Neural Stochastic PDEs: Resolution-Invariant Learning of Continuous Spatiotemporal Dynamics

Abstract

Stochastic partial differential equations (SPDEs) are the mathematical tool of choice for modelling spatiotemporal PDE-dynamics under the influence of randomness. Based on the notion of mild solution of an SPDE, we introduce a novel neural architecture to learn solution operators of PDEs with (possibly stochastic) forcing from partially observed data. The proposed *Neural SPDE* model provides an extension to two popular classes of physics-inspired architectures. On the one hand, it extends Neural CDEs and variants – continuous-time analogues of RNNs – in that it is capable of processing incoming sequential information arriving irregularly in time and observed at arbitrary spatial resolutions. On the other hand, it extends Neural Operators – generalizations of neural networks to model mappings between spaces of functions – in that it can parameterize solution operators of SPDEs depending simultaneously on the initial condition and a realization of the driving noise. By performing operations in the spectral domain, we show how a Neural SPDE can be evaluated in two ways, either by calling an ODE solver (emulating a spectral Galerkin scheme), or by solving a fixed point problem. Experiments on various semilinear SPDEs, including the stochastic Navier-Stokes equations, demonstrate how the Neural SPDE model is capable of learning complex spatiotemporal dynamics in a resolution-invariant way, with better accuracy and lighter training data requirements compared to alternative models, and up to 3 orders of magnitude faster than traditional solvers.

1 Introduction

Stochastic partial differential equations (SPDEs) are the mathematical formalism used to model many physical, biological and economic systems subject to the influence of randomness, be it intrinsic (e.g. quantifying uncertainty) or extrinsic (e.g. modelling environmental random perturbations). Notable examples of SPDEs include the *Kardar–Parisi–Zhang (KPZ) equation* for modelling random interface growth such as the propagation of a forest fire from a burnt region to an unburnt region [12], the *Ginzburg-Landau equation* describing phase transitions of ferromagnets and superconductors near critical temperature [34], or the *stochastic Navier-Stokes equations* modelling the dynamics of a turbulent fluid flow under the presence of local random fluctuations [31]. For an introduction to the theory of SPDEs see Hairer [11]; a comprehensive textbook is Holden et al. [15].

Classical numerical approaches for solving SPDEs include finite difference methods and spectral Galerkin methods [27] among others. To ensure accuracy and stability of numerical solutions of complex SPDEs, computations must be carried out at high resolution using fine discretization grids, rendering the resulting schemes computationally intractable. This limitation motivates the study of data-driven methods that can learn solutions to differential equations from partially observed data. In

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fact, there has been an increased interest in recent years to combine neural networks and differential equations into a hybrid approach, dubbed *neural differential equations* [5, 17, 37].

Neural controlled differential equations (Neural CDEs), as popularised by [3, 18, 32], are continuous-time analogues to recurrent neural networks (RNN, GRU, LSTM etc.). The input to a Neural CDE model is a multivariate time series interpolated into a continuous path $X : [0, T] \to \mathbb{R}^{d_\xi}$; the model consists of a matrix-valued feedforward neural network $f_\theta : \mathbb{R}^{d_h} \to \mathbb{R}^{d_h \times d_\xi}$ parameterizing the vector field of the following dynamical system (and satisfying some minimal Lipschitz regularity to ensure existence and uniqueness of solutions)

$$z_0 = \ell_\theta(u_0), \quad z_t = z_0 + \int_0^t f_\theta(z_s)dX_s, \quad u_t = \pi_\theta(z_t), \tag{1}$$

where $\ell_\theta : \mathbb{R}^{d_u} \to \mathbb{R}^{d_h}$ and $\pi_\theta : \mathbb{R}^{d_h} \to \mathbb{R}^{d_u}$ are feedforward neural networks. The output response $u : [0, T] \to \mathbb{R}^{d_u}$ is then fed to a (possibly pathwise) loss function (mean squared, cross entropy etc.) and trained via stochastic gradient descent in the usual way. In practice, the term "dX_t" means that the solution z_t of the equation (e.g. attention required from a doctor) can change in response to a change of an external stream of information X_t (e.g. heart rate of a patient).

Depending on the level of roughness of the control path X, the integral in eq. (1) can be interpreted in different ways. In [18], X is assumed differentiable and is obtained in practice via cubic splines interpolation of the original time series. In this way, the term "dX_s" can be interpreted as "$\dot{X}_s ds$" so that eq. (1) becomes an ODE of the form $\dot{z}_t = f_\theta(z_t)\dot{X}_t$ that can be evaluated numerically via a call to an ODE solver of choice (Euler, Runge-Kutta, implicit, adaptive stepsize schemes etc.). More generally, if X is of bounded variation then the integral above can be seen as a classical Riemann–Stieltjes or Young integral [38]. Neural SDEs [19, 20, 22, 26] are a special subclass of Neural CDEs where the control is a sample path from a d_ξ-dimensional Brownian motion (which is not of bounded variation), and eq. (1) is understood via stochastic integration (Itô, Stratonovich etc.). Neural RDEs [32] allow to relax even further the regularity assumptions on X by treating the integral using rough integration [10, 30]. In practice, Neural RDEs are particularly well suited for long time series. This is due to the fact that the model can be evaluated via a numerical scheme from stochastic analysis (called the *log-ODE method* [32]) over intervals much larger than what would be expected given the sampling rate of the time series. However, the space complexity of the numerical solver increases exponentially in the number of channels d_ξ, thus model complexity becomes intractable for high dimensional time series.

Despite offering many advantages for modelling temporal dynamics, these models are not designed to process signals varying both in space and in time such as physical fields described by SPDEs. In particular, although these models are time-resolution invariant, they are not space-resolution invariant, and are not well suited to capture nonlinear interactions between the various space-time points typically observed in SPDE-dynamics. Similar to CDEs, the solution u to an SPDE is characterized by an initial condition u_0 and a driving noise X. However, in the case of CDEs, (u_0, X_t, u_t) are vectors, while in the case of SPDEs they are functions.

Neural Operators [21, 23, 24, 28] are generalizations of neural networks capable of modelling mappings between spaces of functions and offer an attractive option for learning with spatiotemporal data [21]. Among all kinds of Neural Operators, *Fourier Neural Operators* (FNOs) [25] stand out because of their easier parametrization while demonstrating similar learning performance compared to other Neural Operator models. However, Neural Operators generally fail to incorporate the effect that an external (possibly random) spatiotemporal signal might have on the system they describe. In the case of SPDEs, the external signal is indeed random (e.g. sample from a Wiener process) and its presence leads to new phenomena, both at the mathematical and the physical level, often describing more complex and realistic dynamics than the ones arising from deterministic PDEs.

Contributions To overcome the above limitations faced by Neural CDEs and Neural Operators, we introduce the *neural stochastic partial differential equation* (Neural SPDE) model, capable of learning solution operators of SPDEs from partially observed data by processing, continuously in time and space, incoming sequential information arriving at an arbitrary resolution. We propose two separate algorithms to evaluate our model: the first reduces the Neural SPDE to a system of ODEs in Fourier space, which can then be solved numerically by means of any ODE solver of choice (emulating a spectral Galerkin scheme); the second rewrites the Neural SPDE as a fixed point

88 problem, which is solved via classical root-finding schemes. For both choices of evaluation, the
89 Neural SPDE model inherits memory-efficient backpropagation capabilities provided by existing
90 adjoint-based and implicit-differentiation-based methods respectively. Finally, we perform extensive
91 experiments on various semilinear SPDEs, including the stochastic Ginzburg-Landau, Korteweg-De
92 Vries, Navier-Stokes equations. The empirical results illustrate several useful aspects of our model:
93 1) it is space and time resolution-invariant, meaning that even if trained on a lower resolution it can
94 be directly evaluated on a higher resolution; 2) it requires a lower amount of training data to achieve
95 similar or better performance compared to alternative models; 3) its evaluation is up to 3 orders of
96 magnitude faster than traditional numerical solvers.

97 The outline of the paper is as follows: in Sec. 2 we provide a brief introduction to SPDEs which will
98 help us to define our Neural SPDE model in Sec. 3, followed by numerical experiments in Sec. 4.
99 In Appendix A, we provide an overview of the computational aspects of SPDEs used to design the
100 model and solve SPDEs numerically. Additional experiments can be found in Appendix B.

2   Background on SPDEs

102 Let $T > 0$ and $d, d_u, d_\xi \in \mathbb{N}$. Let $\mathcal{D} \subset \mathbb{R}^d$ be a bounded domain. Let $\mathcal{H}_u = \{f : \mathcal{D} \to \mathbb{R}^{d_u}\}$ and
103 $\mathcal{H}_\xi = \{f : \mathcal{D} \to \mathbb{R}^{d_\xi}\}$ be two Hilbert spaces of functions from $\mathcal{D}$ to $\mathbb{R}^{d_u}$ and $\mathbb{R}^{d_\xi}$ respectively. We
104 consider a large class of SPDEs of the following type

$$du_t = (\mathcal{L}u_t + F(u_t))\, dt + G(u_t)dW_t, \tag{2}$$

105 where W_t is either an infinite dimensional Q-Wiener process [27, Def. 10.6] or a cylindrical Wiener
106 process [11, Def. 3.54] with values in $\mathcal{H}_\xi$, $F : \mathcal{H}_u \to \mathcal{H}_u$ and $G : \mathcal{H}_u \to L(\mathcal{H}_\xi, \mathcal{H}_u)$ are two
107 continuous operators, $L(\mathcal{H}_\xi, \mathcal{H}_u)$ is the space of bounded linear operators from $\mathcal{H}_\xi$ to $\mathcal{H}_u$, and $\mathcal{L}$ is a
108 linear differential operator generating a *semigroup* $e^{t\mathcal{L}} : \mathcal{H}_u \to \mathcal{H}_u$. For further details on Wiener
109 processes see Appendix A.2, and for a primer on semigroup theory see Hairer [11, Section 4]. A
110 function $u : [0, T] \to \mathcal{H}_u$ is said to be a *mild solution* of the SPDE (2) if for any $t \in [0, T]$ it satisfies

$$u_t = e^{t\mathcal{L}}u_0 + \int_0^t e^{(t-s)\mathcal{L}}F(u_s)ds + \int_0^t e^{(t-s)\mathcal{L}}G(u_s)dW_s, \tag{3}$$

111 where the second integral is a stochastic integral interpreted in the Itô sense [11, Def. 3.57]. Thus, an
112 SPDE can be informally thought of as an SDE with values in the functional space $\mathcal{H}_u$ and driven by
113 an infinite dimensional Brownian motion W. Assuming global Lipschitz regularity on F and G, a
114 mild solution u to (2) exists and is unique [11, Thm. 6.4], at least for short times.

115 We follow Friz and Hairer [9] and consider a regularization $W^\epsilon = \delta^\epsilon * W$ of the driving noise W with
116 a compactly supported smooth mollifier δ^ϵ. It is a classical result (Wong-Zakai [35]) from rough path
117 theory [10, 30] that, for the case of SDEs, the sequence of random ODEs driven by the mollification
118 of Brownian motion converges in probability to a limiting process that does not depend on the choice
119 of mollifier and agrees with the Stratonovich solution of the SDE. Furthermore, the solution map
120 $(u_0, W) \mapsto u$ is continuous in an appropriate rough path topology. This result nicely extends to
121 the setting of SPDEs driven by a finite dimensional noise [9, Thm. 1.3]: if u^ϵ denotes the random
122 PDE solutions driven by $\dot{W}^\epsilon dt$ (instead of $\circ dW_t$), then u^ϵ converges in probability to a limiting
123 process corresponding to the Stratonovich solution of the SPDE. In our setting though, the driving
124 noise is infinite dimensional and the resulting integral cannot be interpreted in the Stratonovich sense
125 becuase otherwise the corresponding Itô-Stratonovich correction would be infinite. Nonetheless,
126 Hairer and Pardoux [14, Thm. 1.1] show that, in the case of the heat operator and under appropriate
127 renormalization and drift correction, the random PDE solution u^ϵ converges in probability to the Itô
128 solution of the SPDE, and that the solution map is continuous in an appropriate regularity structures
129 topology. We note that extending this result to a generic differential operators would require a
130 similarly rigorous proof, which goes beyond the scope of this article and that we leave as future work.

131 As done in Kidger et al. [18] for Neural CDEs, we can rewrite the mild solution of the mollified
132 version of eq. (2) as the following stochastically forced PDE

$$u_t = e^{t\mathcal{L}}u_0 + \int_0^t e^{(t-s)\mathcal{L}}H_\xi(u_s)ds, \quad H_\xi(u_t) := F(u_t) + G(u_t)\xi_t, \tag{4}$$

133 where $\xi = \dot{W}^\epsilon$, $\mathcal{H}_u = L^2(\mathcal{D}, \mathbb{R}^{d_u})$ and $\mathcal{H}_\xi = L^2(\mathcal{D}, \mathbb{R}^{d_\xi})$. We will refer to ξ as *white noise* if W is
134 a cylindrical Wiener process and as *coloured noise* if W is a Q-Wiener process.

In view of machine learning applications, one should think of W as a continuous space-time embedding of an underlying spatiotemporal data stream. In this paper we are only going to consider W to be a sample path from a Wiener process, but we emphasise that the Neural SPDE model extends, in principle, beyond the scope of SPDEs and could be used for example to process videos in computer vision applications, which we leave as future work. Next we introduce the Neural SPDE model.

3 Neural SPDEs

For a large class of differential operators $\mathcal{L}$, the action of the semigroup $e^{t\mathcal{L}}$ can be written as an integral against a kernel function $\mathcal{K}_t : \mathcal{D} \times \mathcal{D} \to \mathbb{R}^{d_u \times d_u}$ such that

$$(e^{t\mathcal{L}}h)(x) = \int_{\mathcal{D}} \mathcal{K}_t(x,y)h(y)\mu_t(dy), \tag{5}$$

for any $h \in \mathcal{H}_u$, any $x \in \mathcal{D}$ and $t \in [0,T]$, and where μ_t is a Borel measure on $\mathcal{D}$. As in Kovachki et al. [21], here we take μ_t to be the Lebesgue measure on $\mathbb{R}^d$ but other choices can be made, for example to incorporate prior information. We assume that $\mathcal{K}$ is stationary so that eq. (4) can be rewritten in terms of the spatial convolution $*$

$$u_t = \mathcal{K}_t * u_0 + \int_0^t \mathcal{K}_{t-s} * H_\xi(u_s)ds. \tag{6}$$

For a large class of SPDEs of the form (2), both F and G are local operators acting on a function $h \in \mathcal{H}_u$. In other words, the evaluations $F(h)(x)$ and $G(h)(x)$ at any point $x \in \mathcal{D}$ only depend $h(x)$, and not on the evaluation $h(y)$ at some other point $y \in \mathcal{D}$ in the neighbourhood of x.

3.1 The model

Let $\mathcal{H}_h = L^2(\mathcal{D}, \mathbb{R}^{d_h})$ for some latent space dimension $d_h > d_u$. Let

$$L_\theta : \mathbb{R}^{d_u} \to \mathbb{R}^{d_h}, \quad F_\theta : \mathbb{R}^{d_h} \to \mathbb{R}^{d_h}, \quad G_\theta : \mathbb{R}^{d_h} \to \mathbb{R}^{d_h \times d_\xi}, \quad \Pi_\theta : \mathbb{R}^{d_h} \to \mathbb{R}^{d_u}$$

be four feedforward neural networks. For any differentiable control $\xi : [0,T] \to \mathcal{H}_\xi$, define the map $H_{\theta,\xi} : \mathcal{H}_u \to \mathcal{H}_u$ so that for any $h \in \mathcal{H}_u$, $x \in \mathcal{D}$, $t \in [0,T]$

$$H_{\theta,\xi}(h)(x) = F_\theta(h(x)) + G_\theta(h(x))\xi_t,$$

A Neural SPDE is defined as follows

$$z_0(x) = L_\theta(u_0(x)), \quad z_t = \mathcal{K}_t * z_0 + \int_0^t \mathcal{K}_{t-s} * H_{\theta,\xi}(z_s)ds, \quad u_t(x) = \Pi_\theta(z_t(x)). \tag{7}$$

We note that globally Lipschitz conditions can be imposed by using ReLU or tanh activation functions in the neural networks F_θ and G_θ. In secs. 3.2 and 3.3 we propose two distinct algorithms to evaluate the Neural SPDE model (7) which are based on two different parameterization of the kernel $\mathcal{K}$.

3.2 Evaluating the model by solving a system of ODEs

Levereraging the *convolution theorem*, we can rewrite the integral in eq. (7) as follows

$$z_t = \mathcal{F}^{-1}\left(\mathcal{F}(\mathcal{K}_t)\mathcal{F}(z_0) + \int_0^t \mathcal{F}(\mathcal{K}_{t-s})\mathcal{F}(H_{\theta,\xi}(z_s))ds\right), \tag{8}$$

where $\mathcal{F}, \mathcal{F}^{-1}$ are the *d-dimensional Fourier transform* (FT) and its inverse (see Def. A.1). If one further assumes that $\mathcal{L}$ is a polynomial differential operator of degree N of the form

$$\mathcal{L} = \sum_{n=0}^{N} \sum_{\substack{n_1,...,n_d \\ n_1+...+n_d=n}} C_{n_1,...,n_d} \frac{\partial^n}{\partial x_1^{n_1}...\partial x_d^{n_d}},$$

where $C_{n_1,...,n_d} \in \mathbb{C}^{d_h \times d_h}$ are complex matrices, then the FT of the kernel associated to $\mathcal{L}$ satisfies

$$\mathcal{F}(\mathcal{K}_t)(y) = e^{tP(iy)} \in \mathbb{C}^{d_h \times d_h},$$

for any $y \in \mathbb{C}^d$, where e is the matrix exponential and P is the following matrix-valued polynomial

$$P(y) = \sum_{n=0}^{N} \sum_{\substack{n_1,\dots,n_d \\ n_1+\dots+n_d=n}} (2\pi)^n y_1^{k_1}\dots y_d^{k_d} C_{n_1,\dots,n_d}.$$

This means that there exists a map $A : \mathbb{C}^d \to \mathbb{C}^{d_h \times d_h}$ such that $\mathcal{F}(\mathcal{K}_t)(y) = e^{tA(y)}$. It follows that

$$z_t = \mathcal{F}^{-1}\bigg(\underbrace{e^{tA}\mathcal{F}(z_0) + \int_0^t e^{(t-s)A}\mathcal{F}(H_{\theta,\xi}(z_s))ds}_{:=v_t} \bigg),$$

where $v_t : \mathbb{C}^d \to \mathbb{C}^{d_h}$ is the solution of the following ODE

$$\dot{v}_t = Av_t + \mathcal{F}(H_{\theta,\xi}(\mathcal{F}^{-1}(v_t))).$$

Hence, z_t can be obtained by applying the inverse FT to the output of an ODE solver on $[0,t]$ with initial condition $\mathcal{F}(z_0)$, vector field $\Psi_{\theta,\xi} := A + \mathcal{F} \circ H_{\theta,\xi} \circ \mathcal{F}^{-1}$, i.e.

$$z_t \approx \mathcal{F}^{-1}\big(\text{ODESolve}(\mathcal{F}(z_0), \Psi_{\theta,\xi}, [0,t])\big)$$

This approach can naturally be seen as a "neural version" of the classical *spectral Galerkin method* for SPDEs as described in Appendix A.3.

We note that this numerical evaluation of the Neural SPDE model (7) allows to inherit memory-efficient adjoint-based backpropagation capabilities as in the evaluation of a Neural CDE. For further details on adjoint-based backpropagation we refer the reader to Chen et al. [5], Kidger [17].

3.3 Evaluating the model by solving a fixed point problem

In our second approach of model evaluation, we make use of three different versions of the FT: the time-only FT $\mathcal{F}_1$ and its inverse $\mathcal{F}_1^{-1}$, the space-only FT $\mathcal{F}_d$ and its inverse $\mathcal{F}_d^{-1}$, and the space-time FT $\mathcal{F}_{d+1}$ and its inverse $\mathcal{F}_{d+1}^{-1}$ (see Def. A.1 for details). Denoting by $\star$ the space-time convolution, the integral in eq. (7) can be rewritten as

$$z_t = \mathcal{K}_t * z_0 + (\mathcal{K} \ \star \ \mathbb{1}_{\geq 0}H_{\theta,\xi}(z_.))_t \,,$$

where $\mathbb{1}_{\geq 0}$ is the indicator function restricting the temporal domain to the positive real line. Using again the convolution theorem we obtain

$$z_t = \mathcal{F}_d^{-1}\left(\mathcal{F}_d(\mathcal{K}_t)\mathcal{F}_d(z_0)\right) + \mathcal{F}_{d+1}^{-1}\left(\mathcal{F}_{d+1}\left(\mathcal{K}\right)\mathcal{F}_{d+1}\left(\mathbb{1}_{\geq 0}H_{\theta,\xi}(z_.)\right)\right)_t \,,$$

where all multiplications are matrix-vector multiplications. Using the trick introduced in [25], one can parameterize $\mathcal{F}_{d+1}(\mathcal{K})(y)$ directly in Fourier space as a complex tensor B, so that eq. (7) becomes

$$z_t = \mathcal{F}_d^{-1}\left(\mathcal{F}_1^{-1}(B)_t \mathcal{F}_d(z_0)\right) + \mathcal{F}_{d+1}^{-1}\left(B\mathcal{F}_{d+1}\big(\mathbb{1}_{\geq 0}H_{\theta,\xi}(z_.)\big)\right)_t,$$

where we used the fact that $\mathcal{F}_d(\mathcal{K}_t) = \mathcal{F}_1^{-1}(\mathcal{F}_{d+1}(\mathcal{K}))_t$. Hence, the solution z can be obtained by solving the fixed point problem $z = \Phi_{\theta,\xi}(z)$, where

$$\Phi_{\theta,\xi}(z)_t := \mathcal{F}_d^{-1}\left(\mathcal{F}_1^{-1}(B)_t \mathcal{F}_d(z_0)\right) + \mathcal{F}_{d+1}^{-1}\left(B\mathcal{F}_{d+1}\big(\mathbb{1}_{\geq 0}H_{\theta,\xi}(z_.)\big)\right)_t.$$

This can be solved numerically using classical root-finding schemes (e.g. by Picard's iteration)

$$z \approx \text{FixedPointSolve}(z_0, \Phi_{\theta,\xi}).$$

Analogously to adjoint-based backpropagation for the evaluation approach mentioned in Sec. 3.2, there is a mechanism that leverages the *implicit function theorem* allowing to backpropagate through the operations of a fixed point solver in a memory-efficient way. See Bai et al. [2] for further details.

We note that the FTs are numerically approximated using the *discrete Fourier transform* (DFT) and selecting a maximum number of frequency modes [1] (see Appendix A.1 for details).

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[1]The DFT approximates the Fourier series expansion truncated at a maximum number of modes. This allows to specify the shape of the two complex tensors A ($k_{\max}^1 \times \dots \times k_{\max}^d \times d_h \times d_h$) in Sec. 3.2 and B ($k_{\max}^1 \times \dots \times k_{\max}^{d+1} \times d_h \times d_h$) in Sec. 3.3. The $k_{\max}^i$ are treated as hyperparameters of the model.

3.4 Space-time resolution-invariance

As depicted in Fig. 1, the input to a Neural SPDE corresponds to a (possibly irregularly sampled) time-indexed sequence of (possibly partially-observed) spatial observations recorded on a space-time grid. The data is then interpolated into a continuous spatiotemporal signal ξ and initial condition u_0. By construction, a Neural SPDE operates in continuous time and space on the tuple of functions (u_0, ξ) and produces a spatiotemporal response u, which is also continuous in space and time; the function u can then be evaluated at an arbitrary space-time resolution, possibly different from the one used during training. In the next section we will demonstrate empirically that even if trained on a coarser resolution, a Neural SPDE can be evaluated on a finer resolution without sacrificing performance, a property known as *zero-shot super-resolution*.

Figure 1: Schematic view of a Neural SPDE.

4 Experiments

In this section, we run experiments on three semilinear SPDEs: the stochastic Ginzburg-Landau equation in 4.1, the stochastic Korteweg-De Vries equation in 4.2, and the stochastic Navier-Stokes equations in 4.3. We note that although the assumption of globally Lipschitz vector fields might be violated for the following SPDEs, well-posedness (i.e. existence of global solutions) can be shown using equation-specific arguments. We consider three supervised operator-learning settings:

- $u_0 \mapsto u$, assuming the noise ξ is not observed;

- $\xi \mapsto u$, assuming the noise ξ is observed, but the initial condition u_0 is fixed across samples;

- $(u_0, \xi) \mapsto u$, assuming the noise ξ is observed and u_0 changes across samples.

We note that learning the operator $u_0 \mapsto u$ of an SPDE without observing the driving noise ξ unavoidably yields poor results for all considered models as only partial information about the system is provided as input. However, we find it informative to include the performances obtained in this setting, as this provides a sanity check that emphasizes the importance of the noise in all the experiments we consider in this paper. Moreover, the ability to process the initial condition u_0 on its own (in absence of noise) testifies that Neural SPDEs can also be used to learn deterministic PDEs. We provide an example on the deterministic Navier-Stokes equations in Appendix B.4.

Neural CDE, Neural RDE, FNO and DeepONet [28, 29] will be the main benchmark models. In addition, we also propose an additional baseline Neural CDE-FNO, which is a hybrid model consisting of a Neural CDE where the drift is modelled by an FNO and the diffusion by a feedforward neural network. The motivation for using a FNO to represent the drift comes from the universal approximation properties of FNOs studied in Kovachki et al. [21, Thm. 4].

An interesting line of work to tackle SPDE-learning is provided in [7, 16]. The authors construct a set of features from the pair (u_0, ξ) following the definition of a model from the theory of regularity structures [13]. They then perform linear [7] and nonlinear [16] regression from these features to the solution of the SPDE at a single time point. Therefore, these models would have to be retrained for any new prediction. In addition, both [7, 16] assume knowledge of the differential operator $\mathcal{L}$ governing the dynamics, while Neural SPDE learns a representation of $\mathcal{L}$ via the parametrization of the associated kernel. For these reasons these recent models are not included in our benchmark.

For all the experiments, the loss function is the relative pathwise L^2 error. The hyper-parameters for all the models are selected by grid-search (see Appendix B.1 for further experimental details). Experiments are run on a Tesla P100 NVIDIA GPU. The code for the experiments is provided in the supplementary material. Additional experiments may be found in Appendix B.

4.1 Stochastic Ginzburg-Landau equation

We start with the stochastic Ginzburg-Landau equation, a reaction diffusion equation in 1D given by

$$\partial_t u - \Delta u = 3u - u^3 + \xi,$$
$$u(t,0) = u(t,1),$$
$$u(0,x) = u_0(x), \quad (t,x) \in [0,T] \times [0,1].$$

This equation is also known as the Allen-Cahn equation in 1-dimension and is used for modeling various physical phenomena like superconductivity [34]. Here ξ denotes space-time white noise with sample paths generated using classical sampling schemes for Wiener processes detailed in A.2.

Table 1: **Ginzburg-Landau equation**. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. *In the first task ($u_0 \mapsto u$) only partial information (u_0) is provided as input; the underlying noise ξ is used to generate the dynamics, it varies across samples, but is not provided as an input to the models.* This explains why the performance of the applicable models is poorer than for all other tasks. In the second task ($\xi \mapsto u$) the initial condition u_0 is kept fixed. In the third task, the initial condition u_0 and the noise ξ change and are both provided as input.

Model	$N = 1\,000$			$N = 10\,000$		
	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
NCDE	x	0.112	0.127	x	0.056	0.072
NRDE	x	0.129	0.150	x	0.070	0.083
NCDE-FNO	x	0.071	0.066	x	0.066	0.069
DeepONet	0.130	0.126	x	0.126	0.061	x
FNO	0.128	0.032	x	0.126	0.027	x
NSPDE (Ours)	0.128	**0.009**	**0.012**	0.126	**0.006**	**0.006**

We consider two data-regimes: a *low data regime* where the total number of training observations is $N = 1\,000$, and a *large data regime* where $N = 10\,000$. In both cases, the response paths are generated by solving the SPDE along each sample path of the noise ξ using a finite difference scheme described in Appendix A.3 using 128 evenly distanced points in space and time and step size $\Delta t = 10^{-3}$. Following the same setup as in Chevyrev et al. [7, eq. (3.6)], we solve the SPDE until $T = 0.05$ resulting in 50 time points and choose as initial condition $u_0(x) = x(1-x) + \kappa \eta(x)$,

$$\eta(x) = a_0 + \sum_{k=-10}^{k=10} \frac{a_k}{1 + |k|^2} \sin(k\pi x), \quad \text{with } a_k \sim \mathcal{N}(0,1). \tag{9}$$

We either take $\kappa = 0$ or $\kappa = 0.1$ to generate a dataset where the initial data is either fixed or varies across samples. We provide extra experiments on this SPDE for larger time horizons T and multiplicative forcing in Appendix B.2.

We report the results in Table 1. The Neural SPDE model (NSPDE) yields the lowest relative error for all tasks, reaching one order of magnitude improvement on the main task $(u_0, \xi) \mapsto u$ in the large data regime compared to all the applicable benchmark models (NCDE, NRDE, NCDE-FNO). In all settings, even with a limited amount of training samples ($N = 1\,000$), the NSPDE model is applicable and achieves $\sim 1\%$ error rate, and marginally improves to $< 1\%$ error when $N = 10\,000$.

4.2 Stochastic Korteweg–De Vries equation

Next, we consider the stochastic Korteweg–De Vries (KdV) equation, a higher order SPDE given by

$$\partial_t u + \gamma \partial_x^3 u = 6u\partial_x u + \xi,$$
$$u(t,0) = u(t,1),$$
$$u(0,x) = u_0(x), \quad (t,x) \in [0,T] \times [0,1].$$

This equation is used to describe the propagation of nonlinear waves at the surface of a fluid subject to random perturbations (another wave equation is studied in Appendix B.3). We refer the reader to Wazwaz [36] for an overview on the KdV equation and its relations to solitary waves.

The stochastic forcing is given by $\xi = \dot{W}$ for W being a partial sum approximation of a Q-Wiener process as per Example 10.8 in Lord et al. [27] with $\lambda_j \sim j^{-5+\varepsilon}$ and $\phi_j(x) = \sin(j\pi x)$ (see eq. (11) in Appendix A.2). Taking small $\varepsilon > 0$ guarantees that W_t is twice differentiable in space for every $t \geq 0$. To generate the datasets, we solve the SPDE with $\gamma = 0.1$ until $T = 0.5$.

Table 2: **Stochastic KdV**. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. $N = 1\,000$ and $T = 0.5$.

Model	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
NCDE	x	0.464	0.466
NRDE	x	0.497	0.503
NCDE-FNO	x	0.126	0.259
DeepONet	0.874	0.235	x
FNO	0.835	0.079	x
NSPDE (Ours)	0.832	**0.004**	**0.008**

Stochastic KdV. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. $N = 1\,000$ and $T = 1$.

Model	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
FNO	0.913	0.112	x
NSPDE (Ours)	0.904	**0.009**	0.012

The stochastic forcing is simulated using 128 evenly distanced points in space and a time step $\Delta t_{\mathrm{ref}} = 10^{-3}$. We then approximate realizations of the solution of the KdV equation using a time step $\Delta t = 10^{-2}$ until $T = 0.5$. Here, the initial condition is given by $u_0(x) = \sin(2\pi x) + \kappa\eta(x)$, where η is defined in eq. (9). Similarly to Sec. 4.1 we either take $\kappa = 0$ or $\kappa = 1$ to generate datasets where the initial condition is either fixed or varies across samples. Each dataset consists of $N = 1\,000$ training observations.

As reported in Table 2, Neural SPDEs outperforms the second best model FNO by a full order of magnitude in the task $\xi \mapsto u$ and the second best model NCDE-FNO by almost two orders of magnitude in the task $(u_0, \xi) \mapsto u$. We also perform the same tasks for a larger time horizons $T = 1$ and report the results of a comparison against FNO in Sec. 4.2.

4.3 Stochastic Navier-Stokes equations

Finally, we consider the vorticity form of the Navier-Stokes equations in 2-dimensions for an incompressible flow

$$\partial_t w - \nu\Delta w = -u \cdot \nabla w + f + \sigma\xi, \tag{10}$$
$$w(0, x) = w_0(x), \quad (t, x) \in [0, T] \times [0, 1]^2,$$

where u is the unique divergence free ($\nabla \cdot u = 0$) velocity field such that $w = \nabla \times u$. These equations describe the motion of an incompressible fluid with viscosity ν subject to external forces [34]. The deterministic forcing f, defined as in Li et al. [25], is a function of space only. The stochastic forcing ξ is given by $\xi = \dot{W}$ for W being a Q-Wiener process which is colored in space and rescaled by $\sigma = 0.05$ (see Appendix A.2). The initial condition is generated according to $w_0 \sim \mathcal{N}(0, 3^{3/2}(-\Delta + 49I)^{-3})$ with periodic boundary conditions. The viscosity is set to $\nu = 10^{-4}$.

Figure 2: **Top panel:** Solution of the vorticity equation for one realisation of the stochastic forcing between the 500th and the $5\,000^{\mathrm{th}}$ time steps. **Bottom panel:** Predictions with the Neural SPDE model given the initial condition at the 500th time step and the forcing between the 500th and the $5\,000^{\mathrm{th}}$ time steps. The model is trained on a 16×16 mesh and evaluated on a 64×64 mesh.

For each realization of the Q-Wiener process (sampled according to the scheme in Appendix A.2) we solve eq. (10) with a pseudo-spectral solver described in Appendix A.3, where time is advanced with a Crank–Nicolson update. We solve the SPDE on a 64×64 mesh in space and use a time step of size 10^{-3}. For the tasks $u_0 \mapsto u$ and $\xi \mapsto u$, we generate the datasets by solving the SPDE up to time $T = 1$ and downsample the trajectories by a factor of 10 in time (resulting in 100 time steps) and 4 in space (resulting in a 16×16 spatial resolution). The number of training samples is $N = 1\,000$. To generate the training set for the task $(u_0, \xi) \mapsto u$, we generate 10 long trajectories of $15\,000$ steps each up to time $T = 15$. We partition each of these 10 trajectories into consecutive sub-trajectories of 500 time-steps using a rolling window. This procedure yields a total of $2\,000$ input-output pairs. We chose to split the data into shorter sequences of 500 time steps so that one batch training could fit in memory on a Tesla P100 NVIDIA GPU.

We report the results in Table 3. Neural SPDEs marginally outperforms FNO in the simpler task $\xi \mapsto u$, but with a significantly larger performance gap in the harder task $(u_0, \xi) \mapsto u$ from the second best model NCDE-FNO. Fig. 2 indicates that the Neural SPDE model is capable of zero-shot super-resolution in space and in time, achieving good performance even when evaluated on a larger time horizon of $5\,000$ time steps and on an upsampled 64×64 spatial grid. Finally, we report in Table 4 the ratios of inference time of the trained Neural SPDEs over the runtime of the solvers, indicating that NSPDEs can be up to 3 orders of magnitude faster than traditional numerical solvers.

Table 3: **Stochastic Navier-Stokes equations in two dimensions**. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. The symbol - indicates that the model does not fit in memory.

Model	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
NCDE	x	0.366	0.843
NRDE	x	-	-
NCDE-FNO	x	0.326	0.178
DeepONet	0.432	0.348	x
FNO	0.188	0.039	x
NSPDE (Ours)	0.155	**0.034**	**0.049**

Table 4: Ratio of the inference time of NSPDE (once trained) over the runtime of the numerical solver for different SPDEs. In each case we consider a single solution. We use the same space and time discretization for both NSPDE and the numerical solver.

Dataset	Speedup
Stochastic Ginzburg-Landau Equation	$59\times$
Stochastic Korteweg-De Vries Equation	$80\times$
Stochastic Navier-Stokes	$300\times$

5 Conclusion and future work

In this paper we introduced the Neural SPDE model capable of learning solution operators of PDEs with (possibly stochastic) forcing from partially observed data. Neural SPDEs provide an extension to two popular classes of physics-inspired models. They extend Neural CDEs and variants in that they are resolution-invariant both in space and in time, and they extend Neural Operators as they can be used to learn solution operators of SPDEs depending simultaneously on the initial condition and driving noise. We performed extensive experiments illustrating how the model achieves superior performance while requiring a lower amount of training data compared to alternative models, and its evaluation is up to 3 orders of magnitude faster than traditional numerical solvers.

Based on our promising empirical results, we think the following are interesting questions for future research: (i) Does the random PDE model in eq. (4) converge to a limiting Itô SPDE? Is the solution map continuous in an a regularity structure topology? Is the limiting process independent on the choice of mollifier? (ii) Is it possible to construct a discrepancy between probability measures supported on spatiotemporal signals, generalizing for example the signature kernel MMD in [33]? Neural SPDEs paired with such discrepancy would allow the design of new generative models for spatiotemporal signals generalizing the results in Kidger et al. [20]; (iii) Can Neural SPDEs be used in broader data science contexts, such as computer vision to process videos?

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Appendix

This appendix is organized as follows. In Appendix A we provide a summary of the computational aspects of SPDEs used for data simulation and model definition, emphasizing the important role of the Fourier Transform (A.1) for simulating noise realizations of Wiener processes (A.2) and building numerical solvers for SPDEs (A.3). In Appendix B we provide further experimental details (B.1) and additional experiments on the stochastic Ginzburg-Landau (B.2) and wave (B.3) equations, and on the deterministic Navier-Stokes PDE (B.4).

A Computational aspects of SPDEs

We start this section with the definition of the *Fourier Transform* (FT). We then define the *Discrete Fourier Transform* (DFT) as an approximation to the FT of a function observed at finitely many locations. Next, we discuss the role played by the FT to sample realizations of Wiener processes, necessary to build spectral solvers for SPDEs. The interested reader is referred to Briggs and Henson [4] and Lord et al. [27] for further details.

A.1 The Fourier Transform

Let V be a vector space over the complex numbers (e.g. $\mathbb{C}^{d_h}$ or $\mathbb{C}^{d_h \times d_h}$). Let $r \in \mathbb{N}$ and let $\mathcal{C} \subset \mathbb{R}^r$ be a compact subset of $\mathbb{R}^r$. In the paper we used either $r = d$ and $\mathcal{C} = \mathcal{D}$ or $r = d + 1$ and $\mathcal{C} = [0, T] \times \mathcal{D}$.

Definition A.1 (*r-dimensional Fourier Transform*). The r-dimensional FT $\mathcal{F}_r : L^2(\mathbb{R}^r, V) \to L^2(\mathbb{R}^r, V)$ and its inverse $\mathcal{F}_r^{-1} : L^2(\mathbb{R}^r, V) \to L^2(\mathbb{R}^r, V)$ are defined as follows

$$\mathcal{F}_r(f)(y) = \int_{\mathbb{R}^r} e^{-2\pi i \langle x, y \rangle} f(x) dx, \quad \mathcal{F}_r^{-1}(g)(x) = \int_{\mathbb{R}^r} e^{2\pi i \langle x, y \rangle} g(y) dy$$

for any $f, g \in L^2(\mathbb{R}^r, V)$, where $i = \sqrt{-1}$ is the imaginary unit and $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on $\mathbb{R}^r$.

In practice, we do not observe a function on $\mathbb{R}^r$ but on a subset $\mathcal{C} \subset \mathbb{R}^r$. Furthermore, functions are observed at finitely many locations in $\mathcal{C}$, and another transform—the discrete Fourier transform (DFT)—is used for numerical computations.

In the sequel we denote by Π_N the set of periodic sequences indexed on $\mathbb{Z}_r$ with period vector $(N_1, \ldots, N_r)$.

Definition A.2 (*r-dimensional Discrete Fourier Transform*). The r-dimensional DFT $\mathcal{D}_r : \Pi_N \to \Pi_N$ and its inverse $\mathcal{D}_r^{-1} : \Pi_N \to \Pi_N$ are defined as follows,

$$\mathcal{D}_r(u)_n = \sum_{k \in \mathbb{Z}^r \cap \mathcal{R}_N} u_k e^{-2\pi i \langle n, N^{-1}k \rangle}, \quad \mathcal{D}_r^{-1}(v)_k = \frac{1}{|\det N|} \sum_{n \in \mathbb{Z}^r \cap \mathcal{R}_N} v_n e^{2\pi i \langle n, N^{-1}k \rangle}$$

with $N = \mathrm{diag}(N_1, \ldots, N_r) \in \mathbb{N}^{r \times r}$, and $\mathcal{R}_N$ the rectangular domain $\mathcal{R}_N = \{x \in \mathbb{R}^r \mid 0 \le x_i < N_i, \ i = 1, \ldots, r\}$.

The DFT of a sequence can be computed exactly and efficiently using the *fast Fourier transform* (FFT) algorithm [8] which reduces the complexity from $\mathcal{O}(M^2)$ to $\mathcal{O}(M \log M)$ where $M = N_1 N_2 \ldots N_r$. Most importantly, the FFT algorithm is implemented in machine learning libraries such as PyTorch, which provide support for GPU acceleration and automatic differentiation capabilities.

Note that if we have a finite sequence, we may still define its DFT by implicitly extending the sequence periodically. In particular, when a compactly supported function is sampled on its interval of support, and the samples are used as input for a DFT, it is as if the periodic extension of the function had been sampled. More precisely, consider an input sequence which corresponds to the evaluation of a function f on a regular grid of $\mathcal{C} = \mathcal{R}_N$. For simplicity, suppose that $N_i = N_1$ for all $i = 1, \ldots, r$ and consider the grid points $x_n = nL/N_1$ for $n \in \mathbb{Z}^r \cap \mathcal{R}_N$. Taking the DFT of the sequence of general term $u_n = f(x_n)$ we obtain for all $n \in \mathbb{Z}^r$,

$$\mathcal{D}_r(u)_n = \sum_{k \in \mathbb{Z}^r \cap \mathcal{R}_N} u_k e^{-2\pi i \langle n, k/N_1 \rangle} = \sum_{k \in \mathbb{Z}^r \cap \mathcal{R}_N} f(x_k) e^{-2\pi i \langle y_n, x_k \rangle},$$

where y_n are the reciprocal frequency points given by $y_n = n/L$ for $n \in \mathbb{Z}^r \cap \mathcal{R}_N$. The DFT of a compactly supported (or approximately compactly supported) function f sampled on the regular grid of points x_k approximates the FT of f at the frequency points y_n (up to a constant multiplicative factor).

The FT is closely related to the notions of *Fourier coefficients* and *Fourier Series* defined hereafter.

Definition A.3 (*r*-**dimensional Fourier series**). Let f be a piecewise smooth function $f : \mathbb{R}^r \to V$ which is periodic in x_i with period $L_i \in \mathbb{R}_+$ for all $i = 1, \ldots, r$. The r-dimensional Fourier series of f is a representation of the form,

$$f(x) \sim \sum_{n \in \mathbb{Z}^r} c_n(f) e^{2\pi i \langle L^{-1} n, x \rangle},$$

where $L = \mathrm{diag}(L_1, \ldots, L_r) \in \mathbb{R}^{r \times r}$ and $c_n(f)$ are complex coefficients, called *Fourier coefficients*, given by

$$c_n(f) = \frac{1}{|\det L|} \int_{\mathcal{R}_L} e^{-2\pi i \langle L^{-1} n, x \rangle} f(x) dx, \ \ n \in \mathbb{Z}^r$$

where $\mathcal{R}_L \subset \mathbb{R}^r$ denotes the rectangular domain of sides $L_1, \ldots, L_r$.

We note that in the definition above, the sign $\sim$ means that the series is a formal series and no statement is made about the convergence of the series (the forms of convergence are studied in Alimov et al. [1]). If f is compactly supported on $\mathcal{R}_L$, we may still define its Fourier coefficients, and in this case $\mathcal{F}_r(f)(y_n) = |\det L| c_n(f)$ at the frequency points $y_n = L^{-1} n$.

Numerical consideration

Consider a function f which has compact support (or is periodic) which is observed at M locations in its support (or its unitary cell $\mathcal{R}_L$). When using the DFT to approximate M points of the spectrum $\mathcal{F}_r(f)(y_k)$ (or M coefficients $c_k(f)$), a so-called *aliasing* error usually occurs: due to the periodicity of the DFT, the kth coefficient of the DFT includes the contributions not only of the kth frequency mode, but also from higher modes of the underlying function f. In general the accuracy of the highest frequency modes is more impacted by this error, and aliasing occurs specifically when we compute nonlinear terms in the physical space. For example, in the main paper we approximate the evaluation on a discretization spatiotemporal grid $D \times \mathcal{T}$ of $\mathcal{F}_{d+1}^{-1}(\mathcal{F}_{d+1}(\mathcal{K}) \mathcal{F}_{d+1}(f))$ by $\mathcal{D}_{d+1}^{-1}(B \mathcal{D}_{d+1}(f|_{D \times \mathcal{T}}))$ where $f = \mathbb{1}_{\geq 0} H_{\theta, \xi}(z)$ and $H_{\theta, \xi}$ is nonlinear. One possibility to mitigate aliasing is to set to zero the DFT terms (arising in nonlinearities) corresponding to the highest frequency modes before we apply the inverse DFT to go back to the physical space. This is precisely what we do when we parametrize only $k_{\max}^1 \times \ldots \times k_{\max}^{d+1} \times d_h \times d_h$ entries of the complex tensor B, and set the others to zero, hence resolving potential aliasing errors. We note that specific rules have been proposed (notably in the literature on pseudo-spectral solvers) to deal with specific nonlinearities. However, in the context of Neural SPDE we learn the nonlinearities, hence the number of frequency modes that we retain is treated as an hyperparameter.

A.2   Stochastic simulation of Wiener processes

After defining Wiener processes we outline the sampling procedure that we used to simulate the datasets in the main paper. For more details on computational aspects of SPDEs the reader is referred to Lord et al. [27].

Throughout this section, H will denote a separable Hilbert space (e.g. $H = L^2(\mathcal{D})$) with a complete orthonormal basis $\{\phi_k\}_{k \in \mathbb{N}}$. Let $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbb{P})$ be a filtered probability space.

A.2.1   Q-Wiener process

Consider an operator $\mathcal{Q} : H \to H$ such that there exists a bounded sequence of nonnegative real numbers $\{\lambda_k\}_{k \in \mathbb{N}}$ such that $Q\phi_k = \lambda_k \phi_k$ for all $k \in \mathbb{N}$ (this is implied by Q being a trace class, non-negative, symmetric operator, for example).

Definition A.4 (*Q*-**Wiener process**). Let Q be a trace class non negative, symmetric operator on H. A H-valued stochastic process $\{W(t) : t \geq 0\}$ is called a Q-Wiener process if

1. $W(0) = 0$ almost surely;

2. $W(t; \omega)$ is a continuous sample trajectory $\mathbb{R}^+ \mapsto H$, for each $\omega \in \Omega$;

3. $W(t)$ is $\mathcal{F}_t$-adapted and has independent increments $W(t) - W(s)$ for $s < t$;

4. $W(t) - W(s) \sim \mathcal{N}(0, (t-s)Q)$ for all $0 \le s \le t$.

In analogy to the Karhunen Loéve expansion, it can be shown that $W(t)$ is a Q-Wiener process if and only if for all $t \ge 0$,

$$W(t) = \sum_{j=1}^{\infty} \sqrt{\lambda_j} \phi_j \beta_j(t) \tag{11}$$

where $\beta_j(t)$ are i.i.d. Brownian motions, and the series converges in $L^2(\Omega, H)$. Moreover the series is $\mathbb{P}$-a.s. uniformly convergent on $[0, T]$ for arbitrary $T > 0$. (i.e. converges in $L^2(\Omega, \mathcal{C}([0, T], H))$).

In the Navier-Stokes example, we drive the SPDE by samples ξ from a Q-Wiener process in two dimensions. Here we follow Lord et al. [27, Example 10.12] and explain how the sampling procedure works in this case. Let $D = (0, L_1) \times (0, L_2)$ and consider an $L^2(D)$-valued Q-Wiener process $W(t)$. If the eigenfunctions of Q are given by,

$$\phi_k(x) = \frac{1}{\sqrt{L_1 L_2}} e^{2i\pi(k_1 x_1/L_1 + k_2 x_2/L_2)}$$

numerical approximation of sample paths from $W(t)$ are easy to obtain through a DFT. Denote by λ_k the eigenvalues of Q (e.g. $\lambda_k = e^{-\alpha|k|^2}$ for some parameter $\alpha > 0$) and let $\mathcal{J}$ be the index set defined by,

$$\mathcal{J} := \{(j_1, j_2) \in \mathbb{Z}^2 \ : \ -J_1/2 + 1 \le j_1 \le J_1/2, \ -J_2/2 + 1 \le j_2 \le J_2/2\}$$

The goal is to sample from the truncated expansion of $W(t)$,

$$W^J(t) = \sum_{j \in \mathcal{J}} \sqrt{\lambda_j} \phi_j \beta_j(t),$$

at the collection of sample points,

$$x_k = (L_1 k_1/J_1, L_2 k_2/J_2)^T, \qquad 0 \le k_1 \le J_1 - 1, \ 0 \le k_2 \le J_2 - 1.$$

Consider the random variable $Z(t_n, x)$ defined by,

$$Z(t_n, x) = \sqrt{\Delta t} \sum_{j \in \mathcal{J}} \sqrt{\lambda_j} \phi_j(x) \xi_j^n, \qquad \xi_j^n \sim \mathbb{C}\mathcal{N}(0, 2),$$

meaning that $\xi_j^n = a + ib$ with $a, b \overset{\text{i.i.d}}{\sim} \mathcal{N}(0, 1)$ such that $Z(t_n, x_k)$ is a complex random variable with independent real and imaginary part with the same distribution as two independent copies of the increment $W^J(t_n + \Delta t, x_k) - W^J(t_n, x_k)$. Furthermore, $Z(t_n, x_k)$ can be expressed in the form,

$$Z(t_n, x_k) = \frac{1}{J_1 J_2} \sum_{j_1 = -J_1/2+1}^{J_1/2} \sum_{j_2 = -J_2/2+1}^{J_2/2} \widetilde{Z}_{j_1, j_2} e^{2i\pi\left(j_1 \frac{k_1}{J_1} + j_2 \frac{k_2}{J_2}\right)} \tag{12}$$

where $\widetilde{Z}_{j_1, j_2} = \sqrt{\Delta t \lambda_{j_1, j_2}} J_1 J_2 \xi_{j_1, j_2}^n$ We recognize that the matrix with entries given by eq. (12) is the 2D inverse DFT of the $J_1 \times J_2$ matrix with entries $\widetilde{Z}_{j_1, j_2}$. Therefore, we can sample two independent copies of

$$W^J(t_n + \Delta t, x_k) - W^J(t_n, x_k), \ 0 \le k_1 \le J_1 - 1, \ 0 \le k_2 \le J_2 - 1$$

by computing a single 2D inverse DFT.

A.2.2 Cylindrical Wiener process

If the operator $Q = I$ is the identity, then Q is not of trace class on H so that the series in eq. (11) does not converge in $L^2(\Omega, H)$. This motivates the definition of cylindrical Wiener processes.

Definition A.5 (**Cylindrical Wiener process**). Let H be a separable Hilbert space. A cylindrical Wiener process (a.k.a space-time white noise) is a H-valued stochastic process $\{W(t) : t \geq 0\}$ defined by

$$W(t) = \sum_{j=1}^{\infty} \phi_j \beta_j(t) \tag{13}$$

where $\{\phi_j\}$ is any orthonormal basis of H and $\beta_j(t)$ are i.i.d. Brownian motions.

In all examples except Navier-Stokes, we drive the SPDE by samples ξ from a cylindrical Wiener process in one dimension. Let $D = (0, L)$ and consider an $L^2(D)$-valued cylindrical Wiener process $W(t)$. As explained in Lord et al. [27, Example 10.31], if we take the basis

$$\phi_k(x) = \sqrt{2/L} \sin(k\pi x/L)$$

numerical approximation of sample paths from $W(t)$ are easy to obtain. The goal is to sample from the truncated expansion,

$$W^J(t) = \sum_{j=1}^{J} \phi_j \beta_j(t), \tag{14}$$

at the collection of sample points $x_k = kL/J$ for $k = 1, \ldots, J$. Observing that a trigonometric identity yields,

$$\mathrm{Cov}\left(W^J(t, x_i), W^J(t, x_k)\right) = (tL/J)\delta_{ik}, \qquad i, k = 1, \ldots, J$$

the increments $W^J(t_n + \Delta t, x_k) - W^J(t_n, x_k) \sim \mathcal{N}(0, \Delta t L/J)$ for all $k = 1, \ldots, k$.

A.3 Numerical solvers

In this section we present an overview of the numerical solvers for SPDEs we used to generate the data for all the experiments. The stochastic Ginzburg-Landau (Sec. 4.1 and appendix B.2), stochastic wave (Appendix B.3) equations have been solved using the finite difference method, while the stochastic Korteweg–De Vries (Sec. 4.2) and Navier Stokes (Sec. 4.3) equations have been solved using the spectral Galerkin method. We use the same setup as in Sec. 2. In particular, we focus on stochastic semilinear evolution equations of the form

$$du_t = (\mathcal{L}u_t + F(u_t)) \, dt + G(u_t)dW_t \tag{15}$$

where W_t is either a Q-Wiener process or a cylindrical Wiener process and $\mathcal{L}$ is a linear differential operator generating a semigroup $e^{t\mathcal{L}}$. We consider nonlinearities F, G regular enough (see Lord et al. [27, Assumption 10.23]) to guarantee existence and uniqueness of mild solutions of eq. (15) [27, Thm. 10.26].

A.3.1 Finite difference method

We illustrate this numerical method for the reaction-diffusion equation

$$du_t = \left(\epsilon \partial_{xx}^2 u + F(u_t)\right) dt + \sigma dW_t, \quad u(0, x) = u_0(x),$$

with homogeneous Dirichlet boundary conditions and where $\epsilon, \sigma > 0$ are constants. We assume for simplicity that u_0, u_t, W_t are real-valued and $\mathcal{D} = (0, a)$. The generalization to higher dimensions is straightforward.

Consider the grid points $x_j = jh$, where $h = \frac{a}{J}$ and $j = 0, ..., J$, for some spatial resolution $J \in \mathbb{N}$. Let $u_J(t)$ be the *finite difference approximation* of $[u(t, x_1), ..., u(t, x_{J-1})]$ (similarly for $W_J(t)$) resulting from the solution of the following SDE

$$du_J(t) = [-\epsilon M u_J(t) + \hat{f}(u_J(t))]dt + \sigma dW_J(t)$$

609 where $\hat{f}(u_J) = [f(u_1), ..., f(u_{J-1})]^T$ and M is the $(J-1) \times (J-1)$ matrix approximating Laplacian
610 (with free boundary conditions) which is given by

$$M = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}$$

611 One could modify M for specific boundary conditions. For instance in the case of periodic boundary
612 one should modify $M_{1,J-1} = M_{J-1,1} = -1$ (see Lord et al. [27, Chapter 3.4] for Dirichlet and
613 Neuman boundary condition modifications of M). To discretize in time, we may apply numerical
614 methods for SDEs (see for example Lord et al. [27, Chapter 8]). Choosing the standard Euler-
615 Marayama scheme with time step Δt yields an approximation $u_{J,n}$ to $u_J(t_n)$ at $t_n = n\Delta t$ defined
616 by

$$u_{J,n+1} = (I + \Delta t \epsilon M)^{-1} \left(u_{J,n} + \hat{f}(u_{J,n})\Delta t + \sigma(W_J(t_{n+1}) - W_J(t_n)) \right)$$

617 The increments $(W_J(t_{n+1}) - W_J(t_n))$ are generated using techniques discussed in Appendix A.2.

A.3.2 Spectral Galerkin method

619 Consider again a separable Hilbert space H. Assume that the differential operator $\mathcal{L}$ in eq. (15)
620 has a complete set of orthonormal eigenfunctions $\{\phi_j\}_{j\in\mathbb{N}}$ and eigenvalues $\lambda_j < 0$, ordered so that
621 $\lambda_{j+1} < \lambda_j$. Then, we can define the semigroup $e^{t\mathcal{L}}$ as follows

$$e^{t\mathcal{L}}h = \sum_{j=1}^{\infty} e^{\lambda_j t}\langle h, \phi_j\rangle\phi_j, \quad h \in H.$$

622 Define the *Galerkin subspace* $V_J = \text{Span}\{\phi_1, ..., \phi_J\}$ and the orthonormal projections $P_J : H \to V_J$
623 as follows

$$P_J h = \sum_{i=1}^{J}\langle u, \phi_j\rangle\phi_j, \quad h \in H.$$

624 Then, the following defines *spectral Galerkin approximation* of eq. (15)

$$du_J(t) = (\mathcal{L}_J u_J(t) + P_J F(u_J(t)))dt + P_J G(u_J(t))dW_J(t), \quad u_J(0) = P_J u_0$$

625 where $u_J := P_J u$ and $\mathcal{L}_J := P_J \mathcal{L}$ and $W_J = P_J W$ is as in (14). Using a Euluer-Marayama
626 discretization as above, we obtain the following discretization

$$u_{J,n+1} = (I + \Delta t \mathcal{L}_J)^{-1}(u_{J,n} + \Delta t P_J F(u_{J,n}) + P_J G(u_{J,n})\Delta W_{J,n}).$$

627 This approach is particularly convenient for problems with additive noise where the eigenfunctions
628 of $\mathcal{L}$ and Q (the covariance of the Q-Wiener process W) are equal, which is the case for all the
629 experiments in this paper generated with this method. The eigenfunctions of the Laplacian with
630 periodic boundary conditions correspond to the Fourier basis exponentials; therefore, one can define
631 the projection P_J in terms of the DFT.

B Further experiments

633 We start this section with additional details on the training of NSPDE and the baseline models,
634 including how the relevant hyperparameters have been selected for each model.

B.1 Additional experimental details

636 For all experiments the dataset is split into a training, validation and test sets with relative sizes
637 $70\%/15\%/15\%$. For all models, a grid search on the hyperparameters is performed using the training
638 and validation sets. We use the Adam optimizer and a scheduler which reads the validation loss and
639 reduces the learning rate if no improvement is seen for a *patience* number of epochs. Additionally,
640 an early stopping method is used to halt the training of the model if no improvement is seen after a
641 *patience* number of epochs. The hyperparameters included in the grid search are stated below and
642 examples of hyperparameter selection results are provided in tables 5 to 9.

NSPDE The hyperparameters included in the grid search are the number of frequency modes used to parametrize the kernel in Fourier space $B = \mathcal{F}_{d+1}(\mathcal{K})$ and the number of forward iterations used to solve the fixed point problem.

FNO The hyperparameters included in the grid search are the number of frequency modes used to parametrize the kernel and the number of layers M. Note that the numbers of frequency modes in the grid search differ from the ones used for the NSPDE model by a factor 2 to ensure that the effective number of retained modes is the same. For both the NSPDE model and FNO, we kept the number of hidden channels fixed to $d_h = 32$ as this systematically yielded better performances than previously included values and enabled to perform the grid search in a reasonable time.

DeepONet The *Deep Operator Network* (DeepONet) [28] is another popular class of neural network models for learning operators on function spaces. The DeepONet architecture is based on the universal approximation theorem of Chen and Chen [6]. It consists of two sub-networks referred to as the *branch* and the *trunk* networks. The trunk acts on the coordinates $(t, x) \in [0, T] \times \mathcal{D}$, while the branch acts on the evaluation of the initial condition u_0 on a discretized grid D. Therefore, the DeepONet is not a space resolution-invariant architecture. The output of the network is expressed as

$$\text{DeepONet}(u_0)(t, x) = \sum_{k=1}^{p} b_k(u_0)\tau_k(t, x) + b_0,$$

where the b_k and the τ_k are the outputs of the branch and trunk network respectively. The trunk network is usually a feedforward neural network, and one can chose the architecture of the branch network depending on the structure of the input domain. We follow Lu et al. [28] and use feedforward neural networks for both the trunk and the branch networks. We perform a grid search on the depth and width of the trunk and branch feedforward neural networks.

NRDE/NCDE/NCDE-FNO The hyperparameters included in the grid search are the number of hidden channels and the type of solver as implemented by torchdiffeq [5]. We note that we used a depth-2 NRDE model (depth-2 already results in $d_\xi = 8\,385$ for forcings observed at 128 spatial points and higher depths models could not fit in memory) and recall that NCDE is a depth-1 NRDE.

Table 5: Grid search NCDE (KdV)

d_h	# parameters	solver	validation loss
8	136464	rk4	0.511
16	272672	rk4	0.510
32	545088	rk4	0.505
8	136464	euler	0.560
16	272672	euler	0.561
32	545088	euler	0.556

Table 6: Grid search NCDE-FNO (KdV)

d_h	# parameters	solver	validation loss
8	5761	rk4	0.140
16	15617	rk4	0.142
32	48769	rk4	0.145
8	5761	euler	0.310
16	15617	euler	0.314
32	48769	euler	0.321

Table 7: Grid search DeepONet (KdV)

Branch & trunk width	Branch depth	Trunk depth	# parameters	validation loss
256	3	4	1935616	0.258
128	3	4	885888	0.269
128	3	3	869376	0.279
128	3	2	852864	0.284
512	3	4	4526592	0.294
512	2	2	3738624	0.295
256	4	4	2001408	0.295
512	4	4	4789248	0.302
256	2	2	1738240	0.304
256	3	3	1869824	0.307
128	4	3	885888	0.311
128	4	2	869376	0.311
256	3	2	1804032	0.313
128	2	2	836352	0.315
256	4	2	1869824	0.316
128	4	4	902400	0.318
256	4	3	1935616	0.319
512	4	3	4526592	0.320
512	4	2	4263936	0.334
512	3	2	4001280	0.350
128	2	4	869376	0.350
512	3	3	4263936	0.359
512	2	3	4001280	0.366
256	2	3	1804032	0.370
128	2	3	852864	0.382
256	2	4	1869824	0.392
512	2	4	4263936	0.395

Table 8: Grid search FNO (KdV)

d_h	depth	modes 1	modes 2	# parameters	validation loss
32	1	16	16	532993	0.163
32	1	16	50	1647105	0.117
32	1	32	16	1057281	0.163
32	1	32	50	3285505	0.117
32	2	16	16	1058337	0.163
32	2	16	50	3286561	0.120
32	2	32	16	2106913	0.163
32	2	32	50	6563361	0.118
32	3	16	16	1583681	0.163
32	3	16	50	4926017	0.120
32	3	32	16	3156545	0.163
32	3	32	50	9841217	0.120
32	4	16	16	2109025	0.163
32	4	16	50	6565473	0.122
32	4	32	16	4206177	0.163
32	4	32	50	13119073	0.120

Table 9: Grid search NSPDE (KdV)

d_h	Picard's iterations	modes 1	modes 2	# parameters	validation loss
32	1	32	32	1055233	0.023
32	1	32	100	3283457	0.011
32	1	64	32	2103809	0.030
32	1	64	100	6560257	0.009
32	2	32	32	1055233	0.018
32	2	32	100	3283457	0.012
32	2	64	32	2103809	0.015
32	2	64	100	6560257	0.010
32	3	32	32	1055233	0.016
32	3	32	100	3283457	0.013
32	3	64	32	2103809	0.022
32	3	64	100	6560257	0.011
32	4	32	32	1055233	0.019
32	4	32	100	3283457	0.012
32	4	64	32	2103809	0.021
32	4	64	100	6560257	0.016

B.2 Stochastic Ginzburg-Landau equation

Recall that the stochastic Ginzburg-Landau equations are of the form,

$$\partial_t u - \Delta u = 3u - u^3 + G(u)\xi, \tag{16}$$
$$u(0, x) = u_0(x), \quad (t, x) \in [0, T] \times [0, 1]$$

subject to either Periodic or Dirichlet boundary conditions. Periodic boundary conditions are given by $u(t, 0) = u(t, 1)$ for all $t \geq 0$ and Dirichlet boundary conditions are given by $u(t, 0) = u(t, 1) = 0$ for all $t \geq 0$. Initial condition we take as in Sec. 4.1 $u_0(x) = x(1 - x) + \kappa\eta(x)$ with $\kappa = 0$ or $\kappa = 0.1$ depending on a task. In both Periodic and Dirichlet case we can take $\eta(x)$ as in eq. (9) though in Dirichlet case one must take $a_0 = 0$ to ensure u_0 being zero at the boundary.

We first reproduce an experiment from Sec. 4.1 on the additive stochastic Ginzburg-Landau equation but with Dirichlet boundary conditions instead of the periodic. We compare it to the benchmark of FNO model which was the most successful among all the benchmarks of Sec. 4. From Table 10 we see that even though Neural SPDE model depends on the spectral methods the errors did not increase compared to the periodic equation in Sec. 4.1 (see Table 1). Our algorithm still outperforms FNO whose relative $L2$ error increased slightly. The fact that Neural SPDE can be applied to non-periodic equations could be perhaps explained by interpolation (L_θ) and projection (Π_θ) neural networks that could correct for non-periodicity of the data.

Table 10: **Additive stochastic Ginzburg-Landau equation with homogeneous Dirichlet boundary conditions**. The experimental setup is the same as in the main paper. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. N is fixed to $1\,000$.

Model	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
FNO	0.132	0.023	x
NSPDE (Ours)	0.135	0.008	0.010

We now take a look at the specific hyperparameter: number of forward iterations in the fixed point solver. We also call this a number of Picard iterations P. Theoretically as P increases Fixed Point Solver should converge to the true solution (see [11]). This suggests that higher P should improve the performance of the Neural SPDE algorithms. In practise we observed in both additive Ginsburg Landau equation from Sec. 4.1 and in KdV equation from Sec. 4.2 that $P = 1$ could already be enough. This could be explained either by dominance of the linear part of the equation

or by overfitting in these cases. Thus we present an experiment on the multiplicative stochastic Ginzbug-Landau equation over a longer (compared to Sec. 4.1) time interval. In the Table 11 we compare NSPDE with $P \in \{1, 2, 3, 4\}$ and again include FNO benchmark (which performed best in the previous experiments). We see that NSPDE with even $P = 1$ outperforms FNO. Relative $L2$ error for $T = 0.05$ increases for both NSPDE and FNO due to more complicated multiplicative noise. In Table 11 we present for each P the best result over other hyperparameters obtained by cross validation. One could clearly see an improvement in error as we increase the number of Picard iterations P (with an exception of the case $T = 0.05$ where $P = 3$ outperformed $P = 4$). This improvement becomes more apparent as the time frame T increases. Heuristically (and qualitatively) this is due to the fact that for the short times solution of the SPDE is relatively close to its linearised version and that nonlinearity of the equation starts to play a bigger role for larger T.

Table 11: **Multiplicative stochastic Ginzburg-Landau equation**. We report the relative L2 error on the test for FNO and NSPDE (Ours) for different number of Picard iterations on the task $\xi \to u$.

Time horizon	FNO	NSPDE ($P = 1$)	NSPDE ($P = 2$)	NSPDE ($P = 3$)	NSPDE ($P = 4$)
$T = 0.05$	0.040	0.023	0.018	**0.016**	0.017
$T = 0.10$	0.068	0.042	0.041	**0.040**	**0.040**
$T = 0.25$	0.105	0.079	0.077	0.073	**0.072**

B.3 The stochastic wave equation

In this section we consider the following nonlinear wave equation with multiplicative stochastic forcing,

$$
\begin{aligned}
\partial_t^2 u - \Delta u &= \cos(\pi u) + u^2 + u\xi, \\
u(t, 0) &= u(t, 1), \\
u(0, x) &= u_0(x), \\
\partial_t u(0, x) &= v_0(x), \quad (t, x) \in [0, T] \times [0, 1].
\end{aligned}
\tag{17}
$$

The nonlinear stochastic wave equation arises in relativistic quantum mechanics and is also used in simulations of nonlinear waves that are subject to either noisy observations or random forcing. We refer a reader to Temam [34] for an overview on the nonlinear wave equation. The above equation can put in a form of eq. (2) by rewriting it as a system for $(u, v) = (u, \partial_t u)$. To generate training datasets, we solve the SPDE using a finite difference method with 128 evenly distanced points in space and a time step size $\Delta t = 10^{-3}$. As in Chevyrev et al. [7, eq. (3.5)], we solve the SPDE until $T = 0.5$. We then downsample the temporal resolution by a factor 5, resulting in 100 time points. Here, the initial condition is given by $u_0(x) = \sin(2\pi x) + \kappa \eta(x)$, where η is defined in eq. (9) and for simplicity initial velocity v_0 is taken deterministic $v_0(x) = x(1 - x)$. Similarly to Sec. 4.1 we either take $\kappa = 0$ or $\kappa = 1$ to generate datasets where the initial condition is either fixed or varies across samples. Each dataset consists of $N = 1\,000$ training observations.

Table 12: **Stochastic Wave equation**. We report the relative L2 error on the test set. The symbol x indicates that the model is not applicable. N is fixed to $1\,000$.

Model	$u_0 \mapsto u$	$\xi \mapsto u$	$(u_0, \xi) \mapsto u$
NCDE	x	0.142	0.432
NRDE	x	0.146	0.445
NCDE-FNO	x	0.029	0.037
DeepONet	0.190	0.143	x
FNO	0.151	0.026	x
NSPDE (Ours)	0.150	**0.023**	**0.026**

 B.4   Deterministic Navier-Stokes PDE

In this final experiment, we demonstrate that our Neural SPDE model can also be used in the setting of PDEs without any stochastic term. We do so by studying the example from [25] on deterministic Navier-Stokes. More precisely, we consider the 2D Navier-Stokes equation for a viscous, incompressible fluid in vorticity form:

$$\partial_t w(t,x) - \nu \Delta w(t,x) = f(x) - u(t,x) \cdot \nabla w(t,x), \qquad t \in [0,T], x \in [0,1]^2 \qquad (18)$$

$$\nabla \cdot u(t,x) = 0, \qquad t \in [0,T], x \in [0,1]^2 \qquad (19)$$

$$w(x,0) = w_0(x), \qquad x \in [0,1]^2 \qquad (20)$$

where $u : [0,T] \times [0,1]^2 \to \mathbb{R}^2$ is the velocity field, $w = \nabla \times u$ is the vorticity with $w_0 : [0,1]^2 \to \mathbb{R}$ being the initial vorticity. Here f is a deterministic forcing term which we take as in [25]. We follow the experimental setup from [25] and use the dataset (available under an MIT license) where $\nu = 10^{-5}$, $N = 1000$ and $T = 20$. We achieve similar performances as FNO with a L2 error of 0.17. A comparison between a true and predicted trajectory is depicted in Fig. 3.

Figure 3: **Top panel:** Initial vorticity and ground truth vorticity at later time steps on a 64×64 mesh. **Bottom panel:** Predictions of the Neural SPDE model.