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PHORTEX: Physically-Informed Operational Robotic Trajectories for Scientific Expeditions

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Abstract: Mobile robots are increasingly used to collect valuable in situ samples during scientific expeditions. However, many phenomena of scientific interest—deep-sea hydrothermal plumes, algal blooms, warm-core eddies, and lava flows—are spatiotemporal distributions that evolve on spatial and temporal scales that complicate sample collection. Here, we consider the problem of charting the space-time dynamics of deep-sea hydrothermal plumes with the state-of-the-art autonomous underwater vehicle (AUV) Sentry. In the hydrothermal plume charting problem, the plume state is driven by complicated and unobserved dynamics in the deep sea. To effectively sample the moving plume, an autonomy system must infer plume dynamics from sparse, point observations, while respecting operational constraints of AUV Sentry that restrict the set of possible trajectories to nonadaptive, uniform-coverage patterns. We frame the plume charting problem as a sequential decision-making problem and formulate a mission planner PHORTEX (PHysically-informed Operational Robotic Trajectories for EXpeditions) that strategically designs full mission trajectories for Sentry, where each mission plan is informed by the observations of the last. PHORTEX is composed of a trajectory optimizer, which maximizes expected samples collected within a moving plume, and PHUMES (PHysically-informed Uncertainty Models for Environment Spatiotemporality), a modeling framework that leverages an embedded simulator of idealized plume physics as an inductive bias to enable dynamics learning from extreme partial observations and a few Sentry deployments. In both simulation and in field trials at a hydrothermal site in the Gulf of California, we demonstrate that Sentry

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http://fieldrobotics.net
using PHORTEX learns to track a moving hydrothermal plume and gather samples that significantly improve upon baseline spatial and temporal diversity for use in downstream science tasks.

**Keywords:** planning under uncertainty, exploration, marine robotics, physics-based learning, environmental monitoring

### 1. Introduction

Transient, dynamic phenomena—deep-sea hydrothermal plumes, algal blooms, warm core eddies, lava flows—are of interest in many disciplines of observational science. *Expeditionary science* encapsulates the observational sciences that require *in situ* sample collection of environmental phenomena for scientific discovery and model development. In such cases, the environmental targets are typically impossible to observe using remote sensing (e.g., satellites) either due to desired spatial and temporal resolution, environment adversity (e.g., the deep sea, within closed structures), or the nature of the scientific target of interest and corresponding sensing equipment (e.g., building a taxonomy of algae requires physically processing water samples). Expeditionary science is, by definition, conducted in partially-observable and often dynamic environments; performing useful and effective data collection in expeditionary science poses a challenge for human and autonomous decision-makers alike.

In this paper, we study a particular problem within the expeditionary sciences: mapping the space-time dynamics of deep-sea hydrothermal plumes using an autonomous mobile robot. Deep-sea hydrothermal plumes are a source of chemicals and particulates that play a significant role in biogeochemical cycling in the deep ocean (Le Bris et al., 2019; Resing et al., 2015; Dick et al., 2013; Vic et al., 2018; Scholz et al., 2019). Understanding the fate of chemicals and particulates in hydrothermal plumes is of significant interest to biogeochemists and physical oceanographers, and is pertinent to topical discussions on mining the ocean floor for rare materials and the use of the ocean as a location for carbon sequestration. However, directly studying plumes in the water column is a substantial challenge. Deep-sea plumes are driven by complex forces that are generally difficult to observe: advective forces (e.g., deep currents, topographic updrafts), diffusion, and turbulent mixing act on plumes as they rise through the water column. A robot tasked with charting a plume must be able to forecast where and when it will intersect with different regions of the plume, but must do so using only incomplete information about these underlying dynamics provided by noisy and indirect sensors. The challenge of plume charting is exacerbated by the inherent difficulty of sensing a plume using chemical sensors; the chemical distribution of a plume can only be observed with point sensors and each individual point measurement provides only a small amount of information about the holistic plume structure.

In addition to the technical challenges of determining a sensing strategy for a highly uncertain and dynamic phenomenon, the deep-sea environment (>200 m depth) can only be accessed by depth-capable equipment that is often significantly constrained by operational and safety policies. For example, depth-capable autonomous underwater vehicles (AUVs) are typically restricted to execute preset trajectories hand-designed by human scientists (e.g., Camilli et al. 2010). In this mode, the AUV cannot react to measurements while executing a set trajectory. These “open-loop” trajectories can result in sparse measurements of the target phenomenon, such as a dynamic plume, or can miss short-lived events entirely (Flaspohler et al., 2019; Preston, 2019). However, this open-loop concept of operations remains the state-of-the-art in practical deep-sea science because preset trajectories are easy to encode, do not require extensive on-platform computing resources, and result in predictable robot actions that can easily be supervised. Here, we consider constraints of a specific robot: the AUV *Sentry*. *Sentry* is operated by the National Deep Submergence Facility (NDSF) at the Woods Hole Oceanographic Institution (WHOI) (Kaiser et al., 2016) and, by operational policy, typically only executes predetermined trajectories, making significant online adaptation of trajectories impossible.

Enabling depth-capable robots such as *Sentry* to perform expeditionary science and study spatiotemporal phenomena using preset, nonadaptive behaviors requires an autonomy system that
can design fixed trajectory patterns strategically to maximize observations of dynamic phenomena. This autonomy system should learn to forward simulate the dynamics of the target environment over a long-horizon from a small history of robot deployments and plan subsequent deployments using these predictions. This is fundamentally a sequential decision-making problem, and is closely related to informative path planning (IPP) problems, in which a robot selects information-gathering behaviors often using a probabilistic model of the environment. Existing methods for IPP (e.g., Hitz et al. 2017; Hollinger and Sukhatme 2013; Flasphober et al. 2019; Levine et al. 2010; Binney and Sukhatme 2012), the related field of experimental design and optimal sensor placement (e.g., Krause et al. 2008; Wang et al. 2019), and general decision-making under uncertainty (e.g., Sunberg and Kochenderfer 2018; Somani et al. 2013; Kocsis and Szepesvári 2006; Silver and Veness 2010) have demonstrated that sequential decision making can be applied to problems in which online, adaptive behaviors are possible, the phenomenon of interest is static, and/or there is an opportunity to train the belief model from many trials, multiple sensors, or highly adaptive trajectories. Each of these typical scenarios is violated for the expeditionary science sampling problem. Here, we propose an autonomy system, PHORTEX (PHysically-informed Operational Robotic Trajectories for EXpeditions), that addresses each of these real-world constraints using a science-informed observational model, physics-based belief representation PHUMES (PHysically-informed Uncertainty Models for Environment Spatiotemporality), and operationally constrained planner (Figure 1). Code for PHORTEX can be found at https://github.com/expeditionary-robotics/phortex.

1.1. Contributions

In this article, we formulate and demonstrate an autonomy system, PHORTEX, to solve the hydrothermal plume charting problem while respecting the strict operational constraints placed on...
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State-of-the-art deep sea robots, like AUV *Sentry*, which are often required to execute preplanned trajectories that cannot be adapted online. PHORTEX implements *deployment by deployment* mapping of dynamic spatiotemporal phenomena, treating each deployment as a single action in a sequential decision-making problem with few steps and performing a one-step myopic optimization over each deployment in turn. Within a single deployment, PHORTEX optimizes flexible chains of trajectory primitives, e.g., uniform coverage “lawnmower” trajectories, defined by a small set of parameters, including relative size, resolution, and position, to enable AUV *Sentry* to track a moving plume. Unlike previous nested-lawnmower approaches for adaptive plume-source localization, our approach leverages model-informed, preplanned trajectories to meet deep-sea safety constraints while charting a dynamic hydrothermal plume.

To inform trajectory planning, we introduce the PHUMES model, which generates long-horizon dynamic plume forecasts from the sparse, complex observations gathered in each deployment. PHUMES overcomes the shortcomings of state-of-the-art probabilistic models for robotic adaptive sampling—typically tasked with interpolation rather than prediction tasks, or requiring a large corpus of data to effectively train—by leveraging an analytical model of buoyant plume dynamics directly within a Bayesian filtering framework. By virtue of being a physically-informed belief representation, PHUMES enables rapid, sample efficient model discovery in severely constrained mission settings and contexts (e.g., no prior environmental data, extreme partial observability, and limited opportunities for sample collection). PHUMES produces forecasts that summarize the dynamic structure of a spatiotemporally evolving plume and can be used to position a robot to encounter plume fluid, while representing the uncertainty in plume predictions. Together, PHORTEX and PHUMES effectively extend modern informative path-planning, plume-hunting, and front-tracking techniques that rely on underway adaptive behaviors into a decision-making framework well-suited for modern scientific expeditions with nonadaptive robots by embedding task and context specific information within the decision-making loop.

We deployed and evaluated PHORTEX with PHUMES on AUV *Sentry* in a real field trial for hydrothermal plume charting. To enable this field trial, we additionally present a method for classifying *in situ* observations taken by instruments on *Sentry* as either plume fluid or ambient seawater and we adapt the PHUMES model—leveraging its underlying plume simulator—to incorporate external sensing equipment available during expeditions. Through both field trials and complementary validation in simulation, we demonstrate that *Sentry* using PHORTEX collected more spatially and temporally diverse plume-derived fluid samples as compared with science-expert designed surveying approaches. Further, these results demonstrate the first iterative offline planning technique for plume charting with deep-sea capable vehicles in the field. This novel capability for deep-sea assets puts deep-sea hydrothermal fields, which comprise 75% of all known vent fields (Beaulieu et al., 2013), in reach for strategic charting and surveying.

2. Background

2.1. Charting Deep-Sea Hydrothermalism

Hydrothermal vents in the ocean were first observed in 1977 at the Galapagos Rift (Corliss et al., 1979), and since have been a concerted focus of geodynamical and biogeochemical studies. Venting sites, energized by magmatic sources, release fluids between 20 °C–400 °C (background deep ocean temperatures are approximately 2 °C) that are imbued with minerals, metals, dissolved gases, and other compounds (Jannasch and Mottl, 1985; Martin et al., 2008). These warm, nutrient-pumping sites in the deep ocean have created oases for unique micro- and macrofauna (Corliss et al., 1979). Detection and characterization of seafloor hydrothermal venting is critical for understanding fundamental interactions between the deep ocean, its underlying basaltic crust, the deep biosphere, and (bio)geochemical fluxes.

Hydrothermal plumes are driven by density differences between super-heated fluid at seafloor geothermal vents and the cold background seawater, creating a buoyancy force that causes the vent fluids to rise. The plume is typically chemical and particulate rich, and while rising through the water
column, mixes with (entains) the background seawater until it reaches a point of neutral buoyancy with the ambient seawater (Speer and Rona, 1989; Jakuba, 2007; Morton et al., 1956; Lavelle et al., 2013). At the neutrally-buoyant layer, fluid from the plume spreads out in a large plane (following an isopycnal of constant density). From this layer, metals, sediment, and other suspended particulates carried by the plume may drop out and be redeposited onto the seafloor, and any persisting chemicals are diffused, reacted, or digested by microbes (Scholz et al., 2019; Dick et al., 2013).

PHORTEX builds upon a wealth of work that has primarily focused on localizing hydrothermal venting plume sources (e.g., Jakuba 2007; McGill and Taylor 2011; Nakamura et al. 2013; Paduan et al. 2018; Mason et al. 2020; Wang et al. 2020; Kim et al. 2020; Ferri et al. 2010). Generally, vent localization approaches use detections of anomalous water masses (as determined from in situ sensors) in the water column to constrain the location of a seafloor vent. This localization can be fully offline, when surveys by vehicles like Sentry with no adaptive capacity are post-processed to infer vent locations (Jakuba, 2007; Nakamura et al., 2013), or can be fully online, when autonomous gliders with adaptive capabilities utilize gradient descent to seek a plume source (Wang et al., 2020). In Branch et al. (2020), an autonomous glider tasked with localizing a vent source adaptively chains uniform coverage trajectories with increasingly fine resolution as the robot position converges on an estimated vent location. We emulate this chaining in PHORTEX, but select trajectories offline before AUV Sentry is deployed to respect the operational constraints of the vehicle. Online algorithmic strategies for hydrothermal plume hunting almost universally assume access to a glider-type robot platform, which are cost-effective and agile systems, but typically smaller, payload-limited, and less depth-capable than vehicles like Sentry. An estimated 90% of known vent fields are deeper than 200 m in the ocean, and over 75% are deeper than 1000 m (Beaulieu et al., 2013). Gliders widely accessible to the research community are typically not rated deeper than 1000 m, which means that deep-sea research is reliant on vehicles like Sentry and depends on advances in offline-suited planning techniques.

This work additionally builds upon “plume hunting” research in robotics, sometimes framed as odor mapping, odor localization, source localization, and source seeking. In these problems, a source emits a substance (e.g., gas, radio, acoustic, odor), and through partial observations of the emitted substance, the source is discovered. The techniques employed can be broadly categorized as biologically-inspired heuristic search (e.g., Reddy et al. 2022; Chen and Huang 2019) or adaptive informative path planning (IPP) (e.g., Salam and Hsieh 2019). Biological or heuristic techniques, including gradient-based algorithms like chemotaxis (Morse et al., 1998), or algorithms that directly mimic a particular animal (Edwards, 2001), tend to be reactive and myopic. In contrast, adaptive IPP can be nonmyopic, and tends to embed knowledge (either heuristically or rigorously) about flow fields (i.e., advection and diffusion) to assist in plume localization. Such techniques also lie on a spectrum, from algorithms that resemble biologically-inspired approaches like infotaxis (Vergassola et al., 2007) to methods that use model order reduction techniques to encode complex numerical models (e.g., Navier-Stokes equations) into a probabilistic model (Peng et al., 2014).

While source discovery remains an important area of research, in this article we instead focus on how science can be advanced at the hundreds of vents that have been successfully localized. Thus, we pose a complementary problem to source discovery: given a venting source, what impact do the venting fluids have on the local environment? In this problem, rather than using detections of a plume as a means of source localization, the detections themselves are the valuable data product for scientific inquiry. By placing instruments throughout an evolving plume structure over multiple length scale (meter to kilometer) and timescale (hours to days) to collect dense in-plume measurements, previously intractable questions with respect to microbial life cycle and transport, carbon cycling, and anomalous water mass formation, can be studied. Work that has used robots to map or chart plume-like structures has been presented as the “front-tracking” problem (Li et al., 2014; Chen and Huang, 2019). In this problem, two water masses converge (such as the warm hydrothermal fluid and the cold background seawater), and the goal is to use a robotic vehicle to track the edge of these water masses or stay within a single type of water mass. Many of the solutions in front-tracking have been posed for shallow-water environments in which multirobot collaboration, online decision-making, or direct human intervention are possible (Pinto et al., 2021; Belkin et al.,...
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2018; McCammon et al., 2021), and so state-of-the-art adaptive sampling schemes in informative path planning and experimental design can be directly applied. To the best of our knowledge, this article is the first to present a water mass tracking solution within an offline optimization strategy for a single agent, and the first to attempt this for the hydrothermal charting problem.

While deep ocean “fronts” (i.e., plumes) cannot be trivially studied using standard robotic front-tracking techniques, recent research in Berget et al. (2023) and Ge et al. (2023) discusses adaptive sampling of near-surface plumes that could be adapted for the deep ocean. In these works, target plumes are extensively simulated prior to an expedition using full 3D time-dependent numerical models that yield data products used to train probabilistic models (for instance, kernels of a Gaussian process). The trained probabilistic models are subsequently refined from online observations during an expedition. Performing a similar procedure for deep ocean hydrothermal plumes is limited by extreme uncertainty over vent characteristics and lack of consistent historical data which could be leveraged to inform numerical models (that is, numerical models are severely lacking validation and a means toward validation). Pioneering studies are being conducted at sites like the Juan de Fuca Ridge (German et al., 2019) to determine how reliably advanced plume simulators can be used to predict plume distributions on the scale of tens of kilometers (at a resolution of hundreds of meters) and assist scientists with planning strategic sampling missions; the results of these studies may make approaches like those in Berget et al. (2023) possible in the next decade of deep ocean science, with corresponding development of deep ocean technology to enable adaptive control.

In summary, PHORTEX addresses the modern context of the deep-ocean robotic science fleet while leveraging key principles from state-of-the-art approaches: using fundamental scientific knowledge to complement a probabilistic model, leveraging in situ observations from multiple types of expedition-based sensing equipment to learn temporal forcings and spatial distributions for an initially unknown site while other science activities are performed, and enforcing the operational constraints placed on state-of-the-art platforms.

2.2. Closing the Loop: Expedition Logistics for Deep-Sea Robotics

Oceanographic research expeditions require the coordination and collaboration of a science party, external engineering teams that maintain and operate the scientific equipment used during studies, and the captain and crew aboard a research vessel (on which everyone lives and works during operations). Deep-sea capable robotic platforms used in oceanographic research are assets independently maintained from a ship, and typically requested on a per-expedition basis. AUV Sentry may be deployed on many expeditions in a given year, with up to 250 days at sea possible (Kaiser et al., 2016). Safety of both people and equipment are of the highest importance. Further, the critical role of Sentry in oceanographic research drives the strict operational policies to prevent vehicle loss or damage.

Within this context, Sentry deployments are designed by the science party and ultimately approved by the Sentry engineering team. In a typical workflow, the science party may provide a set of coordinates they generate based on bathymetric maps, prior knowledge, or previous data (when available). The Sentry team designs survey trajectories based on these coordinates to respect the basic operational constraints of the vehicle (e.g., speed, minimum/maximum altitude from the seafloor). With approval from the Sentry team, science party, and captain, the survey is then executed. A single “dive” of Sentry is multiple hours (typically not less than 5 hours, and up to 30 hours). At the conclusion of a dive, Sentry is recovered from the ocean and data products containing hundreds of thousands of point measurements from multiple heterogeneous sensors are made available to the science team within a few hours after Sentry returns to the deck. Depending on the length of the dive, 12–18 hours of vehicle cycling time (e.g., recharging, instrument maintenance, preparation for the next deployment) are required. Based on the length of an expedition and other ongoing research activities, Sentry may be deployed only a handful of times. These operational constraints make online adaptation impossible and are not unique to Sentry or even deep-sea contexts. As Section 4.2 demonstrates, the constraints have significant implications for the style and form of autonomy that can be deployed on a deep-sea capable robot.
The complexity of these basic operations for *Sentry* alone, in addition to the burden of coordinating with other ongoing scientific projects that are happening simultaneously and day-to-day operational changes, make performing “closed loop science” with robot platforms at sea a challenge. Our work aims to alleviate the burden of closing the loop onboard a research vessel for AUV operations by positioning PHORTEX as both a means of generating interpretable plume forecasts informed from diverse data streams and a means of producing AUV trajectories that target these forecasts and can be verified by science party members and approved by *Sentry* engineers.

3. Problem Formulation

Expeditionary science requires a robot to make a sequence of decisions to collect scientifically useful measurements of an unknown, partially-observable spatiotemporal environment under operational constraints. The utility of a measurement is determined by a given task (e.g., reduce uncertainty over a quantity, find the global optimum in a distribution, track a moving target). For hydrothermal plume charting, the task is to map or “chart” the spatiotemporal structure of a buoyant plume using a dynamically constrained AUV. Such a chart enables scientists to infer relevant scientific properties of generating vents (e.g., chemical flux) and to create detailed models of deep-sea interactions and nutrient cycling. We first describe how general problems in expeditionary science can be formulated as sequential decision-making problems, then describe the specific constraints of the AUV *Sentry*, and finally present a formal description of hydrothermal charting as a partially observable Markov decision process.

3.1. Scientific Expeditions as a Sequential Decision-Making Problem

Generally, the expeditionary science decision-making problem can be formulated as a partially observable Markov decision-process (POMDP). Let $\Pi(\cdot)$ denote the space of probability distributions over the argument. A finite horizon POMDP can be represented as tuple: $(S, A, T, R, O, b_0, H, \gamma)$, where $S$ are the states of the robot and environment, $A$ are the actions that the robot can take (e.g., targets, motion primitives), and $Z$ are the observations that the robot collects when executing an action. At planning iteration $t$, the agent selects an action $a \in A$ and the transition function $T : S \times A \rightarrow \Pi(S)$ defines the probability of transitioning between states in the world, given the current state $s$ and the selected action $a$. The transition function governs both how the state of the robot will evolve, given the chosen action, and the potentially stochastic evolution of the underlying spatiotemporal environment. After the state transition, the agent receives an observation according to the observation function $O : S \times A \rightarrow \Pi(Z)$, which defines the probability of receiving an observation $z$, given the current state $s$ and previous action $a$. The reward function $R : S \times A \rightarrow \mathbb{R}$ serves as a specification of the task, assigning high reward to the states of the world that are useful for a given scientific objective and others low reward. A POMDP is initialized with belief $b_0 \in \Pi(S)$—an initial probability distribution over state—and plans over horizon $H \in \mathbb{Z}^+$ with discount factor $\gamma \in [0, 1]$.

As the robot moves through the world, it selects actions and receives observations. Since the state of the world is not directly observable in a POMDP, the robot maintains a probability distribution over possible states (i.e., a belief) and must update this distribution each time it takes an action and receives an observation. Given the transition and observation models, the belief can be updated directly using the Bayes filter (Thrun, 2002):

$$b_t(s) = \tau(b_{t-1}, a_{t-1}, z_t)(s) \overset{\Delta}{=} P(S_t = s \mid a_0, z_0, \ldots, a_{t-1}, z_{t-1}, z_t)$$

$$= P(S_t = s \mid b_{t-1}, a_{t-1}, z_t)$$

$$= \int_{s' \in S} O(s, a_{t-1}, z_t) T(s', a_{t-1}, s) b_{t-1}(s') ds'$$

$$= \frac{P(z_t \mid b_{t-1}, a_{t-1})}{P(z_t \mid b_{t-1}, a_{t-1})},$$

where $\tau(b, a, z)$ is the updated belief after taking action $a$ and receiving observation $z$. Unfortunately, Equation 3 is often intractable to compute directly and an approximate Bayesian inference procedure...
is required to represent the belief [e.g., a Kalman filter (Welch et al., 1995), a particle filter (Silver and Veness, 2010), or variational methods (Wainwright and Mulligan, 2002; Kucukelbir et al., 2017)].

Due to the stochastic, partially observable nature of current and future states, the realized reward in a POMDP is a random variable. Optimal planning is defined as finding a horizon-dependent policy \( \{ \pi^*_t : \Pi(S) \to \mathcal{A} \}_{t=0}^{H-1} \) that maximizes expected reward: \( \mathbb{E} \left[ \sum_{t=0}^{H-1} \gamma^t R(S_t, \pi_t(b_t)) \mid b_0 \right] \), where \( b_t \) is the updated belief at time \( t \), conditioned on the history of actions and observations. The recursively defined horizon-\( h \) optimal value function \( V^*_h \) quantifies, for any belief \( b \), the expected cumulative reward of following an optimal policy over the remaining planning iterations: \( V^*_0(b) = \max_{a \in A} \mathbb{E}_{s \sim b}[R(s,a)] \) and

\[
V^*_h(b) = \max_{a \in A} \mathbb{E}_{s \sim b}[R(s,a)] + \gamma \int_{z \in \mathbb{Z}} P(z \mid b, a) V^*_{h-1}(\tau(b, a, z)) \, dz \quad h \in [1, H-1]. \tag{4}
\]

The optimal policy at horizon \( h \) is to act greedily according to a one-step look ahead of the horizon-\( h \) value function. However, Equation 4 is intractable for large or continuous state, action, or observation spaces and thus the optimal policy must be approximated. Much of the art of practical decision-making under uncertainty is making well-designed algorithmic and heuristic choices that enable efficient and robust planning. In the remainder of this section, we introduce the plume charting POMDP with AUV Sentry; in Section 4, we describe the specific algorithmic choices that enable PHORTEX to approximately solve it.

### 3.2. Scientific Decision-Making with AUV Sentry

AUV Sentry is capable of autonomously navigating between given waypoints with a closed-loop controller and a state estimator that uses acoustic ranging between the robot and the ship to set latitude, longitude, and depth coordinates. At present, Sentry is not capable of or permitted to use underway or online decision-making, in which waypoints are adaptively set on-the-fly while the robot is executing its mission. The lack of underway abilities is the result of both logistical and policy-based issues. Logistically, solving a POMDP online often requires significant onboard compute which may not yet be supported by onboard computing resources on Sentry. Additionally, Sentry relies on a high-latency acoustic link to communicate with the ship, meaning that data from Sentry cannot be streamed to an external computing resource on the ship for decision making (science data communication between ship and robot is 0.02 Hz assuming no packet loss, and only a subset of sensor data can be made available in any given packet). Additionally, by policy, Sentry trajectories are rigorously vetted before each dive using bathymetric maps of the target region and dynamics validation schemes. Extreme (and warranted) risk aversion to avoid losing or damaging Sentry leads to the policy that underway plan changes cannot be part of normal operating procedures.

Thus, to enable sequential decision-making with Sentry requires the use of deployment-by-deployment autonomy. Unlike underway decision-making, deployment-by-deployment autonomy does not modify the AUV trajectory in real-time, but instead leverages the “down-time” between robot deployments to post-process data, update a belief model about the environment, and plan a new fixed trajectory for the next deployment to execute. This form of autonomy honors the strong requirement that each deployment must pass through a rigorous safety and validation check, while enabling adaptive search behavior based on accrued knowledge between deployments. Each planning “step” or iteration in the POMDP framework is an entire deployment of Sentry. In the following section, the implications of this constraint are codified within a POMDP framework.

### 3.3. Charting Hydrothermalism as a POMDP

The plume charting POMDP can be formalized as follows.

**The state space \( S \).** The state space of the plume-charting POMDP consists of the joint continuous states of the environment (i.e., the plume) and the robot. The environment state is represented by
a $d$-dimensional vector of continuous plume parameters $x_p \in \mathbb{R}^d$ and a current vector $x_c \in \mathbb{R}^2$ that contains the heading and velocity of the prevailing crossflow and vary in time. The robot state is represented by a vector $x_r \in \mathbb{R}^3$ that describes the latitude, longitude, and depth of the robot; robot orientation does not play a significant role in planning sample collection actions and is omitted from the robot space.

The action space $\mathcal{A}$. Given that observations are not accessible until after an entire deployment of Sentry, a single action is an entire dive or deployment of the AUV. The action space for a single deployment consists of sequences of parameterized lawnmower pattern trajectory primitives; by chaining lawnmower trajectories together during a deployment, a relatively expressive action set is available. Each trajectory primitive is parameterized by a set of $b$ real-valued parameters $\theta \in \Theta \subseteq \mathbb{R}^b$. These parameters include scale (height and width that describe the rectangle in which the lawnmower is contained), resolution (the absolute distance between tracklines of the lawnmower), and global position (latitude-longitude-depth coordinate and planar angle of the origin of the primitive). The robot’s action set thus consists of sequences of parameterized trajectories, i.e., $\mathcal{A} = \Theta^m, n \in \mathbb{Z}^+$. The number of trajectory objects $n$ and the altitude or depth for which a trajectory will be executed for a given chain is fixed $a$ priori to planning. The selection of the lawnmower as the base primitive was given by Sentry operators, however any pattern (e.g., spiral, zigzag, free-form line) could be used in place of this primitive, as long as the primitive can be described by a low-dimensional parameterization.

The transition function $T$. The transition function $T(s, a, s')$ is decomposed into a plume transition $T_p$, a current transition $T_c$, and a robot transition function $T_r$.

- The plume state parameters $x_p$, e.g., venting characteristics like plume exit velocity or vent temperature, are assumed to be constant and therefore the plume transition function $T_p$ is given by $T_p(x_p, a, x_p') = \delta_{x_p'=x_p}$ $\forall a \in \mathcal{A}, x_p, x_p' \in \mathbb{R}^d$. Although it is possible for plume parameters to vary on a timescale relevant to a robotic deployment [over the course of hours, Chevaldonné et al. (1991)], the overall impact to plume rise height, bend angle, and cross-sectional area is essentially negligible.

- The current transition function $T_c$ is more complex and driven by tidal cycles, local bathymetry, and deep sea currents. We choose a deterministic current transition function $T_c(x_c, a, x_c') = \delta_{x_c'=h(x_c)}$ $\forall a \in \mathcal{A}, x_c, x_c' \in \mathbb{R}^2$, where the function $h$ evaluates the future current magnitude and heading from the present current and is learned from point observations of current magnitude and heading collected by an external sensor (for details, see Section 6.3). An extension of this model to allow stochastic current transitions could encode the uncertainty present in current dynamics and be learned from observations.

- The robot transition function $T_r$ assumes that the robot’s waypoint controller is deterministically able to execute a planned trajectory: $T_r(x_r, a, x_r') = \delta_{x_r'=\gamma(x_r, a)}$, where the function $\gamma$ evaluates the goal waypoint of the trajectory given by $a$. Although there is some uncertainty in the robot’s transition, in practice localization and control are well-solved problems for Sentry and pose uncertainty contributes minimally to the robot’s task execution compared with uncertainty about the plume state.

The reward function $R$. The reward function for the plume-charting POMDP encodes the robot’s objective of producing a comprehensive map of the plume. To approximate this objective, we introduce a black-box function $\text{in\_plume}(x_p, x_c, x_r, a)$ such that $R((x_p, x_c, x_r)\top, a) = \text{in\_plume}(x_p, x_c, x_r, a)$. In this article, $\text{in\_plume}$ first converts state vectors and actions into a set of observations that describe the presence or absence of plume-derived fluids, then computes the total number of “in plume” samples as the reward measure. Practically, $\text{in\_plume}$ can take any form, including classical submodular reward functions (e.g., upper confidence bound, expected improvement), or purely exploitative/explorative functions. Our choice in this manuscript, an exploitative
function, is intended to enforce during real deployments that any in-plume measurements should be prioritized (even those that may be considered “revisits” spatially, as replicate samples can be scientifically valuable). As each trajectory in $\mathcal{A}$ is a lawnmower of minimum duration, and therefore a minimum dimension, this reward function encourages greedy placement of trajectories that cannot degenerate into a “single point” assumed to contain plume fluid.

The observation space $Z$. The robot carries a variety of scientific and navigational sensors. We use a sensor model that fuses and converts complex, continuous scientific observations into a set of $k$ simplified measurements of plume content in a given fluid parcel $Z_p \in \{0,1\}^k$, discussed in Section 6.2. By performing this filtering step, we significantly reduce the dimensionality and complexity of the observation space. Outside of the robot, external sensors provide a set of $j$ independent observations of current magnitude $Z_g \in \mathbb{R}_+^j$ and heading $Z_h \in (-180, 180)^j$.

The measurement function $O$. The measurement function encodes the relationship between the plume parameters and heterogeneous scientific sensors on the robot, the prevailing current, and the robot location. We make use of a sensor model described in Section 6.2 to process scientific sensor data into a measurement that indicates whether a fluid parcel was derived by a plume, and utilize PHUMES (Section 4.1) to incorporate both current data and the simplified plume measurement to update the plume belief assuming a model for the plume detection accuracy of the scientific sensors. We assume that the robot position is fully-observable and exactly reported by the navigation equipment.

The horizon $H$ and discount factor $\gamma$. In deployment-by-deployment autonomy, every action is a multi-hour long sequence of trajectory primitives, after which observations are provided for updating the robot’s belief. In this setting, the horizon $H$ can be set to be equal to the total number of deployments to be conducted during an expedition (which is typically a small number), and the discount factor $\gamma$ set to 1.0. However, the timing and context of Sentry deployments are highly unpredictable, and the robot is constrained to start and end each deployment at the (unknown) coordinates of the ship. The operational reality is that we cannot know when the next deployment will occur, or where the next deployment will start or stop. These timing and location constraints are typically only known with reasonable certainty within 1–8 hours of the next deployment. As a result, the expected value of a plan for any given deployment is largely independent of all other deployments, and planning for deployments beyond the current deployment is highly uncertain and of limited value. With this in mind, to reduce the computational requirements of the planner, we can set $\gamma = 0$ to break the finite-horizon sequential decision-making problem into a sequence of horizon-1 myopic planning problems. While this choice reduces the capacity of the planner to reason about long-term, multi-dive information gathering actions, the planning problem is significantly simplified, as the recursion for the value function is no longer necessary.

4. Methodology

To solve the plume-charting POMDP described in Section 3.3, we present PHORTEX, which first utilizes a physically-informed probabilistic model (PHUMES) to generate forecasts of spatiotemporal distributions of plume fluid and then optimizes chains of trajectory primitives (e.g., lawnmowers) to maximize the total number of observations of plumes during a single deployment. As observations from the robot’s heterogeneous science sensors are used to refine the PHUMES model, PHORTEX-planned missions become iteratively more effective at targeting the dynamic plume.

4.1. PHUMES: Physically-informed Probabilistic Forecasts

To plan long-horizon trajectories in a dynamic environment, we leverage forecasts (or forward simulations) of the evolution of the spatiotemporal phenomenon. Fundamentally, perfect models of natural environments are not available and must be approximated from data. We learn a
model of deep-sea hydrothermal plumes from observations and represent the current probabilistic understanding of the plume state within the POMDP belief. The key challenge when learning a dynamics model for a hydrothermal plume is sample sparsity—there are few total deployments of an AUV, the observations are made at point locations in time and space, and the observation measurements are noisy and have a complicated relationship to the “real” phenomenon of interest (e.g., measurements of salinity and temperature only imply the location of where plume fluids may be). To overcome this challenge, PHUMES is designed as a physically-informed model, which embeds a light-weight approximate simulator of the environment physics to serve as a strong inductive bias for data-driven model learning.

For the hydrothermal plume charting problem, PHUMES wraps a physics-based plume simulator within a Bayesian uncertainty framework, which represents and updates the uncertainty of the input parameters and conditions of the simulator using observations. The embedded physics-based plume simulator is based on a system of ordinary differential equations (ODEs) informed by scientific literature that describe the three-dimensional, time-averaged location of vented hydrothermal fluids. The simulator, which can be treated as a blackbox, takes as input a small number of physically meaningful input parameters (vent area, fluid exit velocity, fluid temperature, prevailing current, etc.) and deterministically produces a plume “envelope” which describes a volumetric region of space in which plume fluids are expected to be detected.

In the real world, however, the model input parameters are uncertain and challenging to measure. To represent uncertainty in the plume forecasts, PHUMES wraps the deterministic physics simulator in a Markov Chain Monte Carlo (MCMC) procedure that places a probability distribution over the uncertain input parameters and infers their posterior distribution given observations of plume presence or absence in the water column following a deployment. PHUMES starts with an uninformative prior over the input parameters of the ODE model, which results in a vague and uncertain plume envelope forecast. After collecting plume observations with Sentry, PHUMES runs an MCMC sampler to infer the posterior distribution over plume parameters given new data. As the posterior estimates of the scalar plume parameters become more certain, the resulting plume forecast becomes more focused and can be used to more effectively target subsequent Sentry deployments. The posterior estimates of the plume parameters form the robot’s belief about the plume environment. The individual components of the PHUMES model—numerical simulator, input parameters, and inference method—are described in detail in the following paragraphs and are depicted in Figure 2. We give a series of validation results in Section 5, as well as a demonstration of the practical utility of the approximation in our field trials in Section 6.

*Embedded plume simulator.* The initial conditions and parameters of the physics-based plume simulator at the heart of PHUMES directly map to elements of the POMDP plume $x_p$ and current $x_c$ state (Section 3.3). These vectors consist of physically-meaningful plume parameters: $x_p = [V_0, A_0, \tau_0, \alpha, \beta]^{\top}$ and $x_c = [U_a, \Theta_a]^{\top}$ where $V_0 \in \mathbb{R}^{+}$ is the initial exit velocity of fluid at a vent, $A_0 \in \mathbb{R}^{+}$ is the vent orifice area, $\tau_0 \in \mathbb{R}$ is the temperature of the fluid at the vent orifice, $\alpha \in (0, 1)$ is a coefficient expressing the rate at which turbulent mixing occurs horizontally in a water mass, $\beta \in (0, 1)$ is a coefficient expressing the rate at which turbulent mixing occurs vertically in a water mass, $U_a : \mathbb{R} \rightarrow \mathbb{R}^{+}$ is a time-indexed function that maps a time to a global mean-field crossflow magnitude in meters per second in a water volume, and $\Theta_a : \mathbb{R} \rightarrow (-180, 180]$ is a time-indexed function that maps time to a global crossflow direction in a water volume.

The plume simulator, adapted from Tohidi and Kaye (2016) and Xu and Di Iorio (2012), describes in plume-relative cylindrical coordinates, $s$ and $\theta$, the rise and transport of plume fluid in a weakly stratified water mass under advective crossflow at time $t$:

$$\frac{dQ}{ds} = Q \sqrt{\frac{2(1 + \lambda^2)}{ML}} \left( \alpha |M/Q - U_a(t) \cos \theta| + \beta |U_a(t) \sin \theta| \right),$$  (5)

$$\frac{dM}{ds} - U_a(t) \cos \theta \frac{dQ}{ds} = \frac{FQ}{M} \sin \theta,$$  (6)

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Figure 2. PHUMES overview. PHUMES is a model for forecasting the evolution of a spatiotemporal distribution trained on partial observations. For hydrothermal plume charting, PHUMES generates plume forecasts by leveraging an embedded analytical simulator \( f(x_p, x_c) \) that approximates the physics-driven evolution of hydrothermal fluid (e.g., Tohidi and Kaye 2016) given plume \( x_p \) and current \( x_c \) parameters. Probability distributions are placed over the inputs to the model (e.g., vent fluid temperature, vent area, mixing rate), and samples from these distributions are used to generate a forecast \( W \) which contains many possible 3D snapshots in time of the location of plume fluid. This set of samples can be compressed using any statistical summary and ultimately used in the reward function of a trajectory optimizer which designs a deployment trajectory that is executed by a robot. Following a deployment, the set of binary observations of plume presence are used to update the parameter distributions using a Bayesian Markov Chain Monte Carlo (MCMC) procedure. Field observations of plume fluids are compared with simulated observations from samples of the parameter distributions, and these samples are probabilistically accepted or rejected. The resulting posterior update over the parameter distributions is used in the next planning iteration.

\[
\begin{align*}
U \sin \theta \frac{dQ}{ds} + M \frac{d\theta}{ds} &= \frac{FQ}{M} \cos \theta, \\
\frac{dF}{ds} &= -QN^2 \sin \theta,
\end{align*}
\]

where \( Q = Q(s, \theta) \) represents the plume specific volume flux, \( M = M(s, \theta) \) is the specific momentum flux, \( F = F(s, \theta) \) is specific buoyancy flux, \( N \) is the Brunt-Väisälä frequency, and \( \lambda \) is the ratio of the minor and major axis that define the plume cross-sectional ellipse. Abstract notions of buoyancy and momentum flux can be converted to more readily interpretable and observable vent characteristics (e.g., vent area, fluid exit velocity) that are represented in \( x_p \) using the following relationships:

\[
\begin{align*}
Q_0 &= \lambda V_0 \frac{A_0}{\pi}, \\
M_0 &= Q_0 V_0, \\
F_0 &= g 10^{-4}(\tau - \tau_0)Q_0,
\end{align*}
\]

where \( \tau \) is the temperature of nonvented (background) fluid at the equivalent depth of a vent orifice (treated as a constant) and \( g \) is a constant representing acceleration due to gravity. Solutions of the simulator, in \( s, \theta \) coordinates, can be converted to global Cartesian coordinates in a three-dimensional volume by first translating \( s, \theta \) into plume-relative Cartesian coordinates \( x_s, y_s: x_s = \int_0^s \cos \theta \, ds \) and \( y_s = \int_0^s \sin \theta \, ds \), then translating those coordinates to the global location of the vent being modeled in the field (a known location), and rotating those coordinates according to the prevailing crossflow direction at time \( t \), \( \Theta_a(t) \). We will refer to the simulator as \( f(x_p, x_c) \) to
represent that we can treat the simulator as a blackbox that takes plume parameters as input and produces plume envelope forecasts in world Cartesian coordinates as output.

The use of a system of ODEs as opposed to a high-fidelity numerical simulator using partial differential equations (PDEs) is intentional as a choice for the embedded simulator in PHUMES. The computational complexity of most PDE systems used to model environmental phenomenon at the scales studied during expeditionary missions is tremendous. In contrast, ODE systems are less well-resolved, but summarize the structure of an evolving phenomenon in a useful way for positioning a robot to encounter plume fluids and that can be enhanced by a generic probabilistic formulation wrapping the ODE initial conditions and parameters, as will be described next.

Representing uncertainty. Given a simulator that transforms plume parameters to plume forecasts, we can pose a specific inference problem: find the generating plume parameters, in terms of both plume initial conditions, seawater properties, and current properties \((x_p, x_c)\), given a set of observations consisting of plume detection locations in the water column \(Z_p\) and time-varying current magnitude and heading \((Z_g, Z_h)\). To perform this inference, we place prior probability distributions over \(x_p\) and \(x_c\), initialized as uninformative priors \(P(x_p)\) and \(P(x_c)\), and estimate the posterior distributions \(P(x_p | Z_p)\) and \(P(x_c | Z_g, Z_h)\). Note that for computational and practical reasons we infer \(x_p\) and \(x_c\) independently given the specified observation model in Section 3.3.

Generating plume forecasts with PHUMES. As written, the simulator \(f(x_p, x_c)\) provides a single snapshot of the location of plume fluids for a set of given initial conditions and parameters. As elements of \(x_c\) are time-dependent and defined by transition function \(T_c\) (Section 3.3), it is necessary to solve \(N\) simulations for a given deployment, where \(N\) represents a number of discrete time points in the deployment, with a single time point being represented as \(t \in T \subset \mathbb{R}^+\). In practice, \(N\) can be set based on the relative complexity of \(T_c\) and context of the deployment; if the current is fairly constant, for example, it may be appropriate to use a small value for \(N\).

As \(x_p\) and \(x_c\) are uncertain vectors, we would like to generate forecasts that incorporate the possible variance in the location of plume fluids implied by this uncertainty. We draw \(M\) samples of each vector (with index \(m\)): \(x_{p,t}^{(m)} \sim P(x_p)\) and \(x_{c,t}^{(m)} \sim P(x_c(t))\). Solving the plume simulator for each sample yields

\[
W_t^{(m)} = f(x_{p,t}^{(m)}, x_{c,t}^{(m)}) \quad \forall t \in T, \quad \forall m \in M. \tag{12}
\]

The complete set of all forward-simulated samples \(W\) is the robot’s belief \(b\), with the number of samples being \(N \times M\) in size. A summary of the algorithm is provided in Algorithm 1. This belief can be used to evaluate belief-dependent rewards (Araya et al., 2010), including information theoretic rewards, that elicit desired exploration and exploitation behaviors from the planner. For example, the variance of the forecast \(S^2_W\) and mean \(W\) could be computed and used within an upper confidence bound-based reward.

**Algorithm 1.** Forecast Generation for PHUMES

**Input:** Discrete deployment times \(T\), current belief \(b_h = \{P(x_p), P(x_c)\}\), simulator \(f\), number of samples \(M\)

**for** \(t \in T\) 
**for** \(m = 0, \ldots, M\) 
\(x_{p,t}^{(m)} \sim P(x_p)\) 
\(x_{c,t}^{(m)} \sim P(x_c(t))\) 
\(W_t^{(m)} = f(x_{p,t}^{(m)}, x_{c,t}^{(m)})\) 
**end for**
**end for**
**return** \(\{W_t\}_{t \in T}\)
To compute expected reward from the belief $\mathbf{W}$ using the in_plume function, we pass the belief through an estimator [e.g., the maximum a posteriori estimator (MAP), maximum likelihood estimator (MLE), median, etc.] to get a single estimate for plume state that is used downstream by a trajectory optimizer:

$$E_{[x_p, x_c, x_r] \sim \theta}[R([x_p, x_c, x_r]^{\top}, a)] \approx \text{in\_plume}(\Phi(\mathbf{W}), a),$$

where $\Phi(\cdot)$ represents some plume state estimator using the set of samples.

*Updating the parameter distributions.* For each deployment, tens of thousands of observations may be available from external sensing equipment. PHUMES receives the resulting data product $Z$, which consists of binary observations of plume presence from *Sentry* $z_p$ and direct observations of crossflow magnitude $z_g$ and heading $z_h$ from other sensors, as described in Section 3.3.

To find the posterior distributions over $x_p$ and $x_c$, we utilize two different inference schemes. To find $P(x_c \mid Z_g, Z_h)$, a Gaussian process (GP) model is defined over the components of $x_c$, and the posterior estimate is computed using standard regression methods (Rasmussen and Williams, 2004). The kernel parameters that define the covariance function for the GP are simultaneously updated using a maximum-likelihood update.

To compute the posterior estimate for $x_p$, $P(x_p \mid Z_p)$, a random-walk Metropolis-Hastings Markov Chain Monte Carlo (MH-MCMC) method (Metropolis et al., 1953) is used. In MH-MCMC, proposed samples of $x_p$ are evaluated according to an acceptance criterion that uses field observations to probabilistically accept or reject those samples; the set of accepted samples is then used to define the posterior distribution. As the relevant observations collected in the field, $Z_p$, are binary observations of plume detections in the full space-time state of the environment, proposed samples of $x_p$ must be simulated with $f(x_p, x_c)$ to generate a hypothetical binary observation of plume presence for a given robot location and measurement time to enable sample evaluation for the acceptance criterion. For the purposes of these simulations, samples of $x_c$ provided to the simulator are set to be the mean function from the updated GP representing this vector.

After a sample of $x_p$ is simulated, a Brier score (Brier et al., 1950),

$$\frac{1}{|z_p|} \sum_{i=1}^{|z_p|} \left( \rho(f(x_p, x_c(i))) - \rho(f(x_p, x_c(i))) \right)^2,$$

is used to compute an error term between the simulated observation and true field observation weighted by a predictive probability $\rho(\cdot)$ that represents the likelihood of agreement between the two observations. In practice, $\rho(\cdot)$ is set according to an expected false positive rate and false negative rate for instantaneous sensor measurements established in consultation with collaborating scientists; for this paper, these are set to 0.1 and 0.3 respectively. Functionally, when both observations are in agreement, this leads to a low Brier score; when they are in disagreement, the score is high. The acceptance criterion is then defined as the ratio of the negative log prior probability and Brier score of the proposed sample of $x_p$ and the last accepted sample of $x_p$. The proposed sample of $x_p$ is then probabilistically accepted or rejected accordingly, and a new proposed sample of $x_p$ is proposed. As the MH-MCMC inference method is a chaining procedure, each sample of $x_p$ selected is informed by the last (in this case, by being a small perturbation of the previous sample), and the cumulative distribution of all accepted samples is guaranteed to converge to the true underlying distribution for each of the elements in $x_p$ for long enough chains. At the end of the MH-MCMC simulation, the posterior distribution $P(x_p \mid z_p)$, computed after removing a small number of burn-in samples, is set as the new sampling distribution for the next forecast to be generated. Algorithm 2 summarizes the update procedure.

### 4.2. Trajectory Optimization for Path Planning with Fixed Primitives

Given the hydrothermal plume-charting POMDP model introduced in Section 3 and the probabilistic plume predictions generated by PHUMES, we next consider how to select trajectories for AUV *Sentry* that will effectively map the spatiotemporal dynamics of the evolving plume. We first define
Algorithm 2. Inference Update for PHUMES

Input: Discrete deployment times \( T, N = |T| \), current belief \( b_h = \{ P(x_p), P(x_c) \} \), observations \( \{Z_p, Z_h\} \), number of samples for the chain \( M \), number of burn-in samples in the chain \( K \)

function compute_acceptance\((x_{\text{prop}})\)
    \( L_b = [\] \) // container for computing Brier scores
    for \( t \in T \) do
        \( W_t = f(x_{\text{prop}}, \mathbb{E}[P(x_c)]) \)
        \( L_b.\text{append}(\text{compute_brier_scores_per_obs}(W_t, Z^{(t)}_p)) \) // observations within time \( t \)
    end for
    return \( \frac{1}{|Z_p|} \sum_{t} L_b - \log(P(x_{\text{prop}})) \)
end function

// Perform a Gaussian Process update for current parameters in \( x_c \)
\( P(x_c|Z_h) = \text{gp_update}(Z_h) \)

// Initialize chain arrays
\( X = [] \) // set up sample array of size \( M \)
\( x_p \sim P(x_p) \) // initial chain sample
\( X[0] = x_p \) // add sample to the chain
\( A' = \text{compute_acceptance}(x'_p) \)

// Build MCMC chain
for \( m = 1, \ldots, M \) do
    \( x_p = \text{random_perturbation}(x'_p) \) // propose a sample
    \( A = \text{compute_acceptance}(x_p) \)
    \( \rho = \min(1, \exp(A' - A)) \)
    \( u \sim U[0, 1] \)
    if \( u < \rho \) then
        \( x'_p = x_p \) // Accept new sample
        \( A' = A \)
    end if
    \( X[m] = x'_p \)
end for

\( P(x_p|Z_p) = \text{compute_kde}(X[K:]) \) // empirical belief update ignoring burn-in samples

return \( P(x_c|Z_h), P(x_p|Z_p) \) // return posterior belief

A specific planning problem by re-writing the POMDP value function, Equation 4, in terms of the elements of the hydrothermal POMDP; then, we introduce a sequence of approximations that allow the value function to be feasibly optimized to select high-reward actions.

In each deployment, the planner must select an action in the form of a chained lawnmower trajectory (Figure 3). A chained lawnmower is defined by the number, \( n \in \mathbb{Z}^+ \), of lawnmowers in the chain and the parameters of each individual lawnmower, \( \theta_i \in \Theta \) for \( i = 1, \ldots, n \). These parameters include the height, width, resolution, origin, and orientation of the lawnmower and are sufficient to completely specify a lawnmower trajectory. We define the set \( \Theta \) to enforce that the lawnmower trajectories are contained within a predefined, rectangular safe region and that each lawnmower obeys a time-based budget constraint. As previously mentioned, this constrained action set is dictated by the operational practices of AUV Sentry; lawnmower trajectories result largely in Sentry traveling in straight lines with few, intermittent turns, which is a beneficial paradigm for the navigational sensors used onboard [i.e., acoustic Doppler Velocity Logger (DVL), inertial sensors]. Using lawnmower trajectories has the additional benefit of biasing the vehicle to collect spatially diverse datasets that scientists are accustomed to analyzing. Other trajectory patterns could be formulated and used in place of lawnmowers, as long as a small set of parameters can be used to
Figure 3. Trajectory optimization. The trajectory optimizer leverages the PHUMES simulator to select high-reward chains of parameterized lawnmower trajectories. (A) The optimization loop for a single lawnmower object, parameterized by height, width, resolution, origin, and orientation. To evaluate the reward of a specific parameter setting, (1) the lawnmower trajectory object is generated using the specified parameters; (2) the trajectory is uniformly sampled along its length to produce a set of sample locations; (3) the reward of those sample locations is computed using the PHUMES model forecasts of the plume envelope (Equation 13); and (4) the lawnmower parameters are adjusted using gradient-based constrained optimization. (B) This core trajectory optimization loop is used to select parameters for each of a chain of $N$ lawnmowers executed at varying times during the deployment. (C) The chained trajectory is then operationally validated and deployed on AUV Sentry to collect plume observations.

describe the pattern and an appropriate trajectory generation function (which converts parameters to waypoints) can be formulated.

We can reformulate the general POMDP value function defined in Equation 4 for the plume-charting POMDP:

$$V^*_h(b) = \max_{\{\theta_1, \ldots, \theta_n, n|\theta_i \in \Theta, n \in \mathbb{Z}^+\}} E_{(x_p, x_c, x_r)^\top \sim b}[R((x_p, x_c, x_r)^\top, \{\theta_1, \ldots, \theta_n\})] \quad h \in [0, H - 1], \quad (14)$$

where each $\theta_i \in \Theta$ parameterizes one of the lawnmower trajectories in a length-$n$ sequence of chained trajectories, $b$ is the planner’s belief about the state of the plume, currents, and robot, and the reward function is defined as in Equation 13. In this equation, we see the first of two important planning approximations made by PHORTEX. As mentioned in Section 3, we set the discount factor $\gamma$ to zero, removing the second, recursive portion of the value function. This approximation significantly reduces the complexity of approximating the POMDP value function, allowing each deployment to be optimized myopically. As deployments of AUV Sentry are intermittent, time constrained, and start/end at the ship coordinates, the sequence of deployments are largely de-coupled; decisions made in one deployment have very little impact on the achievable reward of the next.

Solving Equation 14 still involves selecting the number of chains $n$ and the joint optimization of all $n$ lawnmower trajectories in the chain. For a standard parameterization of a lawnmower (height, width, resolution, origin, orientation), this results in a challenging high-dimensional, nonconvex, constrained optimization problem in which the dimensionality of the optimization problem changes with the number of lawnmowers selected in the chain. In a typical 15-hour deployment of AUV Sentry that uses $n = 15$, one-hour chained lawnmowers, this results in a 90-dimensional, nonconvex joint optimization problem, which must then further be optimized over the number of lawnmowers $n$. Optimization is additionally complicated because evaluating the reward function is computationally expensive, requiring PHUMES to produce a prediction of plume probability for the locations sampled by a given lawnmower, and by a lack of analytical gradients for the reward function with respect to the lawnmower parameters (gradients are instead computed numerically).

To simplify the planning problem further to address chaining optimization, we make a second approximation. We assume that the number of chained lawnmowers is given, i.e., $n = N$, and
decompose the joint optimization of all chains in a trajectory into $N$-independent optimization problems. In this case $N$ is equivalent to the number of discrete time points used by PHUMES to simulate plume evolution in time, as described in Section 4.1. This approximation allows us to break a high-dimensional, joint optimization problem into a sequence of much lower-dimensional optimization problems, and is a reasonable approximation if the travel cost between subsequent lawnmowers is not significant. The final PHORTEX value function, with the two approximations we described, is given by the following:

$$V_h^*(b) \approx \max_{\theta_1 \in \Theta} \ldots \max_{\theta_N \in \Theta} \mathbb{E}[x_c, x_c, x_c] \rightarrow \mathbb{E}[R((x_p, x_c, x_c)^T, \{\theta_1, \ldots, \theta_N\})] \quad h \in [0, H-1].$$

To evaluate the reward function, we define a trajectory sampler operator $G: \Theta \rightarrow \mathbb{R}^{|W|}$ that takes a trajectory parameter vector as input and produces a set of locations in $\mathbb{R}^3$ that will be sampled when the robot executes the trajectory, where $k$ is the number of sampled points. In practice, our trajectory sampler $G$ produces the lawnmower specified by $\theta$ and then subsamples uniformly along its length with a fixed spacing. The final reward calculation in Equation 13 leverages the function $\text{in_plume}$ that counts whether an observation made at a specific location and time is within the plume envelope at that time. Given a belief consisting of the set $W$ of timestamped plume envelope samples produced by PHUMES, we approximate the expected reward in Equation 15 by using the MAP statistical estimator $\Phi$ to produce a single plume envelope forecast per time stamp $t \in [1, N]$:

$$V_h^*(W) \approx \max_{\theta_1 \in \Theta} \ldots \max_{\theta_N \in \Theta} \text{in_plume}(\Phi(W), \{G(\theta_1), \ldots, G(\theta_N)\}) \quad h \in [0, H-1].$$

We solve Equation 16, which defines multiple, independent, nonconvex, constrained optimization problems, using the trust-constrained method in the scipy optimization library for a fixed number of iterations (Conn et al., 2000). For each trajectory, the defining parameters are initialized to produce lawnmowers of equal height and width that respect the total trajectory length budget and start at the location of the predicted plume center from PHUMES; they are then refined by the optimization procedure to maximize intersection with the moving plume. A summary of the trajectory optimization routine is provided in Algorithm 3.

**Algorithm 3. Trajectory Optimization for PHORTEX**

**Input:** Discrete deployment times $T, N = |T|$, plume envelope samples $\{W_t\}_{t \in T}$, constraint set $\Theta$, trajectory sampler $G: \Theta \rightarrow \mathbb{R}^{|W|}$, reward function $\text{in_plume}$

1. Initialize trajectory chain parameters $\{\theta_n\}_{n=1}^N$
2. for $n = 0, \ldots, N - 1$
   1. $t = T[n]$
   2. // Define reward as a function of input points and time index
   3. $R_n(p) = \text{in_plume}(\Phi(W_t), p), \forall p \in \mathbb{R}^{|W|}$
   4. // Define function mapping from input parameters to total reward
   5. $g: \Theta \rightarrow \mathbb{R} = R_n \circ G$
   6. if $n = 0$ then
      1. $\Theta' = \Theta$
   7. else
      1. // Add constraint such that the trajectories chain, i.e., the nth trajectory starts at the termination point of the (n-1)th trajectory
      2. $p_{n\text{ast}} = \text{termination point of } G(\theta_{n-1})$
      3. $\Theta_n = \{\Theta, \text{initial_point}(\theta_n) = p_{n\text{ast}}\}$
   8. end if
   9. // Optimize given initial state, objective function, and constraint set
   10. $\theta'_n = \text{optimize}(\theta_n, g, \Theta')$
11. end for
12. return $\{\theta'_n\}_{n=1}^N$ // return optimized trajectory chain

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Algorithm 4. PHORTEX

**Input:** POMDP \( \{S,A,T,R,Z,O,b_0,H,\gamma\} \), discrete deployment times \( T \), \( N = |T| \), trajectory sampler \( \mathcal{G} \), horizon \( H \), constraint set \( \Theta \), reward function \text{inplume} \( \text{inplume} \), number of trajectories in a chain \( N \), samples for forecast generation \( M_c \), samples for belief update \( M_u \), burn-in samples \( K \)

\begin{algorithm}
\begin{algorithmic}
\FOR \( h = 0, \ldots, H - 1 \) \DO
\STATE \( W = \text{phumes\_forecast}(T, b_h, f, M_c) \)
\STATE \( a = \text{traj\_opt}(T, W, \Theta, \mathcal{G}, \text{inplume}) \)
\STATE \( Z_h, Z_p \leftarrow \text{execute\_mission}(a) \) // robot executes mission and gathers observations
\STATE \( b_{h+1} \leftarrow \text{phumes\_update}(T, b_h, Z_p, Z_h, M_u, K) \)
\ENDFOR
\end{algorithmic}
\end{algorithm}

### 4.3. Computational Considerations for PHORTEX

PHORTEX is a modular POMDP solver that is implemented for the plume-charting problem in a deployment-by-deployment scenario, in which most computation can be done between AUV missions. The algorithmic sketch of PHORTEX is provided in Algorithm 4. The major components of PHORTEX — PHUMES and trajectory optimization — are convergence-based algorithms, with a direct trade-off between run-time and performance. In practice, the available time between deployments fixes the upper limit on the duration that can be spent updating PHUMES, generating forecasts, and planning a new deployment. In the trials presented in this article, 3–8 hours were available between missions, and the number of MCMC samples and optimizer iterations were selected to ensure that PHORTEX produced high-quality plans while respecting this time constraint.

Within the PHORTEX algorithm, the most computationally intensive process occurs during trajectory optimization and PHUMES belief update, when we convert the solution of the system of ODEs into a time-dependent volumetric representation of plume-location probabilities in order to evaluate the reward function and observation likelihoods respectively. In this process, samples of \( x_p \) and \( x_c \) are used in the simulator \( f(\cdot,\cdot) \) described in Section 4.1 to yield the representation of a plume in \( s,\theta \) coordinates. Solving a system of ODEs is typically cubic in the (small, for our application) number of discrete components of the state. To compute the reward function or compare the model values to true observations \( Z_p \), we project the \( s,\theta \) representation into time-relative spatial Cartesian coordinates. In PHUMES, each sample that is drawn in the MCMC procedure to perform an update requires the solutions of \( N \) ODEs and \( |Z_p| \) projections. In trajectory optimization, only one ODE solution is computed (as the MAP sample of the forecast is used), but many thousands of points may be projected to evaluate the reward function within the internal optimization loop. Evaluating the reward during trajectory optimization additionally requires converting a given trajectory parameter choice \( \theta' \) into Cartesian points using the trajectory generator \( \mathcal{G} \) using geometric sub-sampling. Optimized geometric sub-sampling, memory caching, strategic parallelization, or development of approximate (but deterministic) functions to map \( s,\theta \) to Cartesian coordinates are all techniques which could be adopted to accelerate computation. Future work will investigate how components of PHORTEX can be adapted or approximated to enable expeditionary missions in contexts for which computing time is more severely limited.

### 5. Simulation Experiments

To perform an initial validation of the performance of PHORTEX, we designed a simulated environment that closely replicates our ultimate field deployment described in Section 6. In the simulation, a point robot is tasked with collecting spatially and temporally diverse samples of an advecting plume. Each simulation is a three-dive expedition, in which PHORTEX starts with an uninformative prior over \( x_p \) and executes an initial naive survey (as would occur in a realistic field scenario), then plans two more dives by iteratively updating PHORTEX with collected observations. We perform 10, three-dive simulations for two altitudes: 100 and 150 m. Each single dive in the
Figure 4. Simulated validation environment. This is the generated environment for simulation trials as snapshots for altitudes of 100 and 150 m. As the current magnitude and heading changes, the plume expression changes shape and location over 12 hours. Plume intensity is shown in orange in the top two rows. The bottom row shows a vertical cross-section of the plume envelope, along the crossflow direction, at different points in the tidal cycle, with the 100 and 150 m levels marked as red horizontal lines.

three-dive sequence occurs over 12 hrs of simulated time, on a spatial scale similar to the field deployment (over 50 acres, or 0.25 km²).

In the experimental simulator, the embedded analytical model in PHUMES is used to generate a ground-truth environment that closely matches the conditions of the real-world vent at the field site using available data. The simulated vent produces 300 °C and 34.608 PSU salinity plume fluid at an initial exit velocity of 0.6 m s⁻¹ and has a 0.8 m² orifice area. The simulated environment sets the mixing coefficients to 0.15 and 0.2 for horizontal and vertical mixing, respectively. The current function sweeps a generated plume from due North to due East over the course of 12 hours of simulation time, and the magnitude follows a periodic curve beginning and ending at a set velocity of 0.11 m s⁻¹ and with a minimum of 0.04 m s⁻¹. Snapshots of the true simulated environment are provided in Figure 4.

The robot travels at approximately 0.5 m s⁻¹, collecting binary observations every meter that is traveled. In the first simulated dive, the robot executes a single lawnmower trajectory that is placed to maximize in-plume intersections over the course of execution, representing a “best case” placement for a random lawnmower with respect to performance. This trajectory covers the entire target spatial region of a 500 m by 500 m area at a resolution of 15 m (selected in order to complete the survey in 12 hours). For every simulated three-dive expedition, the first dive is always the same lawnmower. For the second and third dives, trajectories are optimized using PHORTEX and consist of $N = 4$, three-hour long chained lawnmowers. Each lawnmower in the chain has a fixed resolution of 10 m, and the height, width, origin, and orientation of each lawnmower are optimized to collect the most reward based on a plume forecast using the maximum a posteriori (MAP) sample computed with the PHUMES model for the plume parameters. As the state-of-the-art replacement for PHORTEX-designed trajectories is currently human/scientist-informed trajectories, we use the first dive in the series to set a baseline standard against which the second and third dive performances are compared, in lieu of adding a human-in-the-loop to our simulations. As the first trajectory is designed to represent a best case scenario for a single lawnmower, the performance of this lawnmower sets a reasonable standard for comparison.

In these experiments, the PHUMES model must estimate the vent area, vent fluid velocity, and both mixing coefficients from plume observation in the water column, starting with uninformative
priors over each quantity. A noisy current magnitude and heading function is provided to PHUMES, as would typically be available from external sensors in the field. For the PHUMES update, 150 samples from an MH-MCMC chain are used to approximate the posterior distributions over the inference targets (this excludes an initial 50 samples of burn-in).

5.1. Evaluation Metrics

The scientific objective of AUV Sentry is to collect observations of a deep-sea hydrothermal plume that are useful for characterizing the space-time dynamics of the plume and related scientific characteristics (i.e., chemical flux, consumption). To evaluate the performance of PHORTEX for deep-sea plume charting in both simulation and field trials in Section 6, we introduce three key metrics that measure how well Sentry collects such samples.

• Proportion of positive plume observations: the number of observations collected in a dive that are classified as in-plume. This metric captures how effectively the robot targeted the plume during a deployment.

• Spatial utilization: the most distal plume detection and the ratio between the most distal plume detection and the longest distance that the robot traveled from the plume source. This metric captures the spatial coverage of the plume achieved by the robot and the spatial efficiency of the deployment. For example, if detections were made up to 300 m away from the vent, but the robot traveled up to 1 km away, then the survey spent too much time outside of the detectable plume region and would not be as effective as a survey that only traveled 200 m away but stayed well within the detectable plume range.

• Temporal utilization: the proportion of hours in the dive with at least 10% or more plume detections. This metric quantifies how effective the robot was at staying in or revisiting the plume over time. Given the long duration of these missions, it is important to use the entire mission window for the task at hand; moreover temporally diverse observations are of scientific interest.

5.2. Simulation Results

Figure 5 shows example planned trajectories and Figure 6 shows the distribution of the evaluation metrics presented in Section 5.1—proportion in plume, spatial utilization, temporal utilization—for the three dives at each altitude tested in the trials. These figures demonstrate that the PHORTEX-optimized trajectories significantly outperform the uninformed baseline (the initial naive lawn-mower), collecting over twice the proportion of samples in-plume, at least doubling the number of hours that the robot spends in a plume, and improving spatial utilization to nearly 100% from 60%–70%.

PHUMES model validation. The performance of PHORTEX stays consistently high in the second and third dives, suggesting that PHUMES quickly learns a sufficient model for planning from the small number of samples collected by the naive trajectories. To further understand the model learned by PHUMES, we qualitatively inspect the learned models in two exemplar trials at 100 m and 150 m altitudes during the initial naive survey, as presented in Figure 7. In the naive survey, less than 20% of all detections are positive detections, and all detections only occur in the first three hours of the 12-hour mission. Qualitatively, at an altitude of 100 m, the robot essentially “skims” the bottom of the neutrally-buoyant plume; at 150 m, the robot is consistently within the band of the neutrally-buoyant plume.

Regardless of the altitude that the robot explored, both learned models show remarkably similar characteristics—a predicted plume centerline no more than 25 m off from the true environment’s plume centerline, and an envelope width that nearly completely encompasses the true plume distribution without being overly conservative or trivial. This is in contrast with an illustrative sample of a plume forecast drawn from the PHUMES prior distributions (the second row from the
Figure 5. Simulated deployments with PHORTEX-designed trajectories. Shown are representative trajectory examples for two simulated deployments at altitudes of 100 and 150 m. The first dive for every simulated deployment is always a simple lawnmower; the second and third dive are PHORTEX-designed trajectories. PHUMES is incrementally trained after each dive on the 1 m spaced binary plume detections shown in this plot.

Figure 6. Evaluation of the PHORTEX trajectories. The three-dive sequence, consisting of a naive lawnmower followed by two rounds of PHUMES model training and PHORTEX trajectory optimization, are evaluated for proportion of positive plume detections, spatial utilization, and temporal utilization (Section 5.1) for simulations trained with observations gathered at 100 m and 150 m altitudes. Ten simulated trials for each altitude are used to compute the performance distributions. The PHORTEX-designed dives show a clear improvement in all three metrics, gathering more spatially and temporally diverse observations of the dynamic hydrothermal plume. Iterative rounds of PHORTEX model-training and trajectory optimization continue to collect a high proportion of scientifically valuable observations.
Figure 7. Illustration of model learning. Snapshots of the true generating environment are compared with a sample from the prior distribution over PHUMES parameters and the learned models from data collected by naive lawnmowers in both 100 m and 150 m simulation trials. In two exemplar experiments, model learning performance is comparable between the PHUMES models trained on data from different altitudes. The learned model, in comparison to the prior sample, demonstrates a lower neutrally buoyant stem height, is wider, and better explains the data collected at either of the two sampling heights. Snapshots at different times and locations to the training data show that the learned parameters robustly predict future shapes of the plume, even when trained on partial data available from the naive lawnmowers.

top of the figure, in red), which is over 50 m in error from the true plume centerline and fails to emulate the true environmental plume at either 100 m or 150 m altitudes. By nature, the uninformed prior can produce plume structures that are significantly different in form from the true generating environment in both location and scale; following an update step, the posterior distributions inferred by PHUMES are used to generate forecasts, and it is evident that the posterior samples effectively “focus” the plume forecasts to useful distributions for planning.

Additionally, it is of note that despite positive detections of the plume during the initial naive lawnmower being temporally clustered to the first three hours, the predictive quality of the location of the plume by the updated PHUMES forecasts to an “unseen” time (t = 9 hrs) is strong. This demonstrates the advantage of using an embedded dynamics model to generate predictions of the state space to extrapolated times.

To quantify the performance of the plume forecasts generated by the inferred MAP estimates of generating parameters from PHUMES following iterative training, the intersection over area (IoA) and intersection over union (IoU) are computed between the true simulated environment and each of the learned models following the first naive lawnmower and the second PHORTEX-designed trajectory in the deployment sequence (Figure 8). To compare trained model performance over the 10 simulations with the initial, uninformed model performance, 10 samples from the uninformed prior are drawn and simulated; these samples demonstrate the breadth of forecast quality before any training. IoA (or recall) provides a number from 0-1 that expresses the alignment between predicted “in-plume” area of the learned model and the actual location of the plume in the generating environment. IoA does not penalize false positives: a value of 1 implies that all in-plume area in the model is contained by the in-plume area of the environment, and a 0 implies that there is no in-plume area overlap between them. IoU (or precision) also provides a number from 0-1, but penalizes false
Figure 8. Intersection over Area (IoA) and Intersection over Union (IoU) of trained models. For each of models trained from data at 100 m and 150 m altitudes (a total of 20 simulations, 10 for each altitude), the average IoA and IoU (using the method illustrated at the figure top) for a set of prior model samples (initial), PHUMES updated with observations from the naive dive (first update—Naive), and PHUMES trained on the follow-up PHORTEX-designed dive (second update—PHORTEX) are computed. In general, the trained models maintain performance over the two relevant dives, with high IoA and medium-to-high IoU that is consistently above the prior samples. Trials trained on data from 150 m tend to have more performant model estimates (IoA near 1, IoU skewed above 0.8) compared to those trials trained on data from 100 m.

positives: a value of 1 implies perfect alignment between the model and environment, and a 0 implies no alignment. The comparison of these numbers helps to contextualize the performance of model learning.

In Figure 8, the trained PHUMES models are shown to have a narrower variance in performance than the baseline samples, and that they generally exhibit very high IoA (up to 1), and a higher IoU (up to 0.9) than the baseline models (up to 0.75). With a high IoA, there is confidence that the learned models are placing plume predictions in areas where the true plume is present, and with a higher IoU, there is confidence that the structure of the predicted plume envelopes align well (as in, are not trivial) with the true environment. Taken together, a very high IoA with medium to high IoU suggests that trajectories planned with the PHORTEX-trained models are very likely to plan and successfully execute trajectories that intersect with the targeted plumes. There is no degradation of performance with more data as PHUMES is re-trained on newly collected data following the first PHORTEX-designed trajectory, suggesting that from very little data (a single naive dive), an immediately useful model is available.
Notably, there is a distinct difference in the distribution shapes of IoA and IoU between the two altitudes. In particular, training from samples at 150 m appears to be more consistently highly performant (IoA mode is at or near 1; IoU distributions skew towards 0.8) than at the lower altitude, which has more variance in performance characteristics (with IoA skewed around 0.8, and IoU centered just above 0.6). This has interesting implications for choosing deployment altitudes in practical missions, within the constraints of robot abilities. For instance, AUV Sentry cannot swim over a certain altitude and maintain good localization, thus constraining what parts of a plume are accessible; knowing in advance that there is a strategic advantage to choosing one or several altitudes prior to a mission can help make the most of the initial naive lawnmower trajectory.

6. Field Deployment: Charting Deep-Sea Hydrothermal Plumes

In November 2021, an expedition aboard the research vessel, R/V Roger Revelle, was conducted at the Northern Guaymas Basin in the Gulf of California to study a recently discovered hydrothermal ridge (Soule et al., 2018; Geilert et al., 2018). The research cruise had several objectives that aimed to investigate the transport and consumption of methane and other geochemical tracers produced by active hydrothermal vents. To assist in operations, AUV Sentry, remotely-operated vehicle (ROV) Jason, and standard oceanographic equipment were available. The deployment of PHORTEX on the cruise for Sentry operations was coupled with objectives to test in situ instruments and collect microbiota samples. For both of these tasks, charting different regions within a plume was important to test the capabilities of the novel instruments and collect biological samples from a diversity of plume-conditions.

6.1. Site Description and General Conditions

The main site for the study conducted by AUV Sentry using PHORTEX was a hydrothermal ridge located in the northern Guaymas Basin, approximately 1850 m underwater and at the edge of an additionally 300 m deeper graben (a valley with steep sides) (Figure 9). The ridge is approximately 600 m long and features several tall sulfide structures 45–75 m in height with active smoking along their bodies. A smoking “chimney” at the northernmost point of the ridge was targeted for plume-charting. The chimney vent was composed of a cluster of tens of small orifices (<0.1 m diameter) that created an approximately 1.5 m diameter chimney base. The fluid produced was thick with particulates and measured with a temperature wand on ROV Jason to be 340 °C at the source. Fluids ventilated rapidly at approximately 0.7 m s⁻¹ (as measured by video equipment) and were rich in dissolved methane. In contrast, the ambient seawater was methane-poor, considerably less

![Figure 9. Study site in the Guaymas Basin, Gulf of California. The inset map is bathymetric data collected by AUV Sentry during this expedition and shows the approximately 600 m long ridge in yellow. The red star marks the chimney that is of particular study in this article. (A)–(D) show imagery from the ridge and chimney site. (A)–(C) show various forms of plume-producing vents located at the chimney and (D) shows an example of the macrofauna covering the structures along the ridge.](image-url)
turbid, and cold at 4 °C. As vent fluids rise and form a plume at this site, the ambient water is mixed (entrained) at an unknown rate, and advected by mild deep-water currents. Under these conditions, plume expressions could be transported several hundred meters from a known source, and would be expected to rise over 200 m in the water column. In scientific work following this expedition, plume fluids marked by elevated methane and turbidity were identified up to 7 km away from the same venting sites described here (Preston et al., 2022).

6.2. Plume Detection: Treatment of Robotic Science Sensors

The observational data from AUV Sentry are continuous measurements from multiple science sensors. These data must first be processed into a binary product, $Z_p$, the can be used to train the PHUMES model. In the hydrothermal charting task, there is no single sensor that can be used directly as a proxy for whether a parcel of fluid was hydrothermally derived (Jakuba, 2007; Preston et al., 2022). Drawing on the work in Jakuba (2007), the suite of oceanographic sensors on Sentry are processed into a binary data product to indicate whether Sentry was in a plume or in background seawater (an absence of plume-derived fluid). This sensor model converts multiple time-stamped sensor measurements $s_{t,i} \in \mathbb{R}$, $i = 1, \ldots, S$ to a time-stamped binary plume detection $z_{p,t} \in \{0, 1\}$. These binary detections are then used to update PHUMES and plan robot trajectories, as described in Section 4.

Sentry is equipped with a standard suite of oceanographic instrumentation, including an oxygen optode (Aanderaa 4330F), an optical backscatter (OBS) instrument (Seapoint Turbidity Meter), an oxidation-reduction potential sensor (NOAA ORP probe), a conductivity-temperature-depth (CTD) instrument (SeaBird SBE49), and a pressure sensor (Paroscientific 8B7000-I). Additionally, custom instrumentation provided by science teams can be integrated onto Sentry, and two separate experimental spectroscopic methane instruments, Pythia (Michel et al., 2022) and SAGE (Kapit and Michel, 2021a,b), were integrated onto Sentry for this study. Each oceanographic sensor is synced to a shared precision clock on Sentry, and logged to separate files at the manufacturer recommended sampling frequencies. In post-processing, all sensor data is interpolated onto a regular, fixed 1 Hz frequency timestamp.

Each of the sensors onboard Sentry have unique characteristic responses to the chemistry of plume water. For example, ORP exhibits a large negative spike when first encountering plume water followed by a slow rising hysteresis back to a nominal value. Measurements of salinity, temperature, and oxygen are expected to be influenced not only by plume water, but background physical mixing in the ocean (Li et al., 2020; Speer and Rona, 1989; Preston et al., 2022); turbidity, ORP, and methane are signals strongly associated with hydrothermalism and are generally not persistent in background seawater. To account for the different ways in which sensors respond to plume waters, each sensor is processed individually to detect plumes (see Table 1). Weights are assigned to each

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Positive Plume Detection Criteria</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Salinity</td>
<td>Detrended practical salinity outside 3 standard deviations of the entire time series</td>
<td>1</td>
</tr>
<tr>
<td>Temperature</td>
<td>Detrended temperatures above the 75th percentile of entire time series</td>
<td>2</td>
</tr>
<tr>
<td>ORP</td>
<td>Detections less than -0.005</td>
<td>2</td>
</tr>
<tr>
<td>OBS</td>
<td>Optical attenuation above the 75th percentile of entire time series</td>
<td>2</td>
</tr>
<tr>
<td>Oxygen</td>
<td>Detrended concentrations outside one-hour rolling computation of 3 standard deviations</td>
<td>1</td>
</tr>
<tr>
<td>Methane</td>
<td>Normalized concentration above 0.3</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 1. Instruments on AUV Sentry and the criteria used to identify plume fluids for each instrument. The weight is used to indicate relative trustworthiness of a plume detection for each sensor, and is used in a corroboration scheme that sums detections across sensors in order to make a final determination on whether an observation location contained a parcel of plume fluid or consisted of background seawater. Detrended data removes depth-related cross-sensitivity from the measurements; for example, temperature is stratified in the deep ocean, so to ignore the impacts of depth changes in the data stream, those effects are removed by “detrending” the data stream.
Figure 10. Example time series (left) and associated detections (right) from the AUV Sentry sensor suite. Oxygen, temperature, and salinity measurements shown here are reported as deviations from the best line of fit between these quantities and depth (to “detrend” these quantities, as they are physically expected to change with depth and not just presence of hydrothermalism). The time series demonstrates two types of plume detections. The first are “obvious detections” in which most sensors register strong anomalies (this happened twice toward the end of the deployment just before and after 04:00) and are most strongly associated with buoyant-stem derived fluids. The second are “persistent-plume detections” in which the robot traverses through water that is slightly more turbid, warm, or chemical-rich than background water over potentially long horizons (this happened in the middle of the deployment from 00:00 and 02:00). Such detections are most strongly associated with neutrally-buoyant layers. The conservative corroboration detector successfully identifies both forms of plume water.

sensor based on their individual reliability for identifying plume water, as determined by the science party and consulted experts in preparation for the research expedition and analyzed in a related follow-up scientific study in Preston et al. (2022). Observations are then classified as plume water or background water using corroboration across sensors: weighted detections for each sensor are summed together and a conservative detection threshold is used to identify an observation as plume or background. A total corroboration score of 4 or more was used to classify an observation as in-plume. An example of this method is applied to real Sentry measurements in Figure 10. The accuracy of this sensor model is difficult to characterize, as there is no available ground-truth in a field setting by which to verify the assigned classifications. Qualitatively, the classifications were reviewed by the science team and verified for their alignment with expert insight.

6.3. Available Oceanographic Instrumentation

One of the key advantages of using a physically-informed model is that external data and measurements of opportunity can be incorporated in a principled way into the belief representation when available in a field setting. During field work presented in this study, external sensors to Sentry were available through other scientific activities aboard the ship, and we leveraged these additional data in three key ways within our PHUMES instance summarized in Table 2 and visualized in Figure 11. First, the density stratification of the water column at the field site was characterized using a ship-board rosette (a metal frame on which oceanographic sensors are mounted and which is attached to the ship via a cable in order to be raised and lowered through the water using a winch) with a CTD probe (Seabird SBE9). The empirical stratification function is used within the analytical simulator in PHUMES to compute buoyancy flux for the hydrothermal fluid relative to background seawater, and treated as a constant throughout the expedition. As the data had small amounts of noise, a simple Gaussian Process (GP) model with radial-basis function (RBF) kernel
Table 2. Summary of auxiliary data. External equipment and opportunistic data available from other operations during the field expedition that was used to inform the PHUMES model within PHORTEX used for at-sea trials.

<table>
<thead>
<tr>
<th>Platform</th>
<th>Instrument</th>
<th>Data Product</th>
<th>PHUMES Incorporation</th>
</tr>
</thead>
<tbody>
<tr>
<td>ROV Jason</td>
<td>Camera</td>
<td>Vent Area</td>
<td>Informs prior over vent area</td>
</tr>
<tr>
<td>ROV Jason</td>
<td>Camera</td>
<td>Fluid Exit Velocity</td>
<td>Informs prior over fluid exit velocity</td>
</tr>
<tr>
<td>ROV Jason</td>
<td>Temperature wand</td>
<td>Vent Temperature</td>
<td>Sets temperature initial condition</td>
</tr>
<tr>
<td>Rosette</td>
<td>CTD</td>
<td>Water Column Stratification</td>
<td>References for analytical model</td>
</tr>
<tr>
<td>Tiltmeter</td>
<td>TCM3 Logger</td>
<td>Current magnitude, heading</td>
<td>Use trained GP in forecast sampling</td>
</tr>
</tbody>
</table>

Figure 11. Auxiliary data products used in PHUMES. External equipment (ROV Jason, tiltmeter, and rosette) provided opportunistic data products during the field expedition that were incorporated into PHUMES. The ROV Jason was used to determine prior estimates for the plume source parameters. The rosette collected vertical temperature and salinity profiles which are used to compute stratification in the basin. A GP is trained over the data, and the mean is visualized in the lower right panel. The tiltmeter records data of current magnitude and heading; a GP was trained over both functions and is visualized in the lower left panel. Heading is reported in compass-rose orientation.

was fit to each of temperature and salinity using GPytorch (Gardner et al., 2018) (100 iterations, learning rate 0.1), and the trained mean function was used within PHUMES.

Second, the crossflow transition function $T_c$ (Section 3.3) was learned from data collected by a current tiltmeter (Lowell Instruments TCM3), an instrument that is fixed to the seafloor on one end and is allowed to tilt under the effects of crossflow. While it may have been possible to estimate $T_c$ solely from binary observations of plume presence over time, access to the tiltmeter for three days of the cruise significantly relieved a burden on the inference process. We observed a maximum crossflow magnitude of approximately $0.1 \text{ m s}^{-1}$, and both magnitude ($U_a$) and heading ($\Theta_a$) appeared to be semi-cyclic, following a pattern established by tidal charts produced by Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE) for the time period of the...
expedition (Valenzuela, 2021). Time-varying currents of magnitudes between 0.1–0.5 m s\(^{-1}\) sweeping from the northwest to southwest were previously reported in Scholz et al. (2019), corroborating our observations. As with the density curve, a GP with RBF kernel for each of current magnitude and heading was trained using \texttt{GPytorch} (magnitude model: 100 training iterations, learning rate 0.5; heading model: 200 training iterations, learning rate 0.1), and the trained GP was used within the sampling framework for PHUMES to generate forecasts (as described in Section 4.1).

Finally, direct observations from the seafloor, by the remotely operated vehicle (ROV) \textit{Jason}, of venting sources were used to set informed priors over the initial conditions for the plume source parameters (i.e., vent area \(A_0\), vent fluid velocity \(V_0\), fluid temperature at the vent \(\tau_0\)). \textit{Jason} carried a camera system (Sulis 4k) and a temperature wand. Measuring temperature with an ROV is precise, and so we directly used the observation of temperature by \textit{Jason}, 340 °C, as the initial condition for vent fluid temperature in the PHUMES model trained with field data. Vent area and vent fluid velocity were measured with cameras onboard \textit{Jason}. Using a 10 cm spaced set of laser points that \textit{Jason} can toggle on and off \textit{in situ}, the vent area was extrapolated from an estimate of vent diameter from pixel-to-distance conversion in still images. Using this method, an area of approximately 1.7 m\(^2\) was estimated, and used to center a uniform distribution over vent area to be updated with PHUMES. Vent exit velocity was estimated by applying particle imaging velocimetry (PIV) (Zhang et al., 2019) to 4K video of the turbid fluids at the vent. PIV methods track turbulent parcels that have high cross-correlation values between frames of a video. By tracking many parcels over several frames, PIV yields a vector field of velocity estimates that can be averaged to establish a mean estimate for a region. Using \texttt{PIVLab}, an open-source \texttt{MATLAB} library (Thielicke and Sonntag, 2021; Thielicke and Stamhuis, 2014; Thielicke, 2014), we estimated a fluid exit velocity of 0.7 m s\(^{-1}\), and similarly used this as the center of a uniform prior placed on exit velocity for PHUMES to update.

6.4. At Sea Operations

PHORTEX was used to enable deployment-by-deployment autonomy during field operations with AUV \textit{Sentry} that fit within the typical workflow of operations at sea (Figure 12). Functionally, the trajectories planned with PHORTEX were provided to the \textit{Sentry} engineering team for extensive safety validation prior to each deployment. If approved by the \textit{Sentry} team, the chief scientist, and
captain of the vessel, the trajectories were downloaded into the Sentry mission planning software as static waypoints. This confirmation process required a lead time of approximately 6 hrs before a scheduled deployment, and 12–18 hrs were available between deployments to mechanically service Sentry and recharge batteries. The ability of PHORTEX to produce viable trajectories from data within the first 3–8 hrs that Sentry was on-deck following a recovery was critical for keeping this strict timeline. Given the long lead time between trajectory design and actual Sentry deployment, there were many opportunities for the time of a deployment to change due to, for example, developments in weather or changing science/technology priorities. To be robust to these changes, we provided deployment plans that started several hours before and several hours after a given deployment time, and the Sentry team truncated the plan at the appropriate points once a deployment time was known with certainty.

6.5. Field Trials with PHORTEX at Sea

Four deployments of AUV Sentry were performed in the northern Guaymas Basin to evaluate PHORTEX in the field. These deployments represent a planning spectrum, from fully expert-designed surveys to fully PHORTEX designed.

- **Dive E-Multi**: Expert designed, multi-task survey. This was the first deployment of Sentry and the survey was designed to both attempt to find plume fluids and to bathymetrically map the local basin area (the map of which would be used as part of the safety check protocol for future deployments). This dive is representative of a standard nested strategy, in which progressively more targeted (finer resolution) surveys are used to study areas of interest. The dive was designed by a human expert who only had access to the approximate location of the target vent. The deployment lasted 21.3 hrs and collected 76,604 observations.

- **Dive E-Plume**: Expert designed, plume-charting survey. This was the second deployment of Sentry and the survey was hand-designed by the science party onboard the vessel to find and sample plume fluids. The science party had access to the performance of Sentry in Dive E-Multi. The strategy was to sweep the basin above areas with known hydrothermal vents, and fly out into the basin in the direction that the plume fluids would be expected to advect. The deployment lasted 21 hrs and collected 75,430 observations.

- **Dive EP-Plume**: Hybrid expert and PHORTEX plume-charting survey. This was the third deployment of Sentry and the survey consisted of trajectories designed by PHORTEX trained by observations collected only in Dive E-Multi. Two of the trajectory primitives designed by PHORTEX were replaced by “naive” lawnmowers placed over the known vent at two different times in the deployment. Thus, EP-Plume consists of an expert-designed portion, noted EP-Plume (E), and a PHORTEX-designed portion, noted EP-Plume (P). The deployment lasted 22.2 hrs and collected 79,792 observations. Of these, 8.2 hrs and 29,438 observations were collected via the expert strategy.

- **Dive P-Plume**: PHORTEX plume-charting survey. This was the fourth and last deployment of Sentry. The survey was fully designed by PHORTEX using observations only from Dive E-Multi, several days prior to this dive. The deployment lasted 9.9 hrs and collected 35,755 observations. This deployment is notably much shorter than the other deployments due to increasing time constraints as the expedition was coming to a close. This deployment also used Sentry in a “depth-hold” mode: whereas in all other dives Sentry’s depth followed the basin terrain, in this experiment the robot held an absolute depth.

6.6. Field Results

Using the metrics introduced in Section 5.1, we evaluate each of the four dives executed at sea. Each dive took place at different times in the tidal cycle, on different days, and often at different altitudes in the water column, and thus the total plume samples available to collect during each dive
Table 3. Per-dive statistics for field trials of PHORTEX. The spatial utilization is reported as both the most distal plume detection (measured from the plume origin) and the ratio of the most distal plume detection over the farthest distance that the robot traveled from the plume origin. Temporal utilization shows what fraction of the total deployment duration contained hours with at least 10% of all samples as positive plume detections. The deployment EP-Plume is broken further into expert designed (E) and PHORTEX designed (P) portions for direct comparison.

<table>
<thead>
<tr>
<th>Dive</th>
<th>Duration</th>
<th># Samples</th>
<th>Positive Detections</th>
<th>Spatial Utilization</th>
<th>Temporal Utilization</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-Multi</td>
<td>21.3 hrs</td>
<td>76,604</td>
<td>22.3%</td>
<td>300 m (19%)</td>
<td>52%</td>
</tr>
<tr>
<td>E-Plume</td>
<td>21 hrs</td>
<td>75,430</td>
<td>10.9%</td>
<td>900 m (64%)</td>
<td>43%</td>
</tr>
<tr>
<td>EP-Plume</td>
<td>22.2 hrs</td>
<td>79,792</td>
<td>41.8%</td>
<td>600 m (100%)</td>
<td>81%</td>
</tr>
<tr>
<td>EP-Plume (E)</td>
<td>8.2 hrs</td>
<td>29,438</td>
<td>42.3%</td>
<td>250 m (100%)</td>
<td>75%</td>
</tr>
<tr>
<td>EP-Plume (P)</td>
<td>14 hrs</td>
<td>50,354</td>
<td>41.5%</td>
<td>600 m (100%)</td>
<td>93%</td>
</tr>
<tr>
<td>P-Plume</td>
<td>9.9 hrs</td>
<td>35,755</td>
<td>12.8%</td>
<td>450 m (100%)</td>
<td>40%</td>
</tr>
</tbody>
</table>

is variable. With this in mind, we present and evaluate each dive quantitatively, and additionally qualitatively examine each as a case study for how different sampling paradigms perform in the real-world. There is no ground-truth available for the deep sea plume-charting problem; we evaluate each Sentry dive assuming that the binary detections produced by the method in Section 6.2 are honest representations of the presence or absence of hydrothermally-derived fluids in the basin.

The results of the field deployment are presented in Table 3 and visualized in Figure 13. For all PHORTEX-designed dives, PHORTEX was trained only on data collected during the first dive, E-Multi, whereas science experts had complete access to all dive data and other shipboard context when planning missions. This makes the comparable performance of PHORTEX to science experts in the collection of in-plume samples during the two dedicated plume-mapping dives E-Plume (10.9%) and P-Plume (12.8%) noteworthy, as P-Plume occurred a week after the original E-Multi dive. This illustrates and emphasizes the long-range forecasting ability of PHUMES. Performance during EP-Plume, in terms of proportion of in-plume samples, is also comparable (42.3% and 41.5% for expert-designed and PHORTEX-designed, respectively).

Importantly, the samples that PHORTEX collects are more spatiotemporally diverse, evidenced by both spatial utilization and temporal utilization metrics. PHORTEX generally increases both the range of the most distal plume detection (as evidenced in EP-Plume) and effectively utilizes the entire explored range (100% spatial utilization in all cases of using PHORTEX). This is most well illustrated in the EP-Plume dive, in which the expert-designed portion is a lawnmower trajectory placed “on top” of the vent; the PHORTEX-designed trajectory collects samples over twice as far from the plume source. Absolute temporal utilization is similar to slightly more performant compared to expert surveys as shown by comparing E-Plume (43%) and P-Plume (40%) as well as within EP-Plume (75% and 93% for expert-designed and PHORTEX designed, respectively). However, qualitatively, the spread of temporal detections is much improved by PHORTEX as compared to expert-designed surveys, which tend to “bunch” detections in time. This is observed most sharply in EP-Plume, in which 90% of positive detections collected by the expert-designed survey occurred only in the second of the two lawnmowers (hours 20–22), whereas PHORTEX collected similar observation totals throughout the dive. Figure 13 shows the qualitative structure of each dive and showcases the diversity in the resulting datasets.

In this field deployment, PHORTEX was a useful and practical tool for plume-charting. The automated nature of PHORTEX operationally alleviates significant decision-making burden on a science team and the trajectory-design burden on the Sentry team; the ability to ingest data from external sensors and previous Sentry missions, and produce trajectories that can be seamlessly ingested by the safety checking system without human intervention is of considerable benefit in the field. Moreover, by virtue of yielding rich context easily interpretable by the science team, the intermediate products of PHORTEX, like PHUMES forecasts, are useful for other tasks in field operations, such as deploying external instruments.
Figure 13. The four field dives of AUV *Sentry*. All data is plotted according to its detection identity (in-plume or seawater). The left column shows a top-view of the dive trajectories in polar coordinates, in which angle and radius is computed relative to the chimney coordinate of the vent of study. The right column shows a time series versus depth of the detections collected. All but Dive P-Plume were dives conducted in altitude-hold mode with *Sentry*, and so the trajectories show obvious changes in elevation; in contrast Dive P-Plume was held in depth-hold mode, so most observations are gathered within a depth-plane. In Dive EP-Plume the portions of the dive that were expert-designed and PHORTEX-designed are labeled with E and P, respectively. As can be seen in the Dive EP-Plume time series, the two expert-designed trajectories have significantly different performance, despite being in locally similar regions of the spatial domain.

**PHUMES Validation with Field Observations.** While there is no external “ground-truth” that can be used to evaluate the performance of PHORTEX, the PHUMES model trained on external and binary *Sentry* observations can be compared with independent measurements of the vertical distribution of particulates (turbidity) near the hydrothermal ridge to provide a sense of the explanatory power of the PHUMES model. Turbidity is a useful proxy measurement for plume presence because floating particulate matter is primarily produced by hydrothermal activity and the measurement of turbidity (beam attenuation in a transmissometer) is reliable. After training, PHUMES estimated the fluid exit velocity from the target chimney to be 0.58 m s\(^{-1}\), the vent area
Figure 14. Validation of PHUMES model trained at sea. We compare the nominal plume estimate from PHUMES trained on at-sea data and Sentry observations with vertical transects of turbidity from shipboard rosette. The plume envelope is the average plume estimated by PHUMES for a nominal crossflow of $0.12 \text{ m s}^{-1}$. Vertical red lines mark 100 and 600 m laterally from the originating vent, for which vertical rosette casts were conducted (both an upcast and a downcast; two lines per transect). The region that the model estimates contains the plume in the water column is highlighted on the turbidity transects with red boxes (extent) and a red dotted line (center of the plume). There is reasonable agreement between the model estimate and the transect data on the location of this turbid layer.

... (the opening of the vent from which plume fluids rise) to be 0.82 m$^2$, and the vertical and horizontal mixing coefficients to be 0.15 and 0.19, respectively. Simulating these conditions with an initial vent temperature of $340 \, ^\circ\text{C}$ and salinity of 34.908 PSU under a nominal crossflow of $0.11 \text{ m s}^{-1}$, the time-averaged plume height and width are computed. Two vertical profiles of turbidity near vents at the Northern Ridge were collected by the rosette, and turbidity was coherently elevated in the water column. In Figure 14, these two vertical transects, one conducted about 100 m from a known vent, and one conducted 600 m from the same vent, are shown and compared with the plume envelope forecasts by PHUMES. There is good alignment between the model and the coherent region of elevated turbidity in the profiles, indicating that the learned PHUMES model has uncovered a useful structure of the hydrothermal plume and is valuable for planning sample trajectories that will intersect with plume fluids.

7. Discussion and Future Work

PHORTEX is an autonomy system that has been demonstrated for real-world hydrothermal plume charting under the complex operational constraints that exist at sea, showing quantitative gains over typical exploration strategies and providing auxiliary value to shipboard scientific operations. The components of PHORTEX—science-informed sensor processing, a physically-informed predictive model PHUMES, and flexible, constraint-aware trajectory optimization scheme—form a framework that can endow our modern scientific robotic fleet with the ability to detect complex spatiotemporal patterns, forecast their dynamics, and reason over those forecasts in order to complete otherwise impossible sampling tasks. As technological advances in robotics become more accessible for scientific expeditions, future work extending PHORTEX for online and multiagent settings are exciting potential next steps. Moreover, algorithmic advances for PHUMES to enable sample-efficient learning of spatiotemporal distributions, would have wide impacts in robotics for science. The following sections discuss some of the key areas for improving PHORTEX and broader areas of research towards transforming expeditionary robotic science.
PHORTEX and PHUMES extend modern informative path planning frameworks to deployment-by-deployment expeditionary contexts, and easily adapt to other scenarios with compartmentalized design adjustments. PHORTEX and PHUMES are formulated as modular frameworks, and in different expeditionary contexts the trajectory optimization scheme, definition of the reward function, and analytical model at the heart of PHUMES could each be replaced directly. PHORTEX is formulated as a deployment-by-deployment sequential decision-making framework that enables offline optimization of operationally-constrained trajectories. Fundamentally, this framework is general enough to extend to any robot system which may not have access to adaptive behaviors such as subsea AUVs and extraplanetary rovers. Performance of PHORTEX as formulated in this article is best suited for contexts in which a target phenomena changes meaningfully on a similar or slower timescale to the entire mission duration (i.e., hours or days). Future missions utilizing PHORTEX in this setting could be enhanced by adjusting the discount factor and planning horizon, to enable strategic nonmyopic behaviors. For environmental systems that evolve rapidly, online trajectory adaptation is necessary. In online settings, PHUMES can support the computation of information-theoretic reward functions and so online belief-based search (e.g., Flaspohler et al. 2019; Arora et al. 2019; Sun et al. 2017; Sunberg and Kochenderfer 2018) common in adaptive sampling and informative path planning literature could be pursued. PHUMES itself is a Bayesian inference model that centers around a particular choice for numerical simulator. To extend to other scientific settings, a different numerical simulator can be selected. This requires some initial knowledge of how a particular target environment may evolve; this knowledge could be partial (as in, only knowing that certain properties may be conserved), approximate (as is presented in this article as an idealized model of plume dynamics), or complete (as in, having a full-fidelity simulator of a target environment). Scientific expeditions in the ocean and other marine environments, as well as atmospheric studies, are particularly well-suited for formulation with PHUMES to inform mobile robot trajectories given the wealth of numerical simulators which exist to describe these environments.

The future of expeditionary scientific missions requires re-thinking classical action primitives to target dynamic phenomena in offline or open-loop settings common in underwater, subterranean, or extraterrestrial contexts. Parameterized uniform coverage surveys (e.g., lawnmowers, spirals) are the foundation of many field robotics deployments undertaken in observational sciences today. While classically used to study spatially static distributions, PHORTEX demonstrates that uniform coverage trajectories can be used to collect plentiful observations of spatiotemporal distributions when optimized over probabilistic forecasts to assist in strategically placing the robot. The optimization technique does not come without its own challenges, however. In PHORTEX, evaluating the reward of a lawnmower trajectory requires generating the trajectory from parameters, sub-sampling that trajectory, and then using the PHUMES model to predict the plume snapshot for a specific point in time and space. Each of these steps can be computationally expensive. To increase the efficiency of the trajectory optimizer during field deployments, we discretized time coarsely and only generated N MAP plume forecasts from PHUMES (1 snapshot for each lawnmower, generated from the start time of each lawnmower). This substantially improved the speed of the planner, at a loss of targeting accuracy for the moving plume. Developing efficient and accurate techniques that can optimize parameterized trajectories (with additional focus on extending beyond lawnmower primitives) for dynamic environments is an imperative step in effectively studying spatiotemporal phenomena with mobile robots.

Utilizing physics-based models within robotic belief representations for environmental sampling improves sample efficiency, but does not (necessarily) overcome ambiguity challenges when solving an inverse problem. Estimating the plume parameters $x_p$ for deep-sea hydrothermal plumes requires solving an ill-posed inverse problem. The relationship between fluid exit velocity and vent area are significantly entwined in the analytical model proposed in Section 4.1 via Equations 9–11. There are countably infinite solutions on the two-dimensional manifold describing this relationship for a single target flux value. Ambiguity in inverse problems is a classical problem in numerical methods, and not
easily resolved without setting strong assumptions (i.e., fixing an unknown parameter) or changing the experimental procedure (i.e., collecting more/different types of data). For the purposes of robot trajectory planning, parameter ambiguity is not necessarily a problem, as long as the resulting model is sufficient for predicting the plume envelope to strategically place the robot. However, resolving this ambiguity may be important in settings in which the posterior estimates trained by PHUMES are used as a scientific data product to make claims about a target environment. To make PHUMES a useful science product (and not just a useful model for planning trajectories), further development that investigates the calibration of uncertainty in posterior estimates and considers possible modifications to the experimental procedure, would be necessary.

Good expeditionary robots (and the models and planners that drive them) must leverage external data, model products, and other agents to inform their actions. Leveraging sensing equipment external to a robot is well established for environmental studies in which satellite, fixed observatory, or historical observations are available. However, in many environments—subsea, subterreanean, and forests—such observational equipment may not be available or needs to be independently deployed by a science team or by a robot explorer. The use of multiagent systems for environmental studies in spatiotemporal fields (e.g., Salam and Hsieh 2019; Li et al. 2014; Luo and Sycara 2018; Ouyang et al. 2014) is particularly powerful, as robots can carry heterogeneous sensors and collect simultaneous observations in different spatial locations. As fleets of deep-sea capable robots are not generally within reach for the science community, in this article, we leveraged an external crossflow sensor deployed by the science team and other standard shipboard sensing equipment to compensate for information that would have been difficult (or impossible) to collect with AUV Sentry otherwise. This includes not only scientific plume data, but information about robot pose provided by sophisticated shipboard acoustic sensors. Without access to any of these external sensors, additional burdens would need to be placed on the state/environmental model and inference methods used for decision-making. For instance, localization using inertial sensor filtering and bathymetric SLAM techniques (e.g., Barkby et al. 2009; Ling et al. 2023) would need to be additionally performed online and jointly with the water mass dynamics and plume physics. Both operational development and research efforts towards a future of multiagent exploratory fleets would have a transforming effect on deep ocean sciences.

There is a significant desire for embodied intelligence and assistive decision-making in environmental exploration and expeditionary science that roboticists are particularly well situated to address. PHORTEX fundamentally relies on human expertise to inform the scientific models used within PHUMES, generate useful reward functions, set trajectory primitives, and operate deployments on a robot while in the field. Relieving the burden on these human agents — whether by creating aggregated data products or proposing multiple field missions with explanations — could lead to significant gains in the short-term for expeditionary science tasks while robot technology matures. For instance, on the expedition discussed here, a simple utility for graphing acoustically transmitted data at 0.02 Hz between Sentry and the ship was created for “real-time” manual plume detection by observing scientists. The capability of viewing real-time data, which to many academic and industrial roboticists may seem obvious or straightforward, is not necessarily standard in the sciences or on state-of-the-art vessels and autonomous platforms. Research efforts on improving data infrastructure, data visualization, real-time signal processing, human decision-making, and supervised autonomy promise to be extremely impactful to the expeditionary sciences.

PHUMES and the data collected in these trials are actively being used to address key gaps in scientific knowledge about the structure, longevity, and fingerprint of hydrothermal plumes. Tens of thousands of in situ observations were collected in the four field dives that were executed in this study. During these trials, co-located water samples (from samplers mounted on Sentry itself, as well as on the ship-board rosette) were collected and are being analyzed in a laboratory for trace metals, dissolved gasses, and evidence of biological activity. The in situ observations are currently
being used in ongoing work to directly interpolate the results of the laboratory analyses, which will yield a more complete map of the residency of different compounds and creatures supported by plume fluids than could be resolved with the sparse water samples alone. This interpolation effort is supported not just by the data, but also by PHUMES, which following field deployments, is now being used as a simulator for testing scientific hypotheses to explain all of the data that has been collected. Qualitatively, the scientific utility of the data gathered by PHORTEX designed trajectories is equivalent to or better than the data collected by expert-designed trajectories. The difference is rooted in the character of spatial and temporal clustering that occurs in PHORTEX trials—in general, long “streaks” of a plume are observed sequentially using PHORTEX, and streaks are collected throughout a dive. This means that the observations well represent the near-instantaneous gradient of the plume layer being studied, and it’s evolution throughout a mission window. This is considerably more interpretable than in the expert designed trajectories, which tended to collect spatially very dense observations, that were temporally concentrated, which is less information rich scientifically. The utility of “streaks” was investigated in Preston et al. (2022) using data from a separate trial in this same research cruise. Given the rarity of oceanographic scientific expeditions and the ability to perform targeted sampling enabled by PHORTEX, the data set collected is generally a contribution for the larger oceanographic community.

8. Conclusion

This paper presents PHORTEX: PHysically-informed Operational Robotic Trajectories for Expeditions. PHORTEX is an autonomy decision-making framework that plans long-horizon, fixed trajectories to target a partially observable spatiotemporal phenomena by leveraging physics-based dynamical models and Bayesian inference. PHORTEX is motivated by the problem of deep-sea hydrothermal plume charting with AUV Sentry, which requires an autonomous agent to map a spatiotemporally evolving plume structure without using adaptive capabilities underway, while observing the world through a complex, heterogeneous sensor suite. With these operational constraints in mind, PHORTEX implements a “deployment-by-deployment” autonomy loop (model update, trajectory design, and trajectory execution) during field operations. At its core, PHORTEX consists of a trajectory optimizer and the PHUMES model. The PHUMES model uses an embedded plume physics simulator to solve a Bayesian inverse problem and forecasts discrete snapshots of 3D plume volumes in time. The trajectory optimizer plans parameterized, chained lawnmower-pattern primitives using PHUMES forecasts to create multi-hour trajectories that maximize expected plume detections. These trajectories are then validated using Sentry safety checks and deployed.

Using mobile robots to perform science in the deep-sea is predicated upon both state-of-the-art autonomy systems, such as PHORTEX, and on the effective use of resources within the operational constraints of an oceanographic research vessel. Beyond the core PHORTEX method, this paper presents a variety of technical and operational approaches to augment the performance of PHORTEX during field deployments. For instance, we formulated a filtering technique which processed Sentry data into a useful binary measurement of plume occupancy. We additionally made use of nonrobotic platforms and instruments to augment our PHUMES learning.

During a research cruise in November 2021, PHORTEX was used for a sequence of four deployments of AUV Sentry. These experimental results demonstrate that PHORTEX can collect at least as many plume observations as surveys designed by expert human scientists and showed improved spatial and temporal diversity in samples for any given deployment, even when trained on days-old data. We further validated PHORTEX in simulation, showing that PHORTEX-designed trajectories can yield obvious gains over naive lawnmower approaches across the metrics we applied in the field. In both field and simulation trials, we additionally demonstrated that trained PHUMES models yield insightful and physically-realistic forecasts that closely match an underlying environment, even in times or places that are not directly observed by the robot while collecting training data.

PHORTEX is modular and can be easily adapted to other domain-specific and expeditionary science tasks. The binary sensor model can be replaced with any discrete or continuous observation
model; the scientific model leveraged within PHUMES could be trivially swapped for another ODE or highly simplified PDE system (well-suited for e.g., ecological/population studies, fluid or thermal environments); and the reward function and trajectory optimization scheme can be modified based on the operational constraints of a target platform.

Understanding our dynamic and changing environment is a pressing societal challenge, and algorithmic development in the service of expeditionary science presents many compelling challenges in scientific machine learning, decision-making and the integration of research and practice for field robotics. The contribution of this work is to demonstrate the utility of incorporating domain-specific knowledge into autonomy frameworks for science, provide an example of how scientific knowledge and operational constraints can be formulated into a sophisticated (and deployable) autonomy stack, and demonstrate the scientific value of such an approach on the real expeditionary science problem of deep-sea hydrothermal plume charting.

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A. Additional Background and Related Work

The formulation and deployment of PHORTEX combines several technical fields including informative path planning, planning under uncertainty, Bayesian reasoning, and scientific computing. This appendix presents related work in these subdomains to provide a more complete introduction of background concepts, and provide an overview of the current state-of-the-art and significant prior art on which PHORTEX builds.

A.1. Informative Path Planning

PHORTEX solves a class of sequential decision-making problems that are closely related to the problems studied within the informative path planning (IPP) literature. IPP is an approach for approximately solving sequential decision-making problems under uncertainty by approximating the reward of a task with an information-theoretic function to elicit exploration and exploitation behaviors while a robot is underway. Some common reward functions include the upper-confidence bound (Agrawal, 1995; Auer, 2002; Snoek et al., 2012), probability of improvement (Snoek et al., 2012; Kushner, 1964), expected improvement (Snoek et al., 2012; Jones et al., 1998), and predictive entropy search (Hennig and Schuler, 2012; Hernández-Lobato et al., 2014). Canonical offline IPP techniques for pure information-gathering that optimize submodular (i.e., diminishing returns) coverage objectives can achieve near-optimal performance Srinivas et al. (2012); Binney and Sukhatme (2012). Existing methods in IPP (e.g., Hitz et al. 2017; Hollinger and Sukhatme 2013; Flaspohler et al. 2019; Levine et al. 2010; Binney and Sukhatme 2012), the related field of experimental design and optimal sensor placement (e.g., Krause et al. 2008; Wang et al. 2019), and general decision-making under uncertainty (e.g., Sunberg and Kochenderfer 2018; Somani et al. 2013; Kocsis and Szepesvári 2006; Silver and Veness 2010) have demonstrated that sequential decision-making can be applied to sample collection scenarios in which online, adaptive behaviors are possible, the phenomenon of interest is static, and/or there is an opportunity to train the belief model from many trials and multiple distributed sensors. Each of these typical scenarios is violated for the expeditionary science sampling problem—online adaptation is not possible, the phenomenon is dynamic, and there are very few total number of deployments for model training. PHORTEX enables valuable scientific assets like Sentry to be used effectively to conduct expeditionary science in complex, spatiotemporal environments while respecting safety and operational constraints over very short deployment horizons.

A.2. Bayesian Inference in POMDP Solvers

We define the hydrothermal plume charting problem as a POMDP and therefore need to select a belief representation which encodes the history of a robot’s observations and the implications of those observations (and remaining uncertainty) over the explorable space. In approximate POMDP solvers, the choice of belief representation over the partially-observable state is critical for computing rewards and simulating possible actions and observations in decision-making. PHUMES uses a Bayesian formulation, enabling inference over sets of unknown parameters informed by observations. A Bayesian inference problem takes the following general form: let $\mathcal{Z} = \{z_0, \ldots, z_{n-1}\}$ be a set of $n$ observed data points (possibly vector-valued), $X$ be the set of parameters that describe the distribution of the data such that $z \sim \Pi(z|X)$, and $\alpha$ is a hyperparameter on the parameter distribution such that $X \sim \Pi(X|\alpha)$. Then the posterior distribution of the parameters given the data can be expressed as

$$
\Pi(X|\mathcal{Z}; \alpha) = \frac{\Pi(X, \mathcal{Z}; \alpha) \propto \Pi(\mathcal{Z}|X; \alpha)\Pi(X; \alpha)}{\Pi(\mathcal{Z}; \alpha)}.
$$

(1)

Practically, computing the posterior distribution exactly is computationally expensive or intractable due to the potentially large parameter space described by $X$, or complex and possibly
hierarchical structure present between the observations and the parameter space. For the plume-charting problem, the Bayesian inference problem is posed as uncovering the state $S$ defined with parameter vectors $x_p$, $x_c$, and $x_r$ from observations $Z$ collected according to observation model $O$. In this instance, the observations, which are filtered binary measurements at particular locations, are related to the plume parameters $x_p$ and crossflow parameters $x_c$ via the complex spatiotemporal dynamics of plume physics, which can be represented as a systems of partial differential equations (PDEs).

To approximately solve Bayesian inference problems, several techniques can be employed, such as variational inference (Wainwright and Mulligan, 2002), Monte Carlo sampling (MacKay, 1998), or nonparametric model formulations (Rasmussen and Williams, 2004). Gaussian processes (GPs) are one form of nonparametric Bayesian model which has enjoyed considerable adoption in IPP (e.g., Flaspohler et al. (2019); Guestrin et al. (2005); Krause et al. (2008); Srinivas et al. (2012); Luo and Sycara (2018); Ouyang et al. (2014); Wan and Sapsis (2017); Ma et al. (2017); Marchant et al. (2014)). However challenges remain in adopting GPs for nonstationary or otherwise complex (spatiotemporal) distributions as state-of-the-art kernels [e.g., Singh et al. (2010); Garg et al. (2012); Chen et al. (2022); Raissi et al. (2018)] may be difficult to train with the limited data available in a real field setting. In contrast, MC methods are particularly well suited for the Bayesian inference formulation we have posed for hydrothermal charting in PHUMES, as distributions over a small set of physically-meaningful quantities can be easily defined and embedded in a numerical simulator during the sampling procedure. MC methods estimate the true posterior by drawing samples from a proposal density and evaluating those samples with respect to the posterior. In large, complex systems, it is difficult to define a single density that well-describes a target posterior, and so Markov chain MC (MCMC) methods draw samples from a proposal density which is conditioned on the previous sample drawn, and establishing an acceptance criteria to transition between states MacKay (1998); Green (1995); Neal et al. (2011). Since each new state relies on the density of the previous state in MCMC samplers, a “burn-in” period, in which a potentially large number of samples are drawn, is used before virtually independent samples are generated. MC methods will converge to the true estimator of the posterior for large numbers of samples MacKay (1998). In this paper, we make use of an MCMC procedure within our PHUMES algorithm.

A.3. Buoyant Plume Physics

Understanding the physics of plumes is fundamental to interpreting observations gathered during an AUV *Sentry* deployment and using them to quickly learn and improve a forward simulation of a plume. Hydrothermal plumes in the deep sea are typically characterized as buoyancy-driven water masses. On formation at a vent site, emitted fluid is significantly less dense than background seawater (by virtue of being super-heated, with some add-on effects by changes in chemical composition). The less dense water mass rises rapidly in the water column, forming a buoyant stem. As a general rule, a buoyant stem grows in diameter approximately 1 m for every 10 m vertically travelled. Due to rapid cooling, turbulent mixing, and the natural stratification of ocean water, vent-derived fluids will reach a point of neutral-buoyancy with the background seawater. At the point of neutral-buoyancy, the plume-derived fluid spreads out across the isopycnal that describes the ocean layer of equivalent density. In the Atlantic basin, plumes may be expected to rise approximately 300–350 m; in the Pacific basin, this is 150–200 m (Speer and Rona, 1989).

Generalized plume models which have been commonly incorporated in robotic source seeking literature include the Gaussian plume model (Green et al., 1980) and the Gaussian puff model (Ludwig et al., 1977). These models have largely been used to model ground pollution characteristics of smokestack-like sources in open, unstratified atmospheric environments, and typically assume that the advective crossflow dominates plume movement. In the deep sea, a naturally stratified environment, buoyancy forces are the primary advective drivers for plume fluid transport; the change in environment and physics dictates a need for an alternative model. Within the PHUMES framework, a model of plume rise in stratified environments is defined that describes the “envelope”
in which plume fluid may be detected over time, in which a Gaussian assumption is applied which describes the relative concentration of a plume around a centerline describing the steady-state location of a rising plume.

The classical model of plume rise was first popularized by Morton et al. (1956) as a system of conservative equations (here for a stratified fluid) in cylindrical coordinates \((x,r)\) with the \(x\) axis vertical with the vent source at the origin:

Volume:  \[
\frac{d}{dx}(b^2 u) = 2b\alpha u, \tag{2}
\]

Momentum: \[
\frac{d}{dx}(b^2 u^2) = 2b^2 g \frac{\rho_o - \rho}{\rho_1}, \tag{3}
\]

Density deficiency: \[
\frac{d}{dx}(b^2 u \frac{\rho_o - \rho}{\rho_1}) = 2b^2 u \frac{g}{\rho_1} \frac{d\rho_o}{dx}, \tag{4}
\]

where \(\alpha\) is a proportionality coefficient which represents gross mixing (or entrainment) that occurs at the edge of a plume, \(b = b(x)\) is the (symmetric) radius of the plume, \(\rho = \rho(x,r)\) is density inside the plume, \(\rho_o = \rho_o(x)\) is density outside of the plume, \(\rho_1\) is some reference density such that \(\rho_o(0) = \rho_1\), \(g\) is acceleration due to gravity, and \(u = u(x,r)\) is vertical velocity. These equations have been equivalently expressed in terms of mass, salt, heat, and momentum conservation by Speer and Rona (1989) which usefully decomposes density into components of salinity and temperature that can be directly observed by scientific instruments. A version of these equations which additionally account for advective crossflow is used in PHUMES (Tohidi and Kaye, 2016).

Numerical models which describe instantaneous, complicated structure of plume phenomenon in time (e.g., Lavelle et al. 2013; Xu and Di Iorio 2012) have been developed which enhance these spatially-averaged models by directly modeling partial derivatives with respect to time, and incorporating additional dynamical models such as the Navier Stokes equations. Given the computational complexity of these models (on the order of a day on a high-performance computing node to compute a single instance of the evolution of a plume for a simulated hour), we instead focus on leveraging the comparatively simple and fast to compute idealized models described within PHUMES.