Learning Forward Operators for Complex Atmospheric Trace Gas Emission Source Localization with Mobile Sensors

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Abstract

This work investigates the generalized approach to solving the trace gas quantification problem using Machine Learning (ML). Following recent advancements in Physics-informed and Scientific ML to solve PDEs, we utilize Fourier Neural Operator (FNO) frameworks to learn the forward PDE operators for closed loop estimation of the emission source parameters using the Source Receptor Matrix approach.

Problem and Approach

Quantification and localization of methane emissions from oil & gas applications are often formulated as an inverse problem (see Fig. 1).

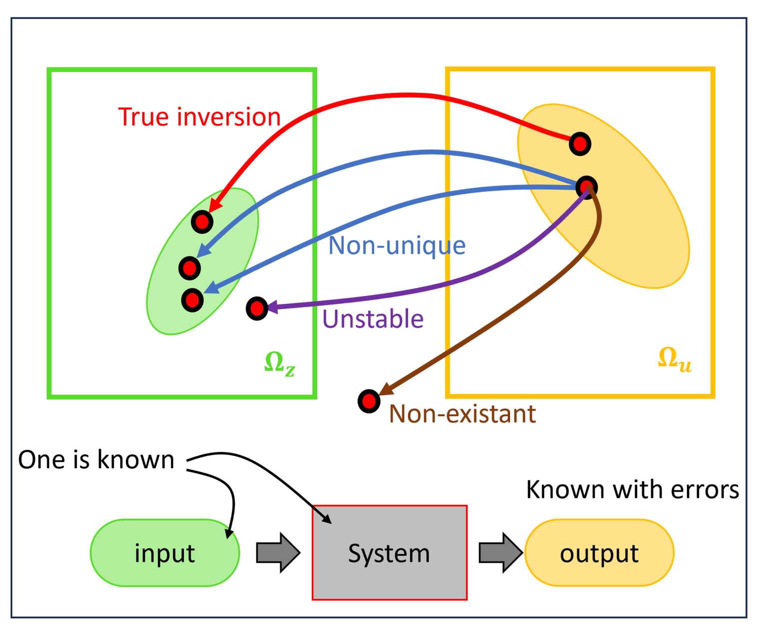


Figure 1: Inverse Problems

Sparse spatio-temporal measurement trajectories are utilized using overly simplified models (e.g. Gaussian Plume) to estimate emissions with sUAS (see Fig. 2). While not valid in many situations with complex fluid interactions (e.g. flow around obstacles), there is no alternative. Therefore, we propose the use of efficient PDE solvers and optimal sensing strategies, namely the FNO, the Source Receptor Matrix (SRM), and the empirical observability Gramian [1].

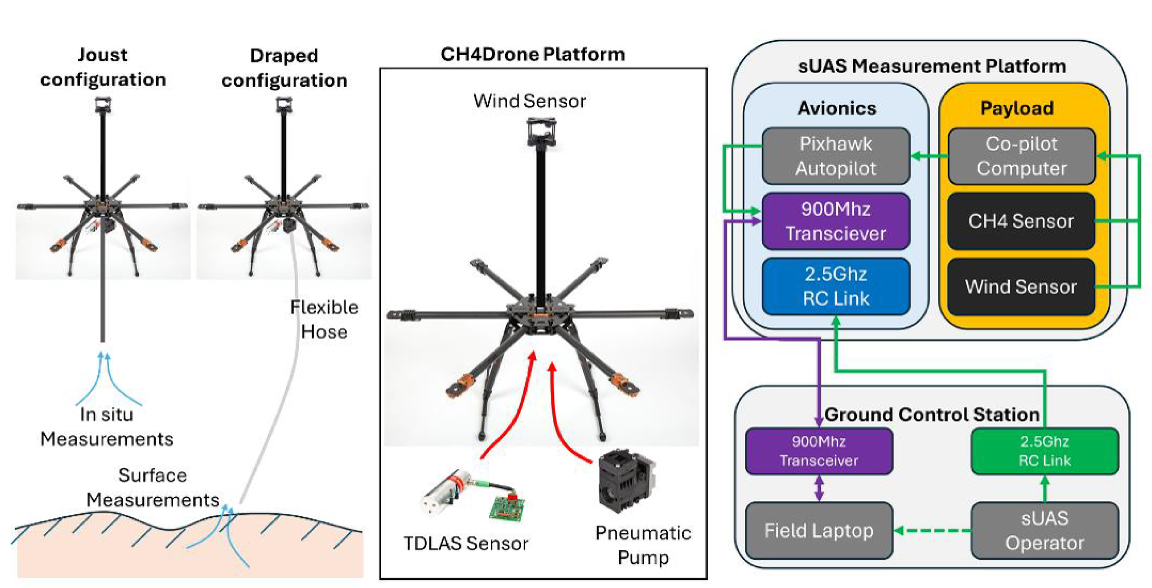


Figure 2: CH4Drone system.

Source Receptor Matrix Method

The source receptor matrix (SRM) approach utilizes a set of measurement trajectories and a set of proposed source locations to estimate the emission rates using linear relationship between the estimated output and the SRM. The SRM can be solved recursively for the location and rate based on the guidance from the optimal sensor placement cost function, which relies on two metrics based on the empirical observability Gramian [2], namely the unobservability index (enforcing rank) and the D-Optimality (shaping estimation ellipsoid) [3].

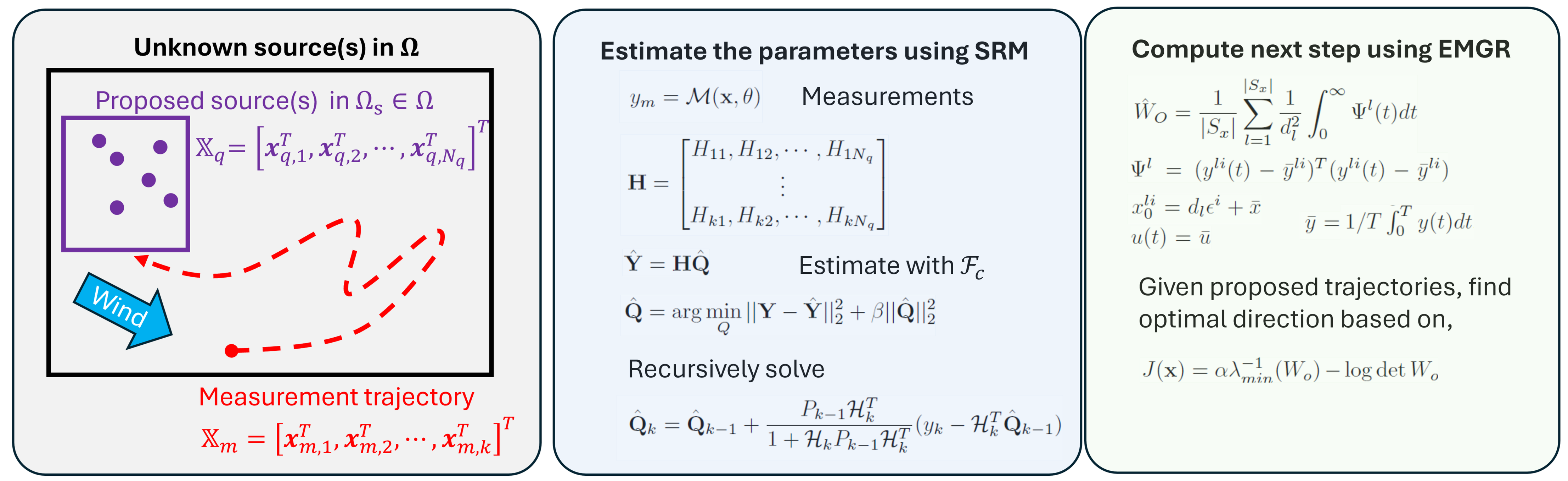


Figure 3: SRM Workflow: 1) Propose unknown source locations, 2) Estimate location and rate based on measurement, and 3) determine guidance based on EMGR.

Training the Forward FNO Models

To approximate a solution to the forward PDEs, a Fourier Neural Operator (FNO) framework was utilized (NeuralOperator) [4]. To train the FNO we generate forward solutions to the coupled Navier-Stokes and Advection Diffusion Equations,

$$\frac{\partial U}{\partial t} = -(U \cdot \nabla)U - \frac{\nabla p}{\rho} + \nu \nabla^2 U, \tag{1}$$

$$\frac{\partial C}{\partial t} = -(U \cdot \nabla)C + D\nabla^2 C + S, \tag{2}$$

subject to initial conditions $u_0 = [u_{0,1}, u_{0,2}]^T$, and obstacle mask $M \in \mathbb{R}^{H \times W}$. The diffusion, D, and kinematic viscosity, ν, parameters are predefined but can be computed from temperature and pressure. To compute efficiently, the equations are numerically solved following [5]. Different to many FNO implementations, here we try to approximate $\mathcal{F}_w : \theta_w \to U$ and $\mathcal{F}_c : \theta_c \to C$ in a steady state fashion. A burn-period was used to initialize the domain before a time-averaged field is computed and used as a snapshot for training (see Fig. 4).

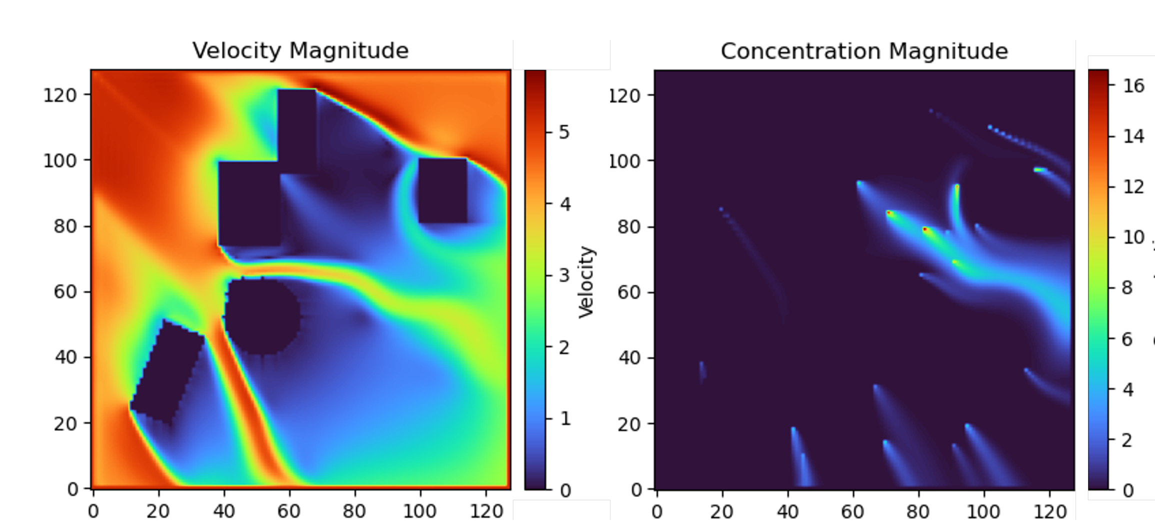
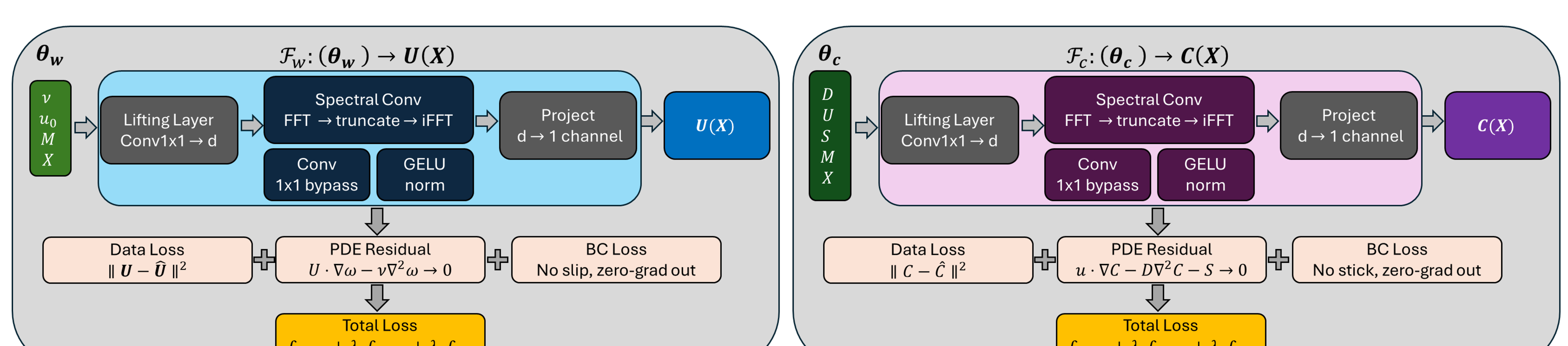


Figure 4: Example dataset snapshot.



Results

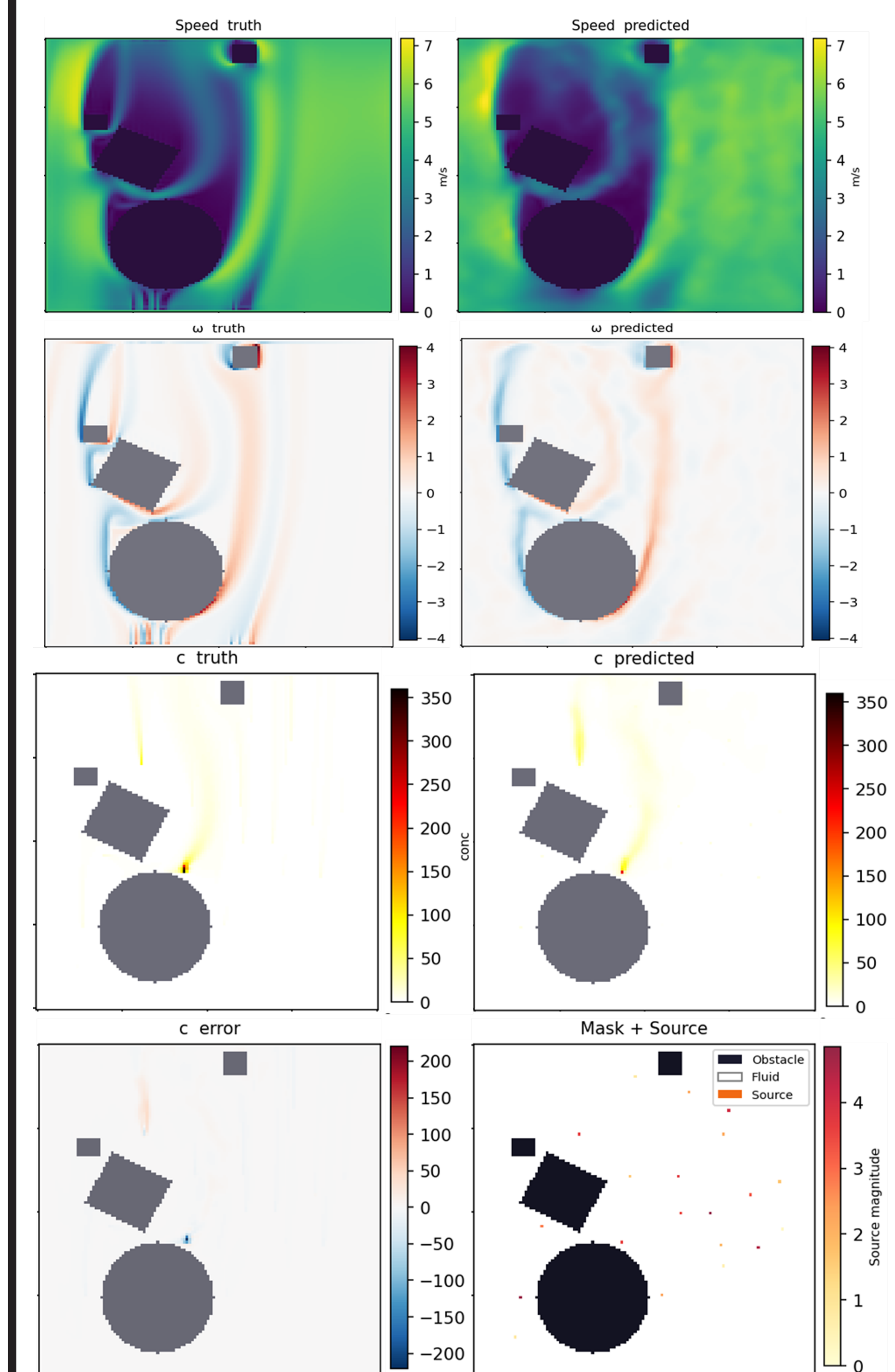


Figure 5: FNO prediction of the velocity, vorticity, and diffusion fields given M and θ.

Future Efforts

Integrate the SRM into simulation before deploying on real CH4Drone system. Investigate the use of adjoint and Neural Inverse Operators (NIO) to improve efficiency. Extend to 3D operator learning and include temperature / pressure as inputs (relate dependence on (1) & (2)).

References

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