State estimation is required whenever we deal with high-dimensional dynamical systems, as the complete measurement is often unavailable. It is key to gaining insight, performing control or optimizing design tasks. Most deep learning-based approaches require high-resolution labels and work with fixed sensor locations, thus being restrictive in their scope. Also, doing Proper orthogonal decomposition (POD) on sparse data is nontrivial. To tackle these problems, we propose a technique with an implicit optimization layer and a physics-based loss function that can learn from sparse labels. It works by minimizing the energy of the neural network prediction, enabling it to work with a varying number of sensors at different locations. Based on this technique we present two models for discrete and continuous prediction in space. We demonstrate the performance using two high-dimensional fluid problems of Burgers’ equation and Flow Past Cylinder for discrete model and using Allen–Cahn equation and Convection-diffusion equations for continuous model. We show the models are also robust to noise in measurements.

Keywords  State estimation · Differentiable implicit layers · Dynamical systems

1 Introduction

State estimation is the ability to recover flow based on a few measurements. It is an inverse problem and arises in many engineering applications such as remote sensing, medical imaging, ocean dynamics, reservoir modeling, and blood flow modeling. Uses of fluid estimation include flow control [1, 2], cardiac blood flow modeling [3, 4, 5], ship wake identification [6], climate prediction [7], optimizing machine design for low-drag vehicles, efficient turbo-machines, etc. Few challenges faced in the processes are limited sensors, sparse label data, moving sensors, ill-posed problems, noisy measurements, etc. This work focuses on learning from moving sparse label data and sensor measurements with a deep learning-based model using an implicit optimization layer for network training. Sparse fluid is encountered in various situations. One reason is that storing high-resolution data generated during direct numerical simulation is challenging due to limited storage space. It makes analysis, sharing, and visualization difficult. Another important reason is that real data is hard to measure on a full scale, like cardiovascular blood flow data obtained from flow magnetic resonance imaging (MRI) [8, 9, 10].

For high dimensional state estimation problems like fluids, popular approaches include library-based approaches or observer dynamical system stochastic approaches. Library-based methods use offline data, and the library consists of generic modes such as Fourier, wavelet, discrete cosine transform basis, or data specific Proper orthogonal decomposition (POD) or Dynamic mode decomposition (DMD) modes, or training data. Library-based approaches using sparse representation assume state can be expressed as the combination of library elements. In an observer dynamical system, we assume the system’s dynamics to produce a full state and update it based on new measurements to reduce estimation error forming a closed feedback loop. The estimate is maintained by Kalman filtering [11, 12, 13]. Tu et al. [14] applied...
We present two models trained using this technique. The first one produces discrete high-dimensional predictions in
space. Second, produce continuous prediction utilizing the information of coordinates. We demonstrate the results
consistent with sparse label data whose position may vary with time, for which POD cannot be performed. Thus it restricts us
from using traditional POD-based approaches. Other deep learning-based approaches like [26,27,28] give accurate predictions
with fewer sensors but require high-resolution labels for training. Gao et al. [29] uses physics-based loss for super-resolution
using sparse data and thus assumes a fixed number of sensors and their positions. In this work, we propose an Energy
network for state estimation with random sensors (ENERS), a technique to learn a model from sparse training labels
capable of predicting full states given a varied number of sensors at random locations. This work, we propose an Energy
network for state estimation with random sensors (ENERS), a technique to learn a model from sparse training labels
capable of predicting full states given a varied number of sensors at random locations. We present two models trained
using this technique. The first one produces discrete high-dimensional predictions in space. Second, produce
continuous prediction utilizing the information of coordinates. We demonstrate the results corresponding to four high
complexity problems: 2-dimensional (2D) coupled Burgers’ equation, transient flow, Allen–Cahn equation, and
Convection-diffusion equation.

The remainder of the paper is organized as follows. In Section 2, details on the problem statement is provided. Details on
the proposed approach are provided in Section 3.1. Section 3 and 4 give details on discrete and continuous formulation
with two numerical examples in each to illustrate the performance of the proposed approach. Finally, Section 5
provides the concluding remarks.

2 Problem statement

Consider a dynamical system obtained by partial discretization of the d-dimensional governing differential equations:
\[ J_t(x,t) = F(x,J(x,t)), \quad J^n = J(x,t_n), \quad x \in \Omega \] (1)
The simulation time domain is discretized by \( L \) steps and the space domain is discretized by \( \omega \) segments resulting in
\[ Z = \{ J^l_m \in \mathbb{R}^{\omega} | l = 0, \ldots, L - 1, \ m = 0, \ldots, M - 1 \} \] (2)
where \( Z \in \mathbb{R}^{L \times M \times \omega} \), \( l \) is time step index, \( M \) = number of system’s state variables, e.g. \( m = 0 \) represents x-velocity and \( m = 1 \) represents y-velocity in § 3.2 of 2D coupled Burgers’ equation. We consider sensor location and data location, represented by integers in discrete domain respectively as
\[ S = \{ \lambda^l_m \in \mathbb{Z}^p \cap [0, \omega - 1]^p | l = 0, \ldots, L - 1, \ m = 0, \ldots, M - 1 \} \] (3)
\[ T = \{ \pi^l_m \in \mathbb{Z}^h \cap [0, \omega - 1]^h | l = 0, \ldots, L - 1, \ m = 0, \ldots, M - 1 \} \] (4)
where \( p \) = number of sensors, \( h \) = number of data nodes, \( S \in \mathbb{Z}^{L \times M \times p} \cap [0, \omega - 1]^{L \times M \times p} \), \( T \in \mathbb{Z}^{L \times M \times h} \cap [0, \omega - 1]^{L \times M \times h} \). The corresponding sensor values and data values are
\[ X = \{ \sigma^l_m \in \mathbb{R}^p | l = 0, \ldots, L - 1, \ m = 0, \ldots, M - 1 \} \] (5)
\[ \Phi = \{ \psi^l_m \in \mathbb{R}^h | l = 0, \ldots, L - 1, \ m = 0, \ldots, M - 1 \} \] (6)
\[ \sigma^l_m = \Lambda^l_m \sigma^l_m \] (7)
\[ \psi^l_m = \Pi^l_m \psi^l_m \] (8)
where \( X \in \mathbb{R}^{L \times M \times p} \), \( \Phi \in \mathbb{R}^{L \times M \times h} \), \( \Lambda^l_m \in \mathbb{R}^{p \times \omega} \) and \( \Pi^l_m \in \mathbb{R}^{h \times \omega} \) are measurement matrices composed of one-hot row vectors. \( \Lambda^l_m \) and \( \Pi^l_m \) are defined as
\[ \Lambda^l_m = \begin{cases} 1 & \text{if } l = j \\ 0 & \text{otherwise} \end{cases} \] (9)
Note that integer sensor locations $\lambda^l_m$ are selected randomly and are kept fixed during training. Similarly, a different set of sensor locations $S$ is selected for testing the network. In this work, we aim to use sensor data from a set of $\gamma$ system states and produce $\gamma$ high dimensional states. Thus we divided the sensor values and data into chunks, each with $\gamma$ states.

$$\chi^k = \{\sigma^k_{mz+i} \in \mathbb{R}^p \mid i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}$$ (11)

$$\phi^k = \{\psi^k_{mz+i} \in \mathbb{R}^h \mid i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}$$ (12)

where $\chi^k \in \mathbb{R}^{\gamma \times M \times p}$ are sensor values for $\gamma$ time steps, $\phi^k \in \mathbb{R}^{\gamma \times M \times h}$ are data values for $\gamma$ time steps, $k = 0, \ldots, N - 1$, $N$ is number of train samples, $z$ is time steps between first state $\sigma^0_z$ of each tensor $\chi^k$.

### 3 Discrete space models

#### 3.1 Proposed approach

![Network architecture of proposed Ensers model.](image)

In this section, we propose a novel deep learning-based framework for state estimation. Prediction of $\gamma$ high dimensional states is done via feed-forward neural network (FNN) $\Gamma$ using optimized reduced state vector $\xi^k \in \mathbb{R}^\varsigma$:

$$\Gamma(\xi^k) = D^k = \{D^k_m \in \mathbb{R}^\omega \mid i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}$$ (13)

where $D^k \in \mathbb{R}^{\gamma \times M \times \omega}$ is a third-order tensor of predicted states. The output vector of FNN has a dimension of $\gamma \times M \times \omega$ which is reshaped into a tensor of shape $\gamma \times M \times \omega$. The reduced state is obtained by solving the following minimization problem using sensor data $\chi^k$ and predicted states by the neural network.

$$\xi^k = \arg\min_{\xi^k} \|\text{vec}(\chi^k -\rho(\xi^k))\|_2^2$$ (14a)
The physics-based loss function is used in the approach because of spare training labels. Training any network with just spare labels will produce garbage values on nodes without labels. Physics-based loss functions have been used to train neural networks for solving PDEs. A popular class of methods is PINNs [41]. The basic idea here is to place a neural network prior to the state variable and then estimate the neural network parameters by using a physics-informed loss function.

3.1.1 Physics-based loss function

The physics-based loss function is used in the approach because of spare training labels. Training any network with just spare labels will produce garbage values on nodes without labels. Physics-based loss functions have been used to train neural networks for solving PDEs. A popular class of methods is PINNs [41]. The basic idea here is to place a neural network prior to the state variable and then estimate the neural network parameters by using a physics-informed loss function. Several improvements to the originally proposed PINN can also be found in the literature. For example, Zhu et al. [42] developed convolutional PINN for time-independent systems. Geneva and Zabaras [43] used physics-constrained auto-regressive model for surrogate modeling of dynamical systems. We use Runge-Kutta methods with q stages for defining loss between γ state predictions. Let

\begin{align}
V^n &= D^{k_0} \\
V^{n+ci} &= D^{k_i}, \quad i = 1, \ldots, q \\
V^{n+1} &= D^{k_{\gamma-1}}
\end{align}

where \(D^{k_i}\) are network prediction. General form of Runge-Kutta methods with q stages applied to Eq. (1):

\begin{align}
V^{n+ci} = V^n - \Delta t \sum_{j=1}^{q} a_{ij} F(V^{n+ci}), \quad i = 1, \ldots, q
\end{align}
Algorithm 1: Training ENSERS

1: **Inputs:** $Z, S, T$. \{Eq. (2), Eq. (3), Eq. (4)\}
2: **Set Hyper-parameters:** $\eta$: outer learning rate, $\eta_0$: inner learning rate at epoch=0, $\bar{\eta}$: inner learning rate, $\beta$: batch size, $I_o$: outer iterations, $I_i$: inner iterations, $\zeta$: physics penalty rate, $\zeta_0$: physics penalty at epoch=0, $N$: number of train samples, $z$, $\gamma$.
3: **Calculate data-set:** $\tilde{\chi}, \phi, \Lambda, \Pi$
4: **Initialize:** Neural network model: $\Gamma(\cdot; \theta)$
5: **for** $t_o = 0$ to $I_o - 1$ **do** \{Outer optimization Loop\}
6: $\eta_i = \eta_0 + t_o \bar{\eta}$ \{Schedule inner learning rate\}
7: $\zeta = \zeta_0 + t_o \bar{\zeta}$ \{Schedule physics penalty\}
8: **for** $k = 0$ to $N - 1$ **do**
9: **Initialize:** $\tilde{\xi}^k$
10: **for** $t_i = 0$ to $I_i - 1$ **do** \{Inner optimization Loop\}
11: $D^k = \Gamma(\tilde{\xi}^k)$ \{Eq. (14d)\}
12: $\hat{Q}^k \leftarrow$ DrawValuesAtSensorLocations($\hat{D}^k$) \{Eq. (14c)\}
13: $\xi = \text{MSE}(\chi^k, \hat{Q}^k)$
14: $\frac{\partial \xi}{\partial \xi^k} \leftarrow$ Backprop($\xi$)
15: $\xi^k = \xi - \eta_i \frac{\partial \xi}{\partial \xi^k}$
16: **end for**
17: $\tilde{\xi}^k = \xi^k$
18: $\hat{D}^k = \Gamma(\tilde{\xi}^k)$ \{Eq. (13)\}
19: $Y^k \leftarrow$ DrawValuesAtDataLocations($\hat{D}^k$) \{Eq. (15c)\}
20: $\mathcal{L} = \text{MSE}(\phi^k, Y^k) + \zeta P(D^k)$ \{Calculate loss\}
21: $\frac{\partial \mathcal{L}}{\partial \theta} \leftarrow$ Backprop($\mathcal{L}$)
22: $\theta \leftarrow \theta - \eta_o \frac{\partial \mathcal{L}}{\partial \theta}$ \{Update weights\}
23: **end for**
24: **end for**
25: **Output:** Trained network $\Gamma(\cdot; \theta^*)$.

Algorithm 2: Testing ENSERS

1: **Inputs:** Trained network $\Gamma(\cdot; \theta^*)$, $S$. \{Eq. (3)\}
2: **Set Hyper-parameters:** $\eta$: inner learning rate, $I_i$: inner iterations, $\hat{N}$: number of test samples, $z$, $\gamma$.
3: **Calculate data-set:** $\tilde{\chi}, \Lambda$
4: **for** $k = 0$ to $\hat{N} - 1$ **do**
5: **Initialize:** $\tilde{\xi}^k$
6: **for** $t_i = 0$ to $I_i - 1$ **do** \{Inner optimization Loop\}
7: $\hat{D}^k = \Gamma(\tilde{\xi}^k)$ \{Eq. (14d)\}
8: $\hat{Q}^k \leftarrow$ DrawValuesAtSensorLocations($\hat{D}^k$) \{Eq. (14c)\}
9: $\xi = \text{MSE}(\chi^k, \hat{Q}^k)$
10: $\frac{\partial \xi}{\partial \xi^k} \leftarrow$ Backprop($\xi$)
11: $\xi^k = \xi - \eta_i \frac{\partial \xi}{\partial \xi^k}$
12: **end for**
13: $\xi^k = \xi^k$
14: $\hat{D}^k = \Gamma(\tilde{\xi}^k)$ \{Eq. (13)\}
15: **end for**
16: **Output:** Predicted states \{$D^k_m$, $m = 0, \ldots, M - 1$\}.

$$V^{n+1} = V^n - \Delta t \sum_{j=1}^{q} b_j F(V^{n+c_j})$$  \hspace{1cm} (17b)
We use the Implicit Runge-Kutta methods with q stages and thus parameters \{a_{ij}, b_{j}, c_j\} are chosen accordingly. Now, shifting second term on right hand side (RHS) in Eq. (17) to left hand side (LHS) and replacing exact operator \(\hat{F}\) with numerical gradient based operator \(\tilde{F}\)

\[
\hat{W}_i = V^{n+c_j} + \Delta t \sum_{j=1}^{q} a_{ij} \tilde{F}(V^{n+c_j}), \quad i = 1, \ldots, q
\]  

(18a)

\[
\hat{W}^c_{q+1} = V^{n+1} + \Delta t \sum_{j=1}^{q} b_{j} \tilde{F}(V^{n+c_j})
\]  

(18b)

\[
P(\chi^k) = \sum_{i=1}^{q+1} ||\vec{v}(\hat{W}_i - V^n)||^2
\]  

(18c)

where \(\hat{W}_i\) are different estimates of \(V^n\), \(P(\chi^k)\) is the physics based loss function. For calculating loss the spatial gradients are approximated using Sobel filter 2D convolutions [44]. See §A for additional details. Note that physics-based loss function is only used during training of network.

In next section, we present two examples to show model proposed is able to learn from sparse moving data labels. We illustrate the performance of the proposed approach with plots of prediction. We show that model is robust against noisy sensor measurements by showing error corresponding to various noise level. Error used as a quantitative metric in plots in defined as

\[
e^k = \frac{||D^{\chi^k}_m - J^{k\chi + \gamma^l}_m||_2}{||J^{k\chi + \gamma^l}_m||_2}, \quad k = 0, \ldots, \tilde{N}
\]  

(19)

where \(e^k \in \mathbb{R}\) represents the error, \(\tilde{N}\) number of testsamples, \(J^{k\chi + \gamma^l}_m \in \mathbb{R}^\theta\) are the true state and \(D^{\chi^k}_m \in \mathbb{R}^\theta\) are the predicted state using the proposed approach. \(||\cdot||_2\) represents the L2 norm.

### 3.2 Experiment: 2D coupled Burgers’ equation

As the first example, we consider the the 2D coupled Burgers’ system. It has the same convective and diffusion form as the in-compressible Navier-Stokes equations. It is an important model for understanding of various physical flows and problems, such as hydrodynamic turbulence, shock wave theory, wave processes in thermo-elastic medium, vorticity transport, dispersion in porous medium. The governing equations for Burgers’ equation takes the following form:

\[
u_t + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = 0,
\]  

(20)

with periodic boundary condition

\[
\mathbf{u}(x = 0, y, t) = \mathbf{u}(x = L, y, t),
\]

\[
\mathbf{u}(x, y = 0, t) = \mathbf{u}(x, y = L, t).
\]  

(21)

Eq. (20) can be written in expanded form as

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0
\]

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} - \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) = 0,
\]  

(22)

where \(\nu\) is viscosity, \(u\) and \(v\) are the \(x\) and \(y\) components of velocity. We consider \(\{x, y\} \in [0, 1]\). The initial condition is defined using truncated Fourier series with random coefficients:

\[
\mathbf{u}(x, y, t = 0) = \frac{2w(x, y)}{\max_{(x, y)}|w(x, y)|} + c,
\]  

(23)
where

\[ \mathbf{w}(x,y) = \sum_{i=-L}^{L} \sum_{j=-L}^{L} a_{ij} \sin(2\pi(ix+jy)) + b_{ij} \cos(2\pi(ix+jy)), \]

(24)

where \( a_{ij}, b_{ij} \sim N(0, I_2) \), \( L = 4 \) and \( c \sim U(-1,1) \in \mathbb{R}^2 \).

### 3.2.1 Data-set and Model Parameters

We use FeNICS [45] computing platform to solve the partial differential equations (22) for generating data-set. We discretize the spatial domain with \( 64 \times 64 \) grid and use a time-step of 0.005. Parameters related to data-set considered are displayed in Table 1. We use noisy measurements to test the approach. Noise level is measured in signal to noise ratio (SNRdB) in decibels (dB) and is represented by \( SNR_{dB} \). Signal after adding noise \( r \) is formulated as:

\[
\begin{align*}
    r &= s + \left( \frac{P}{2 \times 10^{SNR_{dB}/10}} \right)^{0.5} \cdot \mathcal{N} \\
    P &= \sum_{s} s^2
\end{align*}
\]  

(25a)

(25b)

where, \( s \) is noise-free signal, \( \mathcal{N} \) is random variable with standard normal distribution. Plots depicting different noise levels used for testing is shown in Fig. 2.

![Figure 2: Plots of 2D Burgers velocity for visualizing different noise levels. SNRdB represents signal to noise ratio in decibels.](image)

| SNRdB 10 | SNRdB 20 | SNRdB 60 | SNRdB None |
|----------|----------|----------|------------|
| ![Image](image1) | ![Image](image2) | ![Image](image3) | ![Image](image4) |

Table 1: Data-set parameters for 2D Burgers problem.

| \( \gamma \) | \( M \) | \( L \) | \( z \) | \( \omega \) | domain |
|---|---|---|---|---|---|
| 5 | 2 | 50 | 2 | 3969 | \( 63 \times 63 \) |

Table 2: Network architecture of proposed Enisers for 2D coupled Burgers’ problem.

| Layer | Input | Output | Activation |
|---|---|---|---|
| FC | 8 | 64 | Softplus |
| FC | 64 | 64 | Softplus |
| FC | 64 | \( \omega \cdot M \cdot \gamma \) | linear |

Table 3: Training hyper parameters of Enisers for 2D Burgers problem.

| \( \eta_i \) | \( \eta_\theta \) | \( \hat{\eta}_i \) | \( \beta \) | \( I_\theta \) | \( I_i \) | \( \zeta_0 \) | \( \zeta \) | \( I \) | \( h \) | \( \mathcal{N} \) | \( \zeta \) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0002 | 0.1 | 0.006 | 11 | 2001 | 4 | 0.005 | 0.0001 | 32 | 800 | 22 | 8 |

Table 4: Testing hyper-parameters of Enisers for 2D Burgers problem. \( \eta_i \): inner learning rate, \( I_i \): inner iterations

| \( \eta_i \) | \( I_i \) | \( p \) | \( N \) |
|---|---|---|---|
| 5 | 100 | [4, 16] | 12 |
FNN used in the model is a shallow network with three fully connected (FC) layers. We use Softplus \[46\] activation function which has smooth first derivatives. Thus it helps avoid discontinuities because unrolling the inference procedure involves computing $\nabla_\theta \nabla_\xi (L)$. Network architecture is displayed in Table 2. We use 800 data nodes for training from each system variable data which is 20% of high-resolution data. Training hyper-parameters and training data are summarized in table 3. For testing, we use sensor locations different from the ones used during training.

### 3.2.2 Results and Discussions

![Ensers predictions of a 2D coupled Burgers' test case](image.png)

Figure 3: Ensers predictions of a 2D coupled Burgers’ test case. (Top to bottom) x-velocity FEM target solution, x-velocity Ensers prediction, x-velocity L1 error, y-velocity FEM target solution, y-velocity Ensers prediction and y-velocity L1 error.

![Violin plot representing error \(\epsilon\) distribution in prediction vector of x and y velocity for different noise levels in sensor measurements for 2D coupled Burgers’ test case](image.png)

Figure 4: Violin plot representing error \(\epsilon\) distribution in prediction vector of x and y velocity for different noise levels in sensor measurements for 2D coupled Burgers’ test case.
Fig. 5 shows the prediction of Enser for x and y velocity components at various times in simulation with 16 sensors. We see that it produces results that accurately captures the current state of the system at most points in the domain. If a network is trained without a physics-based loss function then it will produce garbage values at points where data is absent. Fig. 4 shows violin plot of error vector $\varepsilon$ defined in Eq. (19) between target and prediction with various noise level in sensor measurement for test case. In Eq. (19), $m$ for x velocity and y velocity are 0 and 1 respectively and $\gamma^* = 2$. The plot represents the distribution of error $\varepsilon$ in the prediction vector. Greater spread corresponding to a point on the y-axis corresponds to more values present in the error vector $\varepsilon$ around that value of the point on the y-axis. We see the model is robust to noise as the mean error in the plot are close for cases of no noise ($SNR_{dB} = None$) and high noise ($SNR_{dB} = 10$).

3.3 Experiment: Flow Past Cylinder

As the second example, we consider the flow past a cylinder problem. It is a well known canonical problem and is characterized by periodic laminar flow vortex shedding. System is governed by incompressible, laminar, Newtonian fluid equations:

$$\frac{\partial(u)}{\partial x} + \frac{\partial(v)}{\partial y} = 0 \tag{26a}$$

$$\frac{\partial(u)}{\partial t} + u \frac{\partial(u)}{\partial x} + v \frac{\partial(u)}{\partial y} = -\frac{1}{\rho} \frac{\partial(p)}{\partial x} + \nu \left( \frac{\partial^2(u)}{\partial x^2} + \frac{\partial^2(u)}{\partial y^2} \right) \tag{26b}$$

$$\frac{\partial(v)}{\partial t} + u \frac{\partial(v)}{\partial x} + v \frac{\partial(v)}{\partial y} = -\frac{1}{\rho} \frac{\partial(p)}{\partial y} + \nu \left( \frac{\partial^2(v)}{\partial x^2} + \frac{\partial^2(v)}{\partial y^2} \right) \tag{26c}$$

3.3.1 Data-set and Model Parameters

A schematic representation of the computational domain is shown in Fig. 5(a). The circular cylinder is considered to have a diameter of 1 unit. The center of the cylinder is located at a distance of 8 units from the inlet. The outlet is located at a distance of 25 units from the center of the cylinder. The sidewalls are at 4 units distance from the center of the cylinder. At the inlet boundary, a uniform velocity of 1 unit along the X-direction is applied. Pressure boundary condition with $P = 0$ is considered at the outlet. A no-slip boundary at the cylinder surface is considered. Coordinate of the snapshot cutout stretches from $[1.5, -2] \times [5.5, 2]$ which is discretized into $64 \times 64$ points in $x$ and $y$ directions (see Fig. 5(b)).

| $\gamma$ | $M$ | $L$ | $z$ | $\omega$ | $v$ | $Re$ | domain |
|----------|-----|-----|-----|---------|-----|------|--------|
| 5        | 3   | 25  | 1   | 4096    | 0.005 | 200  | $64 \times 64$ |

The data-set is generated by using Unsteady Reynolds-averaged Navier Stokes (URANS) simulation in OpenFoam [47]. The overall problem domain is discretized into 63420 elements with finer mesh near the cylinder. Time step $\delta t = 0.02$
We use a shallow network in the model with two fully connected (FC) layers. Network architecture is displayed in Table 6. We use 500 data nodes for training from each system variable data which is 12.2% of high-resolution data. Training and testing hyper-parameters are shown in table 7 and 8 respectively. Sensor locations for testing are different from the ones used during training. For this problem physics-based loss function is extended to include the continuity equation:

\[
P(\chi^k) = \sum_{i=1}^{\omega+1} \| \text{vec}(W_i - V^n) \|_2^2 + \sum_{i=0}^{\gamma-1} \| \text{vec}(\frac{\partial (V_0^n)}{\partial x} + \frac{\partial (V_1^n)}{\partial y}) \|_2^2
\]

Table 6: Network architecture of proposed Ensers for Flow Past Cylinder problem.

| Layer | Input | Output | Activation |
|-------|-------|--------|------------|
| FC    | 8     | 64     | Softplus   |
| FC    | 64    | $\omega \ast M \ast \gamma$ | linear |

Table 7: Training hyper parameters of Ensers for Flow Past Cylinder.

| $\eta_0$ | $\eta_i$ | $\hat{\eta}_i$ | $\beta$ | $I_0$ | $I_i$ | $\zeta_0$ | $\hat{\zeta}_i$ | $p$ | $h$ | $N$ | $\varsigma$ |
|----------|----------|----------------|---------|-------|------|----------|----------------|----|----|-----|----------|
| 0.0003   | 0.1      | 0.002          | 9       | 3001  | 5    | 0.01     | 0.0006         | 16 | 500 | 18  | 8        |

Table 8: Testing hyper parameters of Ensers for Flow Past Cylinder problem. $\eta$: inner learning rate, $I_i$: inner iterations

| $\eta_i$ | $I_i$   | $p$   | $N$ |
|----------|--------|-------|-----|
| 5        | 100    | [4, 16]| 12  |

3.3.2 Results and Discussions

Fig. 7 shows prediction of Ensers for pressure, x and y velocity components with 16 sensors. We see that it produces results that accurately capture the current state of the system at most points in the domain. Fig. 8 shows violin plot of error defined in Eq. (19) between target and prediction with various noise levels in sensor measurement for the test case. In Eq. (19), $m$ for x velocity, y velocity and pressure are 0, 1 and 2 respectively and $\gamma^* = 2$. The plot represents the distribution of error in prediction vectors. We see model is robust to noise as mean error in Fig 8 are close for cases of no noise(SNRdB = None) and high noise(SNRdB = 10).
4 Continuous space models

4.1 Proposed approach

In this section, we propose a novel deep learning-based continuous framework for state estimation. Prediction of $\gamma$ high dimensional states is done via multiple passes from a feed-forward neural network (FNN) $\Gamma$ for every collocation point with coordinate vector $X_r$, using optimized reduced state vectors $\xi^k \in \mathbb{R}^\varsigma$:

$$\Gamma(\Xi^k) = \{D^i_{mr} \in \mathbb{R} \mid i = 0, ..., \gamma - 1, m = 0, ..., M - 1\}, \quad r = 0, ..., \omega$$ (28)

$$\Xi^k_r = \{\xi^k, X_r\}, \quad r = 0, ..., \omega$$ (29)
SNRdb
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
Error
Sensors: 16
U
V
P

SNRdb
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
Error
Sensors: 4
U
V
P

Figure 8: Violin plot representing error $\varepsilon$ distribution in prediction vector of $x,y$ velocity and pressure for different noise levels in sensor measurements for Flow Past Cylinder test case.

where output vector of FNN $\Gamma$ has dimension $\gamma \times M$, $D_{mk}^{ki}$ is predicted states value at $i^{th}$ collocation point, $X_r$ are coordinates of $r^{th}$ collocation point. Output of $\omega$ FNNs are combined to form third-order tensor $D_k \in \mathbb{R}^\gamma \times M \times \omega$. Reduced state is obtained by solving the following minimization problem using sensor data $\chi_k$ and predicted states by the neural network.

$$\xi^k = \arg\min_{\tilde{\xi}^k} \|{\text{vec}}(\chi^k - \rho(\tilde{\xi}^k))\|^2_2$$  (30a)

$$\rho(\tilde{\xi}^k) = \{\tilde{O}^{ki}_m \in \mathbb{R}^p | i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}$$  (30b)

$$\tilde{O}^{ki}_m = \Lambda_m^{kz+i} \tilde{D}^{ki}_m$$  (30c)

$$\Gamma(\tilde{\xi}_r^k) = \{\tilde{D}^{ki}_m \in \mathbb{R} | i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}, \quad r = 0, \ldots, \omega$$  (30d)

$$\tilde{\xi}_r^k = \{\tilde{\xi}_r^k, X_r\}, \quad r = 0, \ldots, \omega$$  (30e)

where $\tilde{O}^{ki}_m \in \mathbb{R}^p$ are values of predicted states at sensor locations $\Lambda_m^{kz+i}$. Note that in practice $\xi^k$ is obtained by a few steps of gradient descent instead of global minimization. The network is trained by minimizing data loss and physics-based loss $P(\chi^k)$ across training samples $N$.

$$\theta^* = \arg\min_{\theta} \sum_{k=0}^{N-1} \|{\text{vec}}(\phi^k - \Upsilon(\chi^k))\|^2_2 + P(\chi^k)$$  (31a)

$$\Upsilon(\chi^k) = \{Y^{ki}_m \in \mathbb{R}^h | i = 0, \ldots, \gamma - 1, m = 0, \ldots, M - 1\}$$  (31b)

$$Y^{ki}_m = \Pi_m^{kz+i} D^{ki}_m$$  (31c)

where $D^{ki}_m \in \mathbb{R}^\omega$ are predicted states from Eq. (28), $Y^{ki}_m \in \mathbb{R}^h$ are values of predicted states at data locations $\pi_m^{kz+i}$, $\Upsilon(\chi^k) \in \mathbb{R}^\gamma \times M \times p$ are predicted states composed of $\gamma$ time steps, $\theta$ are network parameters. Fig. 1 shows the network architecture during training. Equations (28) and (30) together forms the implicit optimization layer shown in the Fig. 1 for the continuous model. Training and testing procedure is shown in Algorithm 3 and 4 respectively.
Algorithm 3: Training ENSERS

1: **Inputs:** Z, S, T. (Eq. 2), Eq. 3, Eq. 4)
2: **Set Hyper-parameters:** η_o: outer learning rate, η_0: inner learning rate at epoch=0, η_1: inner learning rate at epoch=0, β: batch size, I_o: outer iterations, I_i: inner iterations, ξ: physics penalty rate, ξ_0: physics penalty rate at epoch=0, N: number of train samples, z, γ.
3: **Calculate data-set:** Z, θ, A, Π
4: **Initialize:** Neural network model: Γ(·; θ)
5: for t_o = 0 to I_o - 1 do {Outer optimization Loop}
6: η_i = η_0 + t_o η_1 {Schedule inner learning rate}
7: ξ = ξ_0 + t_o ξ_1 {Schedule physics penalty}
8: for k = 0 to N - 1 do
9: **Initialize:** ̂ξ_k
10: for t_i = 0 to I_i - 1 do {Inner optimization Loop}
11: ̂ξ_k^r = (ξ_k, X_r), r = 0, ..., ω
12: ̂D_k = Π(̂ξ_k^r), r = 0, ..., ω {Eq. (30d)}
13: ̂Q̂ = DrawValuesAtSensorLocations(̂D̂k) {Eq. (30c)}
14: Ξ = MSE(̂X̂k, ̂Q̂) {Calculate loss}
15: ̄ξ̂_k = ̂ξ̂_k - η_0 ̂ξ̂_k {Calculate loss}
16: ̂ξ̂_k = ̂ξ̂_k - η_0 ̂ξ̂_k {Update weights}
17: end for
18: ̂X̂_r = X_r
19: ̂ξ̂_k = (ξ̂_k, ̂X̂_r), r = 0, ..., ω
20: ̂D̂_k = Γ(̂ξ̂_k^r), r = 0, ..., ω {Eq. (28)}
21: y_k = DrawValuesAtDataLocations(̂D̂) {Eq. (31c)}
22: Ξ = MSE(φ_k, y_k) + ξP(̂D̂) {Calculate loss}
23: ̂ξ̂_k = Backprop(Ξ) {Calculate loss}
24: θ ← θ - η_0 ̂ξ̂_k {Update weights}
25: end for
26: end for
27: **Output:** Trained network Γ(·; θ).

4.1.1 Physics-based loss function

The physics-based loss function for continuous space models differs from discrete formulation due to how RHS of Eq. 1 is evaluated. In this case, we use automatic differentiation for calculating gradients w.r.t. coordinates used in ̂F. For example in first case of Allen–Cahn equation ̂F is evaluated as:

\[
\hat{F}_r = 0.0001 \frac{\partial^2 u}{\partial X_r^2} + 5u^3 - 5u, \quad r = 0, ..., \omega
\]

(32)

where ̂X_r is coordinate vector concatenated with optimized reduced state vector at end of inner optimization loop, see line 18 in algorithm 3. In second case of Convection-diffusion equation ̂F is evaluated as:

\[
\hat{F}_r = a(x, y) \frac{\partial u}{\partial X_0^0} + b(x, y) \frac{\partial u}{\partial X_1^0} + c \frac{\partial^2 u}{\partial X_0^0} + d \frac{\partial^2 u}{\partial X_1^1}, \quad r = 0, ..., \omega.
\]

(33)

where ̂X_0, ̂X_1 are x and y coordinate respectively, a, b, c, d are defined in Eq. 36.
We consider the Allen–Cahn equation along with periodic boundary conditions. The Allen–Cahn equation is a well-known equation from the area of reaction-diffusion systems. It describes the process of phase separation in multicomponent alloy systems, including order-disorder transitions.

\[ u_t - 0.0001u_{xx} + 5u^3 - 5u = 0, \quad x \in [-1, 1], t \in [0, 1], \]

\[ u(0, x) = x^2 \cos(\pi x), \]

\[ u(t, -1) = u(t, 1), \]

\[ u_x(t, -1) = u_x(t, 1). \tag{34} \]

### 4.2 Experiment: Allen–Cahn equation

We consider the Allen–Cahn equation along with periodic boundary conditions. The Allen–Cahn equation is a well-known equation from the area of reaction-diffusion systems. It describes the process of phase separation in multicomponent alloy systems, including order-disorder transitions.

\[ u_t - 0.0001u_{xx} + 5u^3 - 5u = 0, \quad x \in [-1, 1], t \in [0, 1], \]

\[ u(0, x) = x^2 \cos(\pi x), \]

\[ u(t, -1) = u(t, 1), \]

\[ u_x(t, -1) = u_x(t, 1). \tag{34} \]

#### 4.2.1 Data-set and Model Parameters

Data-set is generated by simulating the Allen–Cahn equation (34) using conventional spectral methods. Starting from an initial condition \( u(0, x) = x^2 \cos(\pi x) \) and assuming periodic boundary conditions \( u(t, -1) = u(t, 1) \) and \( u_x(t, -1) = u_x(t, 1) \), we integrated Eq. (34) up to a final time \( t = 1.0 \) using the Chebfun package [49] with a spectral Fourier discretization with 512 modes and a fourth-order explicit Runge–Kutta temporal integrator with time-step \( \Delta t = 10^{-3} \). For more details on the data-set see [41]. Plots depicting different noise levels used for sensor measurement during testing are shown in Fig. 9.

![SNRdB 10](image1)

![SNRdB 20](image2)

![SNRdB 60](image3)

![SNRdB None](image4)

Figure 9: Data plots of Allen–Cahn equation for visualizing different noise levels. SNRdB represents signal to noise ratio in decibels.

The network considered in the continuous formulation has significantly fewer weights compared to the discrete one. This is because the output of the network is predicted at a single point. Network architecture is shown in table [10]. The input size of the network is equal to the sum of the size of the reduced state \( \zeta \) and the dimension of coordinates. For training we use 10 data nodes \( p \) which is 7.81% of 128 total nodes. Similar to previous cases inner loop learning rate
Table 9: Data-set parameters for Allen–Cahn equation.

| $\gamma$ | $M$ | $L$ | $\omega$ | domain |
|------|-----|-----|---------|--------|
| 5    | 1   | 50  | 1       | 128    |

$\eta_i$ and physics loss penalty $\zeta$ are increased linearly with each epoch. Other training and testing hyperparameters are shown in table 11 and 12 respectively.

Table 10: Network architecture of proposed Ensers for Allen–Cahn equation.

| Layer | Input | Output | Activation |
|------|-------|--------|------------|
| FC   | 7     | 128    | Tanh       |
| FC   | 128   | 128    | Tanh       |
| FC   | 128   | 128    | Tanh       |
| FC   | 128   | $M*\gamma$ | linear |

Table 11: Training hyper parameters of Ensers for Allen–Cahn equation.

| $\eta_o$ | $\eta_i$ | $\hat{\eta}_i$ | $\beta$ | $I_o$ | $I_i$ | $\hat{\zeta}_o$ | $\zeta$ | $p$ | $h$ | $N$ | $\varsigma$ |
|----------|----------|-----------------|---------|-------|------|-----------------|---------|-----|-----|-----|-----------|
| 0.001    | 0.005    | 6e−5            | 10      | 1201  | 8    | 0.01            | 2e−5    | 10  | 10  | 40  | 6         |

Table 12: Testing hyper parameters of Ensers for Allen–Cahn equation. $\eta_i$: inner learning rate, $I_i$: inner iterations

| $\eta_i$ | $I_i$ | $p$ | $N$ |
|----------|------|-----|-----|
| 0.1      | 50   | [6, 16] | 12 |

4.2.2 Results and Discussions

Fig. 10 shows the prediction of Ensers with 16 sensors. A noticeable benefit of the continuous formulation is that prediction is smooth compared to discrete cases. Fig. 11 shows violin plot of L2 error defined in Eq. (19) between target and prediction with various noise levels in sensor measurement for the test case. In Eq. (19), $m = 0$ and $\gamma = 2$. Similar to discrete cases, the model is robust to noise in measurements. Fig. 11 shows a marginal increase in error with noise in the case of 16 sensors. Also, error bars with 6 sensors are similar to 16 sensors with low noise and increase slowly with noise.

4.3 Experiment: Convection-diffusion equations

Next we consider a 2-dimensional linear variable-coefficient convection-diffusion equation on $\omega = [0, 2\pi] \times [0, 2\pi]$,

$$u_t = a(x,y)u_x + b(x,y)u_y + cu_{xx} + du_{yy} \quad (t,x,y) \in [0,0.2] \times \omega$$

$$a(x,y) = 0.5(cos(y) + x(2\pi - x)sin(x)) + 0.6$$
$$b(x,y) = 2(cos(y) + sin(x)) + 0.8$$
$$c = 0.2, d = 0.3$$

Convection-diffusion equations are classical PDEs that are used to describe physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to two processes namely diffusion.
and convection. These equations are widely applied in many scientific areas and industrial fields, such as pollutants dispersion in rivers or atmosphere, solute transferring in a porous medium, and oil reservoir simulation. We consider variables convection and diffusion coefficients Eq. (36) in this experiment.

4.3.1 Data-set and Model Parameters

Data is generated by solving the problem (35) using a high precision numerical scheme with a pseudo-spectral method for spatial discretization and 4th order Runge-Kutta for temporal discretization (with time step size $\delta t = 0.01$). We assume periodic boundary conditions and the initial value

$$u(x, y, 0) = \sum_{|k|, |l| \leq N} \lambda_k, l \cos(k x + l y) + \gamma_k, l \sin(k x + l y)$$

(37)

where $N = 9$, $\lambda_k, l, \gamma_k, l \sim \mathcal{N}(0, 0.02)$, and $k$ and $l$ are chosen randomly. For more details on the data-set see [50]. Noisy data used for sensor measurement during testing is shown in Fig. 12 with various noise levels at a particular time. We use a simulation of length 40 as shown in table 13 along with other data parameters.

| SNRdb 10 | SNRdb 20 | SNRdb 60 | SNRdb None |
|----------|----------|----------|-------------|
|          |          |          |             |

Figure 12: Data plots of Convection-diffusion equation for visualizing different noise levels. SNRdB represents signal to noise ratio in decibels.

| $\gamma$ | $M$ | $L$ | $z$ | $\omega$ | domain |
|----------|-----|-----|-----|---------|--------|
| 5        | 1   | 40  | 1   | 4096    | $64 \times 64$ |

Table 13: Data-set parameters for Convection-diffusion equation.

Network architecture is shown in table 14. Similar to the previous case a deep network with 5 layers and a small output size is used. The activation function is Tanh, which also has a continuous first derivative. For training, we use $p = 1024$
Table 14: Network architecture of proposed Ensers for Convection-diffusion equation.

| Layer | Input | Output | Activation |
|-------|-------|--------|------------|
| FC    | 8     | 128    | Tanh       |
| FC    | 128   | 256    | Tanh       |
| FC    | 256   | 256    | Tanh       |
| FC    | 256   | 128    | Tanh       |
| FC    | 128   | $M\ast\gamma$ | linear |

Table 15: Training hyper parameters of Ensers for Convection-diffusion equation.

| $\eta_i$ | $\eta_{i0}$ | $\bar{\eta}_i$ | $\beta$ | $I_o$ | $I_i$ | $\xi_0$ | $\xi$ | $p$ | $h$ | $N$ | $\bar{\xi}$ |
|----------|--------------|-----------------|--------|------|------|--------|------|-----|-----|-----|-------------|
| 0.0005   | 0.005        | 5e$-5$          | 11     | 1001 | 10   | 0.005  | 1e$-5$ | 32  | 1024| 33  | 6           |

Table 16: Testing hyper parameters of Ensers for Convection-diffusion equation. $\eta_i$: inner learning rate, $I_i$: inner iterations

| $\eta_i$ | $I_i$ | $p$ | $N$ |
|----------|------|-----|-----|
| 0.2      | 50   | [4, 16]| 12  |

training nodes i.e. 25% of total nodes. Training and testing hyperparameters are shown in tables k and ll respectively. Inner loop learning rate $\eta_i$ and physics loss penalty $\xi$ are increased linearly with each epoch.

4.3.2 Results and Discussions

Figure 13: Ensers predictions of a Convection-diffusion equation test case. (Top to bottom) Target solution, Ensers prediction, L1 error.

Fig. 13 shows the prediction of the Ensers with 16 sensors. The model is able to predict the state accurately and with little distortion. Fig. 14 shows violin plot of L2 error defined in Eq. (19) between target and prediction with various noise levels in sensor measurement for the test case. In Eq. (19), $m = 0$ and $\gamma = 2$ i.e. we use middle prediction out $\gamma$ time steps. We see the model is robust to noise as the mean error in the plots are close for cases of no noise($SNR_{dB} = None$) and high noise($SNR_{dB} = 10$) for 16 sensors case and increases slightly nois for 4 sensor cases. Training continuous model for two dimensions takes more time than discrete because of the increased number of collocation points and multiple automatic differentiation required for calculating loss function.

5 Conclusions

In this work, we develop a novel technique to learn a deep learning model from spare moving training labels for which model reduction is nontrivial. The method uses an implicit optimization layer for minimizing the energy of the solution implemented through the technique of unrolled differentiation. We proposed two formulations based on this technique for discrete and continuous prediction in space. For learning from spare training labels we included a physics-based loss function calculated via convolutional filters in the discrete formulation and via automatic differentiation in the continuous formulation. Where most deep learning-based methods assume fixed sensors Ensers is capable of predicting full states given a varied number of sensors at random locations.
Figure 14: Violin plot representing error \( \varepsilon \) distribution in prediction vector of x,y velocity and pressure for different noise levels in sensor measurements for Convection-diffusion equation test case.

We demonstrate the model performance using two-fluid problems of 2D coupled Burgers’ equation and Flow Past Cylinder for the discrete case. For the continuous case, we used two problems namely Allen–Cahn equation and the Convection-diffusion equation. Model is shown to be robust against noisy sensor measurements. Future work can be aimed at quantifying uncertainty in such networks. Another direction can be to train networks for future states only using initial and boundary conditions.

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Reproducibility

The codes associated with the paper will be released on acceptance.

A Convolution operators for gradient and laplacian terms

Sobel Filter used to estimate 1st-order gradient is:

\[
E = \begin{bmatrix}
1 & -8 & 0 & 8 & -1 \\
2 & -16 & 0 & 16 & -2 \\
3 & -24 & 0 & 24 & -3 \\
2 & -16 & 0 & 16 & -2 \\
1 & -8 & 0 & 8 & -1 
\end{bmatrix}
\]  
(38a)

\[
\frac{\partial}{\partial x} = E \times \frac{1}{9 \times 12 \delta x}
\]  
(38b)

Filter used to estimate laplacian is:

\[
\frac{\partial}{\partial y} = E^T \times \frac{1}{9 \times 12 \delta y}
\]  
(38c)

\[
\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \text{filter} = \begin{bmatrix}
0 & 0 & -1 & 0 & 0 \\
0 & 0 & 16 & 0 & 0 \\
-1 & 16 & -60 & 16 & -1 \\
0 & 0 & 16 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 
\end{bmatrix} \times \frac{1}{12 \delta x \delta y}
\]  
(39)
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