PHYSICS-AWARE, PROBABILISTIC MODEL ORDER REDUCTION WITH GUARANTEED STABILITY

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ABSTRACT

Given (small amounts of) time-series' data from a high-dimensional, fine-grained, multiscale dynamical system, we propose a generative framework for learning an effective, lower-dimensional, coarse-grained dynamical model that is predictive of the fine-grained system's long-term evolution but also of its behavior under different initial conditions. We target fine-grained models as they arise in physical applications (e.g. molecular dynamics, agent-based models), the dynamics of which are strongly non-stationary but their transition to equilibrium is governed by unknown slow processes which are largely inaccessible by brute-force simulations. Approaches based on domain knowledge heavily rely on physical insight in identifying temporally slow features and fail to enforce the long-term stability of the learned dynamics. On the other hand, purely statistical frameworks lack interpretability and rely on large amounts of expensive simulation data (long and multiple trajectories) as they cannot infuse domain knowledge. The generative framework proposed achieves the aforementioned desiderata by employing a flexible prior on the complex plane for the latent, slow processes, and an intermediate layer of physics-motivated latent variables that reduces reliance on data and imbues inductive bias. In contrast to existing schemes, it does not require the a priori definition of projection operators from the fine-grained description and addresses simultaneously the tasks of dimensionality reduction and model estimation. We demonstrate its efficacy and accuracy in multiscale physical systems of particle dynamics where probabilistic, long-term predictions of phenomena not contained in the training data are produced.

1 INTRODUCTION

High-dimensional, nonlinear systems are ubiquitous in engineering and computational physics. Their nature is in general multi-scale. E.g. in materials, defects and cracks occur on scales of millimeters to centimeters whereas the atomic processes responsible for such defects take place at much finer scales (Belytschko & Song, 2010). Local oscillations due to bonded interactions of atoms (Smit, 1996) take place at time scales of femtoseconds ($10^{-15}s$), whereas protein folding processes which can be relevant for e.g. drug discovery happen at time scales larger than milliseconds ($10^{-3}s$). In Fluid Mechanics, turbulence phenomena are characterized by fine-scale spatiotemporal fluctuations which affect the coarse-scale response (Laizet & Vassilicos, 2009). In all of these cases, macroscopic observables are the result of microscopic phenomena and a better understanding of the interactions between the different scales would be highly beneficial for predicting the system's evolution (Givon et al., 2004). The identification of the different scales, their dynamics and connections however is a non-trivial task and is challenging from the perspective of statistical as well as physical modeling.

In this paper we propose a novel physics-aware, probabilistic model order reduction framework with guaranteed stability that combines recent advances in statistical learning with a hierarchical architecture that promotes the discovery of interpretable, low-dimensional representations. We employ a generative state-space model with two layers of latent variables. The first describes the latent dynamics using a novel prior on the complex plane that guarantees stability and yields a clear distinction between fast and slow processes, the latter being responsible for the system's long-term evolution. The second layer involves physically-motivated latent variables which infuse inductive bias, enable connections with the very high-dimensional observables and reduce the data require-

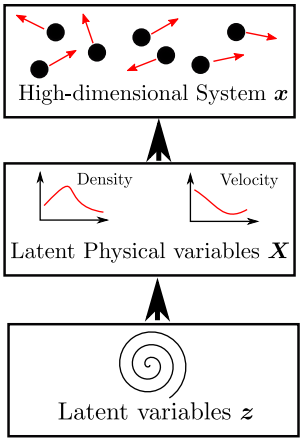

Figure 1: Visual summary of proposed framework. The low-dimensional variables $\boldsymbol{z}$ act as generators of an intermediate layer of latent, physically-motivated variables $\boldsymbol{X}$ that are able to reconstruct the high-dimensional system $\boldsymbol{x}$.

ments for training. The probabilistic formulation adopted enables the quantification of a crucial, and often neglected, component in any model-order reduction process, i.e. the predictive uncertainty due to information loss. We finally want to emphasize that the problems of interest are *Small Data* ones due to the computational expense of the physical simulators. Hence the number of time-steps as well as the number of time-series used for training is small as compared to the dimension of the system and to the time-horizon over which predictions are sought.

2 Physics-Aware, Probabilistic Model Order Reduction

Our data consists of N times-series $\{\boldsymbol{x}_{0:T}^{(i)}\}_{i=1}^{N}$ over T time-steps generated by a computational physics simulator. This can represent positions and velocities of each particle in a fluid or those of atoms in molecular dynamics. Their dimension is generally very high i.e. $\boldsymbol{x} \in \mathcal{M} \subset \mathbb{R}^f$ ($f >> 1$). In the context of state-space models, the goal is to find a lower-dimensional set of collective variables or latent generators $\boldsymbol{z}_t$ and their associated dynamics. Given the difficulties associated with these tasks and the solutions that have been proposed in statistics and computational physics literature, we advocate the use of an intermediate layer of physically-motivated, lower-dimensional variables $\boldsymbol{X}_t$ (e.g. density or velocity fields), the meaning of which will become precise in the next sections. These variables provide a coarse-grained description of the high-dimensional observables and imbue interpretability in the learned dynamics. Using $\boldsymbol{X}_t$ alone (without $\boldsymbol{z}_t$) would make it extremely difficult to enforce long-term stability while achieving sufficient complexity in the learned dynamics (Felsberger & Koutsourelakis, 2019; Champion et al., 2019). Furthermore and even if the dynamics of $\boldsymbol{x}_t$ are first-order Markovian, this is not necessarily the case for $\boldsymbol{X}_t$ (Chorin & Stinis, 2007). The latent variables $\boldsymbol{z}_t$ therefore effectively correspond to a nonlinear coordinate transformation that yields not only Markovian but also stable dynamics (Gin et al., 2019). The general framework is summarized in Figure 1 and we provide details in the next section.

2.1 Model Structure

Our model consists of three levels. At the first level, we have the latent variables $\boldsymbol{z}_t$ which are connected with $\boldsymbol{X}_t$ in the second layer through a probabilistic map $\boldsymbol{G}$. The physical variables $\boldsymbol{X}_t$ are finally connected to the high-dimensional observables through another probabilistic map $\boldsymbol{F}$. We parametrize $\boldsymbol{F}, \boldsymbol{G}$ with deep neural networks and denote by $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$ the corresponding parameters.

In particular, we postulate the following relations:

$$z_{t,j} = z_{t-1,j} \exp(\lambda_j) + \sigma_j \epsilon_{t,j} \quad \lambda_j \in \mathbb{C}, \quad \epsilon_{t,j} \sim \mathcal{CN}(0,1),\ j = 1, 2, \ldots, h \tag{1}$$

$$\boldsymbol{X}_t = \boldsymbol{G}(\boldsymbol{z}_t, \boldsymbol{\theta}_1) \tag{2}$$

$$\boldsymbol{x}_t = \boldsymbol{F}(\boldsymbol{X}_t, \boldsymbol{\theta}_2) \tag{3}$$

We assume that the latent variables $\boldsymbol{z}_t$ are complex-valued and a priori independent. We model their dynamics with a discretized Ornstein-Uhlenbeck process on the complex plane with initial conditions $z_{0,j} \sim \mathcal{CN}(0, \sigma_{0,j}^2)$[1]. The parameters associated with this level are denoted summarily by $\boldsymbol{\theta}_0 = \{\sigma_{0,j}^2, \sigma_j^2, \lambda_j\}_{j=1}^h$. We explain each of the aforementioned components in the sequel.

2.1.1 Stable low-dimensional Dynamics

While the physical systems (e.g. molecular dynamics) of interest are highly non-stationary, they generally converge to equilibrium in the long-term. We enforce long-term stability here by ensuring that the real-part of the λ_j's in Equation (1) is negative, i.e.:

$$\lambda_j = \Re(\lambda_j) + i\ \Im(\lambda_j) \text{ with } \Re(\lambda_j) < 0 \tag{4}$$

which guarantees first and second-order stability i.e. the mean as well as the variance are bounded at all time steps.

The transition density each process $\boldsymbol{z}_{t,j}$ is given by:

$$p\left(z_{t,j} \mid z_{t-1,j}\right) = \mathcal{N}\left(\begin{bmatrix}\Re(z_{t,j})\\ \Im(z_{t,j})\end{bmatrix} \mid \boldsymbol{\mu} = s_j\ \boldsymbol{R}_j \begin{bmatrix}\Re(z_{t-1,j})\\ \Im(z_{t-1,j})\end{bmatrix}, \boldsymbol{\Sigma} = \boldsymbol{I}\frac{\sigma_j^2}{2}\right) \tag{5}$$

with the orthogonal matrix $\boldsymbol{R}_j$ depending on the imaginary part of λ_j:

$$\boldsymbol{R}_j = \begin{bmatrix}\cos(\Im(\lambda_j)) & -\sin(\Im(\lambda_j))\\ \sin(\Im(\lambda_j)) & \cos(\Im(\lambda_j))\end{bmatrix} \tag{6}$$

The decay rate s_j depends on the real part of λ_j:

$$s_j = \exp(\Re(\lambda_j)) \tag{7}$$

i.e. the closer to zero the latter is, the "slower" the evolution of the corresponding process is. As in probabilistic Slow Feature Analysis (SFA) (Turner & Sahani, 2007; Zafeiriou et al., 2015), we set $\sigma_j^2 = 1 - \exp(2\ \Re(\lambda_j)) = 1 - s_j^2$ and $\sigma_{0,j}^2 = 1$. This implies that a priori the latent dynamics are stationary[2] and enables ranking of the slowness of each process j on the basis of $\Re(\lambda_j)$. Hence the only independent parameters are the λ_j. The imaginary part of λ_j can account for periodic effects in the latent dynamics.

The joint density of $\boldsymbol{z}_t$ can finally be expressed as:

$$p(\boldsymbol{z}_{0:T}) = \prod_{j=1}^{h}\left(\prod_{t=1}^{T} p(z_{t,j} \mid z_{t-1,j}, \boldsymbol{\theta}_0) p(z_{0,j})\right) \tag{8}$$

The transition density between states at non-neighbouring time-instants is also available analytically, which is useful for training on longer trajectories or in cases of missing data. Details can be found in Appendix C.

2.1.2 Probabilistic Generative Mapping

We employ fully probabilistic maps between the different layers which involve two conditional densities based on Equations (2) and (3), i.e.:

$$p(\boldsymbol{x}_t \mid \boldsymbol{X}_t, \boldsymbol{\theta}_2) \quad \text{and} \quad p(\boldsymbol{X}_t \mid \boldsymbol{z}_t, \boldsymbol{\theta}_1) \tag{9}$$

[1] A short review of complex normal distributions can be found in Appendix A.

[2] More details can be found in Appendix B.

In contrast to the majority of physics-motivated papers (Zwanzig, 1973; Mori, 1965; Chorin & Stinis, 2007), we note that the generative structure adopted does not require the prescription of a restriction operator and the reduced variables need not be selected a priori but rather are adapted to best reconstruct the observables.

The splitting of the generative mapping into two parts through the introduction of the intermediate variables $\boldsymbol{X}_t$ has several advantages. Firstly, known physical dependencies between the data $\boldsymbol{x}$ and the physical variables $\boldsymbol{X}$ can be taken into account, which reduces the complexity of the associated maps and the total number of parameters. For instance, in the case of particle simulations where $\boldsymbol{X}$ represents a density or velocity field, i.e. it provides a coarsened or averaged description of the fine-scale observables, it can be used to (probabilistically) reconstruct the positions or velocities of the particles. This physical information can be used to compensate for the lack of data when only few training sequences are available (Small data) and can seen as a strong prior to the model order reduction framework. Due to the lower dimension of associated variables, the generative map between $\boldsymbol{z}_t$ and $\boldsymbol{X}_t$ can be more easily learned even with few training samples. Lastly, the inferred physical variables $\boldsymbol{X}$ can provide insight and interpretability to the analysis of the physical system.

2.2 Inference and Learning

Given the probabilistic relations above, our goal is to identify the state variables $\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}$ as well as all parameters $\boldsymbol{\theta}$ of the model. We follow a hybrid Bayesian approach in which the posterior of the state variables is approximated using structured Stochastic Variational Inference (Hoffman et al., 2013) and the MAP point estimates for $\boldsymbol{\theta} = \{\boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2\}$ are obtained.

The application of Bayes' rule leads to the following posterior:

$$p(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta} | \boldsymbol{x}_{0:T}^{(1:n)}) = \frac{p(\boldsymbol{x}_{0:T}^{(1:n)} | \boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})\, p(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})}{p(\boldsymbol{x}_{0:T}^{(1:n)})} \tag{10}$$

$$= \frac{p(\boldsymbol{x}_{0:T}^{(1:n)} | \boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{\theta})\, p(\boldsymbol{X}_{0:T}^{(1:n)} \mid \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})\, p(\boldsymbol{z}_{0:T}^{(1:n)} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})}{p(\boldsymbol{x}_{0:T}^{(1:n)})} \tag{11}$$

where $p(\boldsymbol{\theta})$ denotes the prior on the model parameters. We employ variational inference to resolve the posterior and use the following decomposition for our parametrized variational posterior[3]:

$$q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}) = \prod_{i=1}^{n} \left(\prod_{j=0}^{h} q_{\boldsymbol{\phi}}(\boldsymbol{z}_{0:T,j}^{(i)} \mid \boldsymbol{X}_{0:T}^{(i)}) \right) q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)}) \tag{12}$$

We are approximating the conditional posterior of $\boldsymbol{z}$ given $\boldsymbol{X}$ with a complex multivariate normal which is parameterized using a tridiagonal precision matrix as proposed in Archer et al. (2015); Bamler & Mandt (2017). This retains some of the dependencies but the number of parameters grows linearly with the dimension of $\boldsymbol{z}$ which leads to a highly scalable algorithm. For the variational posterior of $\boldsymbol{X}$ we employ a Gaussian with a diagonal coveriance, i.e.:

$$q_{\boldsymbol{\phi}}(\boldsymbol{z}_{0:T,j}^{(i)} \mid \boldsymbol{X}_{0:T}^{(i)}) = \mathcal{CN}(\boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)}), \left[\boldsymbol{B}_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)}) \boldsymbol{B}_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)})^T\right]^{-1}) \qquad q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\phi}}^{(i)}, \boldsymbol{\Sigma}_{\boldsymbol{\phi}}^{(i)}) \tag{13}$$

We denote summarily with $\boldsymbol{\phi}$ the parameters involved and note that deep neural networks are used for the mean $\boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)})$ as well as the upper bidiagonal matrix $\boldsymbol{B}_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(i)})$. Details on the neural net architectures employed are provided in Section 4 and in Appendix E.

It can be readily shown that the optimal parameter values are found by maximizing the Evidence Lower Bound (ELBO) $\mathcal{F}(q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}), \boldsymbol{\theta})$ whose derivation is given in Appendix D. We compute Monte Carlo estimates of the gradient of the ELBO with respect to ϕ and $\boldsymbol{\theta}$ with the help of the reparametrization trick (Kingma & Welling, 2013) and perform stochastic optimization with the help of the ADAM algrithm (Kingma & Ba, 2014).

[3]We note that this decomposition does not introduce any error due to the conditional independence of $\boldsymbol{x}, \boldsymbol{z}$ given $\boldsymbol{X}$.

2.3 PREDICTIONS

Once state variables and parameters are successfully inferred, the reduced model learned can be used for probabilistic future predictions. In order to do so for a time sequence used for training, we employ the following Monte Carlo scheme to generate a sample $\boldsymbol{x}_{T+P}$, i.e. P time-steps into the future:

1. Sample $\boldsymbol{X}_T$ and $\boldsymbol{z}_T$ from the inferred posterior $q_{\boldsymbol{\phi}}(\boldsymbol{z}_{0:T} \mid \boldsymbol{X}_{0:T}) q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T})$.
2. Propagate $\boldsymbol{z}_T$ for P time steps forward by using the conditional density in Equation (5) or (21).
3. Sample $\boldsymbol{X}_{T+P}$ and $\boldsymbol{x}_{T+P}$ from $p(\boldsymbol{X}_{T+P} \mid \boldsymbol{z}_{T+P}, \boldsymbol{\theta}_{1,MAP})$ and $p(\boldsymbol{x}_{T+P} \mid \boldsymbol{X}_{T+P}, \boldsymbol{\theta}_{2,MAP})$ respectively.

Naturally, the trained model can be used for predictions under new initial conditions, e.g. $\boldsymbol{x}_0$. To achieve this, first the posterior $p(\boldsymbol{z}_0|\boldsymbol{x}_0) \propto \int p(\boldsymbol{x}_0|\boldsymbol{X}_0, \boldsymbol{\theta}_{2,MAP})\, p(\boldsymbol{X}_0 \mid \boldsymbol{z}_0, \boldsymbol{\theta}_{1,MAP})\, d\boldsymbol{X}_0$ must be found and the Monte Carlo steps above can be employed.

3 RELATED WORK

The main theme of our work is the learning of low-dimensional dynamical representations that are stable, interpretable and make use of physical knowledge.

Linear latent dynamics The line of work that most closely resembles ours pertains to the use of Koopman-operator theory (Koopman, 1931) which attempts to identify appropriate transformations of the original coordinates that yield linear dynamics (Klus et al., 2018). We note that these approaches (Lusch et al., 2018; Champion et al., 2019; Gin et al., 2019; Lee & Carlberg, 2020) require additionally the specification of a encoder i.e. a map from the original description to the reduced coordinates which we avoid in the generative formulation adopted. Furthermore only a small fraction are probabilistic and can quantify predictive uncertainties but very often employ restrictive parametrizations for the Koopman matrix in order to ensure long-term stability (Pan & Duraisamy, 2020). To the best of our knowledge, none of the works along these lines employ additional, physically-motivated variables and as a result have demonstrated their applicability only in lower-dimensional problems and require very large amounts of training data or some ad hoc preprocessing.

Data-driven discovery of nonlinear dynamics The data-driven discovery of the governing dynamics has received tremendous attention in recent years. Efforts based on the Mori-Zwanzig formalism can accurately identify dynamics of pre-defined variables, which also account for memory effects, but cannot reconstruct the full fine-grained picture or make predictions about other quantities of interest (Chorin & Stinis, 2007; Kondrashov et al., 2015; Ma et al., 2019). Similar restrictions apply when neural-network-based models are employed as e.g. (Chen et al., 2018; Li et al., 2020). Efforts based on the popular SINDy algorithm (Brunton et al., 2016) require additionally data with respect to the time-derivatives of the variables of interest which when estimated with finite-differences introduce errors and reduce robustness. Sparse Bayesian learning tools in combination with physically-motivated variables and generative models have been employed by (Felsberger & Koutsourelakis, 2019) but cannot guarantee the long-term stability of the learned dynamics.

Infusing domain knowledge from physics Several efforts have been directed in endowing neural networks with invariances or equivariances arising from physical principles. Usually those pertain to translation or rotation invariance and are domain-specific as in Schütt et al. (2017). More general formulations such as Hamiltonian (Greydanus et al., 2019; Toth et al., 2019) and Lagrangian Dynamics (Lutter et al., 2019) are currently restricted in terms of the dimension of the dynamical system. Another approach involves using physical laws as regularization terms or for augmenting the loss function as in (Raissi et al., 2019; Lusch et al., 2018; Zhu et al., 2019; Kaltenbach & Koutsourelakis, 2020). In the context of molecular dynamics multiple schemes for coarse-graining which also guarantee long-term stability have been proposed by Noé (2018) and Wu et al. (2017; 2018). In our approach physically-motivated latent variables are used to facilitate generative maps to very high-dimensional data and to reduce the amount of training data needed.

Slowness and interpretability Finally in contrast to general state-space models for analyzing time-series data such as Karl et al. (2016); Rangapuram et al. (2018); Li et al. (2019), the prior proposed and the use of complex variables enable the discovery of slow features which are crucial in predicting the evolution of multiscale systems and in combination with the variables $\boldsymbol{X}_t$ can provide interpretability and insight into the underlying physical processes.

4 EXPERIMENTS

The high-dimensional, fine-grained model considered consists of f identical particles which can move in the bounded one-dimensional domain $s \in [-1,\ 1]$ (under periodic boundary conditions). The variables $\boldsymbol{x}_t$ consist therefore of the coordinates of the particles at each time instant t and the dimension of the system f is equal to the number of particles. We consider two types of stochastic particle dynamics that correspond to an advection-diffusion-type (section 4.1) and a viscous-Burgers'-type (section 4.2) behavior. The particulars of the microscopic dynamics can be found in Appendix E. We assess the performance of the method by computing first- and second-order statistics as illustrated in the sequel as well as in Appendix G.

4.1 PARTICLE DYNAMICS: ADVECTION-DIFFUSION

We train the model on $N = 64$ time-series of the positions of $f = 250 \times 10^3$ particles over $T = 40$ time-steps which were simulated as described in Appendix E.1. The physical latent variables are associated with the particle density which is represented by discretizing the domain with 25 bins of equal size (see Appendix E). Given the conservation of mass constraint, we make use of real-valued $\boldsymbol{X}_t$ which are then transformed with the softmax function in order to yield the particle density. Furthermore, we made use of $h = 5$ complex, latent processes $\boldsymbol{z}_t$. Details regarding the mappings, the variational posteriors and neural network architectures involved can be found in the Appendix E.1.

In Figure 2 the learned values for the complex variables λ_j are plotted as well as the inferred and predicted time-evolution of 2 associated processes $z_{t,j}$ on the complex plane. We note the clear separation of time-scales in the first plot with two slow processes, one intermediate and two fast ones. This is also evident in the indicative trajectories on the complex plane. A detailed discussion of the generative mappings associated with $\boldsymbol{z}_t$ and their influence on $\boldsymbol{x}$ can be found in the Appendix F.

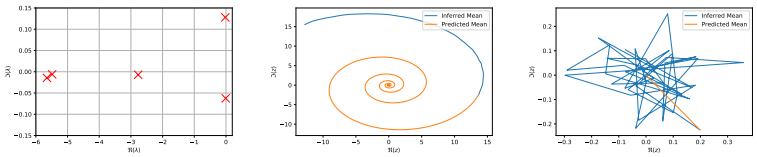

Figure 2: Complex eigenvalues λ (left) and the time evolution of indicative slow (middle) and fast (right) processes $z_{t,j}$ associated with them.

In Figure 3 we compare the true particle density with the one predicted by the trained reduced model. We note that the latter is computed by reconstructing the $\boldsymbol{x}_t$ futures. We observe that the model is able to accurately track first-order statistics well into the future.

A more detailed view of the predictive estimates with snapshots of the particle density at selected time instances is presented in Figure 4. Here, not only the posterior mean but also the associated uncertainty is displayed. We want to emphasize the last Figure at $t = 1000$ when the steady state has been reached which clearly shows that our model is capable of converging to stable equilibrium.

Since the proposed model is capable of probabilistically reconstructing the whole fine-grained picture, i.e. $\boldsymbol{x}_t$, predictions with regards to any observable can be obtained. In Appendix G.1 we assess the accuracy of predictions in terms of second-order statistics, and in particular for the probability of finding simultaneously a pair of particles at two specified positions. Finally, in Appendix H we demonstrate the accuracy of the trained in model in producing predictions under *unseen* initial conditions.

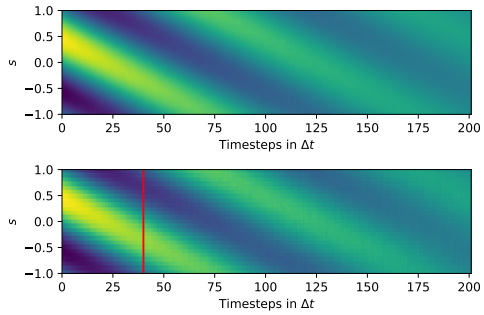

Figure 3: Particle density: Inferred and predicted posterior mean (bottom) in comparison with the ground truth (top). The red line divides inferred quantities from predicted ones.

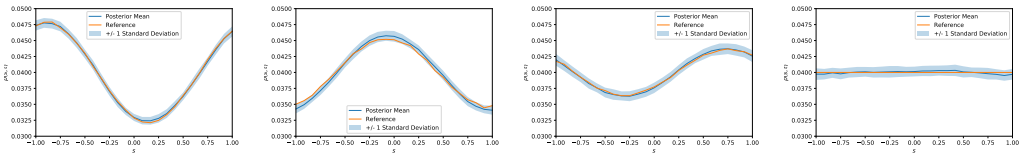

Figure 4: Predicted particle density profiles at $t = 80, 120, 160, 1000$ (from left to right).

4.2 Particle Dynamics: Viscous Burgers' Equation

In this example, we made use of $N = 64$ sequences of $f = 500 \times 10^3$ particles over $T = 40$ time-steps. Details regarding the physical simulator, the stochastic interactions between particles as well as the associated network architectures are contained in Appendix E.2. As in the previous example, we employed the particle density with the softmax transformation for $\boldsymbol{X}_t$ and $h = 5$ complex-valued processes $\boldsymbol{z}_t$ at the lowest model level.

In Figure 5 the learned values for λ_j of the low-dimensional dynamical system are shown where the clear separation of time-scales with three slow and two fast processes can be observed.

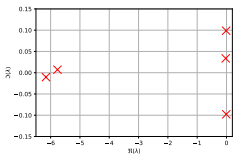

Figure 5: Complex eigenvalues λ for the viscous Burgers' system.

In Figure 6 we compare the evolution of the true particle density with the (posterior mean of) the model-predicted one. We point out the sharp front at the lower left corner which is characteristic of the Burgers' equation and which eventually dissipates due to the viscosity. This is captured in the inferred as well as in the predicted solution.

A more detailed view on the predictive results with snapshots of the particle density at selected time instances is is presented in Figure 7. We emphasize again the stable convergence of the learned dynamics to the steady state as well as the successful capturing and propagation of the shock front.

We compare the accuracy of the predictions for second-order statistics of the fine-grained system in terms of the two-particle probability in Appendix G.2 where excellent agreement with the ground truth, i.e. the one computed by simulating the fine-grained system, is observed.

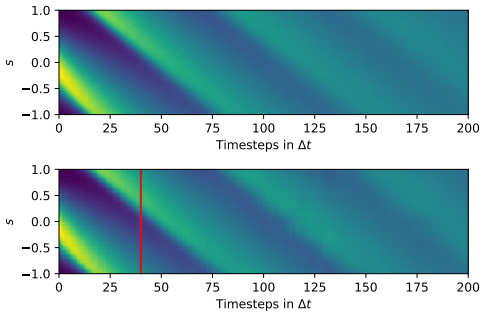

Figure 6: Particle density: Inferred and predicted posterior mean (bottom) in comparison with the ground truth (top). The red line divides inferred quantities from predicted ones.

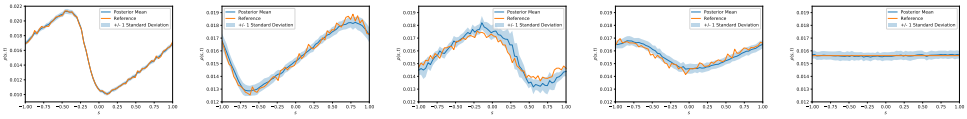

Figure 7: Predicted particle density profiles at $t = 40, 80, 120, 160, 1000$ (from left to right).

5 Conclusions

In this paper, we presented a framework for efficiently learning a lower-dimensional, dynamical representation of a very high-dimensional, fine-grained systems that is predictive of its long-term evolution and whose stability is guaranteed. We infuse domain knowledge with the help of an additional layer of latent variables. The latent variables at the lowest level provide an interpretabable separation of the time-scales and ensure the long-term stability of the learned dynamics. We employed scalable variational inference techniques and applied the proposed model in data generated from very large systems of interacting particles. In all cases accurate probabilistic predictions were obtained both in terms of first- and second-order statistics over a very long time range into the future. Furthermore, the ability of the learned to produce predictions under new, unseen initial conditions was demonstrated. A direct extension of the model would be to augment the list of physical variables $\boldsymbol{X}_t$ in the second layer with the more abstract latent variables $\boldsymbol{z}_t$ i.e. employ a generative map of the form $\boldsymbol{x}_t = \boldsymbol{F}(\boldsymbol{X}_t, \boldsymbol{z}_t)$ instead of Equation (3). This would enable the discovery of new reduced coordinates that are complementary to the physical ones and could provide otherwise inaccessible insight into the multiscale dynamics.

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A COMPLEX NORMAL DISTRIBUTION

In this Appendix, the complex random normal distribution is reviewed. The mathematical definitions introduced follow Andersen et al. (1995):

A p-variate complex normal random variable $\boldsymbol{Y} \in \mathbb{C}^p$ with $\boldsymbol{Y} \sim \mathcal{CN}(\boldsymbol{\mu}_{\mathbb{C}}, \boldsymbol{\Sigma}_{\mathbb{C}})$ is defined by a complex mean vector $\boldsymbol{\mu}_{\mathbb{C}} \in \mathbb{C}^p$ and a complex Covariance Matrix $\boldsymbol{\Sigma}_{\mathbb{C}} \in \mathbb{C}_{+}^{p \times p}$. The density with respect to Lesbegue measures on $\mathbb{C}^p$ can be stated as:

$$f_{\boldsymbol{Y}}(\boldsymbol{y}) = \pi^{-p} \det(\boldsymbol{\Sigma}_{\mathbb{C}})^{-1} \exp\left(-(\boldsymbol{y} - \boldsymbol{\mu}_{\mathbb{C}})^* \boldsymbol{\Sigma}_{\mathbb{C}}^{-1} (\boldsymbol{y} - \boldsymbol{\mu}_{\mathbb{C}})\right) \tag{14}$$

where $*$ indicates the conjugate transpose of a matrix.

This complex normal random variable has similar properties to the well-known, real-valued counterpart. For instance, linear transformations of complex random normal variables are again complex random normal variables.

These properties directly follow from the fact, that for a complex random normal variable there exists an isomorphic transformation to a real valued $2p$-variate normal random variable $W \in \mathbb{R}^{2p}$. This random normal variable is defined with mean

$$\boldsymbol{\mu}_{\mathbb{R}} = \begin{bmatrix} \Re(\boldsymbol{\mu}_{\mathbb{C}}) \\ \Im(\boldsymbol{\mu}_{\mathbb{C}}) \end{bmatrix} \tag{15}$$

and covariance

$$\boldsymbol{\Sigma}_{\mathbb{R}} = \frac{1}{2} \begin{bmatrix} \Re(\boldsymbol{\Sigma}_{\mathbb{C}}) & -\Im(\boldsymbol{\Sigma}_{\mathbb{C}}) \\ \Im(\boldsymbol{\Sigma}_{\mathbb{C}}) & \Re(\boldsymbol{\Sigma}_{\mathbb{C}}) \end{bmatrix} \tag{16}$$

Therefore: $W \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbb{R}}, \boldsymbol{\Sigma}_{\mathbb{R}})$

As an example the real valued isomorphic counterpart of the standard complex random normal distribution $\mathcal{CN}(0, 1)$ is the bivariate normal distribution $\mathcal{N}(\mathbf{0}, \frac{1}{2}\mathbf{I})$.

B CHOICE OF VARIANCE FOR A-PRIORI STEADY STATE

Apart from $\sigma_j^2 = 1 - s_j^2$, we also set the intial variance $\sigma_{0,j}^2 = 1$. This makes the prior stationary and allows direct comparisons between processes $z_{t,j}$ on the basis of the single free parameter i.e. λ_j.The reasoning is explained in more detail below (see also (Turner & Sahani, 2007; Zafeiriou et al., 2015)).

The asymptotic ($t \to \infty$) or stationary[4] distribution of $\begin{bmatrix} \Re(z_{t,j}) \\ \Im(z_{t,j}) \end{bmatrix}$ will be a Gaussian with mean:

$$\boldsymbol{\mu}_{\infty,j} = 0 \tag{17}$$

and covariance:

$$\boldsymbol{C}_{\infty,j} = \frac{1}{2}\frac{\sigma_j^2}{1 - e^{2\Re(\lambda_j)}}\boldsymbol{I} \tag{18}$$

This also explains the specific choice $\sigma^2 = 1 - e^{2\Re(\lambda_j)}$ in more detail to have all latent variables reach the same equilibrium independent of their decay speed:

$$\boldsymbol{C}_{\infty,j} = \frac{1}{2}\boldsymbol{I} \tag{19}$$

Since the initial density has mean $\mathbf{0}$ and covariance $\boldsymbol{C}_0 = \frac{\sigma_{0,j}^2}{2}\boldsymbol{I}$, in order to have an **a priori** stationary process (i.e. where all the marginals are the same) we assume:

$$\sigma_{0,j}^2 = 1 \tag{20}$$

[4]to verify stationarity assume $\begin{bmatrix} \Re(z_{t-1}) \\ \Im(z_{t-1}) \end{bmatrix} \sim \mathcal{N}(\boldsymbol{\mu}_\infty, \boldsymbol{C}_\infty)$ and use the conditional to verify that $\begin{bmatrix} \Re(z_t) \\ \Im(z_t) \end{bmatrix}$ will also follow the same distribution

C TRANSITION PROBABILITY FOR THE LOW-DIMENSIONAL EVOLUTION LAW

The proposed prior model allows for analytic expressions for the the transition density between non-neighbouring states of $\boldsymbol{z}$ as shown below for the transition density between $\boldsymbol{z}_t$ and $\boldsymbol{z}_0$:

$$p\left(z_{t,j} \mid z_{0,j}\right) = \mathcal{N}\left(\begin{bmatrix}\Re(z_{t,j})\\ \Im(z_{t,j})\end{bmatrix} \mid \boldsymbol{\mu} = s_j^t\, \boldsymbol{R}_j^t \begin{bmatrix}\Re(z_{t-1,j})\\ \Im(z_{t-1,j})\end{bmatrix}, \boldsymbol{\Sigma} = \boldsymbol{I}\frac{1-s_j^{2t}}{2}\right) \tag{21}$$

Based on the transition density between neighbouring states in Equation 5 it is possible to derive the marginal mean $\boldsymbol{\mu}_{t,j}$ and Covariance $\boldsymbol{C}_{t,j}$ at each time step t based on an initial condition $\boldsymbol{z}_0 \sim \mathcal{CN}(z_0, \sigma_0^2)$:

$$\boldsymbol{\mu}_{t,j} = s_j^t\, \boldsymbol{R}_j^t \begin{bmatrix}\Re(z_0)\\ \Im(z_0)\end{bmatrix} \tag{22}$$

and

$$\boldsymbol{C}_{t,j} = \frac{1}{2}\left(\sigma_0^2 e^{2\Re(\lambda_j)t} + \sigma_j^2 \frac{1-e^{2\Re(\lambda_j)t}}{1-e^{2\Re(\lambda_j)}}\right)\boldsymbol{I} \tag{23}$$

This is a direct consequence of the properties of the complex normal variables stated previously and the fact that $\sigma_j^2 = 1 - s_j^2$.

D DERIVATION OF ELBO

This section contains details the derivation of the Evidence-Lower-Bound (ELBO) which is the quantity which is optimized with respect to the parameters $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$ during training. In particular:

$$
\begin{aligned}
&\log p(\boldsymbol{x}_{0:T}^{(1:n)}|\boldsymbol{\theta}) \\
&= \log \int p(\boldsymbol{x}_{0:T}^{(1:n)}, \boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})\, d\boldsymbol{X}_{0:T}^{(1:n)}\, \boldsymbol{z}_{0:T}^{(1:n)} \\
&= \log \int \frac{p(\boldsymbol{x}_{0:T}^{(1:n)}|\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta}) p(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})}{q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)})} q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)})\, d\boldsymbol{X}_{0:T}^{(1:n)}\, d\boldsymbol{z}_{0:T}^{(1:n)} \\
&\geq \int \log \frac{p(\boldsymbol{x}_{0:T}^{(1:n)}|\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta}) p(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}, \boldsymbol{\theta})}{q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)})} q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)})\, d\boldsymbol{X}_{0:T}^{(1:n)}\, d\boldsymbol{z}_{0:T}^{(1:n)} \\
&= \mathcal{F}(q_{\boldsymbol{\phi}}(\boldsymbol{X}_{0:T}^{(1:n)}, \boldsymbol{z}_{0:T}^{(1:n)}), \boldsymbol{\theta})
\end{aligned}
\tag{24}
$$

E DETAILS FOR EXPERIMENTS

This appendix contains the details for our experiments involving moving particles that have stochastic interactions corresponding to either an Advection-Diffusion behaviour or viscous Burgers' type behaviour. For all experiments, our high-dimensional system $\boldsymbol{x}$ consists of f moving particles, whose dynamics are approximated by a d-dimensional set of latent physical variables $\boldsymbol{X}$ which are directly related to the discretized particle density at d equally spaced bins. The low-dimensional dynamics corresponds to a h dimensional complex latent space.

First we define our probabilistic mappings needed to reconstruct the high-dimensional system. We start with $p(\boldsymbol{x}_t \mid X_t, \boldsymbol{\theta}_2)$: The nature of the physical latent variables $\boldsymbol{X}_t$ suggests a *multinomial* density, i.e.:

$$p(\boldsymbol{x}_t|\boldsymbol{X}_t) = \frac{f!}{m_1(\boldsymbol{x}_t)!\, m_2(\boldsymbol{x}_t)! \ldots m_k(\boldsymbol{x}_t)!} \prod_{k=1}^{d} \left(\frac{\exp(X_{t,k})}{\sum_{l=0}^{d} \exp(X_{t,l})} \right)^{m_k(\boldsymbol{x}_t)} \tag{25}$$

where $m_k(\boldsymbol{x}_t)$ is the number of particles in bin k. The underlying assumption is that, given the latent physical state $\boldsymbol{X}_t$, the coordinates of the particles $\boldsymbol{x}_t$ are *conditionally* independent. This does *not* imply that they move independently nor that they cannot exhibit coherent behavior (Felsberger & Koutsourelakis, 2019). The practical consequence of Equation (25) is that no parameters need to be learned for $p(\boldsymbol{x}_t|\boldsymbol{X}_t)$.

The second map pertains to $p(\boldsymbol{X}_t \mid \boldsymbol{z}_t, \boldsymbol{\theta}_1)$ which we represent with a multivariate normal distribution with a mean and a diagonal covariance matrix model by a neural networks with parameters $\boldsymbol{\theta}_1$. Details can be found in the following sections.

E.1 PARTICLE DYNAMICS: ADVECTION-DIFFUSION

For the simulations presented $f = 250 \times 10^3$ particles were used, which, at each microscopic time step $\delta t = 2.5 \times 10^{-3}$ performed random, non-interacting, jumps of size $\delta s = \frac{1}{640}$, either to the left with probability $p_{left} = 0.1875$ or to the right with probability $p_{right} = 0.2125$. The positions were restricted in $[-1, 1]$ with periodic boundary conditions. It is well-known (Cottet & Koumoutsakos, 2000) that in the limit (i.e. $f \to \infty$) the particle density $\rho(s, t)$ can be modeled with an advection-diffusion PDE with diffusion constant $D = (p_{left} + p_{right})\frac{\delta s^2}{2\delta t}$ and velocity $v = (p_{right} - p_{left})\frac{\delta s}{\delta t}$:

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial s} = D\frac{\partial^2 \rho}{\partial s^2}, \qquad s \in (-1, 1).. \tag{26}$$

From this simulation every 800th microscopic time step the particle positions were extracted and used as training data for our system. Sample initial conditions are shown in Figure 8:

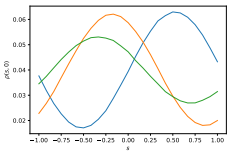

Figure 8: Sample initial conditions for the advection-diffusion type dynamics.

The architecture of the neural networks for the generative mappings described above as well as for the variational posteriors introduced in Section 2.2 can be seen in Figure 9. The neural network used for the generative mapping between the low-dimensional states $\boldsymbol{z}_t$ and the mean and covariance for $\boldsymbol{X}_t$ consists of only one dense layer, whereas the variational posterior on $\boldsymbol{z}_{0:T}$ is parametrized using a dense Layer with ReLu activation followed by another dense layer.

E.2 PARTICLE DYNAMICS: VISCOUS BURGERS' EQUATION

The second test-case involved a fine-grained system of $f = 500 \times 10^3$ particles which perform *interactive* random walks i.e. the jump performed at each fine-scale time-step $\delta t = 2.5 \times 10^{-3}$

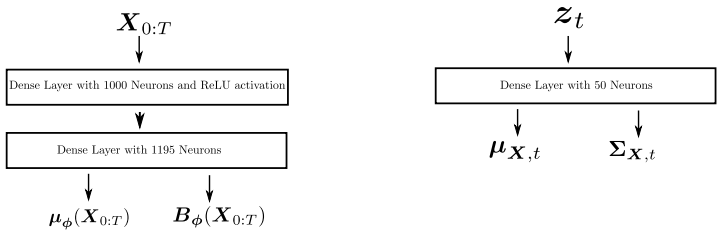

Figure 9: Neural Net architecture used for the particle dynamics corresponding to an advection-diffusion equation.

depends on the positions of the other walkers. In particular we adopted interactions as described in Roberts (1989); Chertock & Levy (2001); Li et al. (2007) so as, in the limit (i.e. when $f \to \infty, \delta t \to 0, \delta s \to 0$), the particle density $\rho(s,t)$ follows a viscous Burgers' equation with $\nu = 0.0005$:

$$\frac{\partial \rho}{\partial t} + \frac{1}{2}\frac{\partial \rho^2}{\partial s} = \nu \frac{\partial^2 \rho}{\partial t^2}, \qquad s \in (-1, 1). \tag{27}$$

From this simulation every 800th microscopic time step the particle positions were extracted and used as training data for our system. Sample initial conditions are shown in Figure 10.

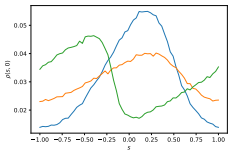

Figure 10: Sample initial conditions for the Burger's type dynamics.

The architecture of the neural networks for the generative mappings described above as well as for the variational posteriors introduced in Section 2.2 can be seen in Figure 11. The neural network used for the generative mapping between the low-dimensional states $\boldsymbol{z}_t$ and the mean and covariance for $\boldsymbol{X}_t$ consists of several dense layers with ReLu activation and Dropout layers to avoid overfitting, whereas the variational posterior on $\boldsymbol{z}_{0:T}$ is parametrized using two dense layers with ReLu activation followed by another dense layer.

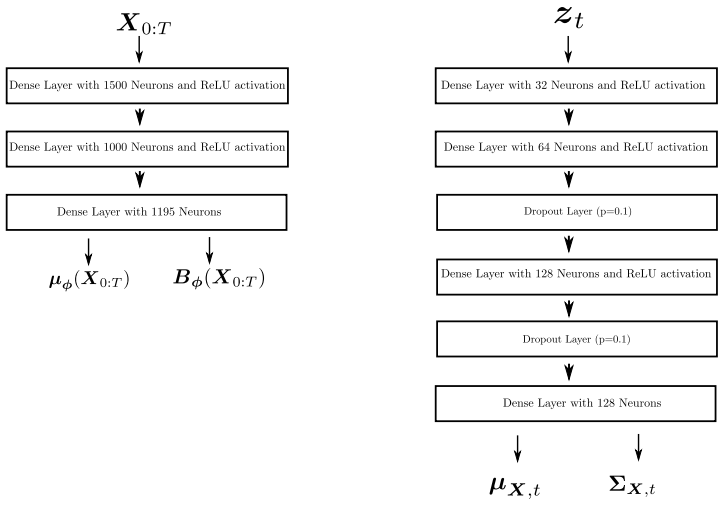

Figure 11: Neural Net architecture used for the particle dynamics corresponding to a viscous Burgers' equation.

F DETAILED ANALYSIS OF THE GENERATIVE MAPPING AND THE SLOW LATENT VARIABLES

In this Appendix we take a closer look at the generative mapping and the (slow) latent variables $\boldsymbol{z}$ learned . For the Advection-Diffusion example, we discovered two slow processes (Section 4.1), $\boldsymbol{z}_1$ and the marginally faster process $\boldsymbol{z}_2$. The rest of the processes were very fast in comparison and took values close to the zero point of the complex plane during the inference as well as during the prediction phase.

In order to visualize the influence through the generative mapping of the two slow processes on the fine-grained system, we set the value for all other processes to zero and then reconstructed the fine-grained state based on different absolute values of $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$. The result are shown in Figure 12; it is clearly visible that those two processes are responsible for reconstructing the fine-grained state as they are able to reproduce various fine-grained geometries. In accordance with their slowness, $\boldsymbol{z}_1$ (the slightly slower process) is responsible for the main part of the geometries, whereas the other slow process generates some smaller scale fluctuations.

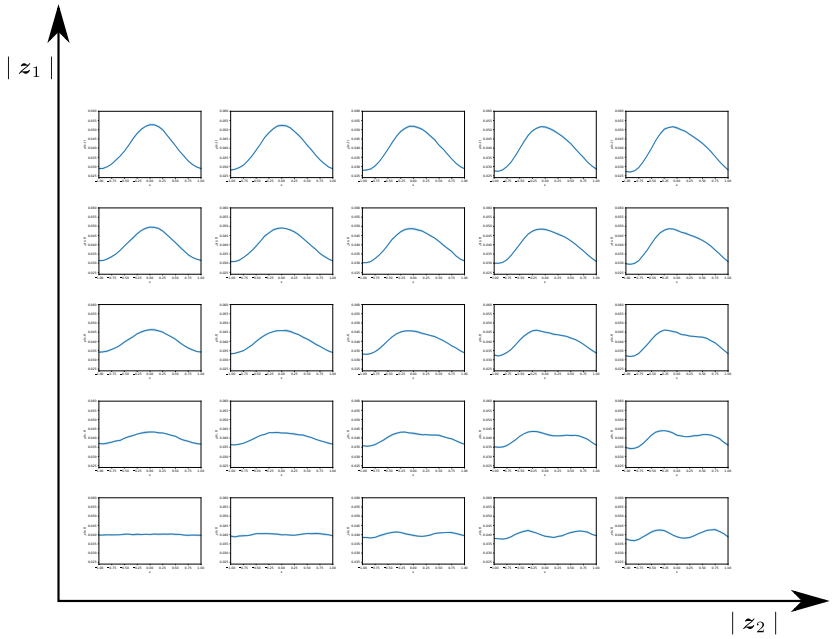

Figure 12: Reconstruction of the fine-grained space with regards to the two slowest processes $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$. All other latent variables were set to zero.

G TWO-POINT PROBABILITY

This appendix contains the predictive estimates for the two-point probability, i.e. the probability of finding two particles simultaneously in two bins (b_1, b_2). This two-point probability can be computed based on the reconstructed fine-grained system and corresponds to a second order statistic.

G.1 PARTICLE DYNAMICS: ADVECTION-DIFFUSION

The estimated two-point probability as well as the comparison to test data is shown for two indicative time-instants in Figure 13 and 14. We note a very good agreement with the ground truth.

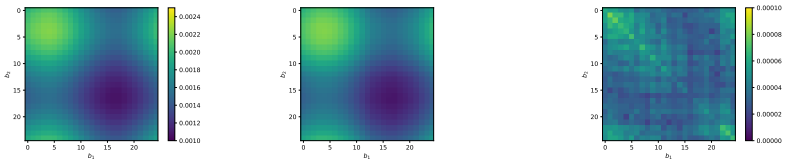

Figure 13: Two-point probability at time step 90: On the left the two-point probability of the data is shown as reference, the figure in the middle contains the predictive posterior mean whereas the figure on the right contains the standard deviation.

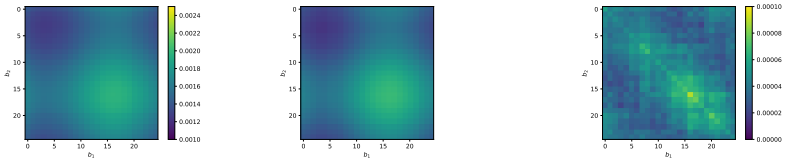

Figure 14: Two-point probability at time step 140: On the left the two-point probability of the data is shown as reference, the figure in the middle contains the predictive posterior mean whereas the figure on the right contains the standard deviation.

G.2 PARTICLE DYNAMICS: VISCOUS BURGERS' EQUATION

The estimated two-point probability as well as the comparison to test data is shown for two indicative time-instants in Figure 15 and 16. We note a very good agreement with the ground truth.

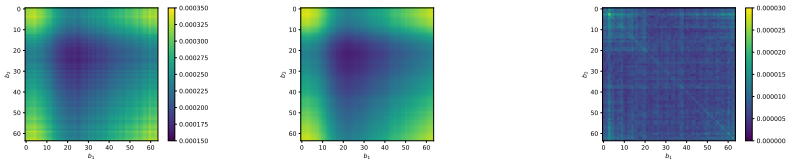

Figure 15: Two-point probability at time step 90: On the left the two-point probability of the data is shown as reference, the figure in the middle contains the predictive posterior mean whereas the figure on the right contains the standard deviation.

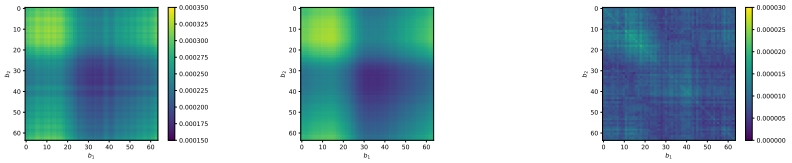

Figure 16: Two-point probability at time step 140: On the left the two-point probability of the data is shown as reference, the figure in the middle contains the predictive posterior mean whereas the figure on the right contains the standard deviation.

H PREDICTION WITH UNSEEN INITIAL CONDITION

This appendix contains predictions with a new initial condition $\boldsymbol{x}_0$ (i.e. not contained in the training data) as described in Section 2.3. Therefore first the posterior of $\boldsymbol{z}_0$ given $\boldsymbol{x}_0$ has to be inferred and then has to be propagated into the future using the learned dynamics. Finally it can be used to reconstruct the full picture of $\boldsymbol{x}$ at any future time-instant.

In Figure 17 the new initial condition in terms of the particle density is shown as well as its reconstruction based on the learned latent variables $\boldsymbol{z}_0$.

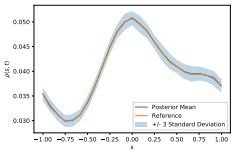

Figure 17: New initial condition in terms of the particle density used for predictions. Reference shows the actual initial conditions, whereas the posterior mean and uncertainty bounds correspond to the reconstruction of the initial condition based on the inferred latent variables $\boldsymbol{z}_0$.

Figure 18 shows predictions of the particle density (i.e. first-order statistics) at different timesteps. We want to emphasise the prediction on the right, which belongs to a prediction at $t = 500$ and shows the steady state of the system. Although the initial condition was not contained in the training data, our framework is able to identify the correct steady state.

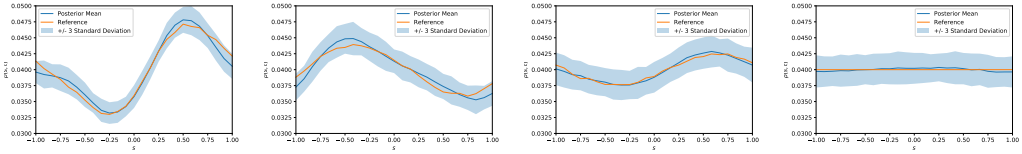

Figure 18: Predictions of the particle density at $t = 25, 75, 125, 500$ (left to right) for on the new initial condition in Figure 17.