Embedding Physics to Learn Spatiotemporal Dynamics from Sparse Data

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Abstract

Modeling nonlinear spatiotemporal dynamical systems has primarily relied on partial differential equations (PDEs) that are typically derived from first principles. However, the explicit formulation of PDEs for many underexplored processes, such as climate systems, biochemical reaction and epidemiology, remains uncertain or partially unknown, where very sparse measurement data is yet available. To tackle this challenge, we propose a novel deep learning architecture that forcibly embedded known physics knowledge in a residual-recurrent Π-block network, to facilitate the learning of the spatiotemporal dynamics in a data-driven manner. The coercive embedding mechanism of physics, fundamentally different from physics-informed neural networks based on loss penalty, ensures the network to rigorously obey given physics. Numerical experiments demonstrate that the resulting learning paradigm that embeds physics possesses remarkable accuracy, robustness, interpretability and generalizability for learning spatiotemporal dynamics.

1 Background

Partial differential equations (PDEs) have played an indispensable role in modeling complex dynamical systems or processes in many disciplines such as fluid mechanics, electromagnetism and biochemistry. However, there still exists a considerable portion of dynamical systems, such as those in epidemiology, neuroscience, climate science and biology, whose governing PDEs are unclear or only partially known. To give prediction on systems like this, there have been attempts to seek alternatives to the physics-based models. For decades, data-driven modeling of dynamical systems has been studied extensively, e.g., symbolic regression [1], equation-free modeling [2], sparse regression [3–5], deep neural networks (DNN) [6–8], physics-informed neural networks (PINN) [9–11], and automated inference of dynamics [12], etc.

The ever-growing data, thanks to rapid advancement of sensing technologies, contributes to the development of data-driven models, especially in the scientific deep learning (DL) community. However, since the lack of interpretability is a common issue faced by black-box DL models, how to construct a data-driven model that learns the underlying dynamics still remains a critical challenge. To tackle this fundamental issue, we propose a novel deep learning architecture that “forcibly” embeds our existing physics knowledge to facilitate interpretable and generalizable learning of the spatiotemporal dynamics in a data-driven manner.

1.1 Related work

Our work is closely related to the following methods while showing distinctions from the existing work in literature.

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**ResNet:** Deep residual network (ResNet) has been one of the most successful DL architectures, which addresses the notorious problem of gradient vanishing/exploding for very deep networks [13]. Studies reveal its close connection with the forward Euler time-stepping scheme [14–17], which provides a new perspective for the architecture design of DL models [18]. That is to consider a DL task in the view of dynamical system and leverage our rich knowledge of numerical methods for network design, e.g., the backward Euler scheme in PolyNet [19] and the Runge-Kutta scheme in FractalNet [20]. Recurrent ResNets [21, 22], whose parameters are shared across time, are also developed to solve sequential prediction problems. Although ResNet has shown success in lots of applications, residual blocks composed of traditional convolutional or fully connected layers face the issue of poor interpretability, hence hindering its applications to spatiotemporal dynamical systems where governing PDEs are potentially available.

**Physics-informed DL:** Recently, there have been attempts to leverage physics principles to inform DNN training. [9] proposed a deep hidden physics model (DHPM) to enable data-driven modeling of spatiotemporal dynamics, where two DNNs are designed to predict the dynamics meanwhile approximating the underlying PDEs. Another representative method is called PINN for solving forward and inverse PDE problems [10, 11, 23]. The network is informed by physics through a weakly imposed penalty loss consisting of residuals of PDEs and initial/boundary conditions (I/BCs). One major limitation of PINN is that its accuracy relies largely on the these soft physical constraints [24, 25] which may not be satisfied well during training given a poor selection of hyperparameters. Furthermore, the use of fully connected layers poses intrinsic limitations to low-dimensional parameterizations. Efforts have been placed to overcome these issues by employing discrete learning schemes via convolutional networks, such as HybridNet [26], dense convolutional encoder-decoder network [27], auto-regressive encoder-decoder model [28], TF-Net [29], PhyGeoNet [30] and PhyDNet [31]. These methods generally show better computational efficiency and accuracy. However, the core learning component of these networks is still a black (or gray) box.

**PDE-Net:** In [32, 33], two versions of PDE-Net are proposed for predicting dynamics of complex systems and uncovering the hidden PDE structures based on measurement data, where the differential operators are approximated by convolutional filters while the nonlinear PDE functional is learned from neural networks (e.g., symbolic neural networks). The interpretability lies in the constraints on (1) the moment matrix of convolutional filters which pose a well-defined multivariate regression problem and (2) the predefined candidate terms potentially appears in the underlying PDEs.

**Product unit neural network (PUNN):** Product unit [34] is a type of computational unit for feedforward NN proposed in the 90’s. Different from the weighted sum unit in conventional NN, the product unit calculates a weighted product, where each input is raised to a power determined by the trainable weight. The underlying idea behind this unit is that it can learn to represent any polynomial functions regarding the input. Although the product unit is proven efficient for some tasks involving higher order representations, it suffers from the increased number of local minima, deep ravines and valleys [35, 36]. In addition, there are few researches extending this idea to the convolutional NN.

### 1.2 Contribution

In summary, the contributions of this work are as follows:

- We propose a physics-embedded recurrent-convolutional neural network (PeRCNN), which forcibly embeds the physics structure to facilitate learning for data-driven modeling of nonlinear systems. The physics-embedding mechanism guarantees the model to rigorously obey the given physics based on our prior knowledge.
- Instead of using activation functions, which results in poor interpretability and generalizability, we achieve nonlinear approximation via elementwise product among the feature maps, leading to the recurrent Π-block that renders PeRCNN with good expressiveness and flexibility at representing complex nonlinear physics.
- The spatial dependency is learned by either convolutional or predefined finite-difference-based filters while the temporal evolution is modeled by a forward Euler time marching scheme.
- Numerical experiments demonstrate that PeRCNN outperforms the existing models (e.g., ConvLSTM, ResNet and DHPM) on the accuracy and generalizability.
2 Methodology

2.1 Problem description

Let us consider a spatiotemporal dynamical system described by a set of nonlinear, coupled PDEs as

\[ u_t = F(x, t, u, u^2, \nabla_x u, u \cdot \nabla x u, \nabla^2 u, \cdots) \]  

(1)

where the state variable/solution \( u(x,t) \in \mathbb{R}^n \) (e.g., \( u = [u, v]^T \) for \( s = 2 \)) is defined over the spatiotemporal domain \( \{x, t\} \subset \Omega \times [0, T] \); \( \nabla x \) is the Kronecker delta with respect to \( x \); and \( F(\cdot) \) is a nonlinear function. The solution to this problem is subject to the initial condition (IC) \( I(u, u; t = 0, x \in \Omega) = 0 \) and boundary condition (BC) \( B(u, \nabla_x u, \cdots; x \in \partial \Omega) = 0 \), where \( \partial \Omega \) denotes the boundary of the system. In this paper, we will mainly focus on regular (rectangular) physical domains. Therefore, the solution \( u \) can be discretized on a \( H \times W \) Cartesian grid at time steps \( \{t_1, \ldots, t_k, \ldots, t_n\} \), where \( n_t \) denotes the total number of time steps. Our motivation is to tackle a challenging problem: establishing a generalizable and robust model for predicting high-res nonlinear spatiotemporal dynamics based on very limited low-res and noisy training data. Provided a scarce and potentially noisy set of measurements over a coarser spatiotemporal grid, the model should give the most likely full-field solution \( \hat{U} \in \mathbb{R}^{2 \times n_t \times H \times W} \) and possesses satisfactory extrapolation ability over the temporal horizon (e.g., for \( t > t_n \)) and generalization to different ICs. It essentially requires the model learns the spatiotemporal dynamics from the underlying data. To this end, we develop an innovative PeCRNN framework.

To demonstrate the basic design principle of PeRCNN, we should recognize that the state variable \( u \) can be updated approximately by the forward Euler scheme, namely,

\[ \hat{u}_{k+1} = \hat{u}_k + \hat{F}(\hat{u}_k; \theta) \delta t \]  

(2)

where \( \delta t \) is the time spacing, \( \hat{u}_k \) is the prediction at time \( t_k \) and \( \hat{F} \) is an approximate function parameterized by \( \theta \) that ensembles a series of operations for computing the RHS of Eq. (1). The form of Eq. (2) makes it possible to design a recurrent network for spatiotemporal prediction of the solution. Noteworthy, the principle of ResNet [13] has led to extensive efforts on leveraging Euler or Runge-Kutta time integration schemes to facilitate DL (e.g., latent modeling of temporal evolution) [14, 17, 18, 20, 32]. In this work, we propose a different recurrent network architecture without the usage of activation functions, which has rarely been studied before.

2.2 Architecture design

In this part, we elaborate the intuitions for designing the network architecture of PeRCNN as shown in Fig. 1(a). PeRCNN consists of two major components: a fully convolutional (Conv) network as initial state generator (ISG) and an unconventional Conv block, namely II-block (product), for recurrent computation. ISG is introduced to produce a fine-resolution initial state \( \hat{U}_0 \) from the noisy and low-resolution measurement \( \hat{u}_0 \) in order to initiate the recurrent computation. In the rest of this paper, we use \( \hat{u} \) to denote the low-resolution measurement while \( \hat{U} \) to represent the fine-resolution prediction by PeCRNN.

Within the II-block, which is the core of PeRCNN, the state variable \( \hat{U}_k \) from the previous time step first goes through multiple parallel Conv layers. The feature maps produced by these layers will then be fused via elementwise product. A \( 1 \times 1 \) Conv layer (or network in network [37]) is appended after the product operation to aggregate (or linearly combine) multiple channels into the output of desired number of channels. The learning target for the block is to represent the spatiotemporal dynamics function \( F \). The equivalent function represented by II-block can be expressed as:

\[ \hat{F}(\hat{U}) = \sum_{c=1}^{N_c} f_c \left( \prod_{l=1}^{N_l} D^{(c,l)} \hat{U} \right) \]  

(3)

where \( N_c \) and \( N_l \) denote the numbers of channels and parallel Conv layers respectively; \( \oplus \) denotes the Conv operation; \( (c,l) \) indicate the filter \( D \) of \( l \)-th layer and \( c \)-th channel; \( f_c \) is the weight in \( 1 \times 1 \) Conv layer while the bias is omitted for the sake of simplicity. This representation promotes the network expressiveness for nonlinear terms like \( u \cdot \nabla u \), compared with the additive form representation \( \hat{F}(\hat{U}) = \sum_{0 \leq i+j \leq N} f_{ij} (D_{ij} \hat{U}) \) commonly seen in related work [31, 32]. It should be noted that
a highway physics-based Conv layer (see Fig 1(a)) could be created when some specific terms are known a priori in the PDEs. We will demonstrate that such a highway connection could accelerate the training speed and improve the model inference accuracy in Appendix C.2.

Instead of using nonlinear activation functions such as Tanh or Sigmoid, we achieve the nonlinearity of our network via elementwise product of the feature maps, for three reasons:

- Though the nonlinear activation function is crucial to the expressiveness of the DL model, it is also a source of poor interpretability. We consider it unfavorable to use these nonlinear functions to build a recurrent block that aims to generalize the unknown physics.

- The nonlinear function $F$ in the form of multivariate polynomial\(^2\) covers a wide range of well-known dynamical systems, such as Navier-Stokes, reaction-diffusion (RD), Lorenz, Schrödinger equations, to name only a few. Since the spatial derivatives can be computed by Conv filters [38], a II-block with $n$ parallel Conv layers of appropriate filter size is able to represent a polynomial up to the $n^\text{th}$ order.

- Compared with the regression models relying on predefined basis functions or prior knowledge (e.g., the highest order) on $F$ [3, 32], the II-block is flexible at generalizing the nonlinear function $F$. For example, a II-block with 2 parallel layers of appropriate filter size ensembles a family of polynomials up to the $2^\text{nd}$ order (e.g., $u$, $\Delta u$, $uv$, $u \cdot \nabla u$), with no need to explicitly define the basis.

**Lemma 1:** By construction, convolutional filter $D$ can approximate any differential operator with prescribed order of accuracy.

**Lemma 2:** Local truncation error of the forward computation resulted from Eq. (2) diminishes as $\delta t$ decreases.

Two Lemmas above are introduced to illustrate that any dynamical system in the form of Eq. (1) with polynomial $F$ can be approximated by the proposed network. Detailed proof for each Lemma is given in Appendix A. In particular, Lemma 1 and Lemma 2 guarantee the accuracy of the approximation $\hat{F}$ (see Eq. (3)) and the forward computation (see Eq. (2)) respectively.

Noteworthy, we mainly consider the nonlinear function $F$ in the form of polynomial. Other terms such as trigonometric and exponential functions are not considered in this work for simplicity. However, incorporating them would require no more effort than adding a particular symbolic activation (e.g., sin, cos, exp, etc.) layer following the Conv operation. What’s more, these functions can be approximated by polynomials based on Taylor series [3].

\(^2\)Polynomial herein encompasses linear derivative terms, e.g., $u \cdot \nabla u + u^2 v$ has $2^\text{nd}$ and $3^\text{rd}$ order terms.
2.3 Embedding physics in the network architecture

The embedding mechanism is employed to strictly impose the prior physical knowledge of the system to PeCRNN, which contributes to a well-posed optimization problem. In this work, two types of physics can be considered for embedding, namely, the prior knowledge on I/BCs and active terms in the governing PDEs. The ICs (or initial states) can be naturally imposed when PeCRNN starts the recurrent computation from \( \hat{u}_0 \). For the BCs (Dirichlet or Neumann type), we borrow the idea from the finite difference (FD) method and apply the physics-based padding to the model’s prediction at each time step (i.e., \( \hat{U}_K \)), as shown by Fig. 1(b). More specifically, for the Dirichlet BCs, we pad the prediction with prescribed values. Likewise, the padding value of the Neumann BCs will be computed based on the boundary values and the gradient information.

In this work, we mainly focus on the periodic Dirichlet BCs for dataset generation and network training, which have been widely adopted in related works [9, 10, 32]. We introduce the periodic padding\(^1\) that utilizes the boundary value from the other side of the grid, for both the prediction and the feature maps. The strength of periodic padding over traditional zero-padding is that it avoids the loss of the nodal information on the physical boundaries.

PeRCNN also has the capability to embed prior-known terms in PDEs via a highway Conv layer (see Fig. 1(a)) with predefined FD-based filters. For instance, in Section 4 where we consider a reaction-diffusion system and assume the diffusion term \( \Delta u \) is known, a Conv layer with discrete Laplace operator (see Appendix Eq. (A.2)) as its filter is created to approximate \( \Delta u \). Note that the associated coefficient for this term is still unknown and placed as part of the trainable variables. By using the residual connection in the recurrent \( \Pi \)-block, we also implicitly embed the term of \( u_t \).

3 Datasets and loss function

3.1 Datasets

In the experiments, we employ three datasets that encompasses two classic nonlinear spatiotemporal dynamical systems: the 2D and 3D Gray-Scott (GS) reaction-diffusion (RD) systems as well as the 2D Burgers’ equation. The GS-RD systems can be described by

\[
\begin{align*}
\dot{u} &= D \Delta u + R(u) \\
\dot{v} &= D \Delta v + R(v)
\end{align*}
\]

where \( \Delta \) is the Laplacian operator; \( u = [u, v]^T \) is the concentration vector; \( D = \text{diag}(\mu_u, \mu_v) \) is the diagonal diffusion coefficient matrix; \( R(u) = [-uv^2 + f(1 - u), u^2 - (f + \kappa)v]^T \) is the nonlinear reaction vector, where \( \kappa \) and \( f \) denote the kill and feed rate, respectively. This model has found wide applications in computational chemistry and biochemistry.

The second dynamical system we consider is governed by the Burgers’ equation, which has wide applications in applied mathematics such as fluid/traffic flow modeling, given by

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}
\]

where \( u = [u, v]^T \) denotes the fluid velocities and \( \nu \) is the viscosity coefficient.

We generate three datasets on a Cartesian grid using the FD method. The spatial derivative \( \Delta(\cdot) \) is computed by 9-point stencil (see Appendix Eq. (A.2)) while \( \partial_x (\cdot) \) by 5-point stencil given by \( W_{\partial_x} = [1, -8, 0, 8, -1]/(12\delta x) \). Four-stage Runge-Kutta scheme is used for time stepping. The parameters employed for each dataset are summarized in Appendix C.1 where the time spacing \( \delta t \) is selected by convergence tests. The 2D GS-RD dataset has parameters of \( \mu_u = 2e - 5, \mu_v = 5e - 6, \kappa = 0.06 \) and \( f = 0.04 \) while the 3D GS-RD dataset has \( \mu_u = 0.2, \mu_v = 0.1, \kappa = 0.055 \) and \( f = 0.025 \). For the 2D Burgers’ dataset, the only parameter \( \nu \) is 0.005.

3.2 Loss function

Given the low resolution measurement \( \hat{u} \in \mathbb{R}^{2 \times n_t \times H' \times W'} \) where \( n_t' < n_t, H' < H \) and \( W' < W \), our goal of the data-driven modeling is to reconstruct the most likely full-field solution \( \tilde{u} \in \mathbb{R}^{2 \times n_t \times H \times W} \). The loss function to train PeRCNN is defined as:

\[
\mathcal{L}(W, b) = \text{MSE} \left( \tilde{U}(\hat{x}) - \hat{u} \right) + \lambda \cdot \text{MSE} \left( \hat{U}_0 - \mathcal{P}(\hat{u}_0) \right)
\]

\(^1\)Periodic padding can be achieved by “circular” mode padding in PyTorch.
where \( \hat{U}(\tilde{x}) \) denotes the network’s prediction at the coarse grid nodes \( \tilde{x} \); \( \hat{u} \) denotes the low-resolution measurement; \( \mathcal{P}(\cdot) \) is a spatial interpolation function (e.g., bicubic or bilinear); \( \lambda \) is the regularizer weighting. The regularization term denotes the IC discrepancy between the interpolated initial state and the network’s prediction, which is found effective in preventing network overfitting.

### 3.3 Evaluation metrics

**Accumulative rooted-mean-square error (RMSE):** Accumulative RMSE, defined by Eq. (7), computes the error of all snapshots before a time step \( t_k \). It is used to evaluate the error propagation of the model prediction.

\[
RMSE(t_k) = \sqrt{\frac{1}{nk} \sum_{i=1}^{k} \left\| \hat{U}_i - U_{i}^{\text{ref}} \right\|_2^2}
\]

where \( U_{i}^{\text{ref}} \) is the reference solution and \( k \in \{1, 2, \cdots, n_t\} \).

**Physics error:** For the data-driven modeling of the physical system, we are also interested in the equation residuals, which reflects to what degree the prediction obeys the underlying physical law. As the prediction is given on a Cartesian grid, we compute the physical error based on the PDEs with the help of FD-based filters after the model is finalized. The physic error (having a different unit compared with the data loss) will serve as reference to evaluate the convergence of model training.

### 4 Results

In the numerical experiments, we study empirically the effects of some major hyperparameters on the prediction, which is presented in Appendix C.2. In addition, ablation study, performed to examine the role each component plays in the learning process, is elaborated in Appendix C.3. In the last, we validate our approach on the aforementioned datasets and compare its performance with baseline models in the context of solution accuracy and generalizability.

#### 4.1 Baselines

We conduct comparison of PeRCNN with other models used widely for data-driven modeling of spatiotemporal systems, i.e., the recurrent ResNet [21, 22], convolutional long-short term memory (ConvLSTM) [39] and DHPM [9]. A very brief introduction to each method is given below for readers to grasp the major characteristics of each model.

**ConvLSTM** [39] is a convolutional variant of LSTM which exploits multiple self-parameterized controlling gates, such as input, forget and output gates, to capture the spatiotemporal correlations among the data. It has been extensively used in applications such as video super-resolution [40, 41], traffic prediction [42] and climate forecasting [39], among many others.

**Recurrent ResNet** is another model adopted widely by researchers [21, 22] for the spatiotemporal prediction of dynamical systems. One main characteristic distinguishes the recurrent ResNet with the conventional ResNet [13] is that the weights are shared across time.

**DHPM** [9] differs from the previous two models as it utilizes fully connected neural networks (FCNNs) and exert hidden (unknown) physics prior on the solution. In DHPM, one deep FCNN is employed to fit the data, i.e., pairs of the spatiotemporal location and solution, while another shallow FCNN is used to impose a hidden physical constraint on the fitted solution.

The range of hyperparameter for tuning for each model is given in Appendix D. In addition to the listed hyperparameters, all other hyperparameters are kept the same, e.g., training/validation/testing dataset split, the number of prediction steps, the optimizer (Adam), the max number of epochs, the Gaussian noise level (10%) and the random seed. In the network architecture design, we assume the solution within the domain is periodic while the dynamical system of interest is accompanied with the ubiquitous diffusion phenomenon. Hence, a diffusion Conv layer with fixed filters will be created in the following PeRCNN models. It is noted that some other baselines such as PDE-Net 2.0 [33] and PhyDNet [31] are also considered in our experiments. However, they are found unable to give meaningful results due to the sparsity and the Gaussian noise in the training data (see Appendix C.4). Hence, they are not adopted as the main baseline models in this study.
4.2 Comparison with existing methods

In this part, we show the performance of PeRCNN compared with the baselines. The training data is downsampled (in time and space) from the fine-resolution dataset polluted with 10% Gaussian noise. Also, 10% validation data is split out from the training data for hyperparameters selection and early stopping. After the model is finalized, extrapolation over time will be performed to examine the generalizability of each model. All the implementations are coded in PyTorch or TensorFlow and run on a NVIDIA Tesla v100 GPU card (32G) in a standard workstation

2D Burgers’ dataset: For the comparison on the 2D Burgers’ dataset, the same settings as described in Appendix C.2 are employed. What’s more, 1200 extra time steps of prediction are performed to evaluate how the trained model generalizes the unknown physics. Figure 3(a) shows the snapshot prediction by each model at $t = 0.095$ and 0.395 s. It is seen that all the models are able to fit the training data and produce satisfactory prediction in the supervised time period. However, when it comes to long-term extrapolation, the model predictions deviate from the ground truth significantly except PeRCNN, which demonstrates that PeRCNN generalizes the unknown underlying physics well. This conclusion is further confirmed by the accumulative RMSE (see Eq. (7)) in Fig. 2(a). We may notice that the accumulative RMSE starts from an initial high value. This is due to the fact that the training data is corrupted by 10% noise and the metrics is computed from one single snapshot at the beginning. The effect of the unrelated noise gradually fades out as more time steps are considered.

2D Gray-Scott dataset For the 2D GS-RD dataset, we consider a data availability scenario when the resolution of training data is relatively low in space but decent in time. The training data for this case encompasses 41 noisy snapshots of on a $26 \times 26$ grid, which ranges from $t = 0$ to 400 s. We assume the dynamical system of interest belongs to RD process; that is to say, there exists a diffusion term ($\Delta u$) with unknown scalar coefficients in $F$. Therefore, we embed the diffusion term

\[^{4}\text{Source codes/datasets are available in Supplementary Material}\]
### Table 1: Number of trainable parameters, computational time, and RMSE for prediction.

| Case  | Model  | No. of Parameters | Time (s) per epoch | Training RMSE | Extrapolation RMSE |
|-------|--------|-------------------|--------------------|---------------|-------------------|
| 2D BE | PeRCNN | 4,134             | 1.97               | 4.6e-2        | 6.7e-2            |
|       | ConvLSTM | 29,666           | 1.84               | 7.0e-2        | 1.5e-1            |
|       | ResNet  | 38,274            | 1.12               | 1.6e-1        | 2.1e-1            |
|       | DHPM    | 59,284            | 0.23               | 3.1e-2        | 4.3e-1            |
| 2D GS | PeRCNN | 7,430             | 3.68               | 1.0e-2        | 5.1e-2            |
|       | ConvLSTM | 110,530          | 3.70               | 1.9e-2        | 1.5e-1            |
|       | ResNet  | 38,274            | 2.16               | 1.0e-1        | 1.6e2             |
|       | DHPM    | 26,624            | 0.11               | 2.7e-2        | 2.9e-1            |
| 3D GS | PeRCNN | 10,118            | 2.43               | 1.9e-2        | 3.7e-2            |
|       | ConvLSTM | 32,034           | 22.73              | 8.3e-2        | 1.6e-1            |
|       | ResNet  | 29,506            | 2.87               | 1.2e-1        | 1.9e-1            |
|       | DHPM    | 26,624            | 0.19               | 1.0e-1        | 4.5e-1            |

into PeRCNN by creating a highway connection with a diffusion filter (see Appendix Eq. (A.2)). The diffusion coefficient ($\tilde{\mu}$) is firstly estimated by solving a linear regression problem of $u_t = \tilde{\mu} \Delta u$ with the available data. Then a lower bound of 0 and upper-bound of $2\tilde{\mu}$ are applied to ensure the stability of diffusion. Herein, the upper bound for diffusion terms is computed to be $6 \times 10^{-5}$, three times the true value. Each model is responsible for predicting 801 fine-resolution snapshots during the training phase while 1700 extra snapshots will be predicted for extrapolation.

Snapshots at different time instants are presented in Fig. 3(b), which reveal the complex maze-like pattern of the GS-RD system. We report that the recurrent ResNet is unable to reconstruct the fine-resolution snapshots even in the training due to the limited data, after trying all the hyperparameter combinations (see Appendix D). It can be seen from the snapshots that PeRCNN is the only model working well for long-time extrapolation in spite of minor discrepancies. We should note that, unlike the previous 2D Burgers' dataset, PeRCNN works well for the filter size of 1 in this 2D GS case. This is because the reaction term of the GS-RD system contains no spatial derivatives. Therefore, prior knowledge on the spatial derivative of system can also be employed when setting the filter size for the model. The error propagation of the prediction by each model is shown in Fig. 2(b). It is observed that PeRCNN outperforms all other models at controlling the error propagation in both training and extrapolation regimes.

**3D Gray-Scott dataset** In the last experiment, we test the models on 3D GS-RD dataset. We aim to examine the performance of our PeRCNN with this computationally intensive spatiotemporal prediction problem. The training data includes 21 noisy snapshots on a $25^3$ grid sampled from $t = 0$ to 150 s. The assumptions on the system and the estimate of the diffusion coefficients in the previous 2D GS-RD example are applied here as well. Each trained model produces 301 fine-resolution snapshots during supervised learning stage while 700 extrapolation steps are predicted after each model is finalized. The predicted isosurfaces of two levels are plotted in Fig. 3(c). The conclusion we draw in the previous example applies here as well since the PeRCNN is the only model that gives a satisfactory long-term prediction. The flat error propagation curve of PeRCNN, as shown in Fig. 2(c), also demonstrates the remarkable generalization capability of PeRCNN. Table 1 summarizes the number of trainable parameters, the training time per epoch, and the RMSE of both training and extrapolation for each model. It is seen that PeRCNN outperforms the other three baselines with much less trainable parameters and higher accuracy.

#### 4.3 Interpret the learned model

One of major drawbacks of the traditional deep neural network is the lack of interpretability because the output of the network is usually expressed as a prolonged nested function. However, since each channel of the input in II-block ($\mathcal{U}_k$) corresponds to a solution component (i.e., $[u, v]$), the multiplicative form of II-block makes it possible to extract (or interpret) the explicit form of learned $\mathcal{F}$ from the learned weights and biases via symbolic computations. The purpose of this subsection is to briefly demonstrate how the learned model can be interpreted as an analytical expression, which would be useful for researcher to disentangle the underlying physics.
We first interpret the learned model from 3D GS-RD case of Section 4.2. Since the parallel Conv layers (in Π-block) have filter size of 1, which means that each output channel would represent the linear combination of \( u \), \( v \) and a constant, the element-wise product of three Conv layers would produce third order polynomials, which correspond to the reaction term of the 3D GS-RD system. The extracted reaction term reads

\[
R(u) = \begin{bmatrix}
-0.0074u^3 - 0.0051u^2v - 0.2uv^2 - 0.0386u^2 + 0.0018u^2 - 0.11uv - 0.055u^2 - 0.016u - 0.022v + 0.025 \\
0.0005u^3 - 0.013u^2v + 0.54uv^2 - 0.087v^3 - 0.0076u^2 + 0.023uv + 0.046v^2 + 0.017u - 0.036v - 0.0097
\end{bmatrix}
\]

The identified diffusion coefficient matrix can be also extracted from the diffusion connection, which reads \( D = \text{diag}(0.18, 0.080) \). Comparing the extracted terms with the ground truth, some distracting terms are observed due to the 10% noise in the training data and the redundancy of the network.

To interpret terms involving partial derivatives (e.g., \( u \Delta u \), \( uu_x \)) it would require us to completely freeze or impose moment matrix constraints on part of the convolutional filters, like in [32]. Here a simple experiment is conducted on the 2D Burgers’ case in Section 4.2, whose governing equation reads Eq. (5). The network employed in the experiment has two Conv layers with two channels. The first Conv layer are associated with \( \partial x \) and \( \partial y \) respectively, by fixing the filters with corresponding FD stencils. The remaining settings are kept the same as the 2D Burgers’ case in Section 4.2 except that noise-free training data is used. The interpreted expression from the whole PeRCNN model is

\[
u_x = \begin{bmatrix}
0.0051u - 0.95u_y(1.07u - 0.0065v - 0.17) + 0.98u_y(0.0045u - 1.01v + 0.17) + 0.053 \\
0.0051u - 0.82u_y(1.22u + 0.0078v - 0.18) - 0.91u_y(0.0063u + 1.08v - 0.17) + 0.058
\end{bmatrix}
\]

It is seen that the equivalent expression of the learned model is close to the genuine governing PDEs, which helps to explain the extraordinary generalization capability of our model. Although the selection of differential operators to be embedded is crucial for identifying the genuine form of the \( \mathcal{F} \) section, we know that each learned model is associated with an equivalent expression, which is known terms in PDEs). This brings distinct benefits for improving the convergence of training and extrapolation along the temporal horizon and on different ICs. The proposed PeRCNN is finally compared with several state-of-the-art models. Results demonstrate that physics-embedded learning paradigm uniquely possesses remarkable robustness against data noise/scarcity and generalizability. Equally important, PeRCNN shows good interpretability due to the multiplicative form of the Π-block. An analytical expression can be extracted from the learned model via symbolic computations. Although PeRCNN shows promise in data-driven modeling of complex systems, it is restricted by the computational bottleneck due to the high dimensionality of the discretized system, especially when it comes to systems in a large 3D spatial domain with long-term evolution. However, this issue is expected to be addressed via temporal batch and multi-GPU training. Furthermore, PeRCNN can also be extended to discover the explicit form of PDEs when combined with sparse representation.

4.4 Generalization to different ICs

In addition to the remarkable extrapolation capability seen in the previous section, we find the trained PeRCNN model can generalize well to different initial conditions. To demonstrate this, we employ the trained model (in Section 4.2) to perform inference with a different initial condition. The boundary condition and PDE’s parameters are kept the same as that of the training data for the generation of FD solution. It should be noted that the DHPM, which roots in fully connected neural network, is incapable of performing inference with different IC. Therefore, it is not considered for the inference.

The prediction given by trained models, as well as the ground truth generated with FD solver, is presented from Fig. A.7-A.9 in Appendix E. It can be seen that PeRCNN result is consistent with the ground truth while the recurrent ResNet and ConvLSTM give wild prediction. From the previous section, we know that each learned model is associated with an equivalent expression, which is independent of initial condition (IC). Therefore, we can assume the learned model parameterizes the dynamics \( \mathcal{F} \) well for predicting the new Burgers’ or GS-RD systems with different IC.

5 Conclusions

A novel DL architecture, called PeRCNN, is developed for modeling of nonlinear spatiotemporal dynamical systems from sparse and noisy data. Our prior physics knowledge is forcibly embedded into PeRCNN which guarantees the resulting network strictly obeys given physics (e.g., I/BCs or known terms in PDEs). This brings distinct benefits for improving the convergence of training and accuracy of the model. To evaluate the generalizability of PeRCNN, the trained model is used for extrapolation along the temporal horizon and on different ICs. The proposed PeRCNN is finally compared with several state-of-the-art models. Results demonstrate that physics-embedded learning paradigm uniquely possesses remarkable robustness against data noise/scarcity and generalizability. Equally important, PeRCNN shows good interpretability due to the multiplicative form of the Π-block. An analytical expression can be extracted from the learned model via symbolic computations. Although PeRCNN shows promise in data-driven modeling of complex systems, it is restricted by the computational bottleneck due to the high dimensionality of the discretized system, especially when it comes to systems in a large 3D spatial domain with long-term evolution. However, this issue is expected to be addressed via temporal batch and multi-GPU training. Furthermore, PeRCNN can also be extended to discover the explicit form of PDEs when combined with sparse representation.
6  Broader impact

The broader impact of our work is two-fold. First, the proposed \( \Pi \)-block can be used as a building block for more sophisticated deep network architecture. It has demonstrated excellent accuracy and generalizability while approximating the nonlinear dynamics. In addition, the interpretability of the proposed network makes it possible to extract an analytical expression from the learned model. Further efforts can be made on the scientific discovery (e.g., distill governing PDEs) from sparse and noisy data using our approach. Overall, the proposed method sheds light on designing new interpretable deep learning architectures preserving our \textit{a priori} knowledge of physics or mathematical structures for scientific discovery in “small” data regimes.

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Appendix

A Proof of Lemmas

Lemma 1: The proof is reproduced from [33]. Consider a bivariate differential operator $\mathcal{L}(\cdot)$, we have

$$\mathcal{L}(u) = \sum_{k_1, k_2 = -\frac{N-1}{2}}^{\frac{N-1}{2}} D[k_1, k_2] \sum_{i,j=0}^{N-1} \frac{\partial^{i+j} u}{\partial x^i \partial y^j} \left|_{(x,y)} \delta x^i \delta y^j + \mathcal{O}(|\delta x|^{N-1} + |\delta y|^{N-1}) \right)$$

$$= \sum_{k_1, k_2 = -\frac{N-1}{2}}^{\frac{N-1}{2}} D[k_1, k_2] u(x + k_1 \delta x, y + k_2 \delta y) + \mathcal{O}(|\delta x|^{N-1} + |\delta y|^{N-1})$$

where $N$ is the size of the filter indexed by $k_1$ and $k_2$. Letting the filter’s entry $D[k_1, k_2]$ be the corresponding Taylor series coefficient, we can see the error of approximation is bounded by $\mathcal{O}(|\delta x|^{N-1} + |\delta y|^{N-1})$.

Lemma 2: Rewriting the update of Eq. (2) as the equality $u_{k+1} = u_k + \mathcal{F}(u_k) \delta t + \mathcal{O}(\delta t^2)$, we can see the truncation error of the forward computation converges to zero as $\delta t$ decreases.

B Discrete Laplace operator

$$W_\Delta = \frac{1}{12(\delta x)^2} \begin{bmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 \\ -1 & 16 & -60 & 16 & -1 \\ 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \end{bmatrix} \tag{A.2}$$

C Supplementary content on numerical experiments

C.1 Parameters of dataset generation

| Dataset  | Dimensions       | $\delta t$ | $\delta x$ |
|----------|------------------|------------|------------|
| 2D GS-RD | 101$^2$ × 2501   | 0.5        | 0.01       |
| 3D GS-RD | 401$^3$ × 1501   | 0.5        | 25/12      |
| 2D Burgers' | 101$^2$ × 1601  | 2.5e-4     | 0.01       |

C.2 Effects of major hyperparameters

The proposed PeRCNN has several major hyperparameters, including the number of parallel convolutional layers, the filter size and whether a highway connection with customized filters exists, which are assumed to affect the performance of the trained model. We are to explore the sensitivity of the model performance w.r.t. these hyperparameters through a series of tests. The 2D Burgers’ dataset (see Appendix C.1) is used as the testbed for the parametric study. The training dataset has 11 low-resolution (51 × 51) snapshots uniformly selected from the time period of $t = 0$ to 0.1 s after 10% Gaussian noise is added to the original dataset. Each PeCRNN model is constructed to produce the prediction on full spatiotemporal resolution, i.e., $\mathbf{U} \in \mathbb{R}^{2 \times 401 \times 101 \times 101}$.

Usage of prior knowledge: One salient feature of PeRCNN is the capability to directly embed our prior knowledge into the network architecture. In this test, the effect of embedding different prior knowledge is examined: (1) no prior knowledge about $\mathcal{F}$ is given, and (2) the diffusion term $\Delta u$ is known a priori in $\mathcal{F}$. An additional physics-based Conv layer (see Fig. 1(a)) is incorporated to account for the diffusion term in $\mathcal{F}$. Both networks have 2 parallel Conv layers with 4 channels, while all the other hyperparameters are kept the same.

The learning curves of these two PeRCNN models are shown in Fig. A.1(a). To evaluate how the predictions respect the true physics, we also plot the associated PDE residual errors. It is observed that, the network embedded with the diffusion term exhibits faster convergence and better accuracy. Thanks to the embedding of
our prior knowledge, the resulting PeRCNN does not need to learn the diffusion process by exploring the data. Thus, incorporating available physics facilitates the learning efficiency and accuracy.

**Filter size:** The relationship between convolution and numerical differentiation has been well studied [38]. The filter (or stencil) size decides the highest order of spatial derivatives a convolution can approximate. In this test, we compare the learning process and model accuracy for PeRCNN with different filter size. We keep the filter size (5, 3 and 1) consistent for all parallel Conv layers for simplicity. Apart from the filter size, each network has 2 parallel Conv layers with 4 channels in addition to the physics-based Conv layer defined by the diffusion term.

Figure A.1(b) compares the learning curves for networks with different filter sizes. We first observe that the network with 1 × 1 filters fails to fit the data since it lacks the capability to represent the spatial correlation between adjacent nodes, i.e., spatial derivatives. However, Section 4.2 shows that the filter size of 1 works quite well for GS-RD systems since the reaction terms contain no spatial derivatives. The filter sizes of both 3 and 5 perform well as indicated by the physics errors, because in the theory of numerical differentiation the 3 × 3 and 5 × 5 stencils are sufficient to approximate the spatial derivatives in the 2D Burgers’ equation.

**Number of Conv layers:** More parallel Conv layers means the capability to approximate the unknown function $\mathcal{F}$ of higher order. However, in most data-driven modeling tasks, prior knowledge on the highest order of the function is usually unavailable. Therefore, the number of Conv layers for PeRCNN are usually determined through numerical tests. In this test, we explore how largely the performance of PeRCNN relies on the number of Conv layers used. The networks with 2, 3 and 4 layers are considered for comparison, with the filter size of 5 and the diffusion term embedded.

Figure A.1(c) compares the learning curves for PeRCNNs with different numbers of Conv layers. It is seen that the loss for the 2-layer network hits a plateau after thousands of epochs while the loss values for the 3-/4-layer networks keep decreasing. The 4-layer network achieves the best training and validation losses as well as the associated physics error. Although two layers would be theoretically sufficient to represent the $\mathcal{F}$ for the 2D Burgers’ equation, we found the redundant parameters in 3-/4-layer networks are beneficial to the optimization due to the better expressiveness.

### C.3 Ablation study

In this section, ablation studies are conducted to investigate the importance of each architecture component in the data-driven modeling task. In addition to the plain version of each model, we also implemented the PeRCNN deprived of the diffusion connection, the ConvLSTM and ResNet equipped with the diffusion connection\(^2\). It should be noted that DHPM is not considered here because it lacks the capability to incorporate partial knowledge (i.e., known terms in PDEs). The numerical test is performed using 2D Burgers’ dataset, with the same settings as in Appendix C.2 except the noise-free training data is employed. To eliminate the effects of ISG, we employed the interpolated fine-resolution snapshot as the initial state for all models.

Figure A.2(a) shows the error propagation curves of different models affected by the existence of diffusion connection and the type of recurrent block. It can be seen that the II-block of PeRCNN, no matter with (w/) or without (w/o) diffusion connection, delivers better overall accuracy and generalizability compared with the ConvLSTM and ResNet block. It demonstrates the advantages of the proposed II-block over the commonly used recurrent block. Furthermore, comparing the error curves between the models w/ and w/o diffusion connection, we can see the benefits of incorporating prior knowledge into the network architecture. The accuracy and generalizability of each model are improved by the diffusion connection to various degree.

The introduction of initial state generator (ISG), essentially a convolutional decoder, is to provide flexibility to the type of available measurement at initial state. In particular, when the available measurement is in low resolution, which happens to the dataset of this test, or polluted by noise, the ISG can adjust its parameters during training so that a suitable (e.g., denoised, fine-resolution) initial state can be generated for subsequent

\(^2\)Diffusion connection is created on the output layer of ConvLSTM and ResNet.
To illustrate the importance of ISG, we compare the performance of PeRCNNs whose initial state is generated via trainable ISG and bicubic interpolation. Figure A.2(b) shows the error curves for each model where $\lambda$ denotes the weight for the regularizer. It can be seen that the PeRCNN w/o ISG starts with a higher error due to the interpolation error while the existence of ISG slightly improves the accuracy of the data-driven model.

C.4 Other baselines considered

In addition to the aforementioned baselines, we also considered some other baselines, such as PDE-Net 2.0 [33] and PhyDNet [31] in our experiments. PhyDNet is a deep network architecture that uses two-branch recurrent block, i.e., physical cell and ConvLSTM cell in parallel, to disentangle the dynamics of a spatiotemporal systems. The branch of PhyCell performs the PDE-constrained prediction in latent space while the ConvLSTM cell accounts for the unknown complementary information in a data-driven manner. However, due to the sparsity (i.e., only one low-resolution snapshot available every 20 or 40 snapshots) and the Gaussian noise of the training data, they cannot deliver meaningful results even in the training region, like shown by Fig. A.3. Therefore, they are not considered as baselines in the main text.

C.5 More snapshots for comparisons

More snapshots of the prediction by the trained models are given in this part to further compare the performance of each method. Figures A.4, A.5 and A.6 show the detailed results for 2D Burgers’, 2D GS-RD and 3D GS-RD datasets in Section 4.2, respectively.

D Range of hyperparameters selection

In Section 4.2, we compare the performance of our PeRCNN with some existing methods, including the ConvLSTM, Recurrent ResNet and DHPM. The hyperparameters for each methods are selected from the ranges summarized in Tables A.2, A.3, A.4 and A.5 respectively, which are determined based on the complexity of the system and the available computational resource. The hyperparameter selection that achieves the lowest validation loss is given in parenthesis.
Figure A.4: Predictions from each model on 2D Burgers’ dataset. Training: (a) and (b); extrapolation: (c)–(f).

Figure A.5: Predictions from each model on 2D GS-RD dataset. Training: (a) and (b); extrapolation: (c)–(f).

Figure A.6: Predictions from each model on 3D GS-RD dataset. Training: (a) and (b); extrapolation: (c)–(f).
Table A.2: Range of hyperparameters for PeRCNN.

| Dataset | Filter size | # layers | # channels (II-block) | # channels (ISG) | Learning rate | $\lambda$ |
|---------|-------------|----------|-----------------------|------------------|--------------|----------|
| 2D BE   | 1~5 (5)     | 2~4 (4)  | 4~16 (8)              | 4~16 (8)         | 0.001~0.01   | 0.001~1 (1) |
| 2D GS   | 1~5 (1)     | 2~4 (3)  | 4~16 (8)              | 4~16 (8)         | 0.001~0.01   | 0.001~1 (0.005) |
| 3D GS   | 1~5 (1)     | 2~4 (3)  | 2~8 (4)               | 4~8 (4)          | 0.001~0.01   | 0.001~1 (0.5)  |

Table A.3: Range of hyperparameters for ConvLSTM.

| Dataset | Filter size | # layers | # channels | Learning rate | Weight decay |
|---------|-------------|----------|------------|---------------|--------------|
| 2D BE   | 3~5 (5)     | 1~2 (2)  | 16~32 (32) | 0.0005~0.01   | e-5~e-3 (e-5) |
| 2D GS   | 3~5 (5)     | 1~2 (2)  | 16~32 (32) | 0.0005~0.01   | e-5~e-3 (e-5) |
| 3D GS   | 3~5 (5)     | 1       | 8~16 (16)  | 0.0005~0.01   | e-5~e-3 (e-5) |

Table A.4: Range of hyperparameters for recurrent ResNet.

| Dataset | Filter size | # layers | # channels | Learning rate | Weight decay |
|---------|-------------|----------|------------|---------------|--------------|
| 2D BE   | 3~5 (3)     | 2~4 (2)  | 16~128 (64)| 0.0001~0.01   | e-5~e-2 (e-4) |
| 2D GS   | 3~5 (3)     | 2~4 (2)  | 16~128 (64)| 0.0001~0.01   | e-5~e-2 (e-3) |
| 3D GS   | 3~5 (3)     | 2~3 (2)  | 8~32 (32)  | 0.0001~0.01   | e-5~e-2 (e-4) |

Table A.5: Range of hyperparameters for DHPM.

| Dataset | $N_1$ width | $N_1$ depth | $N_2$ width | $N_2$ depth | Input for $N_2$ | Learning rate |
|---------|-------------|------------|-------------|-------------|-----------------|--------------|
| 2D BE   | 80~120 (120)| 4~5 (5)    | 10~30 (20)  | 2~3 (2)     | $(\Delta u, \Delta v, uu_x, vv_y)$ | 0.001~0.02 (0.005) |
| 2D GS   | 60~100 (80) | 4~5 (5)    | 10~30 (10)  | 2~3 (2)     | $(\Delta u, \Delta v, u, v)$       | 0.001~0.02 (0.01)  |
| 3D GS   | 60~100 (80) | 4~5 (5)    | 10~30 (10)  | 2~3 (2)     | $(\Delta u, \Delta v, u, v)$       | 0.001~0.02 (0.01)  |

Figure A.7: Inference prediction on a different IC for 2D Burgers’ case.

E Generalization to different ICs

This section shows the result on the generalization of the trained networks to different ICs for 2D Burgers’ (Figure A.7), 2D GS RD (Figure A.8) and 3D GS RD (Figure A.9) systems.
Figure A.8: Inference prediction on a different IC for 2D GS RD case.

Figure A.9: Inference prediction on a different IC for 3D GS RD case.