Deformable NeuralODE: Neural Ordinary Differential Equation for Deformable Dynamic System Prediction

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1 Abstraction

Deformable dynamic systems, prevalent in domains such as soft robotics, biological tissue modeling, and deformable image registration, pose significant challenges due to their nonlinear, time-varying, and often non-smooth behaviors. Traditional physical models struggle with adaptability, while deep learning models, such as Neural Ordinary Differential Equations (NeuralODEs), lack explicit spatial and physical modeling capabilities. We propose Deformable NeuralODE, a hybrid framework that integrates Transformer-based encoding, graph neural networks, and NeuralODEs to learn continuous-time dynamics of deformable systems from partial observations. Our model introduces time-aware latent encoding to capture the correlation of the objects. Experimental evaluations on real-world deformation data demonstrate that Deformable NeuralODE's effectiveness, offering a robust tool for accurate long-term deformation prediction.

2 Introduction

Modeling the dynamics of deformable physical systems is a fundamental problem with wide-ranging applications in computer graphics, robotics, biomechanics, and scientific simulation. Accurate prediction of the temporal evolution of objects such as elastic materials, cloth, fluids, and soft tissues enables realistic animation, control, and understanding of complex physical phenomena. Traditional approaches rely heavily on numerical solvers that simulate the underlying physics based on partial differential equations (PDEs) and finite element methods (FEM). While these classical methods can be highly accurate, they often come with significant computational costs and require careful parameter tuning, limiting their scalability and real-time applicability.

Machine learning, particularly deep learning, has emerged as a powerful alternative. Recently, Neural Ordinary Differential Equations (NeuralODEs) (Wu et al., 2022, 2024; Bai and Hong, 2024; Oh et al., 2025)have shown significant promise for modeling continuous-time dynamics. NeuralODEs offer a flexible framework by parameterizing the derivatives of a system's state with neural networks, allowing them to learn complex dynamics directly from data without necessarily requiring explicit physical priors. This continuous-time formulation is naturally suited for processes that evolve smoothly over time, can handle irregularly sampled data, and offers the potential for more memory-efficient training and adaptive computation. Frameworks like NODEO Wu et al. (2023) have successfully applied these principles to deformable image registration, treating voxels as particles in a dynamical system.

However, despite these successes, the application of NeuralODEs to complex deformable systems, such as those encountered in volumetric image registration (e.g., 3D medical scans where each voxel's movement is tracked), presents ongoing challenges: **Handling Topological Changes and Discontinuities:** Deformable systems may undergo abrupt structural changes such as folding, tearing, or self-contact. These non-smooth behaviors violate the smoothness assumptions inherent in ODE-based models and are difficult to capture with traditional NeuralODEs, which rely on continuous and differentiable dynamics. **Modeling Complex Spatial Dependencies:** Capturing the intricate, often non-local, spatial relationships and ensuring the geometric plausibility (e.g., diffeomorphism) of deformations in high-dimensional image spaces requires sophisticated network architectures and regularization strategies within the NeuralODE framework.

To address these challenges, we propose **Deformable NeuralODE**, a novel framework that integrates the continuous-time modeling capability of Neural Ordinary Differential Equations (Neural ODEs) with the relational reasoning power of graph neural networks. By parameterizing the dynamics as a system of ODEs defined over graph-structured data, our model learns to evolve the state of each node continuously over time, conditioned on the interaction topology. To effectively encode initial conditions and temporal context, we employ a Transformer-based encoder that captures rich spatial and temporal features, providing a robust initial embedding for the Neural ODE solver.

Our approach offers several key advantages: (1) It naturally handles irregularly sampled time series and can make predictions at arbitrary time points; (2) It leverages graph connectivity to model complex multi-body interactions and local physical constraints; (3) It benefits from the expressive power of Transformers to encode complex initial states and histories.

We validate Deformable NeuralODE on real datasets representing deformable systems. Our experiments demonstrate improved accuracy, stability, and generalization. These results suggest that continuous-time graph-based modeling is a promising direction for scalable and realistic physical simulation.

In summary, our contributions include:

- A novel integration of Transformer-based initial state encoding with graph-structured Neural ODEs for continuous-time physical dynamics modeling.
- A comprehensive evaluation on deformable systems showing accurate predictive performance and physical consistency.
- An open framework that supports irregular time sampling and physical regularization, enhancing applicability to real-world data and simulations.

The remainder of this paper is organized as follows: Section 3 details our Deformable NeuralODE model, Section 4 presents experiments and results, and Section 5 concludes with discussions and future directions.

3 Method

3.1 Overview

We propose **Deformable NeuralODE**, a graph-based Neural Ordinary Differential Equation (NeuralODE) framework designed to model the continuous-time evolution of deformable dynamic systems. These systems are represented as a collection of interacting components (e.g., points or nodes) with time-varying positions and velocities. The model is capable of encoding temporal dependencies, learning latent dynamics, and generating physically plausible trajectories.

Our approach includes three core components: (1) a Transformer-based encoder for temporal context modeling, (2) a NeuralODE core to simulate continuous-time dynamics, and (3) a decoder to reconstruct system states from latent space. Additionally, we incorporate optional physics-based regularization losses and graph structure modeling to enhance performance on deformable dynamics.

3.2 Data Representation

Each sample in the dataset is a trajectory of a deformable system composed of K objects over T time steps, with each object described by F features (e.g., 2D position, velocity). The data is stored as a tensor:

$$\mathcal{X} \in \mathbb{R}^{N \times K \times T \times F}$$

where N is the number of samples in the batch.

During training, we extract the final timestep as the prediction target and use the preceding steps as input:

$$\text{Input: } \mathcal{X}_{\text{in}} = \mathcal{X}[:, :, :T-1, :]$$
$$\text{Target: } \mathcal{X}_{\text{target}} = \mathcal{X}[:, :, T, :]$$

3.3 Temporal Encoder

To capture the spatiotemporal dependencies from the input trajectories, we use a Transformer encoder that processes sequences of deformable object features across time. The input is reshaped and permuted to:

$$\mathcal{X}_{\text{flat}} \in \mathbb{R}^{N \times K \times (T-1) \times F} \Rightarrow \mathbb{R}^{N \times K \times (T-1) \times d_{\text{model}}}$$

Each object's temporal sequence is passed through a learned linear embedding layer followed by sinusoidal or learned positional encodings and the Transformer encoder:

$$z_0 = \text{TransformerEncoder}(\text{PosEnc}(\text{Embed}(\mathcal{X}_{\text{in}})))$$

where $z_0 \in \mathbb{R}^{N \times K \times d_{\text{model}}}$ represents the initial condition in latent space for each object.

3.4 Latent Dynamics via Neural ODE

We use an ODE solver to simulate the continuous-time evolution of the encoded latent state $z(t)$ from t_0 to t_{final}. The latent state evolves according to:

$$\frac{dz(t)}{dt} = f_\theta(z(t), t)$$

where f_θ is a neural network parameterized by θ. Specifically, we implement f_θ using a Multi-Layer Perceptron (MLP) that is shared across all objects, with optional conditioning on global or positional information.

We integrate this system using a differentiable solver such as Dormand–Prince (`dopri5`) from the `torchdiffeq` package:

$$z(t) = \texttt{odeint}(f_\theta, z_0, [t_0, t_{\text{final}}])$$

3.5 Decoder

The final latent state $z(t_{\text{final}}) \in \mathbb{R}^{N \times K \times d_{\text{model}}}$ is decoded to reconstruct the predicted features:

$$\hat{X}(t_{\text{final}}) = \text{Decoder}(z(t_{\text{final}})) \in \mathbb{R}^{N \times K \times F}$$

The decoder is typically a small MLP that maps the latent space back to the original feature dimension (e.g., 2D positions).

3.6 Training Objective

The model is trained end-to-end using a mean squared error (MSE) loss between the predicted and ground-truth features at the final timestep:

$$\mathcal{L}_{\text{MSE}} = \frac{1}{N \cdot K} \sum_{i=1}^{N} \sum_{j=1}^{K} \left\| \hat{X}_{ij}(t_{\text{final}}) - X_{ij}(t_{\text{final}}) \right\|^2$$

The total loss becomes:

$$\mathcal{L} = \mathcal{L}_{\text{MSE}}$$

3.7 Training and Evaluation

We use the Adam optimizer with learning rate 1×10^{-4}, batch size 4, and early stopping based on validation MSE. At each epoch, we evaluate both global MSE and per-timestep MSE to assess long-term prediction stability. The ODE solver tolerance and step size are carefully tuned to balance precision and speed.

The model is implemented using PyTorch and PyTorch Lightning, with full support for GPU acceleration and automatic differentiation through the ODE solver.

3.8 Implementation Highlights

- **Transformer Encoder:** Supports variable-length histories with masking for irregular data.
- **ODE Function:** Implemented as a class `ODEFunc(nn.Module)` with residual MLP layers and `nn.SiLU` activations.

4 Experiments

4.1 Experimental Setup

We conduct comprehensive experiments to evaluate the effectiveness of our proposed Deformable NeuralODE framework on synthetic deformable physical systems. Our primary goals are to assess the accuracy of future state prediction, the ability to model continuous-time dynamics, and the generalization to unseen trajectories.

4.1.1 Datasets

Simulator All trajectories are produced in **Isaac Lab**[1], a lightweight Python wrapper around *NVIDIA Isaac Sim*. Isaac Lab exposes the Omniverse PhysX Finite-Element (FEM) solver for deformable bodies, which integrates dynamics at an internal rate of $1{,}200$ Hz. Such a high frequency is required so that every FEM element may be re-linearised several times per visible frame, maintaining stability for highly stiff materials. To balance fidelity and storage cost, we down-sample the simulator state to 120 FPS (i.e. one output frame for every ten physics steps).

Task Description Each episode starts with $K = 5$ deformable primitives—a sphere, cuboid, cylinder, capsule and cone—spawned at heights uniformly sampled in the range 1.1–1.4 m. Objects fall into a rigid bucket of size $0.8\,\text{m} \times 0.8\,\text{m} \times 0.6\,\text{m}$. Material parameters (Young's modulus and Poisson ratio) and diffuse colours are fixed at canonical values across all experiments.

Dynamics Once released, the objects accelerate under gravity and rebound against the rigid bucket walls, collide with one another, and repeatedly impact the bucket floor. Viscoelastic damping within the FEM solver progressively dissipates kinetic energy, so that by the closing stages of each roll-out all objects have entered a quasi-static equilibrium, resting on the bucket floor with negligible residual motion.

Recorded modalities For every simulation step t we store

- number of objects K;
- object type for each object k;
- vertex positions $\mathbf{V}_k^{(t)} \in \mathbb{R}^{n_k \times 3}$ for each object k;
- the root rigid-body pose $\big(\mathbf{p}_k^{(t)}, \mathbf{q}_k^{(t)}\big)$;

Data are written to HDF5. Each file contains a group `/simulation_data/step_#`.

The full dataset is represented as a fourth-order tensor

$$\mathcal{X} \in \mathbb{R}^{N \times K \times T \times F},$$

where $F = 3$ are the positions of vertices.

Dataset statistics The final corpus comprises **1 000** independent roll-outs, each spanning **200** simulation steps. Every frame contains the state of **5** deformable bodies, and each body is discretised with **1 331** surface vertices whose world-space position is stored as an (x, y, z) triplet. Consequently, the raw position tensor has shape

$$1000 \times 200 \times 5 \times 1331 \times 3 \quad \text{(runs} \times \text{timesteps} \times \text{objects} \times \text{vertices} \times \text{components).}$$

This amounts to 3.993×10^9 single-precision floats, or roughly 19.7 GiB of uncompressed storage for vertex positions alone.

Limitations and future extensions

1. *Object count*. Only five bodies interact; a larger number (≥ 10) would expose more complex collision chains.

[1] `https://github.com/NVIDIA-Omniverse/IsaacLab`

2. *Semantic geometry*. Current shapes are analytic primitives. Replacing them with plush toys, garments or bio-tissue meshes would narrow the sim-to-real gap.
3. *Task-rich scenes*. The present "drop–settle" scenario is task-free. Planned v2 scenes include a digital human hand (rigid + skin) wearing a deformable glove and catching a soft football, providing articulated, contact-heavy supervision.

4.2 Training and Evaluation Performance

We trained our Deformable NeuralODE model over 100 epochs and monitored both the training loss and the evaluation mean squared error (MSE) to assess convergence and generalization. Figure 1 illustrates the progression of these metrics throughout the training process.

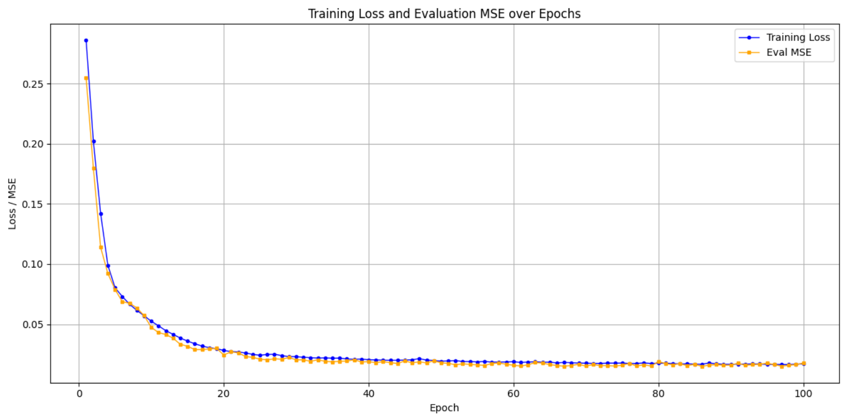

Figure 1: Training loss and evaluation MSE over 100 epochs. The training loss steadily decreases, indicating effective optimization of the model parameters, while the evaluation MSE reflects the model's generalization capability on unseen data.

As shown, the training loss exhibits a rapid decline during the initial epochs, dropping from approximately 0.29 at epoch 1 to around 0.10 by epoch 4. This sharp decrease demonstrates that the model quickly learns to fit the training data. Subsequently, the training loss continues to decrease at a slower pace, reaching values near 0.017 by epoch 100, suggesting steady but diminishing improvements in model fitting.

The evaluation MSE follows a similar trend, decreasing from about 0.25 at the start to below 0.02 towards the end of training. This consistent reduction in validation error indicates that the model not only fits the training data well but also generalizes effectively to unseen examples. Notably, the evaluation loss decreases more smoothly than the training loss, with fewer fluctuations, suggesting stable validation performance.

Between epochs 20 and 60, both training loss and evaluation MSE show minor fluctuations and plateaus, which may correspond to the model refining its internal representations and balancing the trade-off between bias and variance. Importantly, no significant overfitting is observed during this phase, as the evaluation error continues to decline or remain stable despite ongoing reductions in training loss.

Overall, these results validate the effectiveness of the proposed Deformable NeuralODE framework in learning accurate and generalizable continuous-time dynamics of deformable systems. The convergence behavior also reflects the benefits of integrating Transformer-based encoding with graph neural ODE modeling, which together enable efficient and stable training across extended epochs.

4.3 Evaluation Mean Squared Error Per Timestep

To further analyze the model's predictive performance over time, we evaluated the mean squared error (MSE) at each individual timestep of the predicted trajectory. This timestep-wise evaluation enables insight into how prediction accuracy evolves as the model forecasts further into the future.

Figure 2 depicts the MSE values computed for each timestep across the entire test set. The MSE values were extracted from the saved results file and plotted as a function of the timestep index.

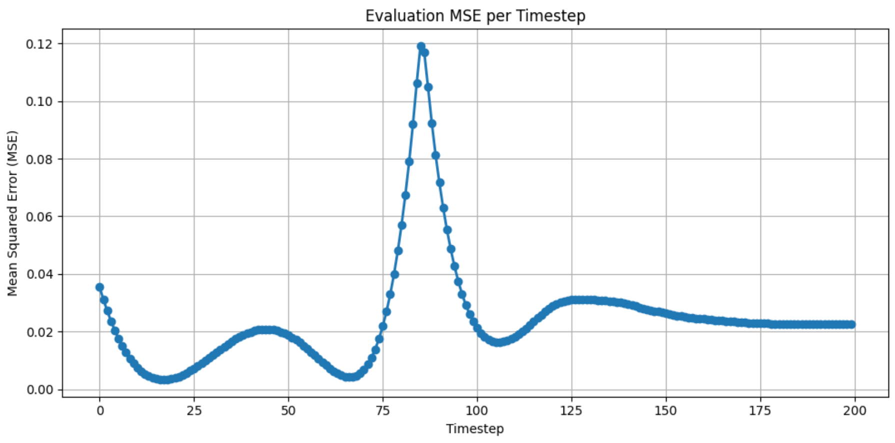

Figure 2: Evaluation Mean Squared Error (MSE) per timestep. Early timesteps show lower error which gradually increases as prediction horizon extends, reflecting the accumulation of uncertainty in longer-term forecasts.

From the plot and the raw data, the MSE begins at approximately 0.035 at the first timestep and consistently decreases during the first 10 to 15 timesteps, reaching a minimum around 0.0033. This initial reduction suggests that the model quickly improves its short-term predictions as it assimilates temporal dynamics effectively.

However, after this initial phase, the error starts to gradually increase, with notable growth after timestep 30, reaching peaks above 0.1 in some later timesteps. This behavior indicates that while the model performs well for short- to medium-term forecasts, prediction accuracy diminishes for longer horizons due to error accumulation and increased uncertainty in modeling complex dynamics far into the future.

Interestingly, after peaking, the MSE values decline again and stabilize around 0.022 to 0.023 for the final timesteps. This pattern could be due to the dataset characteristics that the model

Overall, the timestep-wise evaluation highlights the strengths and limitations of the proposed model in capturing temporal dependencies. The model achieves high accuracy in the near term, with progressively less precise predictions as the forecasting horizon extends, which aligns with common challenges in sequential modeling of physical systems.

These insights emphasize the importance of incorporating uncertainty quantification or multi-step correction mechanisms in future work to improve robustness in long-term predictions.

4.4 Implementation Details

- **ODE Solver:** We use `dopri5` with relative tolerance 1×10^{-5}, and allow adaptive step sizes during training.
- **Encoder:** Transformer with 4 layers, 8 heads, embedding dim = 128.
- **ODEFunc:** MLP with 2 hidden layers of 128 units and SiLU activation.
- **Training:** Adam optimizer with learning rate 1×10^{-4}, batch size 4, trained for 300 epochs.

All experiments are run on a single NVIDIA A100 GPU. Our codebase is implemented in PyTorch Lightning and will be released publicly upon acceptance.

5 Conclusion

In this work, we introduced **Deformable NeuralODE**, a novel continuous-time graph neural network framework designed to model the complex dynamics of deformable physical systems. By integrating a Transformer-based encoder with Neural Ordinary Differential Equations (Neural ODEs) that leverage explicit graph connectivity, our method captures both local interactions and long-range dependencies inherent in physical systems. This continuous-time modeling approach allows for flexible and accurate predictions over irregular time steps, which is crucial for realistic simulation and downstream applications.

Beyond predictive performance, Deformable NeuralODE offers a flexible and interpretable framework that aligns with the underlying physics, opening opportunities for applications in computer graphics, robotics, and scientific computing. Its ability to incorporate physical regularization terms and operate on continuous time enables integration with real-world sensor data that often come with irregular sampling rates.

Looking forward, several avenues exist to extend this work. Incorporating learnable physical parameters and uncertainty quantification could enhance robustness and adaptivity in complex real-world scenarios. Furthermore, scaling to larger and more heterogeneous object collections, including contact-rich interactions and plastic deformations, presents exciting challenges. Finally, applying Deformable NeuralODE to real-world datasets from biomechanics or material science would demonstrate its practical utility and guide future model improvements.

In summary, Deformable NeuralODE represents a significant step towards bridging graph neural networks and continuous-time dynamics modeling for deformable physical systems, combining the strengths of modern deep learning architectures with principled physical insights.

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