EasyChair Preprint

№ 13605

Physics-Informed Data-Driven Simulation of Constrained Multibody Systems

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June 9, 2024

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Abstract

We describe a framework that can integrate prior physical information, e.g., the presence of kinematic constraints, to support data-driven simulation. Unlike other approaches, e.g., Fully-connected Neural Network (FCNN) or Recurrent Neural Network (RNN)-based methods that are used to model the system states directly, the proposed approach embraces a Neural Ordinary Differential Equation (NODE) paradigm that models the derivatives of system states. A central part of the proposed methodology is its capacity to learn the multibody system dynamics from prior physical knowledge and constraints combined with data inputs. This learning process is facilitated by a constrained optimization approach, which ensures that physical laws and system constraints are accounted for in the simulation process. The models, data, and code for this work are available at `https://github.com/jqwang2373/PNODE-for-MBD`.

1 Introduction

In the MBD community, the research has focused on directly capturing the time evolution of the system states [1, 2, 3, 4, 5, 6]. This approach is challenging since the nonlinear nature of the MBD problem means that any alterations in initial conditions or external forces during the simulation necessitate either retraining the model or doubling the input dimensions. As such, incorporating initial conditions and external forces, can exponentially increase the required training data and the associated costs. Moreover, although constraints are a fundamental component of MBD, their integration within deep neural network models remains a complex and open issue. To address these challenges, we extended the existing NODEs [7, 8] and proposed a multibody dynamics parameterized second-order Neural Ordinary Differential Equation method called MBD-NODE. The salient point of MBD-NODE is that we model the derivatives of MBD system states, enabling MBD-NODE to effectively adapt to varying initial conditions and external forces. Furthermore, we have incorporated the augmented Lagrangian method and constraint-equation-based optimization to integrate physical laws and system constraints into the simulation.

2 Methodology

Given the hidden state $\mathbf{Z}(t,\boldsymbol{\mu}) = (\mathbf{z}(t,\boldsymbol{\mu}),\dot{\mathbf{z}}(t,\boldsymbol{\mu}))^T$ for a multibody system with n bodies, the MBD-NODE is defined as:

$$\dot{\mathbf{Z}}(t,\boldsymbol{\mu}) = f_\Theta(\mathbf{z}(t,\boldsymbol{\mu}),\dot{\mathbf{z}}(t,\boldsymbol{\mu}),\mathbf{u}(t),t,\boldsymbol{\mu}), \quad \mathbf{Z}(0,\boldsymbol{\mu}) = (\mathbf{z}_0(\boldsymbol{\mu}),\dot{\mathbf{z}}_0(\boldsymbol{\mu}))^T,$$

where: $\mathbf{Z}(0,\boldsymbol{\mu}) = (\mathbf{z}_0(\boldsymbol{\mu}),\dot{\mathbf{z}}_0(\boldsymbol{\mu}))^T$, is the initial condition, $\mathbf{z}(t,\boldsymbol{\mu}) = (\mathbf{z}^1(t,\boldsymbol{\mu}),...,\mathbf{z}^n(t,\boldsymbol{\mu}))^T \in \mathbb{R}^n$ stores the generalized positions for the n bodies in a coordinate system, $\mathbf{u}(t) = (u^1(t),...,u^m(t))^T \in \mathbb{R}^m$, is the set of external forces/torques applied at time t, $\boldsymbol{\mu} = (\mu_1,\mu_2,\ldots,\mu_{n_{\boldsymbol{\mu}}})^T \in \mathbb{R}^{n_{\boldsymbol{\mu}}}$, are the problem-specific parameters, and $f_\Theta : \mathbb{R}^{2n+n_{\boldsymbol{\mu}}+m} \to \mathbb{R}^n$, is the neural network parameterized by Θ with $2n+n_{\boldsymbol{\mu}}+m$ dimensional input.

To solve the IVP for $\mathbf{Z}(t,\boldsymbol{\mu})$, as shown in Fig. 1, we can use a numerical integrator Φ

$$\mathbf{Z}(t,\boldsymbol{\mu}) = \mathbf{Z}(0,\boldsymbol{\mu}) + \int_0^t f_\Theta(\mathbf{Z}(\tau,\mu),\mathbf{u}(\tau),t,\boldsymbol{\mu})d\tau = \Phi(\mathbf{Z}(0,\boldsymbol{\mu}),f_\Theta,t)\ .$$

For a given initial state $\mathbf{Z}_0 = (\mathbf{z}_0,\dot{\mathbf{z}}_0)$ with its next state $\mathbf{Z}_1 = (\mathbf{z}_1,\dot{\mathbf{z}}_1)$ and the integrator Φ used with time interval Δt, the loss function $\mathrm{L}(\Theta)$ used for the MBD-NODE without constraints describes the mean square error (MSE) between the ground truth state and the predicted state

$$\mathrm{L}(\Theta) = \|\Phi(\mathbf{Z}_0,f_\Theta,\Delta t) - \mathbf{Z}_1\|_2^2 = \|\hat{\mathbf{Z}}_1 - \mathbf{Z}_1\|_2^2\ ,$$

where $\hat{\mathbf{Z}}_1 = (\hat{\mathbf{z}}_1,\hat{\dot{\mathbf{z}}}_1)$ is the predicted state by MBD-NODE.

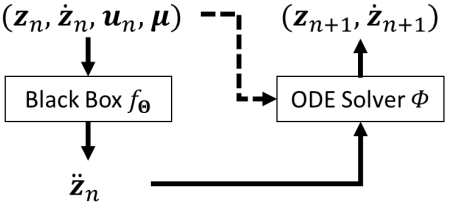

Figure 1: The discretized forward pass for MBD-NODE for general MBD.

3 Experiment and Analysis

We used a single mass-spring-damper system as a case study to illustrate our approach. As demonstrated in Fig. 2, we conducted a comparative analysis of the MBD-NODE against LSTM and FCNN. The MBD-NODE predictions, showcased in Fig. 2(a), align closely with the actual observed behavior of the system, indicating a high level of accuracy. In contrast, the LSTM model, depicted in Fig. 2(b), shows a noticeable stagnation and fails to accurately capture the system's eventual cessation of movement. Meanwhile, the FCNN model, as seen in Fig. 2(c), struggles particularly during extrapolation tests. It tends to generate predictions that veer off tangentially, leading to a significant deviation from the expected trajectory. Notably, the MBD-NODE outperforms these models, achieving the lowest Mean Squared Error (MSE) of approximately 8.6e-4.

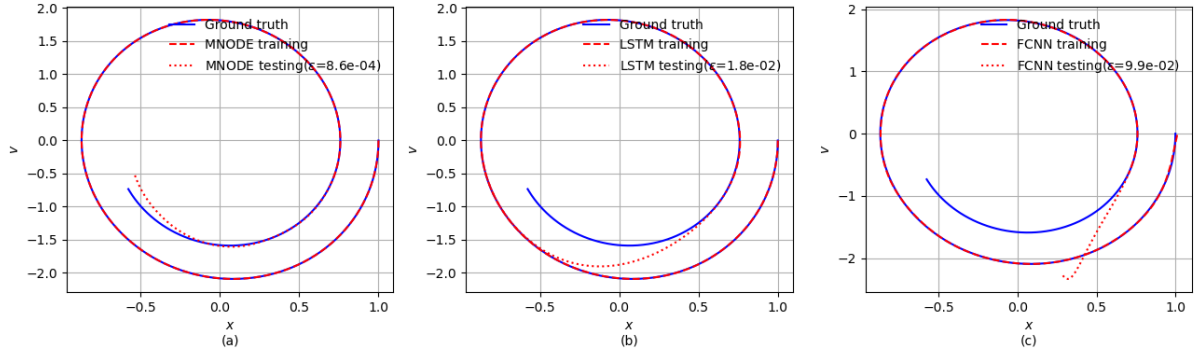

Figure 2: The phase space x vs v for the single mass-spring-damper system. Dashed lines represent performance on the training data and the dotted lines on the test data.

4 Conclusion and Future Work

We outlined MBD-NODE, a method built on the framework of NODE for the data-driven modeling of general MBD problems. Although the results reported are in conjunction with a mass-spring-damper system, we have compared the method against several state-of-the-art data-driven modeling methods using five numerical examples covering various features of multibody dynamics problems in practice, such as energy conservation, energy dissipation, multiscale dynamics, chaotic behavior, and kinematic constraints. Overall, results demonstrate superior performance of the proposed MBD-NODE method. Due to space limitations, these results will be presented at the June meeting.

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