Uncertainty Quantification Using Graph-based Conformal Prediction for Mesh-based Simulation

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Abstract

This paper presents a novel framework for uncertainty quantification in mesh-based simulations using graph-based conformal prediction. Our approach integrates conformal prediction with graph-structured data to provide statistically rigorous uncertainty estimates while preserving the spatial and topological relationships inherent in mesh simulations. Our preliminary experimental results on a diverse dataset of 125 fluid flow trajectories demonstrate a trade-off between precision (i.e., coverage) and reliability (i.e., prediction interval) as interval widths (prediction uncertainty) grew with higher user-defined performance level.

1 Introduction

Uncertainty quantification is critical for engineering simulations as it impacts the reliability and understanding of the simulated system of interest. In fields such as structural analysis, fluid dynamics, and material science, where simulations are often used to inform design, optimization, and safety evaluations, unaddressed uncertainty can lead to costly errors or even catastrophic consequences in a real-world scenario (Oberkampf et al. 2002).

This paper presents a graph-based conformal prediction approach aimed at effectively quantifying uncertainty in mesh-based simulations. These simulations are powerful tools, but are highly susceptible to errors and variability. Such errors can propagate through interconnected systems, amplifying inaccuracies. The challenges are further intensified by the high-dimensional and graph-structured nature of mesh data, which demands methods capable of capturing both local variations and global dependencies. The proposed method addresses these issues by generating reliable prediction intervals, offering a robust solution to manage uncertainty in mesh-based simulations.

Using the conformal prediction framework, our approach provides statistically rigorous high-confidence predictions that account for both the uncertainty of the model and the inherent variability in mesh-based simulations. This capability is crucial for enhancing the trustworthiness and robustness of engineering simulations, ensuring that decisions based on these models are both reliable and well-founded.

The paper is organized as follows: Section 2 reviews existing research on uncertainty quantification in graphs and meshes, highlighting key advancements and limitations that frame the challenges and opportunities of applying conformal prediction techniques in graph-based environments. Section 3 introduces the foundational concepts of conformal prediction on graphs and describes the implementation of graph-based conformal prediction for mesh simulations, focusing on how the approach addresses the unique properties of mesh data. Section 5 presents experimental results, showcasing the method's performance and reliability across various mesh-based simulation scenarios. Finally, Section 6 summarizes the key findings, discusses the implications of this work for uncertainty quantification in mesh-based simulations, and outlines potential directions for future research.

2 Related Work

There is a growing interest in uncertainty quantification (UQ) on graphs and meshes, particularly in areas utilizing discrete data structures, such as computational physics, machine learning, and scientific simulations. The motivation for UQ stems from the inherent variability in inputs, model parameters, and the approximations introduced by numerical methods. Below, we summarize key works that provide a foundation for our research on conformal prediction and UQ in mesh-based simulations.

Wang et al. (2024) provide a comprehensive survey on UQ in Graph Neural Networks (GNNs), addressing both aleatoric (data-related) and epistemic (model-related) uncertainties. They classify UQ methods into Bayesian and frequentist approaches and discuss applications such as node selection and out-of-distribution detection. This work provides valuable insights into challenges and opportunities in UQ for graph-based learning. Hauth et al. (2024) investigate UQ techniques for neural networks modeling complex spatiotemporal processes, focusing on graph convolutional neural networks (GCNNs). They compare Hamiltonian Monte Carlo (HMC) and Stein Variational Gradient Descent (SVGD), including a projected variant, applied to recurrent neural networks and neural ordinary differential equations. Their results indicate that SVGD offers comparable uncertainty estimates to Monte Carlo methods but with increased variance. However, the projected SVGD method restricts the active weight space, potentially introducing stability issues in complex likelihood landscapes. Jiang et al. (2024) introduce a framework for explaining GNN predictions that incorporates uncertainties in both graph data and model parameters. By quantifying both aleatoric and epistemic uncertainties, their approach enhances the reliability of post-hoc explanations, which is critical for real-world applications requiring high trustworthiness.

Karimi and Samavi (2023) focus on conformal prediction (CP), a technique that constructs prediction intervals ensuring the true label lies within the set with high probability. Their probabilistic approach to CP offers a direct method for quantifying uncertainty and is compared to Bayesian and evidential methods. This work emphasizes the importance of reliable uncertainty estimates, particularly in high-stakes fields like medical AI, and serves as a key reference for leveraging CP in scientific simulations. Pfaff et al. (2020) present MeshGraphNets, a framework that integrates graph neural networks with mesh-based simulations to model complex physical systems, such as fluid dynamics and structural mechanics. MeshGraphNets dynamically adjust mesh resolution during simulations, enhancing both accuracy and computational efficiency. This framework forms the foundation for modeling mesh-based data in this study, offering a scalable and adaptable approach to scientific simulations. By combining conformal prediction with the capabilities of MeshGraphNets (Pfaff et al. 2020), this study aims to advance the state-of-the-art in UQ for mesh-based simulations.

3 Conformal Prediction for Mesh-Based Simulations

Conformal prediction (CP) is a statistical approach to construct prediction intervals with user-defined coverage probabilities, making it particularly valuable for reliable uncertainty quantification in graph-structured data (Shafer and Vovk 2008; Zargarbashi, Antonelli, and Bojchevski 2023). This section introduces the core concepts of CP and its application to mesh-based simulations, particularly in computational fluid dynamics.

Fundamentals of Conformal Prediction on Graphs

Consider a graph $G = (V, E)$, where V denotes the set of nodes and $E \subseteq V \times V$ represents the set of edges. Each node $v_i \in V$ has a feature vector X_i and a label y_i. The goal is to predict a confidence set $C(X_i)$ for y_i such that:

$$\mathbb{P}(y_i \in C(X_i)) \geq 1 - \alpha \tag{1}$$

where $\alpha \in (0, 1)$ is the significance level controlling the probability of the true label being included in $C(X_i)$.

Nonconformity Score

The nonconformity score $A_i = A(X_i, y_i)$ quantifies how well a prediction aligns with observed data (Vovk, Gammerman, and Shafer 2005). For graph-based data, it typically incorporates both node attributes and graph topology. In Graph Neural Networks (GNNs), a basic nonconformity score can be:

$$A(X_i, y_i) = |f(X_i; \theta) - y_i| \tag{2}$$

where $f(X_i; \theta)$ is the model's prediction for node i, with θ representing the model parameters.

Calibration

Calibration ensures valid coverage guarantees in conformal prediction by using a calibration dataset $\mathcal{D}_{\text{cal}}$ to approximate the distribution of nonconformity scores. The p-value p_{test} for a test instance v_{test} is calculated as:

$$p_{\text{test}} = \frac{|\{i \in \mathcal{D}_{\text{cal}} : A_i \geq A(X_{\text{test}}, \hat{y}_{\text{test}})\}|}{|\mathcal{D}_{\text{cal}}| + 1},$$

where A_i measures the deviation of calibration samples, and $\hat{y}_{\text{test}}$ is the predicted label. Higher p_{test} values indicate more typical predictions. The denominator adjustment $|\mathcal{D}_{\text{cal}}| + 1$ ensures p_{test} lies strictly in $(0, 1)$, enabling construction of prediction intervals with coverage $1 - \alpha$.

In graph-based data, calibration captures complex dependencies between nodes, accommodating diverse patterns of nonconformity. This is particularly useful in scenarios with interconnected data, ensuring reliable uncertainty quantification and robust coverage guarantees.

prediction interval Construction

The prediction interval $C(X_{\text{test}})$ for a test node X_{test} is constructed by including all labels $\hat{y}$ that satisfy:

$$p_{\text{test}} \geq \alpha$$

This ensures that the prediction interval meets the desired confidence level, $1 - \alpha$, thereby providing robust coverage guarantees. The rationale behind this is that p_{test} represents the proportion of calibration samples with nonconformity scores at least as large as that of the test instance. By thresholding p_{test} at α, we ensure that the true label is excluded from the prediction interval with a probability of at most α. This direct connection between the conformity score and the prediction interval provides both rigor and interpretability.

Graph-Specific Adaptations

For graph-based tasks, nonconformity scores should incorporate neighborhood information:

$$A(X_i, y_i) = |f(X_i, X_{\mathcal{N}(i)}; \theta) - y_i| \tag{3}$$

where $\mathcal{N}(i)$ represents the neighbors of node i. This modification captures the local graph structure, enabling more context-aware predictions.

Application to Mesh-Based Simulations

Mesh-based simulations, particularly in computational fluid dynamics, use graph-structured data to represent physical domains. The nodes denote discrete points and the edges capture spatial relationships or interactions. Graph neural networks (GNNs) have proven effective for modeling such simulations, achieving state-of-the-art performance in predicting flow properties and capturing complex physical phenomena.

Integrating conformal prediction into GNN frameworks ensures that prediction intervals include the true physical state with a specified confidence level. This approach provides reliable uncertainty quantification, particularly in complex fluid dynamics scenarios where traditional error estimates may fail. By offering robust uncertainty bounds, conformal prediction enhances prediction reliability and interpretability. For example, in aerodynamic design, it provides accurate estimates of lift and drag coefficients, aiding critical decision-making and highlighting model limitations, thereby advancing computational fluid dynamics.

4 Empirical Results

Dataset Descriptions

The dataset used in this study models fluid flow over complex geometries and consists of graph-structured data generated from numerical simulations. It includes 125 unique trajectories of fluid flow, with each trajectory representing a distinct sample, as described in (Ju, Lupoiu, and Kanfar 2023).

Figure 1 provides an example of the ground truth data, illustrating the spatial distribution of x-velocity over three time steps in a fluid simulation. The figure highlights the graph-structured nature of the data, where nodes represent discrete points in the mesh, and edges capture spatial relationships. This visualization demonstrates the evolution of fluid flow across the domain and emphasizes the dataset's capability to capture both local and global dynamics, offering a strong basis for uncertainty quantification in graph-based simulations.

On average, each sample contains 1923 nodes, 11,070 edges, and 3612 mesh cells, representing detailed and complex geometries. To ensure numerical stability during training, the node and edge features have been normalized. Additionally, data augmentation techniques, such as small perturbations to mesh positions, have been applied to enhance model generalization.

This comprehensive dataset serves as a robust foundation for integrating graph neural networks (GNNs) with conformal prediction in fluid simulation tasks. Its diverse and challenging scenarios enable a rigorous evaluation of both predictive performance and uncertainty quantification in highly structured graph data.

Experimental Design

The experimental setup is designed to evaluate the performance of MeshGraphNet, for fluid flow simulations enhanced with conformal prediction (Pfaff et al. 2020) (Ju, Lupoiu, and Kanfar 2023). The dataset consists of 125 fluid flow trajectories represented as graph-structured data, with nodes capturing localized physical properties (e.g., velocity, pressure) and edges encoding spatial relationships. The data is split into training, calibration, and test sets, with the calibration set used to compute conformal prediction intervals.

Conformal prediction is applied using a trained MeshGraphNet model and leverages a calibration set to compute residuals, defined as the absolute differences between the true values (y) and the model's predictions ($\hat{y}$). These residuals are used to construct prediction intervals at various confidence levels, corresponding to alphas (α) of 0.3, 0.25, 0.2, 0.15, 0.1, and 0.05, which translate to confidence levels of

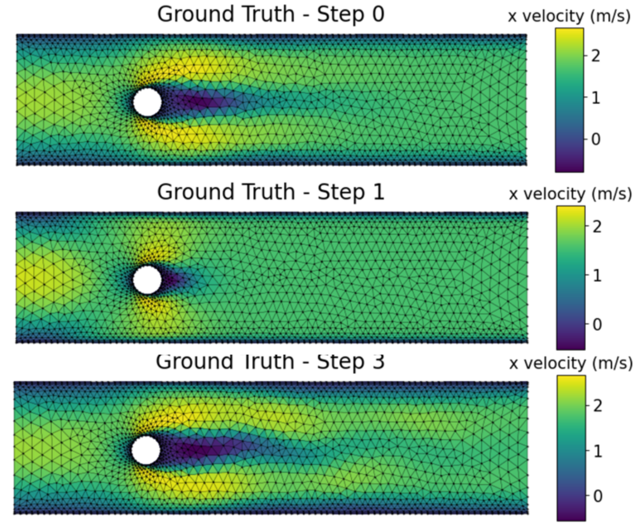

Figure 1: Ground truth visualization of x-velocity (m/s) at three time steps in the fluid flow simulation. The mesh structure represents spatial relationships, and the color scale depicts velocity magnitude.

70%, 75%, 80%, 85%, 90%, and 95%, respectively. The interval radius is determined by the $(1-\alpha)$-quantile of the residuals, ensuring that the true values are captured within the intervals with the specified confidence level.

The MeshGraphNet model is trained using normalized node and edge features to ensure numerical stability, with predictions evaluated on the test set. The calibration procedure calculates the radius of prediction intervals for each confidence level, providing rigorous uncertainty quantification. This experimental design allows for a comprehensive evaluation of the predictive accuracy and reliability of the MeshGraphNet model, along with the interpretability and efficiency of the conformal prediction intervals in fluid flow simulation tasks.

5 Results & Discussions

The experimental results, summarized in Table 1 and visualized in Figures 2 and 3, demonstrate the effectiveness of conformal prediction in providing reliable uncertainty quantification for fluid flow simulations using MeshGraphNet.

The predictive accuracy of MeshGraphNet was evaluated using Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and R^2. These metrics remain consistent across all experiments, with an MAE of 0.4266, RMSE of 0.9720, and R^2 of 0.4081. While the RMSE reflects reasonable predictive accuracy, the R^2 score indicates moderate explanatory power, suggesting opportunities for improving the model's ability to capture highly non-linear flow dynamics.

The coverage versus $1-\alpha$ plot (Figure 2) shows that the achieved coverage consistently meets or slightly exceeds the desired confidence levels for all tested values of α. For instance, at $\alpha = 0.05$ (confidence level 95%), the achieved

α	**Coverage**	**Interval Width**
0.30	0.7488	0.7869
0.25	0.7969	1.0636
0.20	0.8441	1.4114
0.15	0.8776	1.9731
0.10	0.9204	2.7306
0.05	0.9630	4.4744

Table 1: Impact of varying α on coverage and prediction interval width.

coverage is 96.30%, while at $\alpha = 0.10$ (confidence level 90%), it is 92.04%. This consistency reflects the robustness of the conformal prediction framework in ensuring calibrated uncertainty quantification.

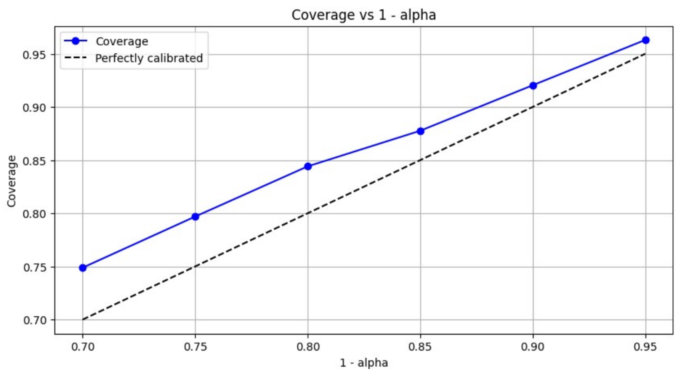

Figure 2: Coverage versus $1 - \alpha$. The achieved coverage meets or exceeds the desired confidence levels, demonstrating reliable calibration.

The interval width versus $1 - \alpha$ plot (Figure 3) illustrates the trade-off between confidence levels and interval width. As $1 - \alpha$ increases, the interval widths grow to accommodate higher reliability. For example, the interval width at $\alpha = 0.30$ (confidence level 70%) is 0.79, while at $\alpha = 0.05$ (confidence level 95%), it increases to 4.47. This behavior is expected and highlights the balance between precision (narrower intervals) and reliability (higher coverage).

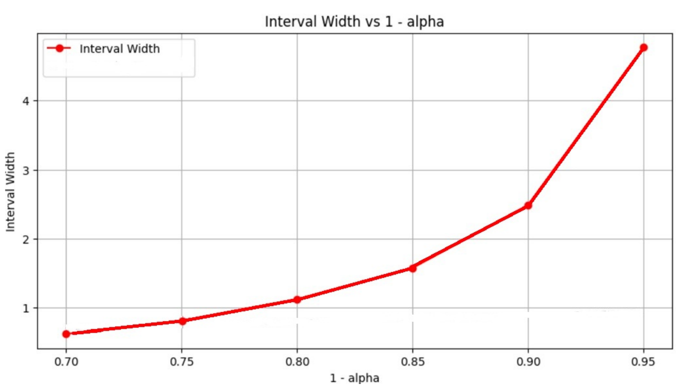

Figure 3: Interval Width versus $1 - \alpha$. The interval widths increase with higher confidence levels, balancing precision and reliability.

6 Conclusions and Future Work

This preliminary study integrated conformal prediction with MeshGraphNet for uncertainty-aware fluid flow simulations. The framework combines graph neural networks (GNNs) with rigorous uncertainty quantification, achieving coverage exceeding desired confidence levels and aligning with theoretical guarantees. A trade-off between precision (i.e., coverage) and reliability (i.e., prediction interval) was observed, as interval widths grew with higher confidence levels.

Future work includes incorporating adaptive interval widths, extending the framework to dynamic and real-time simulations, as well as exploring domain-specific applications like heat transfer and structural mechanics, could broaden its utility.

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