Physics-Constrained Learning of PDE Systems with Uncertainty Quantified Port-Hamiltonian Models

Kaiyuan Tan, Peilun (Tommy) Li, Thomas Beckers

Department of Computer Science, Vanderbilt University, USA

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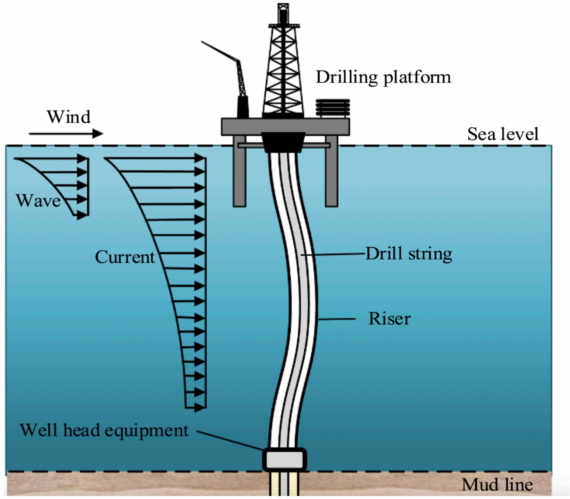
Motivation



[Bending drill string on oil rig [zhang et al]]

[Festo]

Modeling PDE systems is challenging due to high complexity

Need for expressive, reliable, well-generalizing, and flexible models

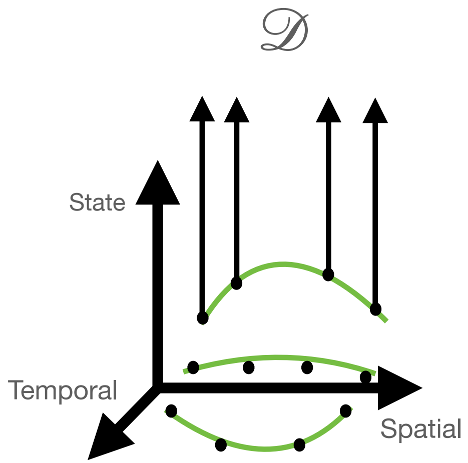
Problem Statement

(partially) unknown function

PDE system

$$0 = f(x, \frac{\partial x}{\partial t}, \frac{\partial x}{\partial z}, \ldots)$$

+ known boundary conditions



Dataset

$$\mathscr{D} = \{(t_1, z_1, x(t_1, z_1), u(t_1)), \ldots, (t_{N_t}, z_{N_z}, x(t_{N_t}, z_{N_z}), u(t_{N_t}))\}$$

Need a model that

- represents a large class of systems -> Expressive
- allows uncertainty quantification -> Reliable
- consistent with physics -> Generalizes well
- Requires minimal expert knowledge -> Flexible

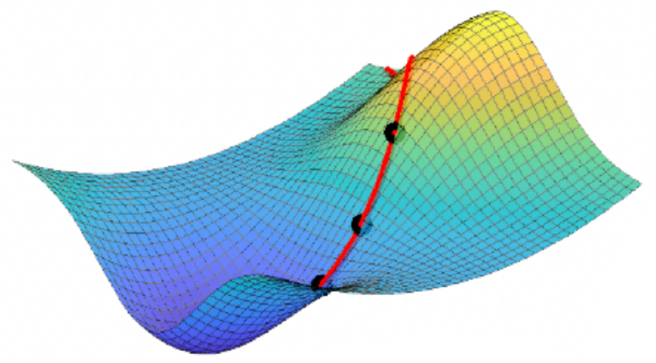
Related Work

	Generalizability	Uncertainty Quantification	Minimal Expert Knowledge	Expressive
Physics based models	✓	✓		✓
Pure, Data-Driven Methods (NN, GPs…)		✓	✓	
Physics-Informed Neural Networks (PINNs)	✓	✓		✓
GP-dPHS (This work)	✓	✓	✓	✓

Distributed Port-Hamiltonian systems + Gaussian Processes

Physics Model

Hamiltonian $\xrightarrow{\text{Ports, Dissipation}}$ port-Hamiltonian System $\xrightarrow{\text{PDE}}$ Distributed port-Hamiltonian System



Interconnection **Dissipation** **Hamiltonian**

$$\frac{\partial x}{\partial t}(t,z) = (J - R)\delta_x \mathscr{H} + Gu$$

Input

$$y = G\delta_x \mathscr{H}$$

$$w = B_{\mathcal{Z}}(\delta_x \mathscr{H}, u)$$

Output **Boundary Condition**

- Skew-adjoint constant differential operator J ensures energy conservation
- R is a constant differential operator that defines dissipation

Extension to PDEs

	ODE model	PDE model
Dynamics	$\dot{x}(t) = [J(x) - R(x)]\frac{\partial H}{\partial x} + G(x)u$	$\frac{\partial x}{\partial t}(t,z) = [J - R]\delta_x \mathscr{H} + Gu$ $w = B_{\mathcal{Z}}(\delta_x \mathscr{H}, u)$
Energy	$H(x)$	$\mathscr{H}(x) = \int_{\mathcal{Z}} H(z,x)dV$
Interconnection	Skew-symmetric $J(x)$	Matrix differential operator J
Training data	$\mathscr{D} = \{t_i, x(t_i), u(t_i)\}_{i=0}^{i=N_t-1}$	$\mathscr{D} = \{t_i, z_j, x(t_i, z_j), u(t_i)\}_{i=j=0}^{i=N_t-1, j=N_z-1}$
Output	Samples of state over time	Samples of state over time and spatial

dPHS example

Vibration of a string with nonlinear stress-strain curve

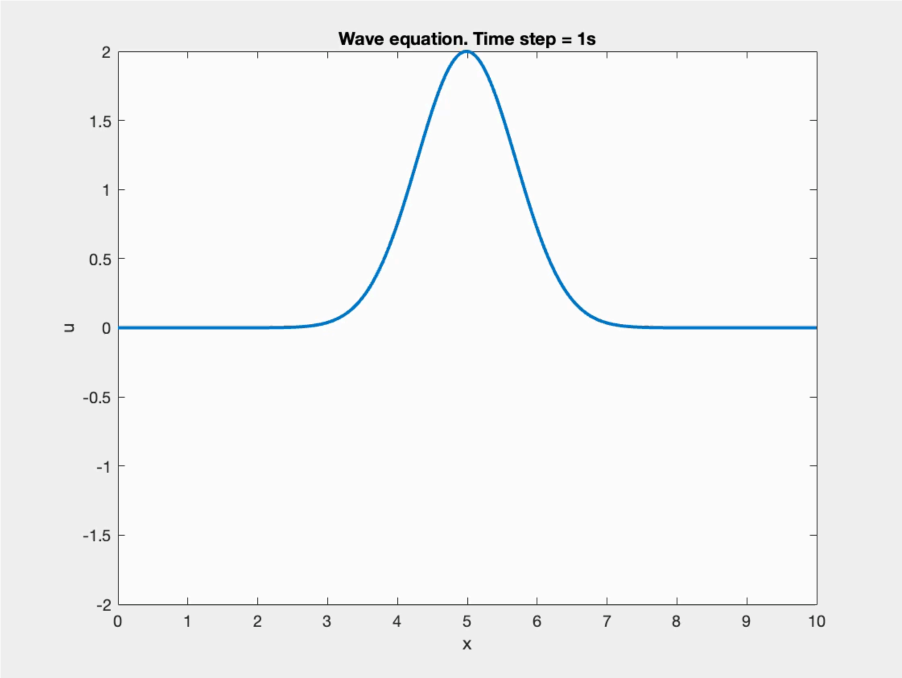
$$\frac{\partial^2 x}{\partial t^2} - f\left(\frac{\partial x}{\partial z}\right)\frac{\partial^2 x}{\partial z^2} = 0,$$

In dPHS form

$\frac{\partial x}{\partial t}$

$$\frac{\partial}{\partial t}\begin{bmatrix} p(t,z) \\ q(t,z) \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 \end{bmatrix}}_{J-R} \delta_{pq}\mathscr{H}(p,q)$$

$\frac{\partial x}{\partial z}$



Example ground truth Hamiltonian functional

$$\mathscr{H} = \int_Z \int s(q)q(t,z)dq + p(t,z)^2 dz$$

Gaussian process

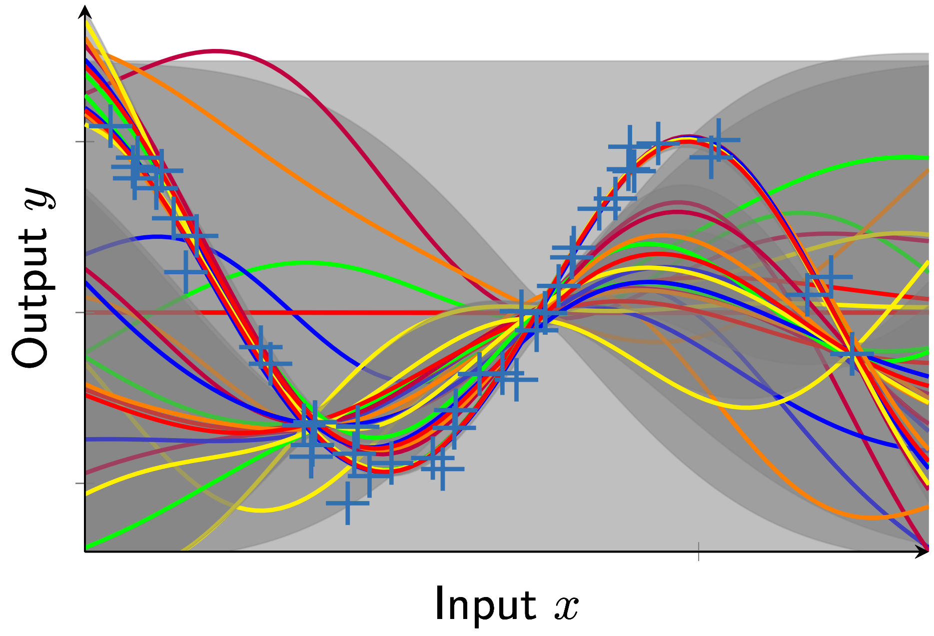
Prior: Gaussian distribution over function space

$$f(x) \sim GP(m(x), k(x, x'))$$

Mean function

Covariance

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$



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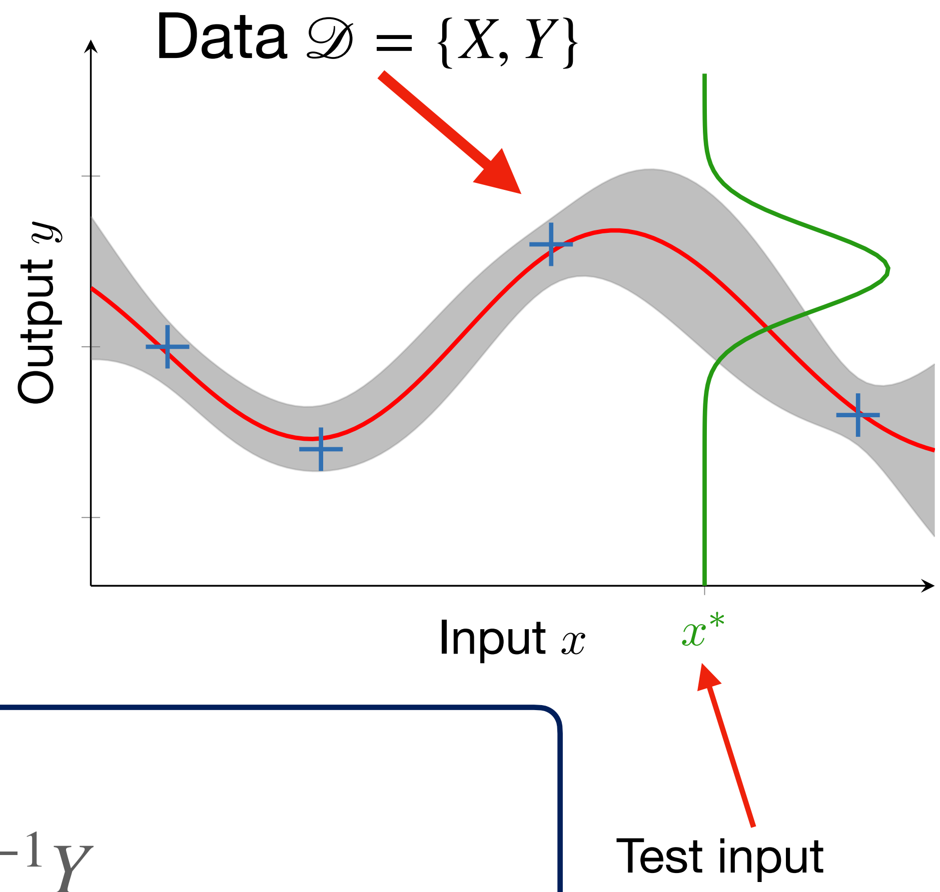

Posterior

$$\mu(y^* \mid x^*, \mathscr{D}) = k(x^*, X)[K(X, X) + \sigma^2 I]^{-1} Y$$

$$\Sigma(y^* \mid x^*, \mathscr{D}) = k(x^*, x^*) - k(x^*, X)[K(X, X) + \sigma^2 I]^{-1} k(x^*, X)^\top$$

C.E. Rasmussen. Gaussian Processes for Machine Learning. 2006

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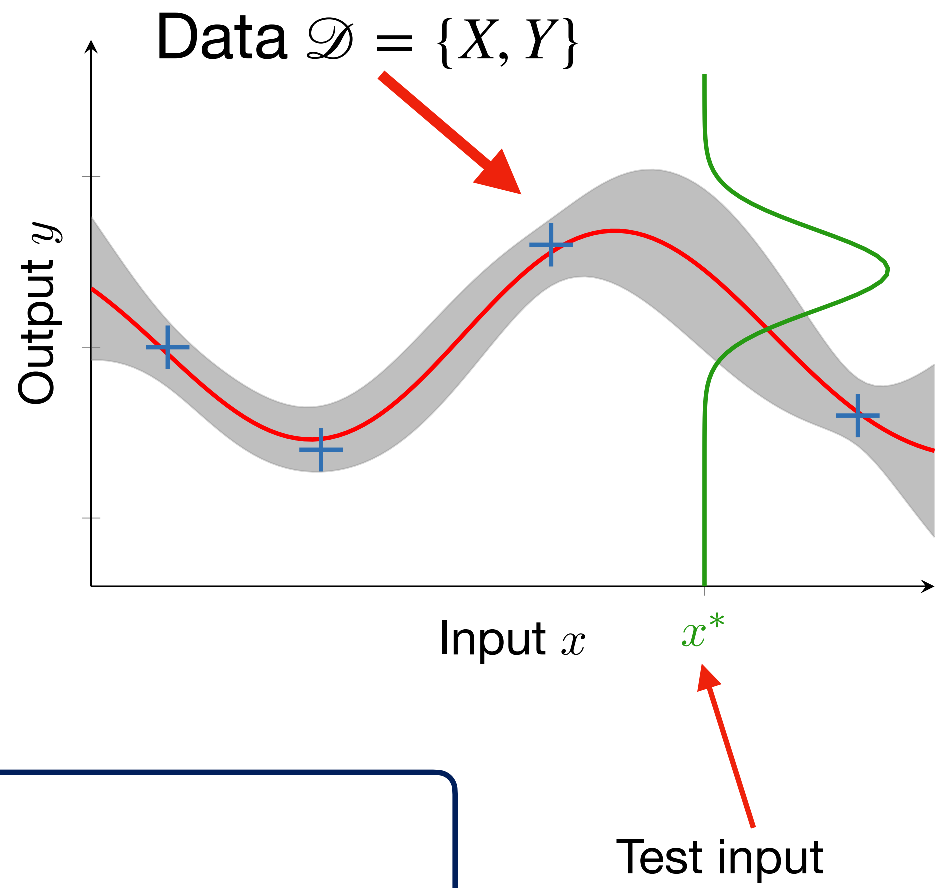

Closed under linear operators

$$f(x) = \mathscr{G}_x g(x) \sim GP(\mathscr{G}_x \mu_g, \mathscr{G}_x k_g \mathscr{G}_x^\top)$$

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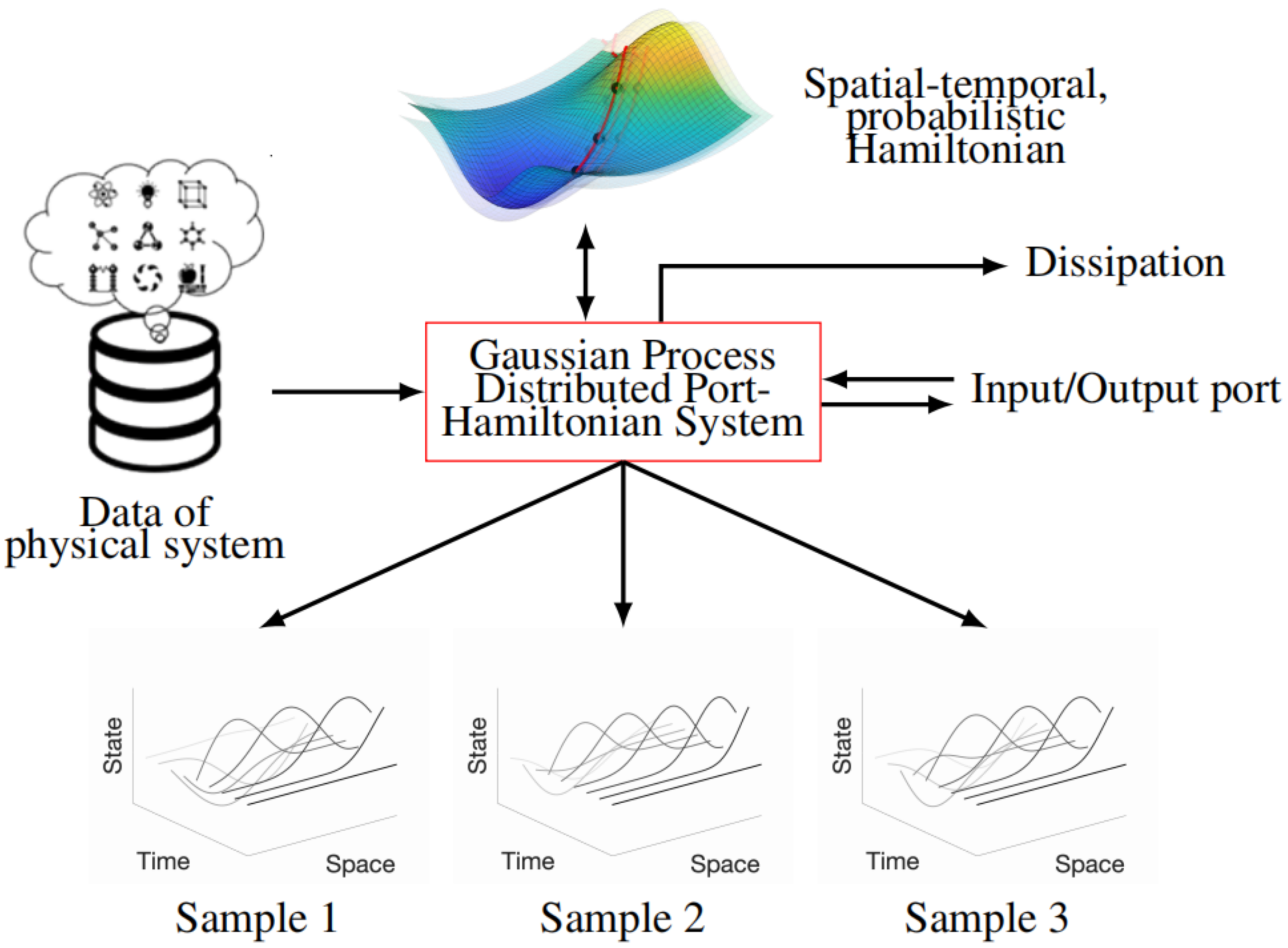
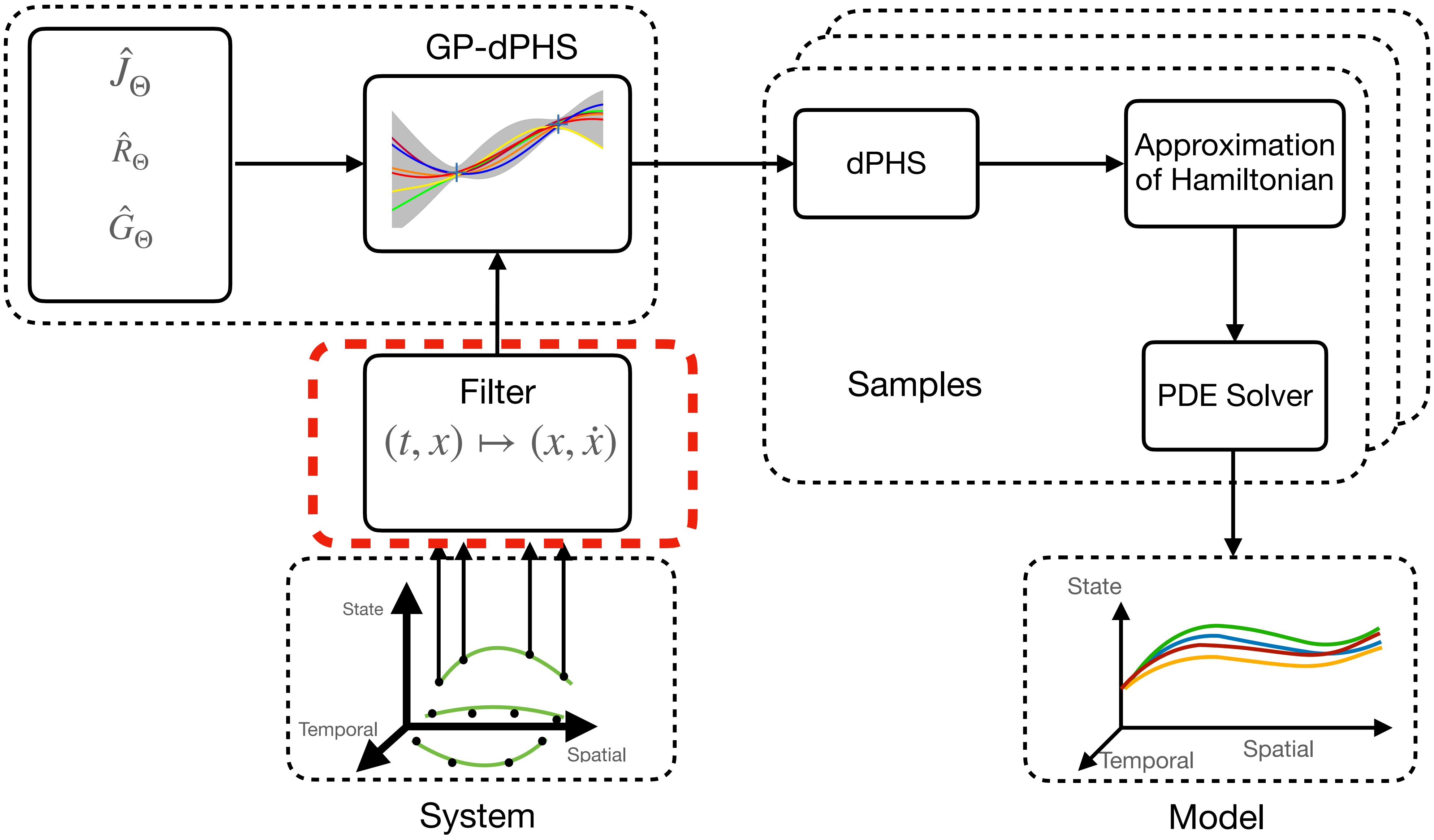
GP-dPHS



- **Idea:** encode the distributed Port-Hamiltonian system form into a GP function

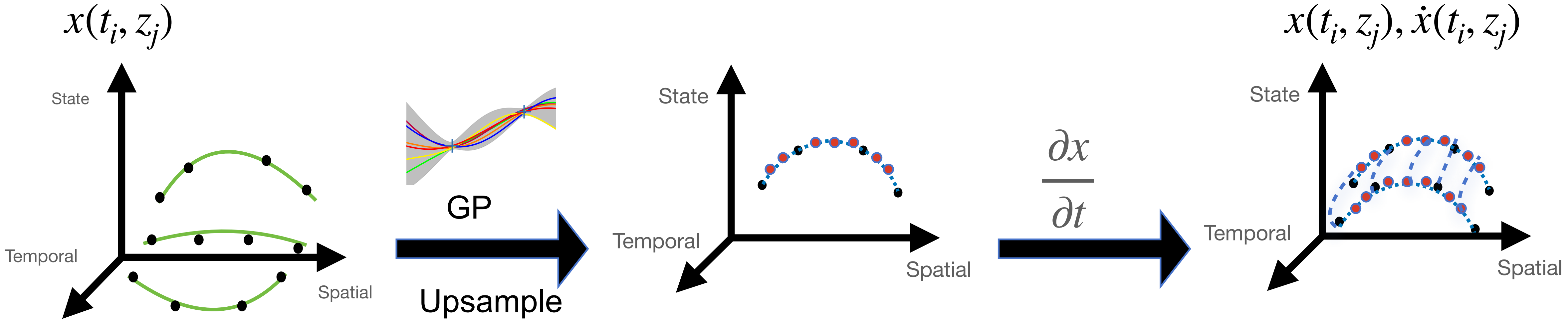
- GP-dPHS includes all possible dPHS under the GP prior on Hamiltonian

GP-dPHS



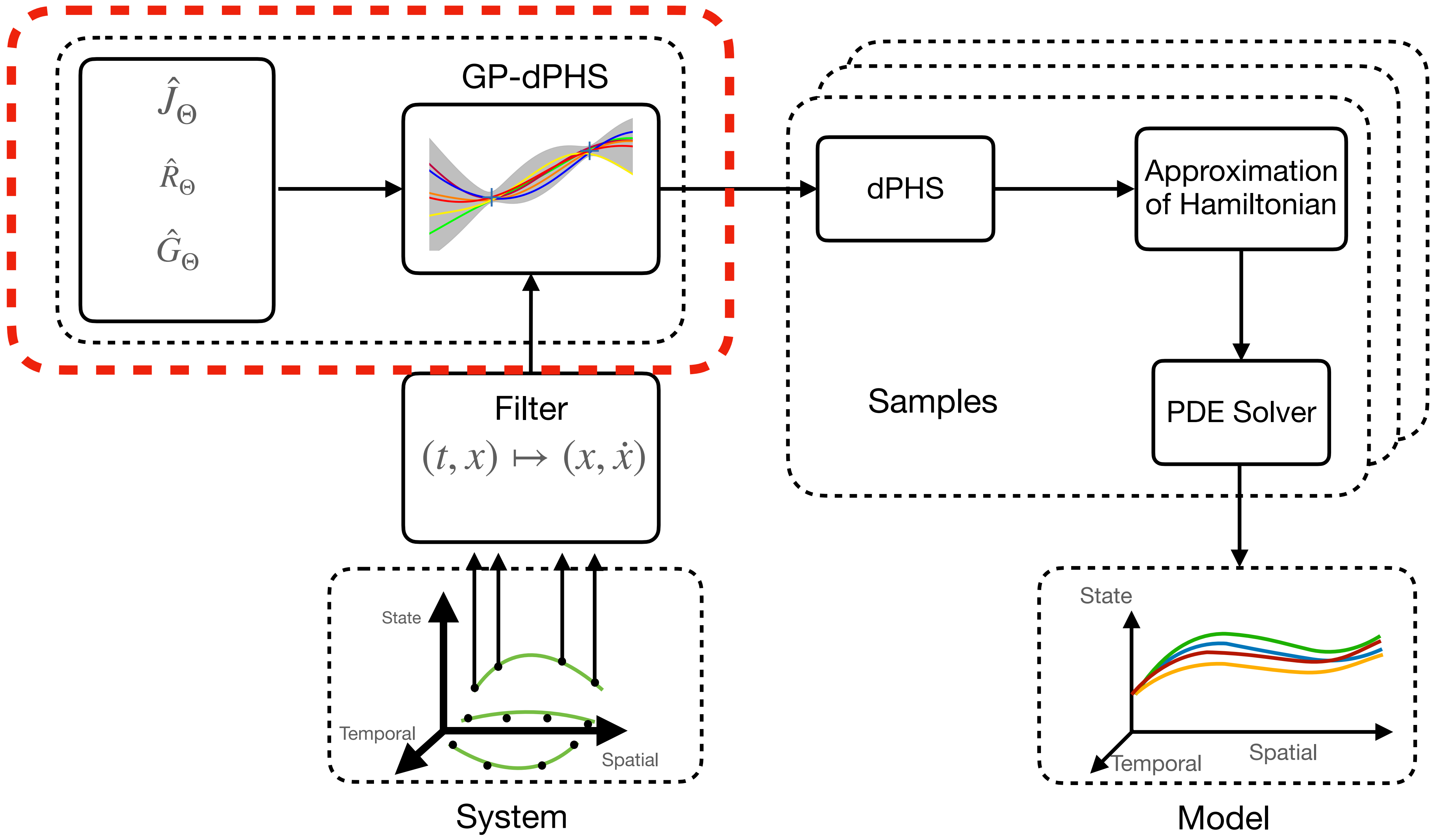
$\hat{J}_\Theta$
$\hat{R}_\Theta$
$\hat{G}_\Theta$
GP-dPHS
dPHS
Approximation of Hamiltonian
Samples
PDE Solver
Filter
$(t, x) \mapsto (x, \dot{x})$
State
Temporal
Spatial
System
State
Temporal
Spatial
Model

Data Generation



- Use GP regression based on raw data
- Upsample data points from GP
- Take time derivative to obtain training data

GP-dPHS



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Training

GP prior on Hamiltonian

$$\frac{\partial x}{\partial t} = \boxed{[\hat{J}_\Theta - \hat{R}_\Theta]\delta_x}\hat{\mathscr{H}} + \hat{G}_\Theta u \longrightarrow \dot{x} \sim GP(\hat{G}_\Theta u, k_{dphs}(x, x'))$$

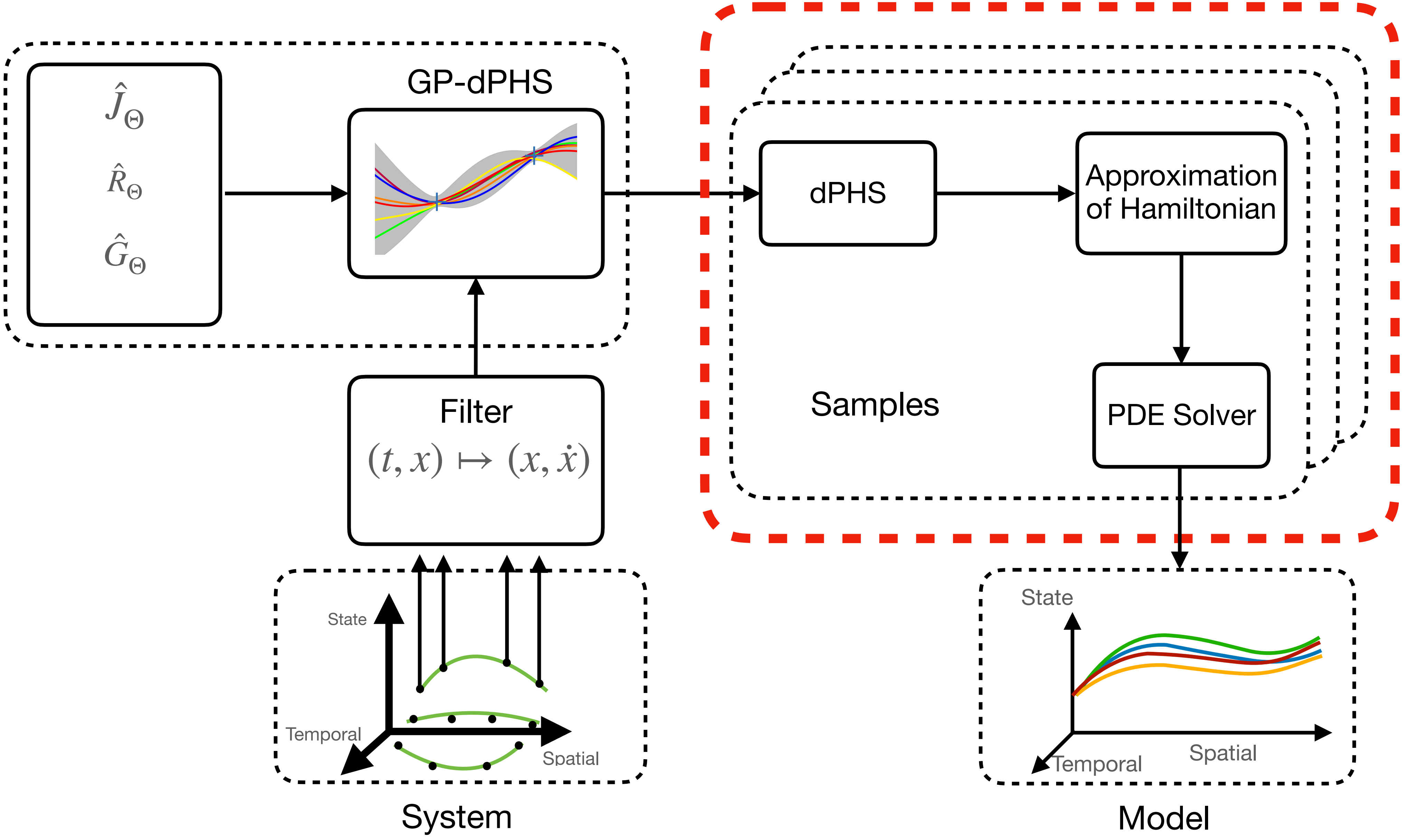
Linear operator

Port-Hamiltonian Kernel

$$k_{dphs}(x, x') = \sigma_f^2 (\hat{J}_\Theta - \hat{R}_\Theta)\delta_x \underbrace{\exp\left(-\frac{||x - x'||^2}{2\varphi_l^2}\right)}_{\text{Squared exp. kernel}} \overbrace{\delta_{x'}^\top (\hat{J}_\Theta - \hat{R}_\Theta)^\top}^{\text{Parametrized estimates}} .$$

Optimizing parameters by means of negative log marginal likelihood function

GP-dPHS



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3. Prediction

dPHS

$$\begin{bmatrix} \dot{X} \\ \hat{f}(x^*) \end{bmatrix} = \mathcal{N}\left(0, \begin{bmatrix} K_{dphs} & k_{dphs}(X, x^*) \\ k_{dphs}(X, x^*)^\top & k_{dphs}(x^*, x^*) \end{bmatrix}\right)$$

$$\dot{x} = \hat{f}(x, \omega)$$

Not callable
(computational expensive)

Approximation of Hamiltonian

$$\begin{bmatrix} \dot{X} \\ \hat{\mathscr{H}}(x^*) \end{bmatrix} = \mathcal{N}\left(0, \begin{bmatrix} K_{dphs} & k_{\dot{x}\mathscr{H}}(X, x^*) \\ k_{\dot{x}\mathscr{H}}(X, x^*)^\top & k_{\mathscr{H}\mathscr{H}}(x^*, x^*) \end{bmatrix}\right)$$

$$\hat{\mathscr{H}}(x^*, \omega) \xrightarrow{\text{Approx.}} \hat{\mathscr{H}}^*(x^*)$$

PDE Solver

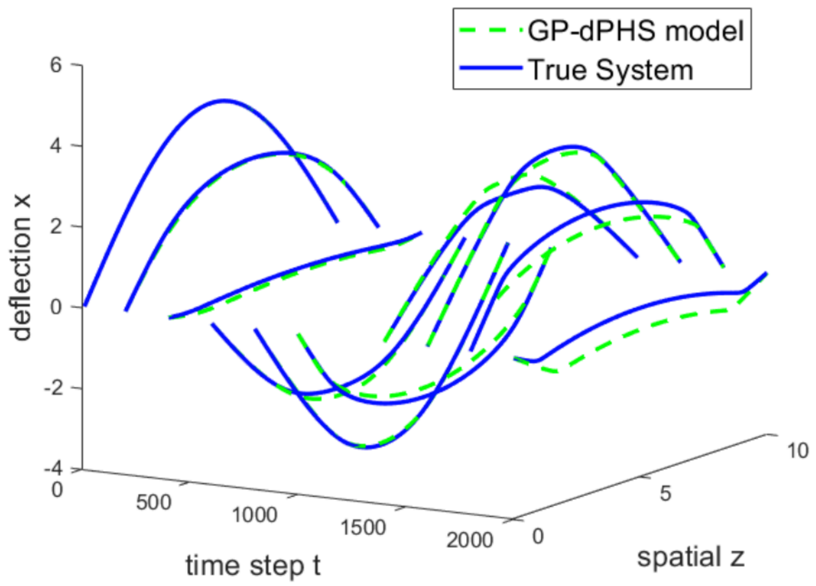
$$\dot{x} = [\hat{J}_\Theta - \hat{R}_\Theta]\delta_x \hat{\mathscr{H}}^* + \hat{G}_\Theta u \xrightarrow{\text{Solver}} x(t, z)$$

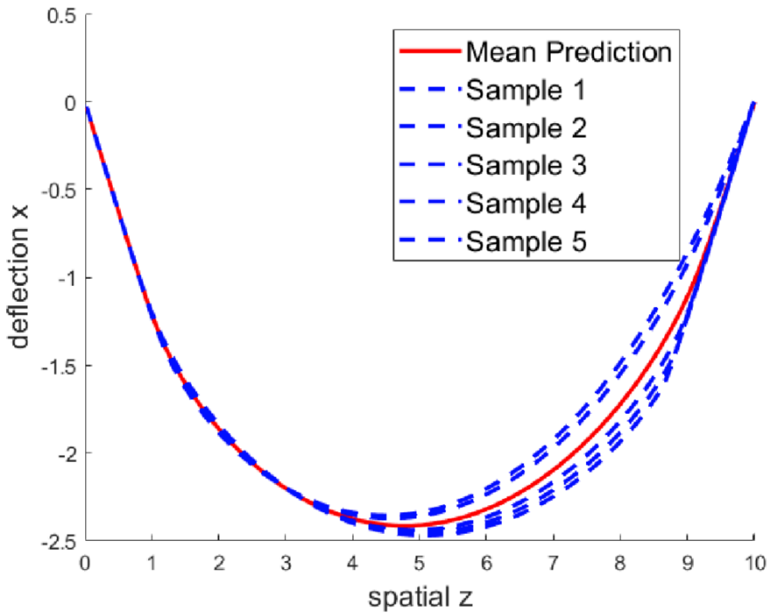
Approximation of H: Callable and structure preserving

GP-dPHS example

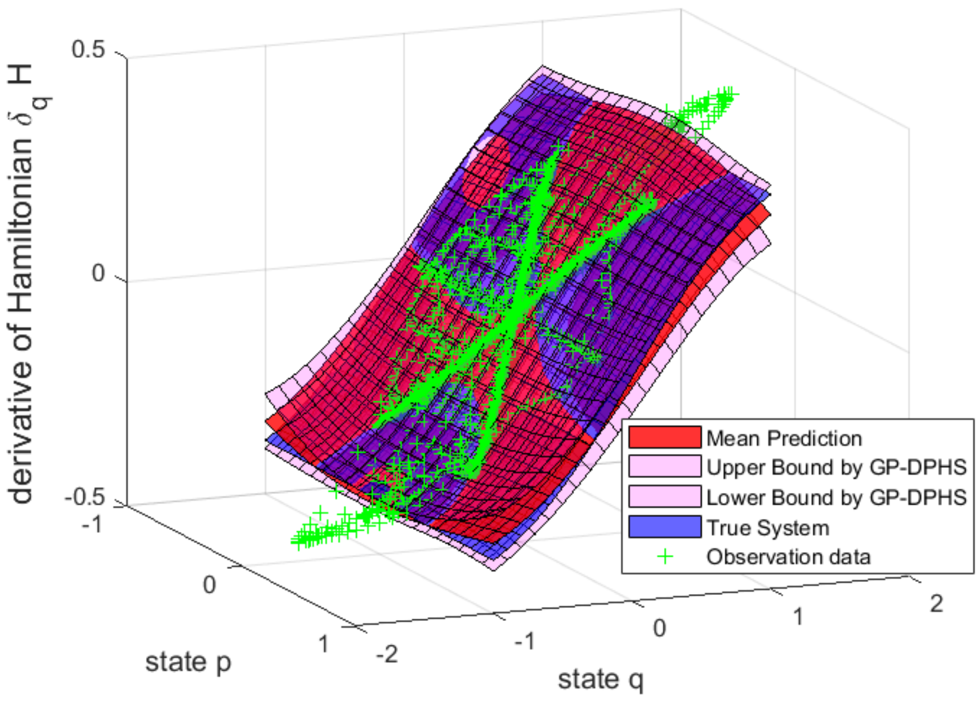
Vibration of a string with
nonlinear stress-strain curve

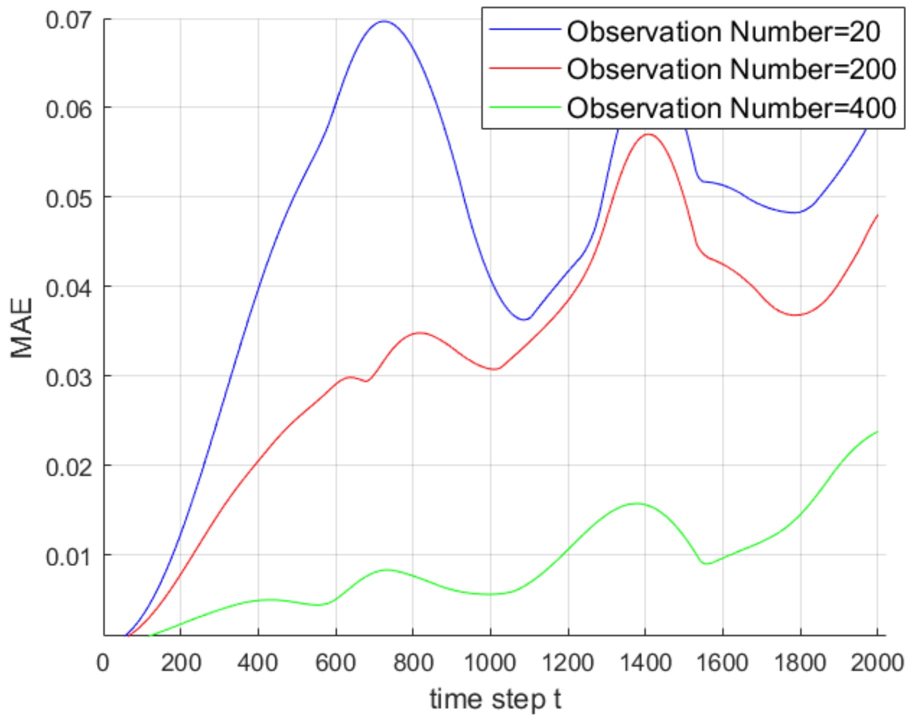
$$\frac{\partial}{\partial t}\begin{bmatrix} \overset{\frac{\partial x}{\partial t}}{\downarrow} \\ p(t,z) \\ q(t,z) \\ \underset{\frac{\partial x}{\partial z}}{\uparrow} \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 \end{bmatrix}}_{J-R} \delta_{pq}\mathscr{H}(p,q)$$





GP-dPHS example

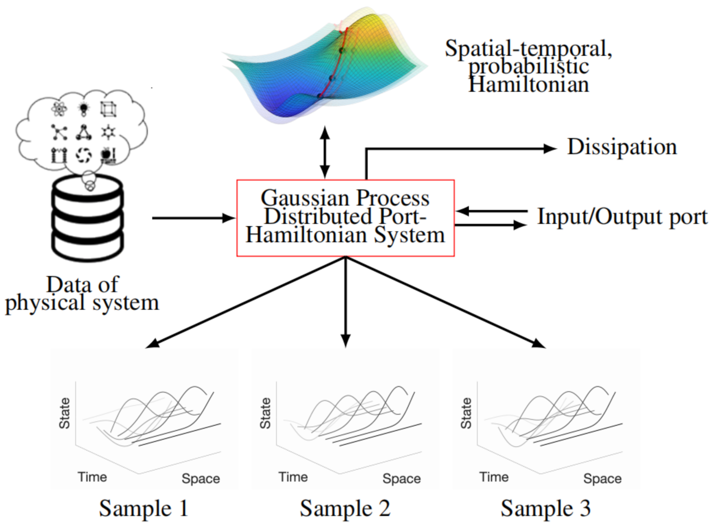




- True $\delta_q \mathscr{H}$ is within the quantified upper and lower bounds
- More data leads to less mean absolute error (MAE)

Conclusion

Gaussian Process + Distributed Port-Hamiltonian System



- Physics-constrained data-driven model for PDE systems
- Expressive and generalizable model for nonlinear systems
- Probabilistic nature enables uncertainty quantification

Contact Info: kaiyuan.tan@vanderbilt.edu

Website: www.tbeckers.com

K. Tan, P. Li, and T. Beckers, Physics-Constrained Learning for PDE Systems with Uncertainty Quantified Port-Hamiltonian Models. L4DC, 2024