ConvLSTM-Based Deep Learning for Predicting Temperature Contours in CFD Simulations

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***Abstract*—Computational Fluid Dynamics (CFD) is a powerful tool for analyzing fluid flow and heat transfer, but its high computational cost poses limitations for large-scale and real-time applications. To address this, we propose a deep learning approach using Convolutional Long Short-Term Memory (ConvLSTM) networks for predicting temperature contours in CFD simulations. This study focuses on transient heat transfer within a 2D rectangular enclosure subjected to a uniform heat flux of 500 W/m² on both vertical walls. A high-resolution CFD dataset, generated using Ansys Fluent 18, captures temperature evolution across 10,000 spatial nodes over time. The ConvLSTM model is trained to learn both spatial and temporal dependencies, enabling accurate prediction of temperature distributions at future time steps. By preserving the spatiotemporal dynamics of the system, this method provides a robust, data-driven surrogate model that significantly reduces computational overhead while maintaining high predictive accuracy. The approach offers a scalable solution for real-time thermal analysis and control in complex engineering systems.**

1. Introduction

Predicting temperature distribution in fluid domains is a critical task in thermal management, energy efficiency design, and many engineering applications involving heat transfer. Traditionally, Computational Fluid Dynamics (CFD) has been the go-to numerical tool for solving such complex flow and heat transfer problems. However, the high computational cost associated with high-resolution CFD simulations often restricts their applicability in real-time scenarios or large-scale parametric studies.

With the recent surge in machine learning and deep learning techniques, data-driven surrogate modeling has emerged as a promising alternative for accelerating CFD-based predictions. Among these, Recurrent Neural Networks (RNNs) and their variants have shown great success in learning temporal patterns from sequential data. Particularly, the Convolutional Long Short-Term Memory (ConvLSTM) network extends this capability by incorporating spatial feature learning through convolutional operations, making it well-suited for spatiotemporal problems such as temperature contour prediction in CFD simulations.

In this study, we develop a ConvLSTM-based deep learning framework to predict the temporal evolution of temperature contours in a 2D rectangular enclosure subjected to a uniform heat flux. The dataset, generated from high-fidelity CFD simulations using Ansys Fluent 18, captures temperature variations across 10,000 spatial nodes over multiple time steps. The proposed model leverages ConvLSTM's ability to simultaneously learn spatial correlations and temporal dependencies, thus enabling accurate multi-step temperature forecasting.

This approach not only reduces the need for repeated CFD simulations but also provides a significant computational speed-up while preserving the essential physical behavior of the system. The goal is to develop a robust, scalable, and interpretable surrogate model for real-time thermal analysis and predictive control in engineering systems involving complex heat transfer.

2. Literature Survey

1. Machine Learning-Based Predictions of Flow and Heat Transfer Characteristics in a Lid-Driven Cavity Authors: Hussein Kokash, Khalil Khanafer, Mihai Burzo Source: Energies 2024, 17, 5220 Summary: This study explores machine learning (ML) techniques for predicting heat transfer characteristics in a lid-driven cavity with a rotating cylinder. The research compares different ML regression models and physicsinformed neural networks (PINNs) to evaluate their accuracy against computational fluid dynamics (CFD) simulations. The results show that the random forest model consistently performs well at different Reynolds numbers, while PINNs trained with CFD data exhibit lower errors compared to purely theoretical PINNs. 2. CFD and Machine Learning-Based Simulation of Flow and Heat Transfer Characteristics of Micro Lattice Structures Authors: Disha Deb et al. Source: IOP Conf. Ser.: Earth Environ. Sci. 850 (2021) 012034 Summary: This paper presents a CFD-based dataset used for training ML models to predict final fluid temperature and pressure drop in micro-lattice structures. The study evaluates six different lattice structures and highlights the potential of ML in predicting thermal

performance. The ML model's predictions align closely with simulated results, indicating its applicability in practical industrial settings. 3. Enhancing CFD Solvers with Machine Learning Techniques Authors: Paulo Sousa, Carlos Veiga Rodrigues, Alexandre Afonso Source: Computer Methods in Applied Mechanics and Engineering, 2024 Summary: This study integrates ML surrogate models into CFD solvers to accelerate pressure computation in incompressible flow simulations. The ML-enhanced solvers achieve an eightfold reduction in execution time while maintaining accuracy in drag coefficient and Strouhal number predictions. The research highlights hybrid CFD solvers that combine physics-informed methods with data-driven surrogate models. 4. Data-Driven Modeling of Geometry-Adaptive Steady Heat Conduction Based on CNNs Authors: Jiang-Zhou Peng, Xianglei Liu, Nadine Aubry, Zhihua Chen, Wei-Tao Wu Source: Case Studies in Thermal Engineering, 2021 Summary: This study proposes a CNN-based model for predicting steady-state heat conduction in objects with arbitrary geometries. Using a signed distance function (SDF) to represent geometry, the model generalizes well to unseen geometries and is over an order of magnitude faster than traditional numerical methods.

3. Dataset Discussion

The dataset used in this study is generated using Computational Fluid Dynamics (CFD) simulations performed in Ansys Fluent 18. The computational domain represents a rectangular enclosure subjected to heat transfer, where both side walls are heated with a constant heat flux of 500 W/m². The dataset is structured to capture the thermal and flow characteristics of the enclosure, providing a high-resolution representation of temperature and velocity fields across the domain.

Dataset Structure

The high-fidelity dataset is obtained through CFD simulations with the following setup:

- **Computational Domain:** Rectangular enclosure.
- **Boundary Conditions:**
  - Left and right walls: **500 W/m² constant heat flux**.
  - Top and bottom walls: **Adiabatic (no heat transfer)**.
  - Fluid inside the enclosure: **Natural convection-driven flow**.
- **Mesh Resolution:**
  - **10,000 spatial points (high-fidelity data)**.
  - Structured or unstructured grid depending on numerical accuracy.
- **Simulation Parameters:**
  - Governing Equations: **Navier-Stokes and Energy equations**.
  - Solver: **Finite Volume Method (FVM)**.
  - Turbulence Model: **Laminar or turbulence model depending on Rayleigh number**.

Data Representation and Features

The dataset consists of numerical solutions for the following field variables:

- **T**emperature (T): Capturing heat distribution across the domain.
- **V**elocity Components (u, v): Representing convective flow patterns.
- **P**ressure (P): Recording pressure variations due to convection.

Each variable is stored as a spatial field, discretized over 10,000 points. The CNN-based Reduced-Order Model (ROM) aims to downsample this dataset to 1,000 spatial points, preserving essential features while reducing computational complexity.

Training Data Selection

Since the model is trained using a single dataset, the selection of an appropriate time step and spatial resolution is critical. The dataset needs to sufficiently represent the steady-state or transient flow physics, ensuring that key thermal and flow features are preserved after dimensionality reduction.

Challenges and Considerations

- **High Dimensionality of CFD Data**
  Large spatial grids combined with many time steps result in memory-intensive datasets. Requires efficient data loading, preprocessing, and storage strategies.
- **Spatiotemporal Learning Complexity**
  ConvLSTM models must extract meaningful spatial patterns and temporal trends simultaneously. Needs careful tuning of convolutional kernel size, sequence length, and number of layers.
- **Long Training Times**
  Deep models on large CFD datasets demand high computational power and longer training durations. Use of GPUs or HPC environments is essential for practical training time.
- **Risk of Overfitting**
  Due to high model capacity and limited unique simulation conditions, there's a risk of overfitting to training data. Regularization techniques such as dropout and early stopping are necessary.
- **Generalization to Unseen Scenarios**
  The model may fail to perform well on new boundary conditions or flow regimes not represented in training data. Training on diverse datasets or including physics-based constraints can help.

- **Boundary Prediction Artifacts**
  Model performance may degrade near enclosure walls due to limited neighborhood context. Consideration for specialized boundary handling or padding techniques is important.
- **Hyperparameter Tuning Complexity**
  Choosing optimal values for learning rate, number of filters, batch size, etc., requires extensive experimentation. Automated tuning (e.g., RandomizedSearch or Bayesian Optimization) is recommended.
- **Loss of Physical Interpretability**
  Unlike CFD solvers, neural networks are black-box models and lack inherent physical transparency. Use of explainability tools (e.g., feature maps, saliency, SHAP) is beneficial.
- **Data Preprocessing Burden**
  Lag features, moving averages, normalization, and reshaping into spatiotemporal sequences are required. Proper pipeline setup is essential for model input compatibility.
- **Evaluation and Validation**
  Standard metrics (MAE, RMSE, R^2) must be supplemented with contour comparison and error maps. Cross-validation must respect temporal ordering to avoid data leakage.

4. Approach

The methodology adopted in this study is designed to develop a data-driven surrogate model capable of predicting temperature contours in a transient CFD simulation using ConvLSTM networks. The approach is divided into several key stages:

Data Generation and Collection

The dataset used for this study is generated through high-fidelity CFD simulations in Ansys Fluent 18. The simulation setup involves a 2D rectangular enclosure subjected to a uniform heat flux of 500 W/m² on both vertical walls. The resulting data includes transient temperature fields over 10,000 spatial nodes across multiple time steps. These high-resolution temperature distributions form the basis for training the deep learning model.

Data Preprocessing

To prepare the CFD data for model input, several preprocessing steps are performed:

- The temperature field is reshaped into a grid format for each time step.
- Min-max normalization is applied to scale the temperature values between 0 and 1.
- Sequential temperature frames are organized into input-output pairs using sliding windows to capture temporal patterns.
- Padding and interpolation techniques are used to maintain uniform input dimensions, especially for edge nodes.

Model Architecture Design

A ConvLSTM network is employed to simultaneously learn spatial and temporal patterns from the CFD dataset. The architect includes:

- One or more stacked ConvLSTM layers for capturing dynamic spatiotemporal behavior.
- Batch normalization and dropout layers for regularization and stability.
- A final convolutional layer to reconstruct the predicted temperature contour.

Post-Processing and Visualization

To interpret the model output:

- Error contour maps and residual heatmaps are generated.
- Temporal evolution plots are used to assess prediction stability.
- Feature activation maps (optional) may be used to visualize learned spatial features.

Model Saving and Deployment

- Save the trained models using the `Pickle` format for reuse and inference.
- Explore potential deployment strategies for real-time temperature prediction applications.

4. Results and Discussion

Training Loss Analysis

The training loss curve, shown in Figure **??**, represents the average Mean Squared Error (MSE) over 50 epochs for a model predicting temperature contours over 50 steps. The loss starts at approximately 10^{-1} and drops sharply to around 10^{-3} within the first 10 epochs, reflecting rapid initial convergence. The loss then gradually decreases, stabilizing near 5×10^{-4} after 30 epochs. This trend indicates effective learning of the temperature distribution patterns, with the model achieving a low error rate. The plateau in loss suggests that additional epochs may yield minimal further improvement, pointing to a well-optimized training process.

Further insights into the model's performance are derived from the sample temperature contour predictions visualized at epoch 50, which

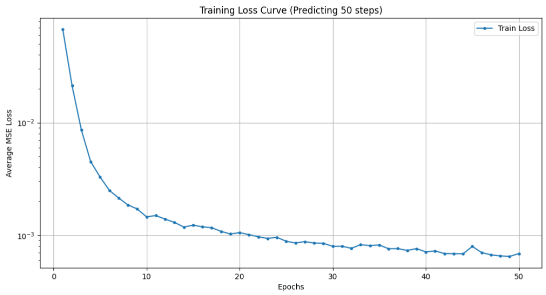

Figure 1. Training loss curve

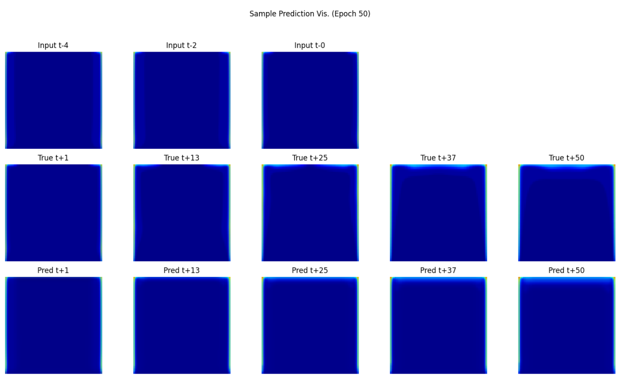

Figure 2. Sample Prediction (time step = 5

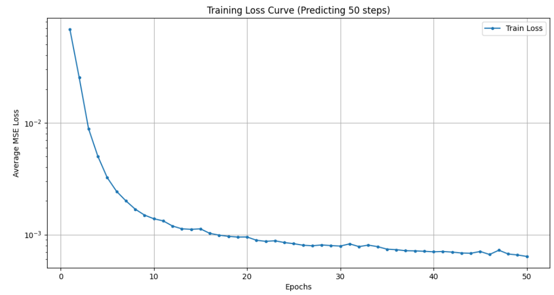

Figure 3. Training loss curve

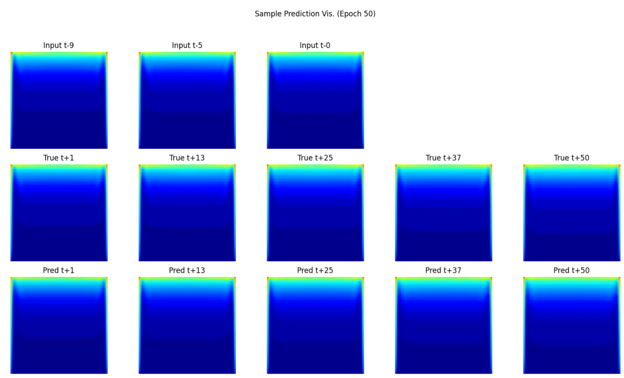

Figure 4. Sample Prediction (time step = 10

compare input sequences, true temperature contours, and predicted contours over the 50-step prediction horizon. Two distinct input sequences are analyzed: the first spans from $t-14$ to $t-0$, and the second extends from $t-19$ to $t-0$. These sequences serve as the foundation for the model's forecasts, with the resulting true contours (e.g., $t+1$, $t+13$, $t+25$, $t+37$, $t+50$) and predicted contours (e.g., $Predt+1$, $Predt+13$, $Predt+25$, $Predt+37$, $Predt+50$) represented through color gradients. In these visualizations, darker blue shades indicate lower temperatures, while lighter shades signify higher temperatures, providing an intuitive representation of the thermal distribution. The predictions exhibit a strong alignment with the true contours, particularly for short-term steps such as $t+1$, where the gradient patterns and temperature distributions closely match, demonstrating the model's proficiency in short-term forecasting. However, as the prediction horizon extends to longer time steps, such as $t+37$ and $t+50$, subtle discrepancies emerge, most notably in the transitions between color gradients. These deviations suggest a gradual reduction in predictive accuracy over extended periods, likely due to the increasing complexity and uncertainty associated with long-term dependencies in the temperature data. This observed trend is consistent with the training loss curve's stabilization, reinforcing the notion that while the model excels at short-term predictions, its ability to accurately capture long-term temperature dynamics may be limited. The close correspondence between predicted and true contours at early steps underscores the model's robustness and generalization capability within the training data's scope. However, the growing divergence at later steps highlights a potential area for improvement, possibly attributable to the model's architecture or the training dataset's temporal coverage. To address these limitations, future research could explore the integration of advanced recurrent or attention-based architectures, such as Long Short-Term Memory (LSTM) networks or Transformer models, which are better suited for modeling long-range dependencies. Additionally, expanding the training dataset with more extensive temporal sequences or incorporating external variables (e.g., environmental factors) could enhance the model's ability to predict

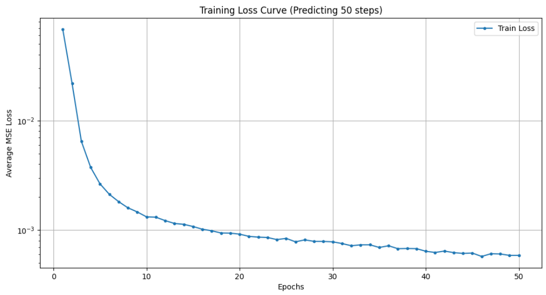

Figure 5. Training loss curve

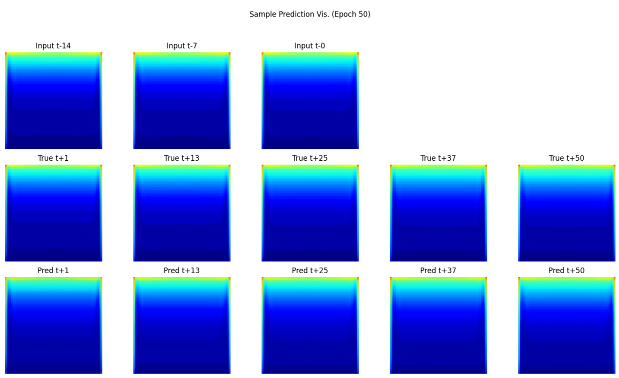

Figure 6. Sample Prediction (time step = 15

temperature contours over longer horizons. These enhancements would aim to refine the model's performance, ensuring greater accuracy and reliability across the entire 50-step prediction range.

5. Conclusion

In conclusion, the model demonstrates a robust performance in predicting temperature contours over a 50-step horizon, as evidenced by the rapid initial decline in the average Mean Squared Error (MSE) to 10^{-3} within 10 epochs and subsequent stabilization near 5×10^{-4} after 30 epochs, reflecting effective learning and optimization. The strong alignment of predicted and true contours for short-term steps, such as $t + 1$, underscores the model's proficiency in capturing immediate temperature distributions. However, the increasing discrepancies observed at longer horizons, such as $t{+}50$, indicate limitations in modeling long-term dependencies, likely due to the complexity of extended temporal dynamics. These findings suggest that while the current model is well-suited for short-term forecasting, future enhancements could involve adopting advanced architectures like Long Short-Term Memory (LSTM) networks or Transformers, and expanding the training dataset with additional temporal sequences or environmental

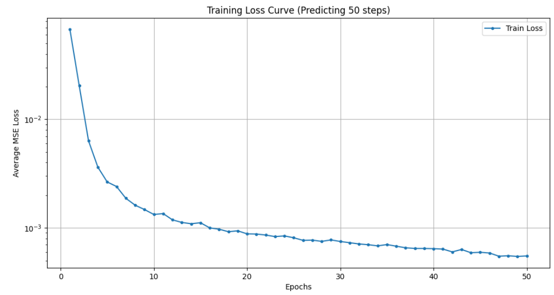

Figure 7. Training loss curve

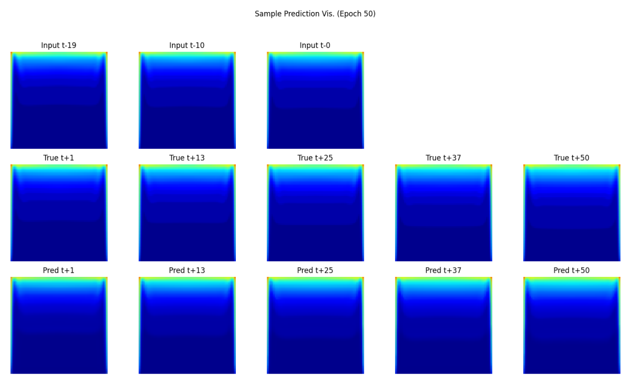

Figure 8. Sample Prediction (time step = 20

variables. Such improvements would aim to enhance the model's accuracy and reliability across the entire prediction range, paving the way for more effective temperature contour forecasting in practical applications.

References

[1] Matthias Eichinger, Alexander Heinlein, and Axel Klawonn. Surrogate Convolutional Neural Network Models for Steady Computational Fluid Dynamics Simulations. *Electronic Transactions on Numerical Analysis*, 56:235-255, 2022.

[2] A. Trullo, M. Pasini, F. Bonaccorso, S. Bianco, R. Caramazza, P. Napoletano, D. De Falco, F. Piccialli A graph-based machine learning approach for predicting the compressive strength of concrete *Scientific Reports*, 14, 9732 (2024).

[3] B. Bogosel, S. Bordeu, C. Fiterau, L. Grigori, and S. Li. Data-driven reduced-order modelling for parameter identification in groundwater remediation. *Proceedings of the Royal Society A*, 479(2278):20230058, 2023.

[4] Jian-Ping Lyu, Xiao-Wei Yu, and Hong-Nan Li. Multifidelity Bayesian optimization for structural reliability analysis with limited data. *CMES-Computer Modeling in Engineering & Sciences*, 134(2):1489-1510, 2023.