

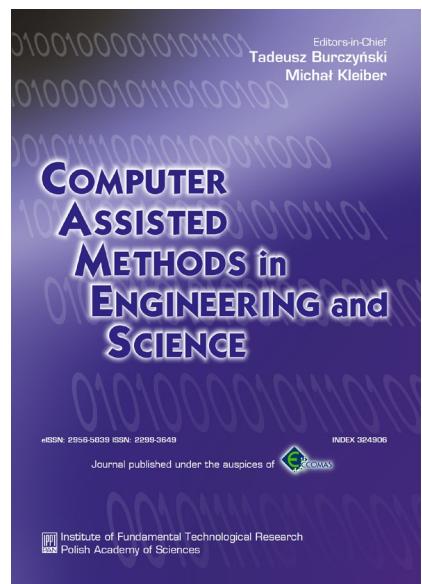
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# Goal-oriented optimal sensor placement for PDE-constrained inverse problems in crisis management

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## Abstract

This paper presents a novel framework for goal-oriented optimal static sensor placement and dynamic sensor steering in PDE-constrained inverse problems, utilizing a Bayesian approach accelerated by low-rank approximations. The framework is applied to airborne contaminant tracking, extending recent dynamic sensor steering methods to complex geometries for computational efficiency. A C-optimal design criterion is employed to strategically place sensors, minimizing uncertainty in predictions. Numerical experiments validate the approach's effectiveness for source identification and monitoring, highlighting its potential for real-time decision-making in crisis management scenarios.

**Keywords**— Airborne contaminant transport, Advection-diffusion equation, Large-scale inverse problems, Optimal experimental design, Dynamic sensor steering

## 1 Introduction

The growing capabilities of unmanned systems (UxS), such as unmanned aerial vehicles (UAVs, drones), autonomous underwater vehicles (AUVs), and unmanned ground vehicles, e.g., mobile robots, have made these systems indispensable tools in crisis management situations (see Figure 1 for examples). Such autonomous sensor platforms facilitate the collection of valuable information in regions where manned missions would be too dangerous or simply impossible due to inaccessibility for humans. However, during the routing of a sensor platform in the complex environment of a crisis situation, the question arises as to at which locations (additional) measurements provide an information gain and thereby constitute added value for decision makers.

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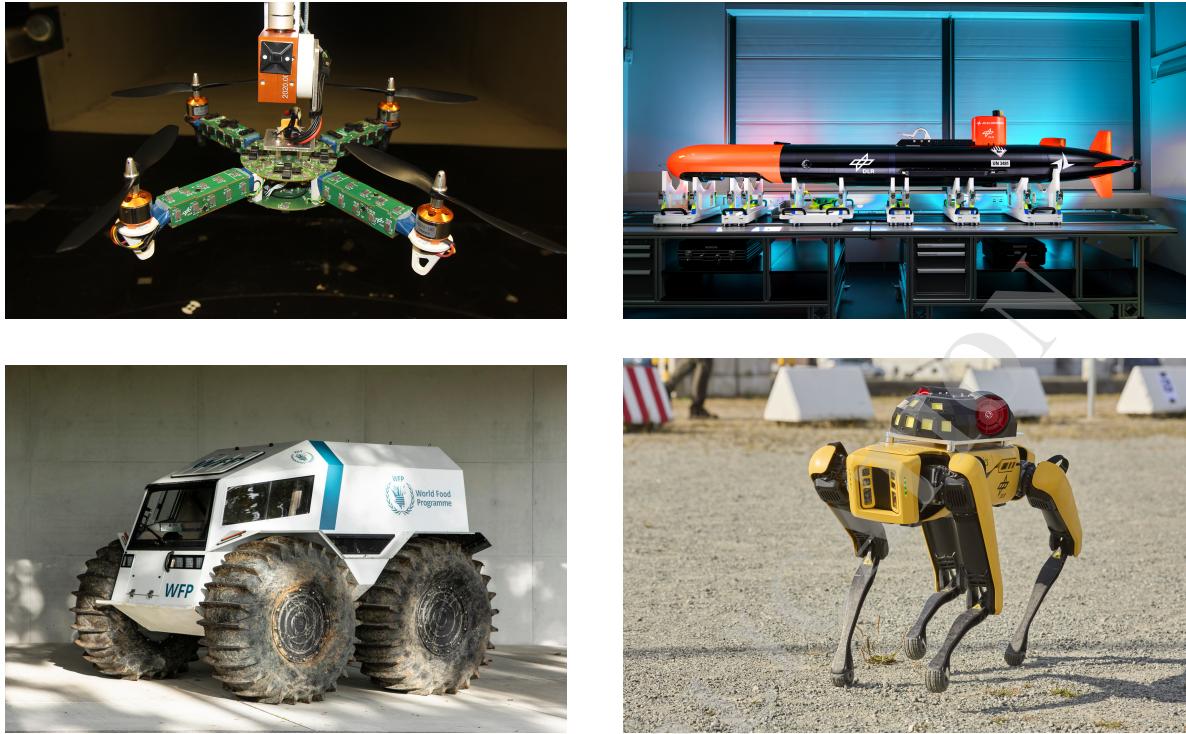


Figure 1: Unmanned systems operated as autonomous sensor platforms at German Aerospace Center (DLR). Images: DLR, CC BY-NC-ND 3.0

This very question leads to the need for a goal-oriented optimal sensor placement and in the dynamic case to a sensor steering problem. The task of selecting optimal measurement locations to infer system knowledge falls within the classical field of optimal experimental design (OED). Goal-oriented optimal experimental design generalizes this concept by determining the optimal design not for the parameters themselves, but for a derived quantity of interest (QoI). This approach offers two major advantages. First, it enables a more application-specific formulation, as the optimal design targets the QoI directly rather than the entire parameter space of the inverse problem. Second, it substantially reduces computational cost, since the QoI typically has far fewer degrees of freedom in its discretized representation.

This contribution addresses the problem in the mathematical setting of inverse problems constrained by partial differential equations (PDEs). A selected sensor steering strategy is developed and applied to the specific challenge of mapping airborne contaminant dispersion in the region of interest using discrete sensor measurements. By specifying the region of interest in both space and time, the problem naturally falls within the framework of goal-oriented optimal sensor placement.

Current methods for contaminant source identification and spread prediction rely heavily on an informative sensor placement. The selection of measuring points (sensor positions) is crucial, yet many existing studies focus solely on stationary sensors. This work bridges this gap by incorporating recent advances in sensor selection and experimental design to derive an algorithm for optimal sensor steering. Our research focuses on developing a systematic approach to select sensor positions that maximize the accuracy of contaminant source identification and prediction. By integrating current methodological advancements, our aim is to provide a practical solution for rescue workers and first responders, allowing informed decisions in high-

stakes situations. Whereas the numerical examples presented in this work focus on the specific application of airborne contaminant transport, the goal-oriented optimal sensor placement strategy is independent of the considered physical model and, hence, can be easily transferred to other crisis management applications.

Starting point for this work is the recent publication by Wogrin et al. [23] that pioneers a dynamic sensor steering method in the context of airborne contaminant transport. In this work, we extend this approach to a significantly more complex geometry. Moreover, the inverse problem solution follows a more advanced approach that uses a Laplacian-like operator of trace class as prior information within a Bayesian inverse problem framework [20, 16]. To achieve approximate real-time capability, low-rank approximations of the Hessian matrix are precomputed in an offline phase [13, 15], enabling efficient problem solving in the online phase using a preconditioned inexact Newton-CG solver [19].

In the calculation of an optimal (stationary) sensor layout, Alexanderian et al. [3] used a reduced model for the contaminant transport to determine an A-optimal design that minimizes the average point-wise posterior variance of the inferred parameter vector. Following extensions proposed in [18] and [5], we focus on a goal-oriented design, i.e., the uncertainty associated with the prediction of the contaminant concentration in a specific region and time is minimized. To demonstrate the feasibility of sensor steering, a relaxed optimality criterion compared to the A-optimal criterion is chosen for this test case. Specifically, we use the C-optimal criterion, which focuses on minimizing the posterior variance of a particular linear combination of the inversion parameters. This approach eliminates the need to estimate the trace of the full covariance matrix and allows us to directly assess the impact of the covariance matrix on the parameter of interest. Alternatively, a D-optimal goal-oriented design in infinite dimensions maximizes the expected information gain [24, 3]. For a broader perspective on optimal experimental design for infinite-dimensional Bayesian inverse problems governed by PDEs, the interested reader is referred to [1]. The remainder of this paper is organized as follows. Section 2 provides background and mathematical formulations of the forward problem of contaminant transport, the inverse problem of source identification, as well as sensor positioning strategies and goal-oriented optimization. The combination of methodological developments into an algorithm for goal-oriented optimal sensor placement and steering is described in Section 3. Numerical results are presented in Section 5 for three test cases of goal-oriented optimal sensor placement, namely (a) to identify an instantaneous contaminant source in a user-defined area of interest, (b) to monitor an area of special interest over a predefined time window, and (c) to steer a moving sensor. Finally, Section 6 offers a conclusion and an outlook.

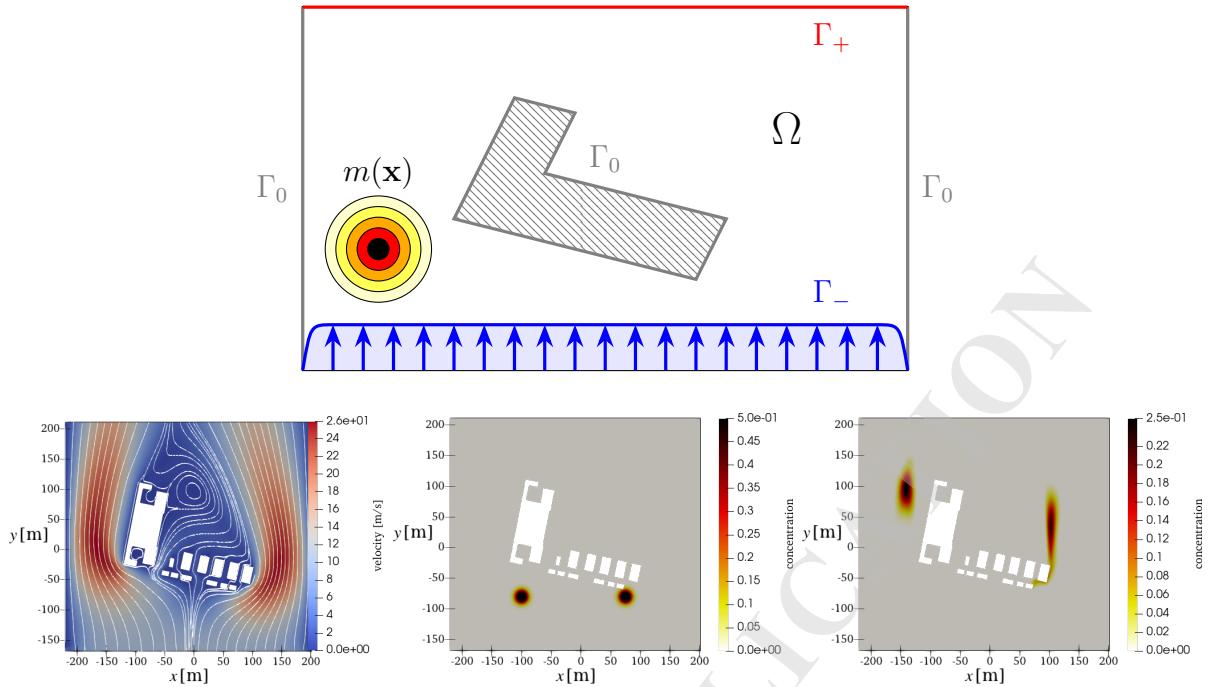


Figure 2: Forward simulation of airborne contaminant transport on a campus geometry. Computational domain  $\Omega$  with highlighted inflow ( $\Gamma_-$ ), outflow ( $\Gamma_+$ ), and characteristic ( $\Gamma_0$ ) boundaries as well as the initial contaminant source  $u(0, \cdot) = m(\cdot)$  (above). Estimated wind vector field  $\mathbf{v}$  (left), initial condition (middle), and simulated concentration at  $t = 10$  s (right).

## 2 Background

### 2.1 Forward problem: Contaminant distribution evolution

A mathematical description of the transport of a substance (contaminant) concentration  $u$  in a bounded open domain  $\Omega \subseteq \mathbb{R}^n$  for  $n \in \{2, 3\}$ , which is shown in Figure 2, is given by the following equation:

$$\begin{aligned}
 r_\kappa(u) := u_t - \kappa \Delta u + \mathbf{v} \cdot \nabla u &= 0 && \text{in } (0, T) \times \Omega, \\
 \kappa \nabla u \cdot \mathbf{n} &= 0 && \text{in } (0, T) \times (\Gamma_+ \cup \Gamma_0), \\
 u &= 0 && \text{in } (0, T) \times \Gamma_-, \\
 u(0, \cdot) &= m && \text{in } \Omega.
 \end{aligned} \tag{1}$$

The parameter-dependent forward problem shown in Equation 1 is formulated for realizations of the parameter  $m$ . A visualization of the contaminant dispersion is provided in Figure 2.

The underlying transport process is governed by a wind vector field  $\mathbf{v}$ , which is assumed to be sufficiently smooth, bounded — i.e.,  $\mathbf{v} \in L^\infty(\Omega, \mathbb{R}^n)$  — and divergence-free — i.e.,  $\nabla \cdot \mathbf{v} = 0$ . The example wind vector field used hereinafter is shown in Figure 2 (left). Based on the orientation of the wind vector relative to the outward-pointing boundary normal  $\mathbf{n}$ , the domain boundary  $\partial\Omega$  is partitioned into three disjoint subsets: the outflow boundary  $\Gamma_+ \subset \partial\Omega$ , where  $\mathbf{v} \cdot \mathbf{n} > 0$ ; the characteristic (or tangential) boundary  $\Gamma_0 \subset \partial\Omega$ , where  $\mathbf{v} \cdot \mathbf{n} = 0$ ; and the inflow boundary  $\Gamma_- \subset \partial\Omega$ , where  $\mathbf{v} \cdot \mathbf{n} < 0$ , following the convention in [10].

## 2.2 Inverse problem: Source identification

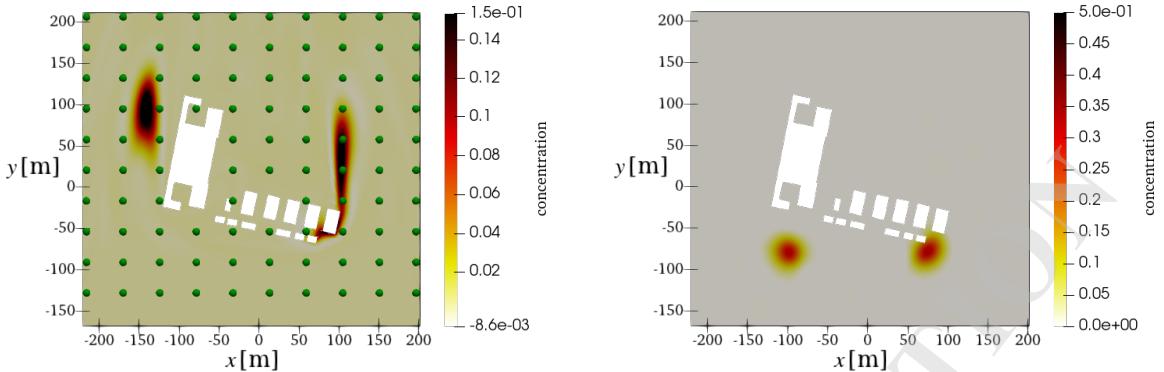


Figure 3: Inverse Problem. Measurements at 96 equidistantly spaced sensor positions (left) and reconstructed initial condition (solution of the inverse problem, right).

Whenever measurements of the concentration at discrete locations and times are available, an obvious question is whether the initial condition can be reconstructed on the basis of the given measurements. The respective inverse problem is illustrated in Figure 3, see also [20]. As function space for the initial condition, we consider an admissible subset of square-integrable functions. For instance, we define  $D := H_{\Gamma_-}^{1,2}(\Omega) := \{m \in H^{1,2}(\Omega) \mid m|_{\Gamma_-} = 0\}$ , where  $H^{1,2}(\Omega)$  denotes the Sobolev space of square-integrable functions whose weak derivatives  $\partial_i u$  exist and are square-integrable. The gradient is denoted as  $\nabla u = (\partial_1 u, \partial_2 u)$ , and the norm on  $H^{1,2}(\Omega)$  is defined as

$$\|u\|_{H^{1,2}(\Omega)} := \left( \int_{\Omega} u^2 + \|\nabla u\|_2^2 \, d\mathbf{x} \right)^{1/2}.$$

In this setting, the estimation of the initial value leads to an optimization problem, which will be addressed in the following. The first step is to describe sensor measurements within this formulation.

To incorporate sensor measurements, let  $T_0 > 0$  be fixed and consider space-time points  $(t_i^{\text{obs}}, x_i^{\text{obs}})$ ,  $i = 1, \dots, q$ , with  $t_i^{\text{obs}} \in [T_0, T]$  and interior points  $x_i^{\text{obs}} \in \Omega = \bar{\Omega} \setminus \partial\Omega$ . For the transient problem in Equation 1 on a smooth domain  $\Omega$ , the diffusion term induces strong smoothing on the parameter field  $m$ . By standard parabolic regularity (see, e.g., [11]),  $u(t, \cdot)$  embeds in the space of continuous functions  $C^0(\bar{\Omega})$  on the closure of  $\Omega$  for any  $t > 0$ . Since continuity is only required near the observation points, define  $\bar{\Omega}_o := \bigcup_{i=1}^q B_{r_0}(x_i^{\text{obs}}) \subset \Omega$ , where  $r_0 > 0$  is chosen such that  $u \in C^0([T_0, T] \times \bar{\Omega}_o)$  admits a continuous representation. This ensures the formulation remains valid for less regular domains  $\Omega$ . Finally, we define a well-posed and bounded *space-time observation operator*  $\mathcal{B} : C^0([T_0, T] \times \bar{\Omega}_o) \rightarrow \mathbb{R}^q$  by  $u \mapsto \sum_{i=1}^q \delta_{(t_i^{\text{obs}}, x_i^{\text{obs}})}(u) \mathbf{e}_i = (u(t_i^{\text{obs}}, x_i^{\text{obs}}))_{i=1}^q$ , where  $\mathbf{e}_i$  is the standard basis of  $\mathbb{R}^q$ . Using this observation operator, the final *parameter-to-observable map*  $\mathcal{F} : D \rightarrow \mathbb{R}^q$  is defined by

$$\mathcal{F}(m) := \mathcal{B} \circ \mathcal{K}(m), \quad \text{with } \mathcal{K}(m) := u \text{ such that } r_{\mathcal{K}}(u) = m. \quad (2)$$

Here  $\mathcal{K}$  is the *parameter-to-state map*, mapping parameter space  $D$  to state space, often referred to as 'model' in this context [8]. An example problem in which  $\mathcal{K}$  maps the initial condition  $u_0$  to the solution of  $u(t = 10 \text{ s}, \cdot)$  is illustrated in Figure 2.

The next step is to model sensor noise, which is usually present in real-world measurements. To this end, it is assumed that the observations  $\mathbf{d} = \mathcal{F}(m) + \boldsymbol{\epsilon}$  contain centered additive Gaussian noise  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \Gamma_{\text{noise}})$  due to measurement uncertainties. For the sake of simplicity, it is further assumed that the sensor noise at the different sensor positions is uncorrelated and of equal magnitude, represented by the diagonal matrix  $\Gamma_{\text{noise}} = \text{diag}(\sigma^2, \dots, \sigma^2)$ . Moreover, the conformity of the simulation with the measured values, also called *misfit*,  $\mathbf{y} = \mathcal{F}(m) - \mathbf{d}$ , is evaluated in the following norm

$$\|\mathcal{F}(m) - \mathbf{d}\|_{\Gamma_{\text{prior}}^{-1}}^2 = 1/\sigma^2 \sum_{i=1}^q (u(t_i^{\text{obs}}, x_i^{\text{obs}}) - d_i)^2.$$

In summary, the inverse problem consists in using available measurements  $\mathbf{d}$  to infer the values of the unknown parameter field  $m$ . Alternatively, the maximum a-posteriori point  $m_{\text{map}}$  can be characterized by the solution of the minimization problem

$$m_{\text{map}} = \arg \min_{m \in D} J(m) := \frac{1}{2} \|\mathcal{F}(m) - \mathbf{d}\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \|m - m_{\text{prior}}\|_{\Gamma_{\text{prior}}^{-1}}^2, \quad (3)$$

with the prior information encoded as a Tikhonov regularization term.

Unfortunately, the system is heavily under-determined under real conditions, as sensor measurements are only available at a few locations, but an initial condition is to be reconstructed for the entire domain. In order to transform this into a well-posed problem, some prior knowledge is needed and a formulation as a Bayesian inverse problem provides a suitable framework. In this setting, a Gaussian prior  $\mathcal{N}(m_{\text{prior}}, \Gamma_{\text{prior}})$  with mean  $m_{\text{prior}}$  and covariance  $\Gamma_{\text{prior}}$  is chosen for parameter regularization. Then, the posterior density of  $m$  satisfies by Bayes' theorem:  $\pi_{\text{post}}(m|\mathbf{d}) \propto \pi_{\text{like}}(\mathbf{d}|m) \pi_{\text{prior}}(m)$ . Here,  $\pi_{\text{like}}(\mathbf{d}|m) \propto \exp(\frac{1}{2} \|\mathcal{F}(m) - \mathbf{d}\|_{\Gamma_{\text{noise}}^{-1}}^2)$  is the likelihood function under the observational Gaussian noise  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \Gamma_{\text{noise}})$ . Due to the linearity of  $\mathcal{F}$ , the posterior distribution is again a Gaussian distribution  $\mathcal{N}(m_{\text{map}}, \Gamma_{\text{post}})$  with covariance and mean

$$\Gamma_{\text{post}} = (\mathcal{F}^* \Gamma_{\text{noise}}^{-1} \mathcal{F} + \Gamma_{\text{prior}}^{-1})^{-1} \quad \text{and} \quad m_{\text{map}} = \Gamma_{\text{post}} (\mathcal{F}^* \Gamma_{\text{noise}}^{-1} \mathbf{d} + \Gamma_{\text{prior}}^{-1} m_{\text{prior}}). \quad (4)$$

The formal adjoint operator  $\mathcal{F}^* : \mathbb{R}^q \rightarrow D^*$  is required for this framework. For the mapping  $\mathcal{F} : D \rightarrow \mathbb{R}^q$  between Hilbert spaces, the formal adjoint operator  $\mathcal{F}^*$  is characterized by the relation  $\langle \mathcal{F}(m), \mathbf{y} \rangle_{\mathbb{R}^q} = \langle m, \mathcal{F}^*(\mathbf{y}) \rangle_{L^2(\Omega)}$  for all  $\mathbf{y} \in \mathbb{R}^q$  and  $m \in D$ , and its existence follows from Riesz's representation theorem [4]. The posterior covariance or Hessian  $\mathcal{H} := \mathcal{F}^* \Gamma_{\text{noise}}^{-1} \mathcal{F} + \Gamma_{\text{prior}}^{-1}$  of the objective function  $J$ , see Equation 3, contains a wealth of information about the system. In line with the Bayesian framework [20], the covariance or inverse Hessian matrix can be employed to predict the uncertainty of the system and is of particular significance for optimal sensor placement in the following chapter.

The mean value  $m_{\text{map}}$  is a reliable estimate for the initial value and thus represents the solution of the inverse problem Figure 3. In order to calculate  $m_{\text{map}}$  from Equation 4, a further specification of the adjoint operator  $\mathcal{F}^*$  is necessary. By applying partial integration to the weak form of Equation 1, the adjoint state  $p$  can be derived and satisfies the following equation:

$$\begin{aligned} -p_t - \kappa \Delta p - \text{div}(p\mathbf{v}) &= -1/\sigma^2 \sum_{i=1}^q y_i \delta_{(t_i^{\text{obs}}, x_i^{\text{obs}})} && \text{in } (0, T) \times \Omega, \\ (\mathbf{v}p + \kappa \nabla p) \cdot \mathbf{n} &= 0 && \text{in } (0, T) \times (\Gamma_+ \cup \Gamma_0), \\ p &= 0 && \text{in } (0, T) \times \Gamma_-, \\ p(T, \cdot) &= 0 && \text{in } \Omega. \end{aligned} \quad (5)$$

for given  $\mathbf{y} \in \mathbb{R}^q$ . Finally, the adjoint operator  $\mathcal{F}^*$  can be explicitly determined, resulting in  $\mathcal{F}^*\mathbf{y} = p(0, \cdot)$ .

### 2.3 Goal-oriented optimal experimental design: Sensor placement

So far, a model for the forward problem and an estimate of the initial condition, given a fixed sensor configuration, have been derived, but the question of how such a sensor arrangement ought to be chosen remains unanswered. As mentioned in the previous chapter, the covariance of the posterior, or more specifically, the Hessian matrix, plays a crucial role in developing an indicator for the uncertainty in the system. In classical Bayesian optimal experimental design (OED), a design functional  $\Phi$  serves as a quantitative criterion for the uncertainty described by the covariance matrix and is used to guide the selection of an optimal experimental setup. Specifically, the problem

$$\min_{\mathbf{w} \in \mathbb{W}} \left( \Phi[\Gamma_{\text{post}}(\mathbf{w})] + \mathcal{R}(\mathbf{w}) \right), \quad (6)$$

is solved, where  $\mathbb{W}$  denotes the set of all valid sensor configurations, and  $\mathcal{R}$  is a suitable regularization term. As in [2], a finite set of candidate sensor placements  $(t_i^{\text{obs}}, x_i^{\text{obs}}) \in [T_0, T] \times \Omega$  for  $1 \leq i \leq q$  will be considered. An example of a spatial grid with 96 sensors can be seen in Figure 3. For this set of candidate locations, a weight vector  $\mathbf{w} \in [0, 1]^q$  is defined with the  $i$ -th entry corresponding to the  $i$ -th location in space and time. In fact, the weight vector decides which measurements are realized or taken into account. In the case of stationary sensors located at positions  $\mathbf{x}_s^{\text{obs}}$ , measurements collected from these spatial points over the entire time horizon, denoted as  $(\cdot, \mathbf{x}_s^{\text{obs}})$ , are constantly weighted, included in the misfit. Hence, the number of independent entries in the weight vector reduces to the number of possible stationary sensor positions. If we consider a mobile sensor, we have a trajectory  $\gamma : \{t_0^{\text{obs}}, \dots, t_s^{\text{obs}}\} \rightarrow \{\mathbf{x}_0^{\text{obs}}, \dots, \mathbf{x}_s^{\text{obs}}\}$ . For points on the trajectory  $(t_i^{\text{obs}}, \mathbf{x}_i^{\text{obs}})$  the sensor weight is  $\mathbf{w}_i = 1$ . All weights away from the trajectory are set to 0. To adjust the forward model to the chosen sensor configuration, we consider the diagonal matrix  $W \in \mathbb{R}^{q \times q}$  with  $W_{ii} = \mathbf{w}_i$ . If we denote the parameter-to-observable map for all sensor positions as  $\mathcal{F}$ , then for each design  $\mathbf{w} \in \mathbb{W}$ , we have  $\mathcal{F}(\mathbf{w}) = W\mathcal{F}$ . Taking this further and using  $W$  to modify the noise matrix, the influence of a selected sensor layout is also captured in the likelihood function

$$\pi_{\text{like}}(\mathbf{d}|m, \mathbf{w}) \propto \exp \left\{ -\frac{1}{2} (\mathcal{F}(m) - \mathbf{d})^T W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} (\mathcal{F}(m) - \mathbf{d}) \right\}.$$

In consequence, the posterior covariance and mean also depend on the sensor layout via (cf. Equation 4)

$$\Gamma_{\text{post}}(\mathbf{w}) = (\mathcal{F}^* W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} \mathcal{F} + \Gamma_{\text{prior}}^{-1})^{-1} \quad \text{and} \quad m_{\text{map}}(\mathbf{w}) = \Gamma_{\text{post}}(\mathcal{F}^* \Gamma_{\text{noise}}^{-1} W \mathbf{d} + \Gamma_{\text{prior}} m_{\text{prior}}). \quad (7)$$

In Bayesian optimal experimental design, the objective is to construct experiments that minimize the posterior uncertainty in the unknown parameter field  $m$ . This approach belongs to the broader class of inverse uncertainty quantification methods. Goal-oriented optimal experimental design extends this framework by additionally incorporating forward uncertainty quantification into the design objective. This is achieved by introducing a goal quantity of interest (QoI), denoted by  $\rho$ . Following [5, Section 3], we consider a QoI defined as the action of a bounded linear operator  $\mathcal{P}$  on the parameter field, i.e.,  $\rho = \mathcal{P}m$ . Due to the linearity of  $\mathcal{P}$ , the prior distribution of  $\rho$  is Gaussian. In particular,  $\rho \sim \mathcal{N}(\rho_{\text{prior}}, \Sigma_{\text{prior}})$ , with mean  $\rho_{\text{prior}} = \mathcal{P}m_{\text{prior}}$  and covariance  $\Sigma_{\text{prior}} = \mathcal{P}\Gamma_{\text{prior}}\mathcal{P}^*$ . The resulting Bayesian inverse problem is well defined, and the posterior

distribution of the QoI given measurements  $\mathbf{d}$  is also Gaussian,  $\pi_{\text{post}}(\rho \mid \mathbf{d}) \sim \mathcal{N}(\rho_{\text{post}}, \Sigma_{\text{post}})$ . The posterior mean and covariance are given by

$$\Sigma_{\text{post}} = \mathcal{P} \Gamma_{\text{post}} \mathcal{P}^* \text{ and } \rho_{\text{post}} = \mathcal{P} m_{\text{map}},$$

where  $\Gamma_{\text{post}}$  and  $m_{\text{map}}$  are the derived quantities from Equation 7.

### 3 Discretization, preconditioning, and sparsification

#### 3.1 Finite element discretization

To solve the PDE problems (Equation 1 and Equation 5) numerically, a finite element discretization is employed using  $n_{\text{dof}}$  Lagrange basis functions  $\mathcal{V}_h = \text{span}\{\phi_1, \dots, \phi_{n_{\text{dof}}}\}$ . Moreover, we find an identification between a vector in  $\mathbb{R}^{n_{\text{dof}}}$  and finite elements  $I : \mathbb{R}^{n_{\text{dof}}} \rightarrow \mathcal{V}_h$  via  $I(a) = \sum_{i=1}^{n_{\text{dof}}} a_i \phi_i$ . This leads to discretized versions of the parameter-to-observable map  $\mathcal{F}_h : \mathbb{R}^{n_{\text{dof}}} \rightarrow \mathbb{R}^q$  defined by  $\mathcal{F}_h(m_h) = \mathcal{B}(u_h)$ , where  $u_h$  solves Equation 1 weakly, and its adjoint operator  $\mathcal{F}_h^* : \mathbb{R}^q \rightarrow \mathbb{R}^{n_{\text{dof}}}$  given by  $\mathcal{F}_h^* \mathbf{y} = p_h(0, \cdot)$ , where  $p_h$  solves Equation 5 weakly. The identification is an isometry, i.e.,  $\langle I(a), I(b) \rangle_{L^2(\Omega)} = \langle a, b \rangle_M =: a^T M b$ , where the mass matrix  $M_{ji} := \int_{\Omega} \phi_i(\mathbf{x}) \phi_j(\mathbf{x}) d\mathbf{x}$ ,  $M \in \mathbb{R}^{n_{\text{dof}} \times n_{\text{dof}}}$  is used to define the corresponding scalar product. For further details of the finite element discretization, we refer to [20] and [21].

#### 3.2 Preconditioning of discrete inverse problem

To solve the discrete inverse problem, the prior distribution needs to be carefully chosen. A Laplacian-like operator of trace class  $\mathcal{A} := (\eta I - \gamma \Delta)$ , with Robin boundary condition,  $\gamma \nabla m \cdot \mathbf{n} + \beta m = 0$  in  $(0, T) \times \partial\Omega$ , is applied with the constant  $\beta$  proposed in [9]. This definition serves as a suitable covariance operator, e.g.,  $\Gamma_{\text{prior}} = \mathcal{A}^{-2} = (\eta I - \gamma \Delta)^{-2}$ . In addition, its discrete counterpart is given by the mapping  $\Gamma_{\text{prior,h}} : \mathbb{R}^{n_{\text{dof}}} \rightarrow \mathbb{R}^{n_{\text{dof}}}$  via  $\Gamma_{\text{prior,h}} = (M^{-1} \mathcal{A})^{-2} = \mathcal{A}^{-1} M \mathcal{A}^{-1} M := R^{-1} M$ , with matrix representation  $A_{ij} = \int \phi_i(x) \mathcal{A} \phi_j(x) dx$ .

Combining this covariance operator together with an appropriate prior mean  $m_{\text{prior}}$  (in our applications, e.g.,  $m_{\text{prior}} = 0$ ) renders the inverse problem well-posed and its solution can be found by solving the following equation for  $m_{\text{map}}$

$$\mathcal{H}_h(\mathbf{w}) m_{\text{map}} = \mathcal{F}_h^* \Gamma_{\text{noise}}^{-1} (W \mathbf{d}) + \Gamma_{\text{prior,h}}^{-1} m_{\text{prior}}, \quad (8)$$

for the discrete version of the Hessian, that is,  $\mathcal{H}_h(\mathbf{w}) = \mathcal{F}_h^* W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} \mathcal{F}_h + \Gamma_{\text{prior,h}}^{-1}$ . Since determining the Hessian matrix directly is computationally expensive for large-scale problems ( $O(n_{\text{dof}})$ -PDE solutions), an iterative conjugate gradient (CG) method is employed. This approach requires only the action of the Hessian-vector on a given vector  $m_k \in \mathbb{R}^{n_{\text{dof}}}$  at each iteration. Specifically, the Hessian action is computed by the following steps: first, solve the forward equation  $\mathbf{d} = \mathcal{F}_h(m_k) = \mathcal{B}(u_h)$ , then, solve the adjoint equation  $\mathcal{F}_h^* (W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} \mathbf{d}) = p_h(0, \cdot)$ , next, compute  $\tilde{m}_k = \Gamma_{\text{prior,h}} m_k$ , and finally obtain the Hessian action as  $\mathcal{H}_h(\mathbf{w}) m_k = p_h(0, \cdot) + \tilde{m}_k$ .

Since two PDE solutions have to be determined in each iteration, a reduced model of the Hessian matrix is created in advance so that the inverse problem can be solved quickly. Using the Cholesky decomposition

of the prior covariance,  $\Gamma_{\text{prior},h}^{-1} = (M^{-1}A)(M^{-1}A)^*$ , one obtains the preconditioned Hessian matrix as

$$(\mathcal{A}_h^{-1})^* \mathcal{H}_h(\mathbf{w}) \mathcal{A}_h^{-1} = (\mathcal{F}_h \circ \mathcal{A}_h^{-1})^* W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} (\mathcal{F}_h \circ \mathcal{A}_h^{-1}) + I, \quad (9)$$

for  $\mathcal{A}_h^{-1} = (A^{-1}M)$ . This preconditioned system  $\mathcal{F} \circ \mathcal{A}^{-1}$  has fast decaying eigenvalues and so, we follow [20, 14] in constructing a low rank approximation of the prior-preconditioned misfit part of the Hessian, i.e.,  $\tilde{\mathcal{H}}_h^{\text{misfit}}(\mathbf{w}) := (\mathcal{F}_h \circ \mathcal{A}_h^{-1})^* W^{\frac{1}{2}} \Gamma_{\text{noise}}^{-1} W^{\frac{1}{2}} (\mathcal{F}_h \circ \mathcal{A}_h^{-1})$  by solving the symmetric eigenvalue problem [13, 15]:

$$\mathcal{H}_h^{\text{misfit}}(\mathbf{w}) v_i = \lambda_i M \Gamma_{\text{prior},h}^{-1} v_i = \lambda_i R v_i$$

for an orthogonal basis  $V_r = (v_1, \dots, v_r) \in \mathbb{R}^{n_{\text{dof}} \times r}$  and  $\lambda_1 \geq \dots \geq \lambda_r$  with respect to the scalar product induced by  $M \Gamma_{\text{prior},h}^{-1}$ , i.e.,  $\langle a, b \rangle_{M \Gamma_{\text{prior},h}^{-1}} =: a^T M \Gamma_{\text{prior},h}^{-1} b$ . Applying the Sherman-Morrison-Woodbury formula, we write

$$\mathcal{A}_h(\mathcal{H}_h(\mathbf{w}))^{-1} \mathcal{A}_h = (\tilde{\mathcal{H}}_h^{\text{misfit}}(\mathbf{w}) - I)^{-1} \approx I + V_r D_r(\mathbf{w}) V_r^T \quad (10)$$

where  $D_r = \text{diag}(\lambda_1/(1+\lambda_1), \dots, \lambda_r/(1+\lambda_r))$  is a low rank approximation of the Hessian. Detailed information on this can be found in [14] and [2]. Using this approximation, the solution of equation Equation 8 can be determined with a preconditioned Newton-CG method, see [20, 19].

### 3.3 Sparsification of sensor layouts and optimality criteria

Obviously, the trace of the posterior covariance will be minimal exactly when every sensor weight is set to 1, which corresponds to using every available piece of information to reduce the level of uncertainty. Thus, to derive a sparse sensor configuration, a penalty term must be introduced into the optimization problem (Equation 6). A common choice for the regularization term in Equation 6 is the  $\ell_1$ -norm, which leads to a convex minimization problem with a unique minimizer. Specifically, the regularization term is defined as

$$\mathcal{R}(\mathbf{w}) := \alpha \|\mathbf{w}\|_1 = \alpha \mathbf{1}^\top \mathbf{w}, \quad (11)$$

where  $\alpha > 0$  is the regularization parameter and  $\mathbf{1}$  is a vector of ones. Finally, a binary sensor configuration  $\{0, 1\}^q$  is obtained by considering only sensor locations with weights above a certain threshold.

It should be noted that the resulting binary vector is not the optimal binary weight vector. Obtaining such an optimal solution requires solving the  $\ell_0$ -regularized problem considered in [2]. The key idea in that approach is to employ a regularization term based on the number of nonzero entries in  $\mathbf{w}$ , i.e.,

$$\mathcal{R}(\mathbf{w}) := \alpha \sum_{w_i \neq 0} 1.$$

To approximate this discontinuous penalty, a sequence of strictly convex functions  $f_j(\mathbf{w})$  is introduced such that  $f_j(\mathbf{w}) \rightarrow \sum_{w_i \neq 0} 1$  as  $j \rightarrow \infty$ . At each iteration, the optimization problem

$$\min_{\mathbf{w} \in \mathbb{W}} (\Phi[\Gamma_{\text{post}}(\mathbf{w})] + f_j(\mathbf{w}))$$

is solved and the optimizer obtained at iteration  $j$  is used as the initial value for iteration  $j + 1$ . This procedure entails substantially higher computational cost. Moreover, as observed empirically in [2, Section 6.1.4], the sensor configurations obtained using this  $\ell_0$ -approximation strategy offer only marginal

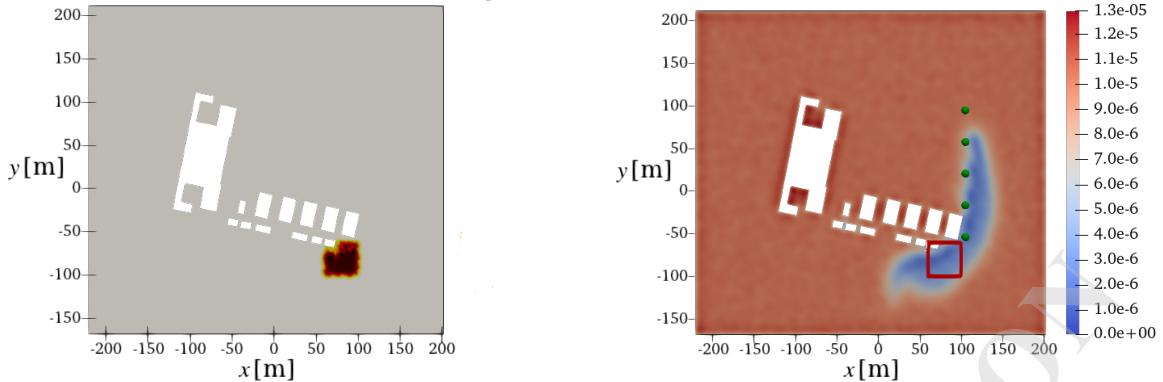


Figure 4: Region of interest  $P$  defining the QoI (left) and point-wise variance  $\sigma^2(x)$  of  $m_{\text{map}}$  obtained with five selected sensors (green spheres, right)

improvement compared with those produced by  $\ell_1$ -regularization followed by a simple thresholding step. Since a highly efficient method is required for the sensor steering presented in Subsection 5.3, we therefore employ an  $\ell_1$ -regularization approach.

The A-optimality criterion for sensor placement minimizes the integrated point-wise posterior variance in linear Bayesian inverse problems:  $\int_{\Omega} \text{Var}[m(x)] dx = \text{tr}(\Gamma_{\text{post}}(\mathbf{w}))$ . To compute the discrete variance field  $\sigma^2(x) := \text{Var}[m(x)]$ , one can extract the diagonal of the inverse Hessian matrix in the finite element basis, assigning each diagonal entry to its corresponding node. However, this exact calculation is computationally expensive ( $O(n_{\text{dof}})$ ), so the reduced-order model (Equation 10) is used for visualization. Figure 4 (right) shows the variance field  $\sigma^2(x)$  of  $m_{\text{map}}$  obtained with a C-optimal sparse sensor layout.

Moreover, the prior covariance is computed using approximate random sampling [20]. Last, but not least, computing the trace of the inverse Hessian is costly. Therefore, we relax A-optimality to a C-optimal design, which requires only the evaluation of the Hessian's action on a fixed vector  $c \in \mathbb{R}^{n_{\text{dof}}}$  [1]. In this case, the design criterion becomes  $\Phi(\mathbf{w}) = c^T \Gamma_{\text{post}}(\mathbf{w}) c$ .

## 4 Goal-orientation and sensor steering

### 4.1 Goal-oriented optimal experimental design

In the next step, the presented method is adjusted to achieve goal-oriented C-optimal experimental designs for stationary sensors. The operator  $\mathcal{P} : D \rightarrow \mathbb{R}$  is first selected so that the design, namely the sensor placement, is optimized to observe initial conditions in an area  $P \subset \Omega$ , shown in Figure 4. This simplification via forward uncertainty quantification, defined by the operator  $\mathcal{P}$ , leads to a C-optimal design for the problem in Equation 7, as described in [1].

The indicator function of a subset, that is the function  $\mathbf{1}_A : \Omega \rightarrow \{0, 1\}$ , which for a given subset  $A$  of  $\Omega$ , attains the value 1 at points in  $A$  and the value 0 at points outside of  $A$  is used to define our operator  $\mathcal{P}$ . If an optimal design for the initial conditions  $m$  is desired, the operator  $\mathcal{P}$  does not depend on the solution  $u$ , or more specifically, it does not depend on the operator  $\mathcal{F}$ . Concretely, the operator for the QoI is given by  $\mathcal{P}(m) := \langle m, \mathbf{1}_P \rangle_{L^2(\Omega)} = \int_P m(\mathbf{x}) d\mathbf{x}$ . By identifying the dual space of  $L^2(\Omega)$  and defining the adjoint

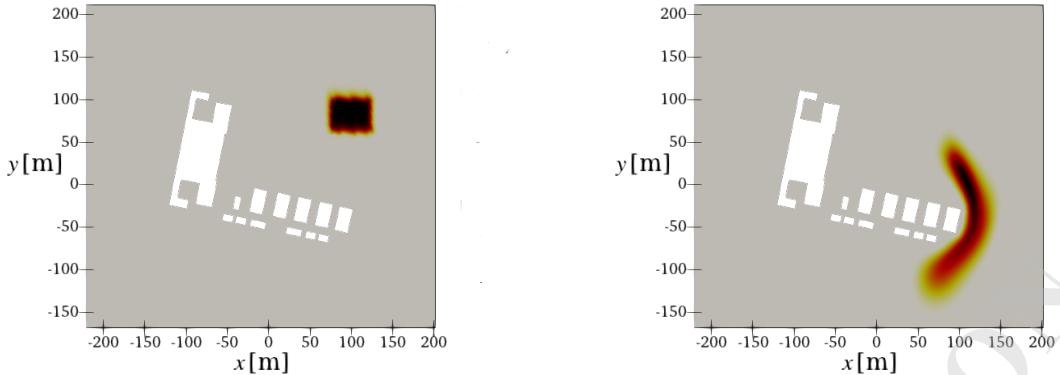


Figure 5: Illustration of an example QoI  $\mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P}$  (kept constant over time, left) and solution  $\mathcal{K}^*(\mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P})(t = 0, \cdot)$  of transport problem induced by adjoint operator  $\mathcal{K}^*$  (right).

operator, it follows that  $\mathcal{P}^* = \mathbf{1}_P$ , and the design function for the optimal experimental design takes the form  $\text{tr}[\Gamma_{\text{post}}(\mathbf{w})] = \langle \mathbf{1}_P, \Gamma_{\text{post}}(\mathbf{w}) \mathbf{1}_P \rangle_{L^2(\Omega)}$ . In a finite element setting, the function  $\mathbf{1}_P$  is represented by a vector  $c \in \mathbb{R}^{n_{\text{dof}}}$  via the usual projection, i.e.,  $\mathbf{1}_P - c_h \perp \mathcal{V}_h$  into the finite element space  $\mathcal{V}_h = \{\phi_1, \dots, \phi_{n_{\text{dof}}}\}$ . According to [1, Section 4.1], the design function is given by  $\Phi(\mathbf{w}) = c_h^T M \mathcal{H}_h^{-1}(\mathbf{w}) c_h$ . Together with a suitable regularization term, e.g.,  $\alpha \|\mathbf{w}\|_{l^1}$ , an optimal design can be obtained by minimizing the objective  $c_h^T M \mathcal{H}_h^{-1}(\mathbf{w}) c_h + \alpha \|\mathbf{w}\|_{l^1}$  which is illustrated in Figure 4. If this procedure is generalized to determine an optimal sensor placement for the contaminant concentration over a specific spatial region and time interval, the operator  $\mathcal{P}$  must be extended accordingly. Specifically, by defining  $\mathcal{P}$  via a subset of space-time, e.g.,  $[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P$ , the operator  $\mathcal{P}$  is then constructed as

$$\mathcal{P}(m) = \int_0^T \int_{\Omega} \mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P} \mathcal{K}(m)(t, \mathbf{x}) dt d\mathbf{x} = \int_{T_0^{\text{QoI}}}^{T_{\text{final}}^{\text{QoI}}} \int_P u(t, \mathbf{x}) dt d\mathbf{x}.$$

Again, the adjoint of  $\mathcal{P}$  is needed. For this, we calculate

$$\begin{aligned} \mathcal{P}^*(1)(\hat{m}) &= \langle \mathcal{K}(\hat{m}), \mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P} \rangle_{L^2(\Omega)} \\ &= \langle \hat{m}, \mathcal{K}^* \mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P} \rangle_{L^2(\Omega)}, \end{aligned}$$

and therefore the map  $c$  is obtained by  $c := \mathcal{P}^*(1) = \mathcal{K}^*(\mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P})$ , since  $\hat{m}$  was arbitrary. More precisely, the map  $c$  satisfies the following PDE:

$$\begin{aligned} -c_t - \kappa \Delta c - \text{div}(\mathbf{v} c) &= \mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P} && \text{in } (0, T) \times \Omega, \\ (\mathbf{v} c + \kappa \nabla c) \cdot \mathbf{n} &= 0 && \text{in } (0, T) \times (\Gamma_+ \cup \Gamma_0), \\ c &= 0 && \text{in } (0, T) \times \Gamma_-, \\ c(T, \cdot) &= 0 && \text{in } \Omega. \end{aligned} \tag{12}$$

In Figure 5 (left) an example of a constant-over-time QoI  $\mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P}$  is shown. The corresponding map  $c(t = 0)$  is visualized in Figure 5 (right). Returning to the definition, the objective for the goal-oriented sensor design reads

$$\begin{aligned} \Phi(\mathbf{w}) &= \mathcal{P} \mathcal{H}^{-1}(\mathbf{w}) \mathcal{P}^*(1) = \mathcal{P}(\mathcal{H}^{-1}(\mathbf{w}) c) \\ &= \langle \mathcal{K}(\mathcal{H}^{-1}(\mathbf{w}) c), \mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P} \rangle_{L^2(\Omega)} \\ &= \langle \mathcal{H}^{-1}(\mathbf{w}) c, \mathcal{K}^*(\mathbf{1}_{[T_0^{\text{QoI}}, T_{\text{final}}^{\text{QoI}}] \times P}) \rangle_{L^2(\Omega)} = \langle c, \mathcal{H}^{-1}(\mathbf{w}) c \rangle_{L^2(\Omega)}. \end{aligned}$$

Thus, the time-dependent case is reduced to the fact that an optimal design for initial conditions for the transported QoI  $c$  must be found and coincides with the first case.

For the numerical evaluation of this objective function and its gradient, which are required to minimize the regularised design function using the L-BFGS-B solver, we start again with the inverse low-rank approximation of the Hessian from Equation 10 and proceed to compute the design function as follows

$$\Phi(\mathbf{w}) = \langle c, \mathcal{H}^{-1}(\mathbf{w})c \rangle_{L^2} \approx c_h^T \mathcal{A}_h^{-1} (I - V_r D_r V_r^T) \mathcal{A}_h^{-1} c_h.$$

For a shorter notation, we set  $\hat{q}_h := (I - V_r D_r V_r^T) \mathcal{A}_h^{-1} c_h$ ,  $q_h := \mathcal{A}_h^{-1} \hat{q}_h$  and obtain  $\Phi(\mathbf{w}) \approx c_h^T q_h$  and so the calculation of the trace consists only a projection in the low rank subspace and solutions of an elliptic problem  $\mathcal{A}$  resp.  $\mathcal{A}_h$ , for which very fast solving strategies exists. To calculate the derivative, we follow [2] and conclude for this simplified case

$$\frac{\partial}{\partial \mathbf{w}_i} \Phi(\mathbf{w}) = (\mathcal{F}^i(q))^2 \approx (\mathcal{F}_h^i \circ \mathcal{A}_h^{-1}(\hat{q}))^2 \quad (13)$$

So, this calculation can be replaced by a surrogate model for the preconditioned forward operator. In principle, this procedure can be extended to a stronger, A- or D-optimal design.

## 4.2 Dynamic sensor steering based on goal-oriented optimal sensor placement

A method will now be presented which is capable of dynamically controlling a sensor in such a way that a greater knowledge of the actual contaminant concentration can be generated. We assume that some knowledge about the concentration is already available due to certain stationary sensors, i.e., that the true contaminant already possesses an appreciable concentration at the sensor location, to permit a solution to the inverse problem. This situation can be seen in Figure 6. We then set the QoI so that its center point is at the maximum of the reconstructed initial condition. The optimum design is then calculated on this basis and the sensor is steered to the position with the highest weight  $\mathbf{w}$ . The next measurement is then awaited and the procedure is started again from the beginning. The method is shown schematically in Figure 7. In this way, we obtain a trajectory  $\gamma : \{t_0^{\text{obs}}, \dots, t_s^{\text{obs}}\} \rightarrow \{\mathbf{x}_0^{\text{obs}}, \dots, \mathbf{x}_s^{\text{obs}}\}$  for the steered sensor.

## 5 Numerical results of optimal experimental designs

In order to simulate scenarios on real-world domains, we use a highly automated process for grid generation. Building imprints as obstacles for two-dimensional contaminant transport are imported directly from Open Street Map (OSM), and locally refined triangular meshes are generated for the region of interest [7]. The forward model is implemented with stabilized linear Lagrange finite elements in the software framework **FEniCs** [6]. The **FEniCs** extension **hIPPYlib** (Inverse Problem PYthon library [20]) was used in the implementation of the inverse problem.

In the three following inverse problem OED examples, we use the forward simulation of Equation 1 illustrated in Figure 2 as the ground truth. Two radially symmetric functions

$$m_{\mathbf{x}_s}(\mathbf{x}; \mathbf{x}_s, r) = \min \left\{ 0.5, \exp \left( -\ln(\epsilon) \|\mathbf{x} - \mathbf{x}_s\|_2^2 / r^2 \right) \right\}, \epsilon = 0.001$$

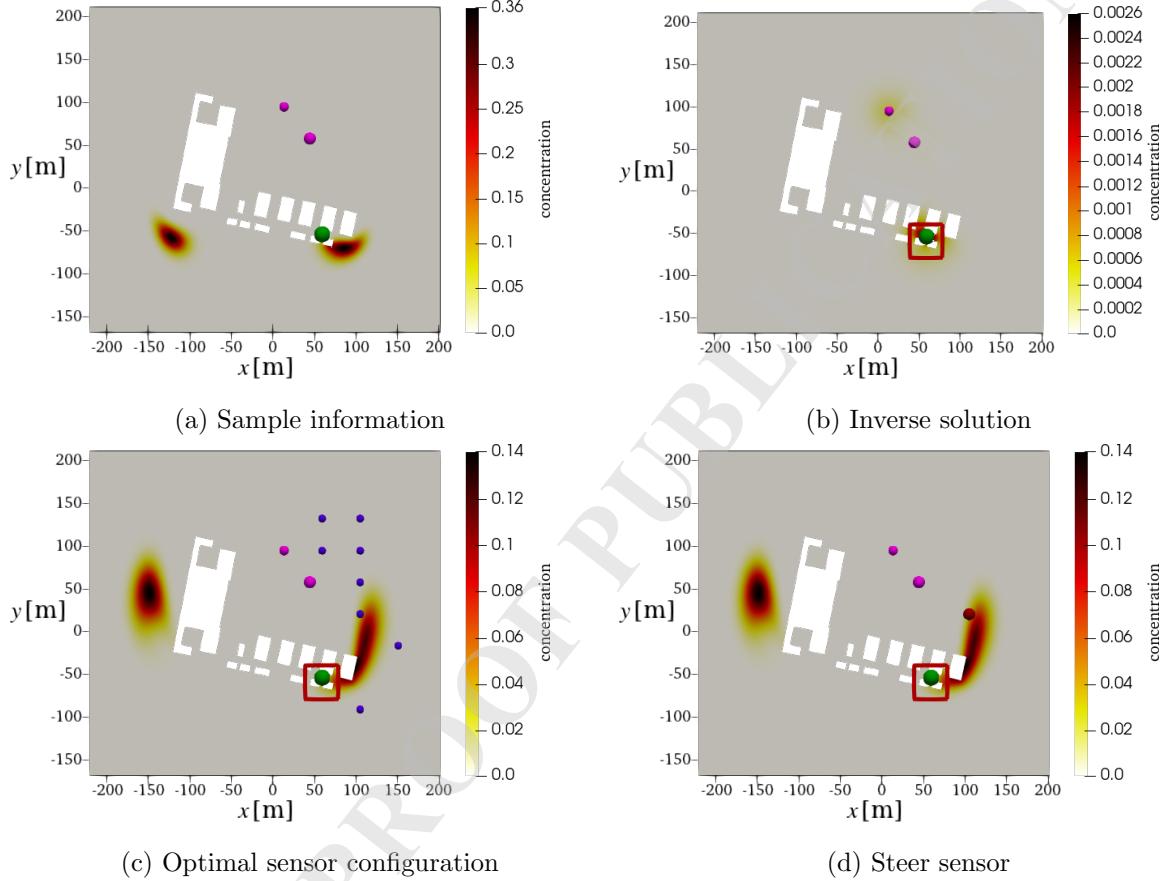


Figure 6: Dynamic sensor steering test case with stationary sensor (green) and mobile sensor (purple trajectory). (a) True concentration field at  $u(\cdot, t = 2.2\text{ s})$  during the second steering time step, (b) Maximum-a-posteriori estimate  $m_{\text{map}}$  of inverse problem and algorithmically selected zone of interest (red square), (c) optimal sensor design, (d) target position of the mobile sensor (red sphere), true concentration field  $u(\cdot, t = 7\text{ s})$  in background of (c) and (d) to visualize transport problem dynamics

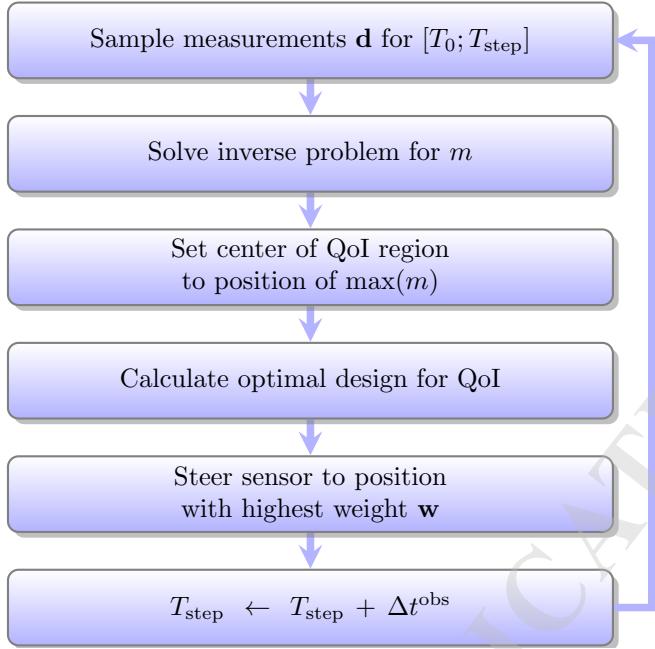


Figure 7: Algorithm for dynamic sensor steering based on goal-oriented sensor placement [22, 23].

describe the initial concentration field,

$$u_0(\mathbf{x}) = m_{\mathbf{x}_s}(\mathbf{x}; \mathbf{x}_s = [-100 \text{ m}, -80 \text{ m}], r = 25 \text{ m}) + m_{\mathbf{x}_s}(\mathbf{x}; \mathbf{x}_s = [75 \text{ m}, -80 \text{ m}], r = 25 \text{ m}). \quad (14)$$

The initial concentration field is transported by the vector field  $\mathbf{v}$ . For the considered test cases, we estimate a stationary wind vector field as solution of the incompressible Navier-Stokes equations with wind entering the given geometry from the south at a velocity of  $\mathbf{v} = 10 \text{ m s}^{-1}$ . This condition is realized using a Dirichlet boundary condition. In the inner boundaries that represent the imprints of the buildings, a no-slip condition is applied. The remaining edges correspond to free boundary conditions. For the chosen Reynolds number of 50, we obtain the laminar wind field visualized in Figure 2. Moreover, the diffusion coefficient is selected as  $\kappa = 1 \text{ m}^2 \text{ s}^{-1}$  resulting in a transport problem with a moderate Peclet number. Finally, the time step size for the implicit Euler time-stepping scheme is set to 0.05 s. In the parametrization of the prior, the constants were chosen as  $\eta = 8$  and  $\gamma = 800$ , yielding the operator  $\mathcal{A} := 8I - 800\Delta$ .

In order to make this problem computationally feasible, reduced-order models (ROMs) of the forward and adjoint operators are derived. Considering the forward operator  $\mathcal{F}_h : \mathbb{R}^{n_{\text{dof}}} \rightarrow \mathbb{R}^q$ , it is observed that it constitutes a linear mapping from a high-dimensional to a lower-dimensional space. Thus, a singular value decomposition is performed to construct a ROM; see also [13, 15]. The decomposition provides singular values  $\lambda_1 \geq \dots \geq \lambda_r$ , an  $L^2$ -orthogonal basis  $U_r = (u_1, \dots, u_r) \in \mathbb{R}^{n_{\text{dof}} \times r}$  and an orthogonal basis  $V_r = (v_r, \dots, v_r) \in \mathbb{R}^{q \times r}$ . During the online phase, for example, when the precomputed reduced-order model (ROM) is used for sensor steering, the selected initial condition is projected, such that only matrix-vector multiplications are required:

$$\mathcal{F}_h(m_h) \approx V_r D_r U_r M m_h,$$

where  $m_h \in \mathbb{R}^{n_{\text{dof}}}$  and  $D_r = \text{diag}(\lambda_1, \dots, \lambda_r)$ .

As discussed in Equation 9 and Equation 13, it is also viable to construct a ROM directly for the

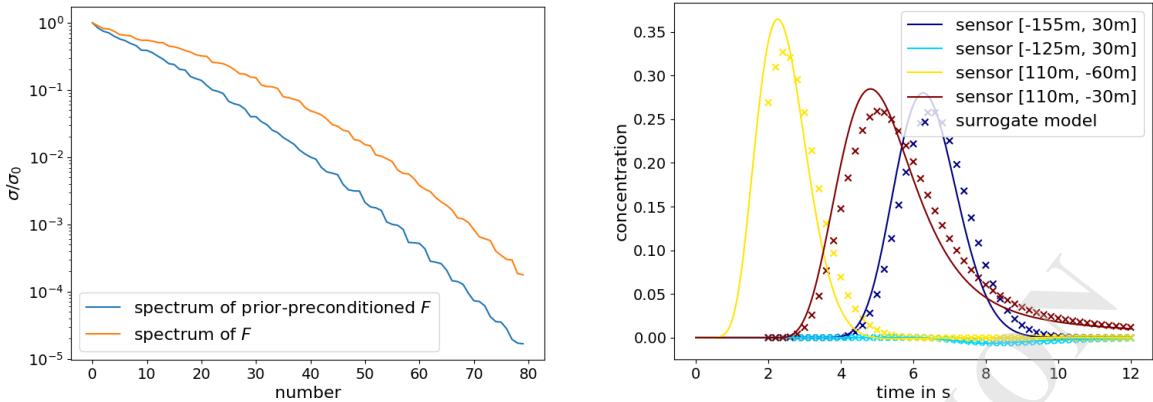


Figure 8: Reduced-order modeling. Decay of singular values of  $\mathcal{F}_h$  and of preconditioned  $\mathcal{F}_h \circ \mathcal{A}$  (left), comparison of ROM and forward model  $\mathcal{F}_h$  evaluated at sensor positions (right).

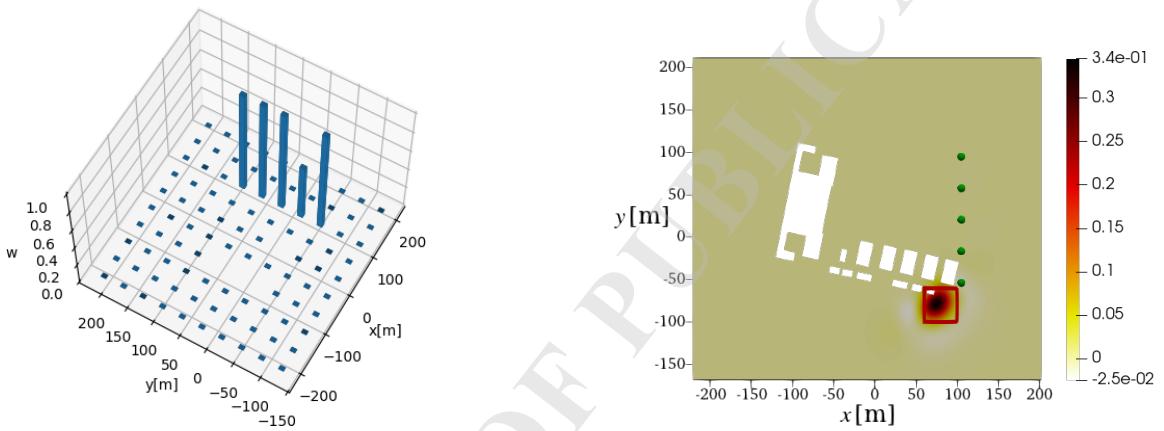


Figure 9: OED 1. Weights of optimal sensor configuration to monitor  $P_1$  (left) and reconstructed initial condition (right, ground truth shown in Figure 2).

preconditioned forward operator. The singular values of the operators  $\mathcal{F}_h$  and  $\mathcal{F}_h \circ \mathcal{A}$  are compared in Figure 8 (left). It is observed that the singular values of the preconditioned operator decay faster and therefore less computations have to be performed to construct a ROM with acceptable accuracy. Figure 8 (right) shows that the ROM approximates the forward operator fairly well. Furthermore, the computed singular value decomposition is reused to approximate the adjoint operator  $\mathcal{F}_h^* : \mathbb{R}^q \rightarrow \mathbb{R}^{n_{\text{dof}}}$  with a ROM as well, namely,  $\mathcal{F}_h^*(y) \approx M U_r D_r V_r y$ , for  $y \in \mathbb{R}^q$ .

To assess the benefits of the reduced model in the context of forward evaluations, we first performed a single evaluation of the full-order model, which required approximately 1s on our hardware. To simulate a scenario relevant to optimal sensor placement, the reduced model was used to evaluate the full-order model at 96 spatial positions over 90 time instances, resulting in a total of  $q = 8640$  measurements. In total, we calculated 200 spectral values. On average, each evaluation of the reduced model took 6.25 ms, yielding a relative speedup of approximately 160 compared to the full-order model.

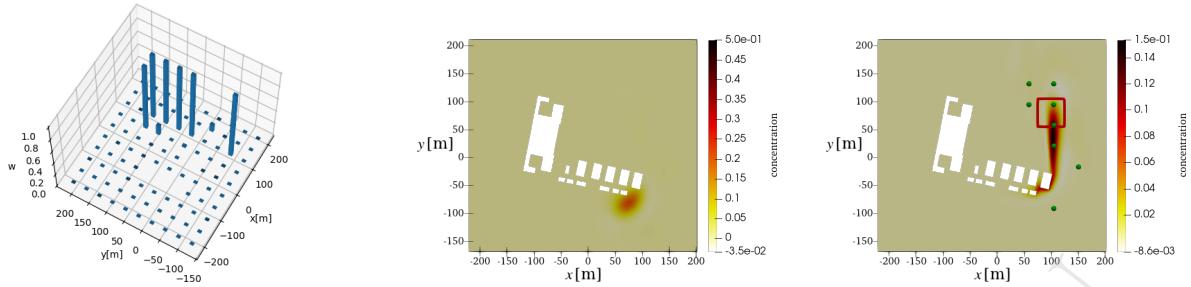


Figure 10: OED 2. Weights of optimal configuration to monitor concentration evolution in  $\mathcal{P}_2$  (left), reconstructed initial condition (middle), prediction of concentration for  $T = 10$  s (right)

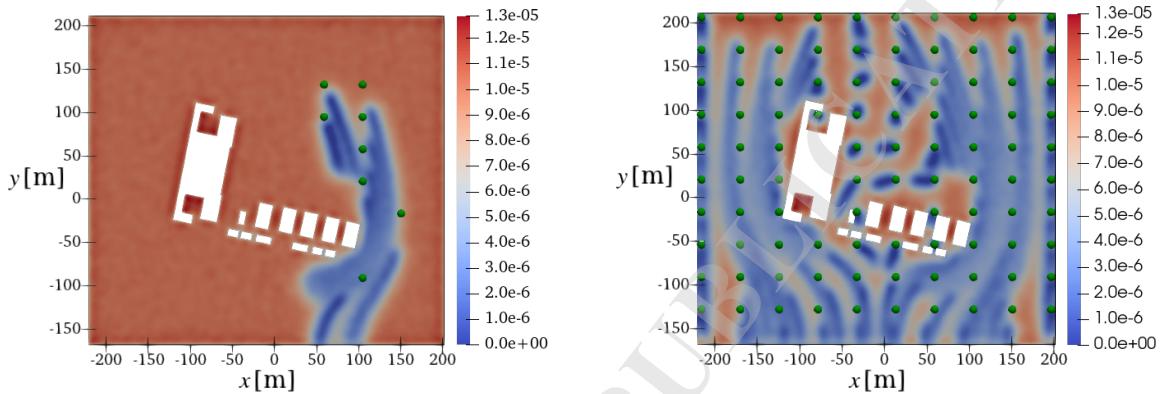


Figure 11: OED 2. Point-wise variance  $\sigma^2$  as measure of the uncertainty of the inferred parameter for the optimal configuration for  $\mathcal{P}_2$  (left) compared to the full sensor grid (right)

### 5.1 OED 1. Sensor configuration to reconstruct initial condition in critical area

As first example for a goal-oriented optimal experimental design, we address the problem of identifying an optimal sensor layout to recover the initial condition in a defined subset of the computational domain  $P_1 := \{(x, y) \in \Omega \mid 75 \leq x \leq 125, -100 \leq y \leq -60\}$ . In a practical application,  $P_1$  might represent a critical area of a chemistry plant site where hazardous material is stored. The inverse problem is posed under the assumption that only stationary sensors are used. These sensors sample the concentration at a rate of 5 Hz, beginning at  $T_0 = 2$  s. Measurements taken after 12 s are not taken into account. A noise variance of  $\sigma^2 = (0.005)^2$  is assumed, resulting in a signal-to-noise ratio of approximately  $\text{SNR} \approx 100$ . Moreover, a regularization parameter of  $\alpha = 0.1$  is applied to obtain a sparse sensor configuration, see Equation 11. The selected domain where the quantity of interest (QoI) is inferred is indicated in Figure 4 (left), along with the optimal sensor configuration (Figure 4 (right)). Moreover, the point-wise variance, which represents the uncertainty in the reconstruction, is also illustrated in Figure 4. The solution to the inverse problem represented by  $m_{\text{map}}$  is visualized in Figure 9. The numerical result demonstrates a reconstruction quality in  $P_1$  comparable to that achieved using the full configuration with 96 sensors (Figure 3) in contrast to 5 optimally selected sensors in OED 1.

## 5.2 OED 2. Configuration to monitor concentration evolution in critical area

In the second scenario, our aim is to secure a specific area for a given time period. To achieve this, the quantity of interest (QoI) is defined to depend on the state  $u$ . To create a meaningful scenario, we shift  $P_2 := \{(x, y) \in \Omega \mid 75 \leq x \leq 125, 60 \leq y \leq 100\}$  upwards. The goal of OED 2 is to ensure that concentration values can be predicted correctly in region  $P_2$  during the time from 5 s to 12 s. This formulation results in the following operator:

$$\mathcal{P}_2(m) = \int_{T_0^{\text{QoI}}=5 \text{ s}}^{T_{\text{final}}^{\text{QoI}}=12 \text{ s}} \int_{P_2} \mathcal{K}(m)(t, \mathbf{x}) dt d\mathbf{x} = \int_{T_0^{\text{QoI}}=5 \text{ s}}^{T_{\text{final}}^{\text{QoI}}=12 \text{ s}} \int_{P_2} u(t, \mathbf{x}) dt d\mathbf{x}.$$

The sensor weights  $\mathbf{w}$  in Figure 10 are calculated using a regularization parameter of  $\alpha = 1.0$ . In this case as well, the source relevant to the QoI is reconstructed accurately using the optimized sensor configuration. The reconstructed initial condition and the corresponding prediction are shown in Figure 10. As illustrated in Figure 11, the reduction in uncertainty is concentrated primarily in the region relevant to QoI compared to the complete sensor configuration.

## 5.3 OED 3. Dynamic sensor steering for source identification

Finally, the sensor steering method described in Subsection 4.2 is tested in a numerical application case with  $\kappa = 10 \text{ m}^2 \text{ s}^{-1}$ . To steer the sensor, a much finer sensor grid totaling 1511 possible sensor locations is used. In this formulation, the moving sensor is allowed to take one step on this grid per cycle, which needs 0.2 s and thus corresponds to the measurement frequency of 5 Hz. This corresponds to a speed of approximately  $40 \text{ m s}^{-1}$  for the moving sensor. To demonstrate the capabilities of the sensor steering approach, we placed a single stationary sensor just behind one of the obstacles. However, due to the transport characteristics in this region, information solely from this stationary sensor results in an inaccurate reconstruction of the source, which grossly underestimates the degree of contamination further from the buildings. In addition to the stationary sensor, measurements from a mobile sensor are available. The measurement process begins at time  $T_0 = 2 \text{ s}$ , with data collected at a frequency of 5 Hz. The state  $u$  at  $T_{\text{step}} = T_0 = 2 \text{ s}$  is shown in Figure 12 (a). At this point, the stationary sensor receives very limited information and is thus unable to provide an accurate source estimate. However, computing the optimal sensor design based on the current quantity of interest (QoI), defined as the integral over a square measuring 40 m on each side, centered on the maximal point of the reconstructed initial condition, yields favorable estimates for informative measurement positions. The mobile sensor is then directed toward the location associated with the highest weight  $\mathbf{w}$ , as determined by the C-optimal design criterion, computed over the observation period  $[T_{\text{step}}, T_{\text{step}} + 2 \text{ s}]$  with the same sampling rate of 5 Hz, wherein we take as sensor weights in the time leading up to  $T_{\text{step}}$ , the actual past locations of the sensor. In the subsequent time steps, illustrated in Figure 12 (c), the sensor continues to move toward regions of increasing concentration. In Figure 12 (d), corresponding to  $T_{\text{step}} = 4.6 \text{ s}$ , the mobile sensor has found the core of the contaminant. Finally, Figure 12 (e) and (f) demonstrate that the mobile sensor continues to accurately pursue the contaminant in further time steps. Comparing the performance of the stationary sensor with that of the combination of a stationary sensor and a dynamically steered one, we find, as depicted in Figure 13, that the mobile sensor achieves substantially improved reconstruction

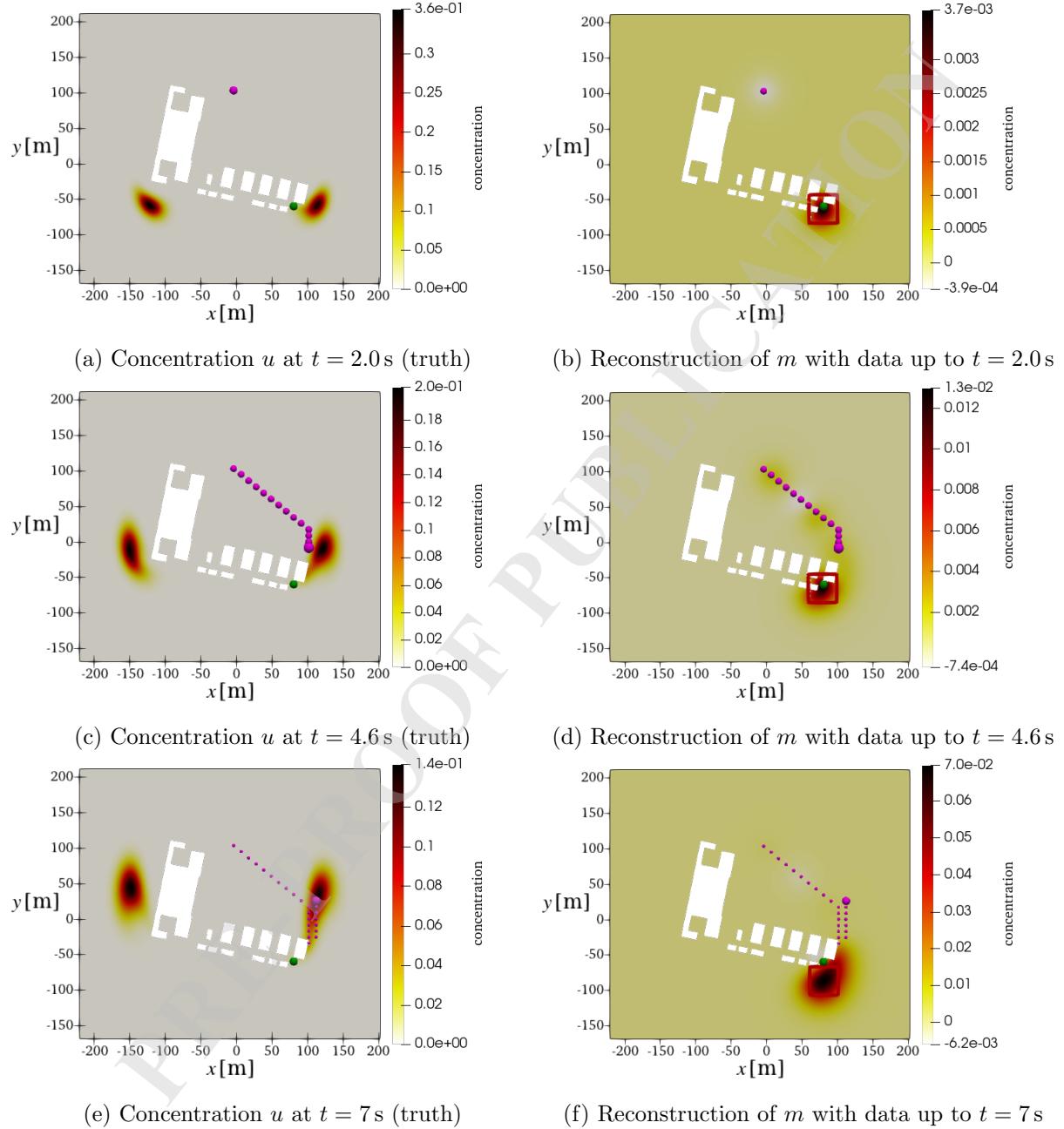


Figure 12: OED 3. Data fusion of stationary sensor (marked in green) and mobile sensor (marked in purple). Mobile sensor steered to maximize information gain (trajectory marked with small purple spheres)

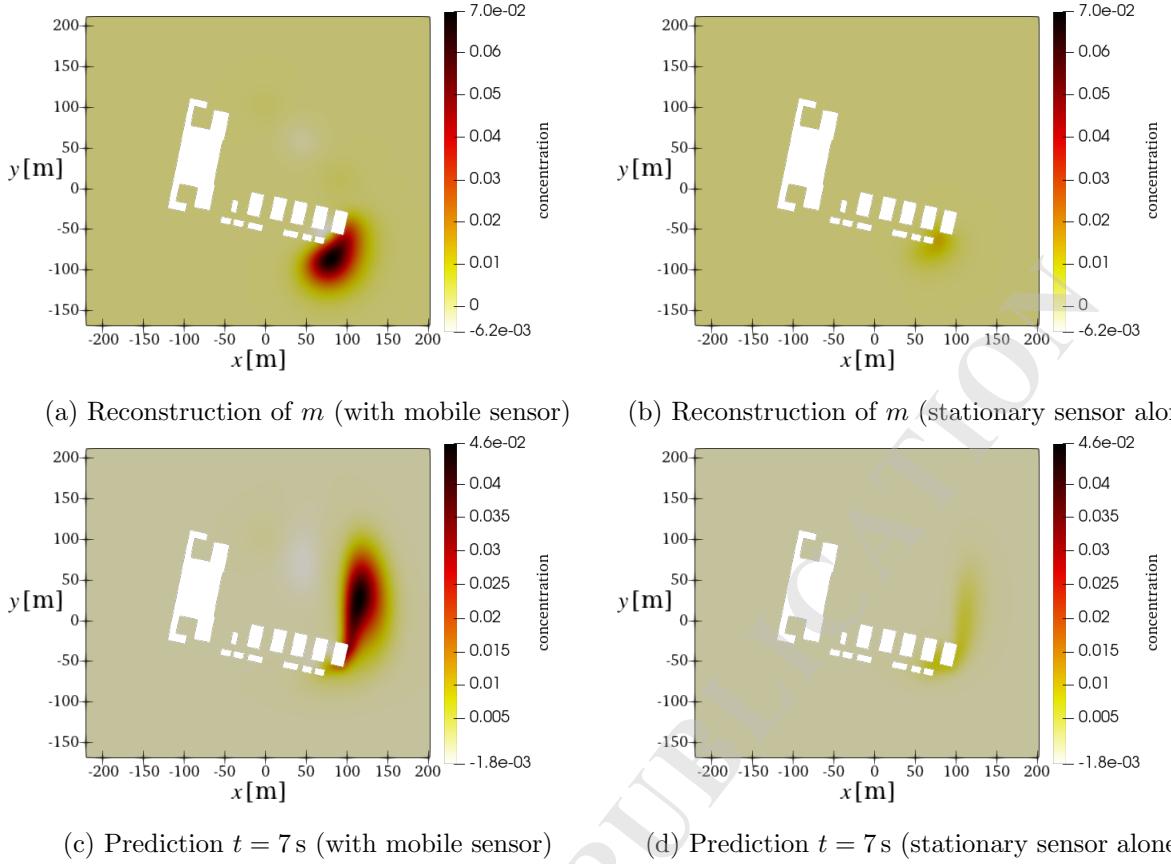


Figure 13: OED 3. Comparison of predictions based on data fusion of mobile sensor and stationary sensor (left column) and stationary sensor alone (right column)

accuracy after just 7 s, in contrast to the stationary sensor, which fails to produce a reliable estimate even after 12 s.

## 6 Conclusion and Outlook

This paper investigated a novel approach for goal-oriented optimal static sensor placement and dynamical sensor steering for PDE-constrained problems. Adopting previous work by Wogrin et al. [23, 22] on dynamic sensor steering, we leverage a Bayesian approach for the solution of the inverse problem, accelerated by offline-computations of low-rank approximations for the Hessian matrix and an online preconditioned inexact Newton-CG method. The resulting framework was then applied to a more complex geometry extracted from real-world map data. We showcased the strengths of the proposed workflow on three application cases from the field of airborne contaminant transport: In the first example, we derived an optimal placement of stationary sensors to recover the initial condition inside a spatially constrained rectangular region. The results showed that our proposed method only requires five sensors to reconstruct the initial condition locally with an accuracy comparable to the full configuration of 96 sensors. In our second example, we extended the QoI in the sense that a region of interest is monitored not only at a specific time instance, but over a fixed time period. From a practical point of view, this corresponds to the goal of securing a specific area for a given time period. Using only eight sensors, the evolution of the concentration was accurately

reconstructed and the uncertainty was minimized in the area of interest. Lastly, we investigated a dynamic sensor steering problem. Here we showed, that while we are still able to roughly predict the general shape of the initial condition with an unfavorably placed stationary sensor, adding a mobile sensor we obtain much better agreement with the true solution while simultaneously reducing the required measurement time to one-third of the stationary case. This proves that the presented method is able to successfully handle the complexity of a moving sensor and steer the sensor to achieve a fast and reliable reconstruction of the (in practice unknown) initial condition.

While we believe this work to be an important step towards optimally steering unmanned sensor platforms in crisis situations, there still remain several points for improvement and further investigation of the proposed algorithm. One potential area for improvement concerns the mathematical formulation and solution of the inverse problem. In many applications, it is reasonable to assume that the initial condition is sparse. Integrating this additional knowledge into the solution procedure is expected to speed up the time to solution and further improve real-time capabilities of the method [17]. Moreover, we plan to extend the sensor steering to Reinforcement Learning based approach, where the position and size of the QoI in each step is determined by an agent that was previously trained based on trial-and-error interactions with the forward model [12].

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