)$ and the functional $\ell(w; s)$. Gateaux differentiating $a(c, w)$ with respect to w we get $\langle a'_w(c, w), v \rangle = \frac{d}{d\epsilon} a(c, w + \epsilon v)|_{\epsilon=0} = a(c, v)$, where we have used linearity of the bilinear operator in each argument. Similarly, Gateaux differentiating $\ell(w; s)$ with respect to w we get $\langle \ell'_w(w; s), v \rangle = \ell(v; s)$. Therefore, the derivative of the Lagrangian with respect to w becomes

$$\langle \mathcal{L}'_w, v \rangle = a(c, v) - \ell(v; s) = 0, \ \forall v \in V. \tag{6}$$

[3]As discussed earlier in Section II-A such a representation exists and is unique.

Note that this equation is exactly the VBVP (2). Given a source function s, the solution of (6) allows us to find the corresponding concentration c.

Next, the Gateaux derivative of the Lagrangian (5) with respect to c in an arbitrary direction h is set to zero. The two terms containing c in the Lagrangian are $\mathcal{J}(c,s)$ and $a(c,w)$. Using equation (4), the Gateaux derivative of $\mathcal{J}(c,s)$ with respect to c is $\langle \mathcal{J}'_c, h\rangle = \int_\Omega h\,(c - c^m)\ \chi_E\ d\Omega$. Moreover, similar to the previous case the Gateaux derivative of the bilinear form $a(c,w)$ with respect to c is given by $\langle a'_c(c,w), h\rangle = a(h,w) = a^*(w,h)$, where $a^*(w,h)$ is the adjoint operator of the bilinear form $a(h,w)$. Therefore, the derivative of the Lagrangian with respect to c becomes

$$\langle \mathcal{L}'_c, h\rangle = \langle \mathcal{J}'_c, h\rangle + a^*(w,h) = 0,\ \forall h \in V. \tag{7}$$

Because of the appearance of the adjoint operator, this equation is called the adjoint equation and the procedure of calculating the desired gradient is referred to as the Adjoint Method. Given the concentration c obtained from (6), the solution of (7) yields the corresponding multiplier w.

Finally, given the multiplier w obtained from (7), the desired Gateaux derivative of the Lagrangian (5) with respect to s in a direction q is $\langle \mathcal{L}'_s, q\rangle = \langle \mathcal{J}'_s, q\rangle - \langle \ell'_s(w;s), q\rangle$. Combining equations (6) and (7) with this expression, the Adjoint Method to calculate the gradient of the Lagrangian (5) with respect to the source s can be summarized in the following procedure:

$$\text{AD-PDE:}\quad a(c,v) - \ell(v;s) = 0 \quad \forall v \in V, \tag{8a}$$
$$\text{Adjoint Eq:}\quad \langle \mathcal{J}'_c, h\rangle + a^*(w,h) = 0\ \forall h \in V, \tag{8b}$$
$$\text{Gradient:}\quad \langle \mathcal{L}'_s, q\rangle = \langle \mathcal{J}'_s - \ell'_s(w;s), q\rangle. \tag{8c}$$

The set of equations (8) can be used to determine the gradient of the cost functional $\mathcal{J}(\mathcal{F}(s),s)$ that is necessary to solve the SI problem (3). Since the variables c and s of this optimization are functions that live in the infinite dimensional function spaces V and S, respectively, in order to solve this problem numerically it is necessary to approximate V and S by finite dimensional subspaces $V_d \subset V$ and $S_d \subset S$ determined by appropriate sets of basis functions. This approximation allows us to parametrize the concentration and source functions by a finite number of parameters that depend on the basis functions that constitute V_d and S_d. We discuss this parametrization in Section IV, while in Section V we develop the numerical aspects of our solution, namely we provide the first and second order information needed for the optimization and discuss initialization.

IV. Finite Dimensional Approximation

In order to obtain a finite dimensional approximation V_d of the function space V we use Proper Orthogonal Decomposition (POD). For a survey of popular Model Order Reduction methods, see e.g., [13]. At the same time, we propose a novel nonlinear representation of the source term s as a combination of compactly supported nonlinear tower functions. This representation reduces the dimension of S_d drastically, compared to classical approaches that utilize the Finite Element Method (FEM).

Algorithm 1 Proper orthogonal decomposition

1: Given the set of snapshots $C = \{c_i(\mathbf{x})\}_{i=1}^K$;
2: Construct the covariance matrix $\mathbf{C}$;
3: Solve the eigenvalue problem $\mathbf{CQ} = \mathbf{\Lambda Q}$ such that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_K \geq 0 \text{ and } \mathbf{Q} = [\mathbf{q}^1\ \mathbf{q}^2\ \ldots\ \mathbf{q}^K];$$

4: The POD bases $\{\psi_k\}_{k=1}^K$ are given via $\psi_k = \sum_{i=1}^K q_i^k c_i$.
5: For $N < K$ the reduced order model c_d is given as $c_d \in V_d = \text{span}\,\{\psi_k\}_{k=1}^N$.

A. Model Order Reduction

A key component in POD is the availability of a set of solutions of the PDE, also known as snapshots. Such snapshots can be obtained using the FEM, which provides the solution of the AD-PDE (1) for a given source term s. Let $C = \{c_i(\mathbf{x})\}_{i=1}^K$ denote a set of K snapshots obtained by solving the AD-PDE (1) for different realizations of the source term, i.e., each $c_i(\mathbf{x})$ corresponds to the solution of the VBVP (2) for a given $s_i(\mathbf{x})$. The objective of POD is to generate a set of optimal basis functions that span the space of snapshots C. As explained in [14], the problem of generating these optimal bases can be recast as an eigenvalue problem for the covariance matrix $\mathbf{C} \in \mathbb{R}^{K\times K}$ defined by $[\mathbf{C}]_{ij} = 1/K \int_\Omega c_i\, c_j\, d\Omega$. The details of this procedure are presented in Algorithm 1.

As shown in [14, thm. 1], the i-th eigenvalue λ_i of matrix $\mathbf{C}$ contains the average energy in the i-th mode. Moreover for a given number $N < K$ of basis functions, the POD bases have the maximum possible energy and are optimal. Thus, for a given fraction η, we can select the number N of required bases as the smallest number such that $\sum_{i=1}^N \lambda_i / \sum_{i=1}^K \lambda_i \geq \eta$.

B. Parametrization

Using the basis functions ψ_k that constitute V_d, cf. Algorithm 1, we can represent the variable pairs $\{w,v\}$ and $\{c,h\}$ by a finite number of parameters that can be used for numerical optimization. Specifically, we define

$$w_d = \boldsymbol{\psi}\,\mathbf{w},\ v_d = \boldsymbol{\psi}\,\mathbf{v},\ c_d = \boldsymbol{\psi}\,\mathbf{c},\ \text{and}\ h_d = \boldsymbol{\psi}\,\mathbf{h}, \tag{9}$$

where $\boldsymbol{\psi} = [\psi_1\ \ldots\ \psi_N]$ and $\mathbf{w},\mathbf{v},\mathbf{c},\mathbf{h} \in \mathbb{R}^N$.

To parametrize the source function s we follow a different approach. Specifically, we propose a novel nonlinear representation of this term as a combination of compactly supported tower functions. The motivation for this representation is that each compactly supported source area can be approximately described by a very small number of parameters corresponding to the intensity and shape of the source. In this paper we focus on rectangular sources, although other geometric shapes can also be used for this purpose.

In particular, let M be the number of basis functions used to approximate the source term in the domain $\Omega \subset \mathbb{R}^l$ and consider two parameters $\{\underline{\mathbf{x}}_j, \bar{\mathbf{x}}_j\}$ for each basis function, where $\underline{\mathbf{x}}_j, \bar{\mathbf{x}}_j \in \mathbb{R}^l$ and $j \in \{1,\ldots,M\}$. We define the compactly supported tower functions as $\phi_j(\mathbf{x};\underline{\mathbf{x}}_j,\bar{\mathbf{x}}_j) = 1$ if $\underline{\mathbf{x}}_j \leq \mathbf{x} \leq \bar{\mathbf{x}}_j$ and zero otherwise, where the inequalities are component-wise and $\underline{\mathbf{x}}_j \leq \bar{\mathbf{x}}_j$. Then, we can approximate

the desired source term by $s_d(\mathbf{x}) = \sum_{j=1}^{M} \beta_j \phi_j(\mathbf{x}; \underline{\mathbf{x}}_j, \bar{\mathbf{x}}_j)$, where we require $\beta_j \geq 0$ so that $s_d \in S$. We denote by $\mathbf{p} = (\beta_1, \underline{\mathbf{x}}_1, \bar{\mathbf{x}}_1, \ldots, \beta_M, \underline{\mathbf{x}}_M, \bar{\mathbf{x}}_M)$ the parameters associated with the source term. For example if $\Omega \in \mathbb{R}^2$, then $\mathbf{p} \in \mathbb{R}^{5M}$. We assume that we know an upper bound M on the number of sources that exist in the domain. If such a bound is not available, then a sufficiently large M can be used.

Substituting the above approximations c_d and s_d of the concentration and source functions c and s in (3), we obtain a finite dimensional counterpart of the SI problem as

$$\begin{aligned} &\min_{\mathbf{c},\mathbf{p}} J(\mathbf{c}, \mathbf{p}) \\ &\text{s.t. } \mathbf{M}(\mathbf{c}, \mathbf{p}) = \mathbf{0}, \\ &\qquad \beta_j \geq 0,\ \mathbf{l} \leq \underline{\mathbf{x}}_j \leq \bar{\mathbf{x}}_j \leq \mathbf{u}, \end{aligned} \tag{10}$$

where $j \in \{1, \ldots, M\}$ and $\mathbf{l}, \mathbf{u} \in \mathbb{R}^l$ are the lower and upper bounds on the coordinates of domain. Moreover, $J : \mathbb{R}^{N \times 5M} \to \mathbb{R}$ is defined as $J(\mathbf{c}, \mathbf{p}) = \mathcal{J}(c_d, s_d)$ and $\mathbf{M} : \mathbb{R}^{N \times 5M} \to \mathbb{R}^N$ is defined as $\mathbf{M}(\mathbf{c}, \mathbf{p}) = \mathcal{M}(c_d, s_d)$, where the dimensions are given for 2D case.

V. Numerical Optimization

The optimization problem (10) can be solved using a variety of available nonlinear optimization algorithms. Any such algorithm requires first and possibly second order information, i.e., the gradient and Hessian, as well as appropriate initialization since the problem is nonlinear. In this section we develop those necessary components in order to solve (10) numerically. All calculations are done in reduced space, by incorporating the AD constraint directly in the analysis; see Section III. As a result, only the bound constraints in (10) need to be considered explicitly for numerical optimization.

A. First Order Information

In Section III we discussed the Adjoint Method to obtain the gradient of problem (3) when the variable s is a function that lives in the infinite dimensional function space S. Here, we employ the approximations V_d and S_d of Section IV to obtain a finite dimensional counterpart of equation (8). First we substitute the approximations (9) into equation (8a) to get $a(c_d, v_d) - \langle \ell(s_d), v_d \rangle = 0,\ \forall v_d \in V_d$, which after simplification yields $\sum_{k=1}^{N} c_k a(\psi_k, \psi_i) - \langle \ell(s_d), \psi_i \rangle = 0$ for all $i \in \{1, \ldots, N\}$. Writing the above equations for all $i \in \{1, \ldots, N\}$ in matrix form we obtain

$$\mathbf{A}\mathbf{c} = \mathbf{b}, \tag{11}$$

where $\mathbf{A} \in \mathbb{R}^{N \times N}$. Thus the finite dimensional model in equation (10) is given explicitly as $\mathbf{M}(\mathbf{c}, \mathbf{p}) = \mathbf{A}\mathbf{c} - \mathbf{b}(\mathbf{p}) = \mathbf{0}$. The uniqueness of the solution for the AD-PDE (1) problem translates to the invertibility of matrix $\mathbf{A}$.

Similarly, for the adjoint equation (8b) utilizing equation (9) we get $\langle \mathcal{J}_c', \psi_i \rangle + \sum_{k=1}^{N} w_k a^*(\psi_k, \psi_i) = 0$ for all $i \in \{1, \ldots, N\}$. Again writing the equations for all i in matrix form we obtain

$$\mathbf{A}^T \mathbf{w} = -\mathbf{d}, \tag{12}$$

where the transpose sign appears because of the adjoint operator in the equations.

Algorithm 2 Adjoint Method for gradient

1: Given the vector of parameters $\mathbf{p}$;
2: Solve $\mathbf{A}\mathbf{c} = \mathbf{b}$ for the concentration coefficients;
3: Solve $\mathbf{A}^T\mathbf{w} = -\mathbf{d}$ for the Lagrange multipliers;
4: Compute the desired gradient $\nabla_{\mathbf{p}} \bar{J}$.

Given values for the source parameters $\mathbf{p}$, the linear systems of equations (11) and (12) can be used to obtain the concentration and Lagrange multipliers. This information can be used in (8c) to calculate the desired gradient. In order to simplify the notation and without loss of generality, we assume a single source in a 2D domain given by $s_d(\mathbf{x}) = \beta\, \phi(\mathbf{x}; \underline{\mathbf{x}}, \bar{\mathbf{x}})$, where $\underline{\mathbf{x}} = (\underline{x}_1, \underline{x}_2)$ and $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2)$. Substituting the approximations (9) and s_d in the Lagrangian (5) we get $\mathcal{L}(c_d, s_d, w_d) = \mathcal{J}(c_d, s_d) + a(c_d, w_d) - \ell(w_d; s_d)$. Then, to obtain the finite dimensional counterpart of (8c) we need to take the derivatives of $\mathcal{L}(c_d, s_d, w_d)$ with respect to the parameters $\mathbf{p}$ of the source term s_d. The terms that contain s_d are $\mathcal{J}(c_d, s_d)$ and $\ell(w_d; s_d)$. For the term $\mathcal{J}(c_d, s_d)$, from equation (4) the only part involving the parameters of s_d is the regularization term $\int_\Omega s_d\, d\Omega = \beta\ (\bar{x}_1 - \underline{x}_1)(\bar{x}_2 - \underline{x}_2)$. Thus $\partial \mathcal{J} / \partial \underline{x}_1 = -\tau\beta(\bar{x}_2 - \underline{x}_2)$; similarly for the other parameters in $\mathbf{p}$. Same as before, substituting $s_d(\mathbf{x})$ in $\ell(w_d; s_d)$ we get $\ell(w_d; s_d) = \int_{\underline{x}_1}^{\bar{x}_1} \int_{\underline{x}_2}^{\bar{x}_2} \beta\ w_d(\mathbf{x})\ dx_2\ dx_1$. The derivative with respect to β is straightforward and for the other parameters we use Leibniz rule, e.g., $\partial \ell / \partial \underline{x}_1 = -\beta \int_{\underline{x}_2}^{\bar{x}_2} w_d(\underline{x}_1, x_2)\ dx_2$. Then by equation (8c), $\partial \bar{J} / \partial \underline{x}_1 = \partial \mathcal{J} / \partial \underline{x}_1 - \partial \ell / \partial \underline{x}_1$, where $\bar{J}(\mathbf{p}) = \mathcal{J}(\mathcal{F}(s_d), s_d)$. The other derivatives can be calculated exactly the same way. The process for calculating the desired gradient $\nabla_{\mathbf{p}} \bar{J}$ given $\mathbf{p} = (\beta, \underline{x}_1, \underline{x}_2, \bar{x}_1, \bar{x}_2)$ is described in Algorithm 2.

If there are multiple sources, i.e., if $M > 1$, we can calculate the gradients for each basis function separately. This follows from the rule for differentiating sums. Moreover if $\Omega \subset \mathbb{R}^3$, we can exactly follow the same steps to calculate the gradient.

B. Second Order Information

Including second order information in the optimization, can make the solution of the SI problem (10) more efficient and accurate. Such information can be in the form of the Hessian $\mathbf{H} = \nabla_{\mathbf{pp}} \bar{J}$ of the cost function itself, or in the form of Hessian-vector products $\mathbf{H}\mathbf{u}$, for some vector $\mathbf{u}$, that is used in the optimization procedure, see e.g., [15, ch. 7]. We use the procedure to calculate the Hessian-vector multiplication here since it provides an organized approach to incorporate the model into the Hessian calculations. Specifically using the Lagrangian (5), we can devise a procedure to calculate the product $\mathbf{H}\mathbf{u}$ for a given vector $\mathbf{u}$ as explained in Algorithm 3, see, e.g., [16]. The derivatives appearing in this algorithm can be calculated in the exact same way as previous derivations.

C. Initialization

Appropriate initialization is critical for the solution of nonlinear optimization problems, such as (10), since otherwise the solution can get trapped in undesirable local minima. In

Algorithm 3 Hessian-vector multiplication

1: Given the vector $\mathbf{u}$;
2: Compute $\mathbf{h}_2 = \mathbf{M_p u}$;
3: Solve $\mathbf{A h}_1 = \mathbf{h}_2$;
4: Compute $\mathbf{h}_3 = \nabla^2_{\mathbf{cc}} L\ \mathbf{h}_1$;
5: Solve $\mathbf{A}^T \mathbf{h}_4 = -\mathbf{h}_3$;
6: Calculate $\mathbf{H\,u} = \mathbf{M}_\mathbf{p}^T\, \mathbf{h}_4 + \nabla^2_{\mathbf{pp}} L\ \mathbf{u}$.

this paper, we employ a result on the point source sensitivity (SS) analysis of the SI cost functional presented in [17] for initialization of our method. According to this idea, given the set of measurements E in Section II-B, we can obtain an approximate localization via a solution of the adjoint equation. Specifically, we solve the linear system of equations $\mathbf{A}^T \bar{\mathbf{w}} = -\bar{\mathbf{d}}$, where $\bar{w}_i = \int_\Omega c^m\ \psi_i\ d\Omega$ for $i \in \{1, \ldots, N\}$, to get the finite dimensional Lagrange multiplier function as $\bar{w}_d = \boldsymbol{\psi}\, \bar{\mathbf{w}}$. Then an approximate localization of the source is obtained through thresholding as $\hat{w}_d(\mathbf{x}) = \bar{w}_d(\mathbf{x})$ if $\bar{w}_d(\mathbf{x}) \leq \alpha\, \bar{w}_d^{\min}$ and zero otherwise, where $\bar{w}_d^{\min} = \min_{\mathbf{x}\in\Omega} \bar{w}_d(\mathbf{x})$ and $\alpha \in (0, 1)$. Note that the thresholding parameter α determines the number of possible source locations. As shown in the simulations, this initialization has a great impact on the computation time and final error. Moreover, it plays an essential role in solving the SI problem for nonconvex domains.

VI. Simulations

In this section we provide numerical simulations to support the applicability of the proposed procedure. We solve the constrained nonlinear optimization problem (10), utilizing MATLAB optimization toolbox that employs an interior-point algorithm which accepts the Hessian-vector multiplication information; see e.g., [15].

In order to quantify the performance of our method, we report the uncovered source ratio e_{un} and the false detection ratio e_{fd}. The first term measures the fraction of the true source $\bar{s}_d$ that is left out by the estimated source s_d and the second term considers the parts of the estimated source s_d that do not overlap with the true source $\bar{s}_d$. In mathematical terms we have $e_{\text{un}} = \|\bar{s}_d - s_d\|_{\mathcal{X}_F} / \|\bar{s}_d\|_{L^2}$ and $e_{\text{fd}} = \|s_d\|_{\mathcal{X}_{\Omega\setminus F}} / \|\bar{s}_d\|_{L^2}$, where F is the support set of $\bar{s}_d$ and $\mathcal{X}_F$ denotes its indicator function defined in Section II-B. Note that any value $e_{\text{un}} < 1$ indicates an overlap between the true and estimated sources. Moreover, we define the signal to noise ratio in dBs as $\text{SNR} = 20 \log \left(\|c(\mathbf{x})\|_{\chi_E} / \|\epsilon(\mathbf{x})\|_{\chi_E} \right)$.

In the simulations, we focus on 2D domains, i.e., $\Omega \subset \mathbb{R}^2$. In addition, we use a lattice of m equidistantly placed sensors to acquire the measurements. We initialize the iterations via the SS approach with $\alpha = 0.7$; see Section V-C. To initialize the algorithm, we place a small square inside each region provided by the SS method. Moreover, we select the regularization parameter τ such that the weights of the data fidelity $\|c - c^m\|^2_{\chi_E}$ and regularization $\mathcal{R}(s)$ terms in the objective (4) are roughly the same.

A. Advection-Diffusion Transport

In this section we assume that the true sources are rectangular and the domain Ω is a 1×1 square area. Moreover, we set the upper bound for the intensity parameter β to 10.

First we solve the SI problem for a single source in a diffusion-dominated case, i.e., we set $D = 1$ and $\mathbf{q} = \mathbf{0}$ in equation (1). In order to compare the simulation time for different sizes of the FE mesh used to create the POD snapshots, we use two different sizes of $n = 41 \times 41 = 1681$ and $n = 101 \times 101 = 10201$. Moreover the POD parameters are $K = 100$ and $\eta = 0.95$, which yield $N = 11$ and $N = 12$ for the two grid sizes respectively.

We set the true parameters of the source as $\bar{\mathbf{p}} = (2, 0.3, 0.6, 0.4, 0.8)$. In table I, we have reported several results with different measurement numbers and SNR values. Generally the reconstruction accuracy measured by the uncovered e_{un} and false detection e_{fd} ratios increases as the number of measurements m increases and deteriorates via the addition of noise. Nevertheless, the most important observation is that increasing the FE mesh size by a factor of 6 has a very low impact on the computation time.

Next we apply our method to identify twin sources inside the domain of interest. For this simulation, we assume a constant velocity of $\mathbf{q} = (0.01, -0.025)$ for advection and we set $D = 3 \times 10^{-3}$. The forward models for all of the simulations with advection are generated using the DiffPack C++ library [18]. We use an unstructured mesh with $n = 1681$ and we set $K = 100$ and $\eta = 0.99$, which yield $N = 42$.

Using an array of 7×7 noiseless measurements to initialize the algorithm with the SS technique and setting $\tau = 10^{-3}$, the algorithm takes 19.37 sec to solve the problem. The uncovered and false detection ratios are $e_{\text{un}} = 0.593$ and $e_{\text{fd}} = 0.583$. Notice that the number of POD bases used here is almost 4 times larger than in the previous case. As it turns out, this parameter has the primary impact on the runtime, since it determines the size of the linear systems (11) and (12) that are solved in each evaluation of the gradient and Hessian. In simulations, it appears that the runtime grows linearly by N.

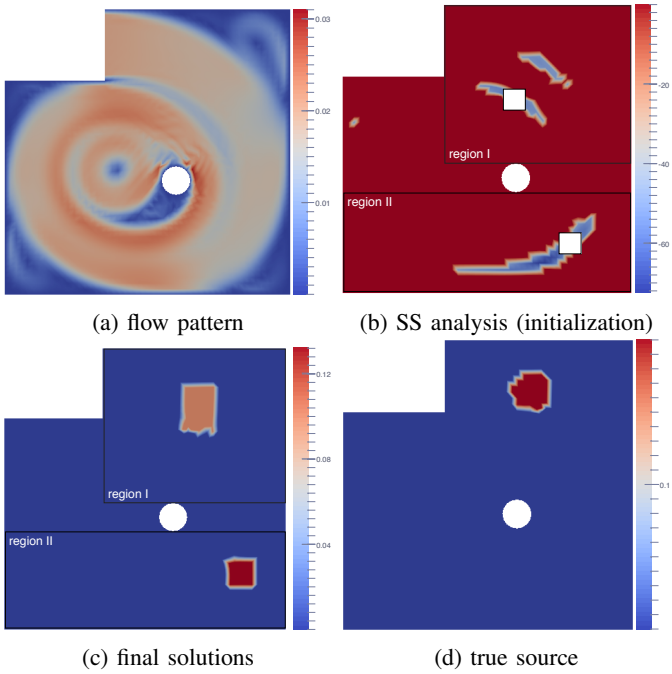
B. Source Identification in Nonconvex Domain

In this section, we study a general advection-diffusion problem in a nonconvex domain. Note that since in the optimization problem (10) we can only specify a convex feasible region, addressing non-convex domains requires additional consideration. We assume that the flow enters the domain with constant inlet velocity of $\mathbf{q}_{\text{in}} = (0.01, 0)$ from the top left edge and solve for the flow pattern using a fluid dynamics model with an unstructured mesh of $n = 2492$ points. Figure 1a depicts the described domain and flow pattern. We use the resultant velocity together with $D = 1 \times 10^{-5}$ in AD-PDE (1). For POD we set $K = 100$ and $\eta = 0.99$, which yield $N = 44$. We also assume a circular source with the radius of 0.07 and the center of $(0.65, 0.825)$ shown in Figure 1d.

The key idea to obtain a solution for this non-convex domain is to search for the source locally in convex subregions of the domain that contain the possible source locations determined by the SS method. Specifically, assuming a 15×15 array of

TABLE I: Exp. A-I - the results of parameter study for the diffusion-dominated SI problem

n	m	SNR (dB)	τ	$\mathbf{x}_0$	$\mathbf{x}$	e_{un}	e_{fd}	time (sec)
41×41	4×4	∞	5×10^{-7}	$(1, 0.375, 0.575, 0.425, 0.625)$	$(1.57, 0.288, 0.577, 0.455, 0.745)$	0.60	0.41	2.71
41×41	7×7	∞	1×10^{-7}	$(1, 0.375, 0.6, 0.425, 0.65)$	$(1.41, 0.257, 0.610, 0.447, 0.805)$	0.43	0.42	1.72
101×101	10×10	∞	5×10^{-7}	$(1, 0.375, 0.575, 0.425, 0.625)$	$(1.48, 0.291, 0.595, 0.439, 0.748)$	0.58	0.33	5.17
101×101	10×10	1.77	1×10^{-6}	$(1, 0.325, 0.625, 0.375, 0.675)$	$(1.26, 0.268, 0.605, 0.408, 0.745)$	0.65	0.27	2.41



(a) flow pattern (b) SS analysis (initialization)

(c) final solutions (d) true source

Fig. 1: Exp. B - the contour plots for the advection-diffusion SI problem.

noiseless measurements and utilizing the SS method, we divide the domain into two simple rectangular areas enclosing the top left and bottom regions as depicted in Figure 1b. For the first case containing the true source, the solution of the SI problem for $\tau = 7$ takes 21.9 sec, with $e_{\text{un}} = 0.72$ and $e_{\text{fd}} = 0.37$. The final solution for both cases is depicted in Figure 1c.

Assuming it is known that a single source is present in the domain and referring to the Definition 2.1 of the SI problem, we are interested in the solution that predicts the measurements the best in the least squares sense. Denoting the concentration prediction for these two source estimates with c_d^1 and c_d^2 respectively, we have $\left\|c_d^1 - c^m\right\|_{\chi_E} = 0.087$ and $\left\|c_d^2 - c^m\right\|_{\chi_E} = 0.210$. These values indicate that indeed the first solution is a better approximation of the true source.

VII. Conclusion

In this paper we proposed a computationally efficient algorithm to address the Source Identification (SI) problem in a steady-state transfer phenomenon. Given a set of noisy measurements of the concentration, we formulated an optimization problem that estimates the source function generating the measured concentrations in the domain. We used proper orthogonal decomposition to obtain a finite dimensional approximation of the function space of the concentration. Moreover, a set of nonlinear basis functions were proposed to model the source term. These approximations allowed us to formulate the SI problem as a nonlinear optimization problem with a very small number of unknowns. Our method presents a significant improvement in terms of computational cost compared to methods that use linear basis functions. At the same time, we are able to solve SI problems in non-convex domains, which has significant practical implications. The simulation results demonstrate the effectiveness of the proposed approach.

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