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Exploring the potential applicability of deep learning methods in computing wall distributed aerodynamics and thermal effects in rarefied flows

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Abstract

With advancements in aerospace technology, artificial intelligence methods are increasingly being employed in flow field and aerodynamic computations, offering significantly higher computational efficiency compared to traditional CFD approaches. However, most existing studies on aerodynamic forces focus on using geometric conditions as inputs to guide calculations, paying limited attention to the generalization capabilities of models across diverse flow regimes. This study investigates the potential and practical applicability of deep learning methods for computing distributed aerodynamic and thermal effects on surfaces in rarefied flows. A deep learning-based surrogate model is proposed to directly characterize the relationship between near-wall flow states and the local distribution of aerodynamic and thermal effects on surfaces. Furthermore, a trainable weighted subnetwork and a cascaded model output structure are incorporated to improve the model's generalization capability and interpretability across a wider range of flow regimes and enhance the model's prediction accuracy for regions with high thermal flux and aerodynamic forces. The proposed model successfully predicts aerodynamic and thermal effects in flows with large Knudsen numbers ranges, offering accurate and interpretable results that provide valuable insights for further research and development.

Keywords: rarefied flow, aerodynamic forces, thermal effects, deep learning

Introduction

Accurately predicting surface aerodynamic and thermal effects is essential for the design of thermal protection systems, material selection, and overall performance evaluation in applications such as hypersonic flight, spacecraft re-entry, and landing. Among the commonly used numerical methods, the Navier-Stokes (NS) equations offer relatively high computational efficiency but are unsuitable for rarefied flow regimes. In contrast, the Direct Simulation Monte Carlo (DSMC) method provides accurate solutions for rarefied flows but incurs prohibitively high computational costs, limiting its feasibility for engineering optimization and real-time prediction[1–3].

In recent years, deep learning methods have garnered significant attention in fluid mechanics due to their potential to replace various aspects of traditional physical models by learning dependencies from high-fidelity experimental and simulation data. These methods have been successfully applied to predict flow states[4,5], aerodynamic forces[6,7], and heat flux distributions[8,9], substantially improving computational efficiency.

However, most existing studies remain constrained by geometric priors, such as signed distance functions, or are limited to fixed inflow conditions, resulting in poor generalization and reduced adaptability to complex flow environments. To address these limitations, researchers have explored predictive modeling approaches based on local flow field parameters., Xu et al. [10]proposed that local wall-normal heat flux could be represented as a nonlinear function of nearby wall shear stress and wall pressure fluctuations using a multi-layer neural network. They employed a convolutional neural network (CNN) to predict local heat flux and leveraged gradient maps to analyze spatial correlations between heat flux and surrounding flow features. Erwan et al. [11] introduced a data-driven wall function estimation method, training a fully connected feedforward neural network to infer wall friction from local flow conditions. Upon integration into an industrial CFD solver, their model significantly improved wall friction predictions in Reynolds-Averaged Navier-Stokes (RANS) simulations.

Building on this foundation, the present study further investigates deep learning models driven by local flow field parameters. By simplifying the underlying relationships, we develop a surrogate model that

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directly maps the near-wall flow state to local aerodynamic and thermal effects. Additionally, a trainable weighted sub-network is introduced to enhance the model's generalization capability across a broader range of flow regimes while improving interpretability. Furthermore, a hierarchical output processing structure, informed by predicted physical phenomena, is designed to improve both prediction accuracy and robustness. The proposed model accurately predicts aerodynamic and thermal effects across a wide range of Knudsen numbers, providing valuable insights for future research and applications.

Method

This study investigates the application of deep learning methods to learn from classical CFD algorithm results, leveraging these relationships to enhance prediction efficiency. The development of the surrogate model begins with the selection of a high-fidelity (HiFi) dataset. The dataset utilized in this study is generated using the PWS developed at Beihang University, a DSMC-based approach that has been validated for both aerodynamic and thermal computations[12]. The dataset comprises flow fields and aerodynamic effects resulting from multiple engine jets impinging on a flat plate in a vacuum environment at varying distances. From these computational results, flow variables at nodes positioned a certain distance from the wall are extracted, along with their corresponding heat flux density and shear stress components along the y and z axes on the wall, as illustrated in Figure 1(a). A deep learning model is then trained to infer the latter from the former.

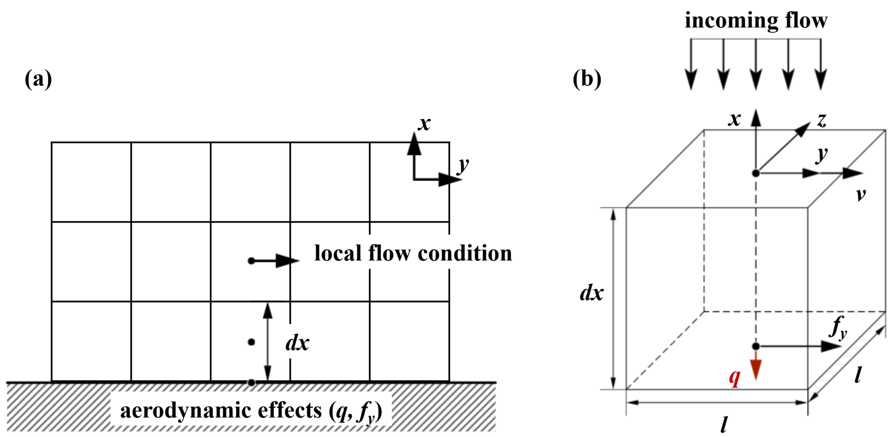

Figure 1 Use of near-wall data for train and prediction: a. input–output datasets extracted at a given position in the flow from HiFi simulations, b. the simplified model for local nondimensionalization

To minimize the influence of far-field conditions and surface geometry, thereby enhancing the model's generalization capability, the proposed deep learning approach relies on a set of input variables, I_p, obtained from the first off-wall node:

$$I_p = \left\{ U_i^*, \rho^*, p^*, T^*, Ma, \left(\frac{\partial U_i^*}{\partial x_i}\right), \left(\frac{\partial \rho^*}{\partial x_i}\right), \left(\frac{\partial p^*}{\partial x_i}\right), \left(\frac{\partial T^*}{\partial x_i}\right), \left(\frac{\partial Ma}{\partial x_i}\right), \left(\frac{\partial \left(U_i^*\right)^2}{\partial x_i}\right), \right\} \tag{1}$$

$$i = 1,2,3 \tag{2}$$

where U represents velocity, ρ is density, p is pressure, T is temperature, and Ma is the Mach number. Based on the assumption that aerodynamic heating effects are strongly correlated with I_p at the first off-wall node, a simplified model is constructed, as shown in Figure 1(b). This model simplifies the aerodynamic process as the interaction between a uniform inflow (characterized by I_p) and the bottom surface of a micro body. To ensure consistency across different flow regimes, the flow parameters are nondimensionalized using the density ρ and temperature T from the inlet conditions of the micro-body:

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$$U_i^* = \frac{U_i}{(RT)^{1/2}}, f_y^* = \frac{f_y}{\rho RT}, q^* = \frac{q}{\rho (RT)^{3/2}}, \rho^* = \log_{10}\rho, p^* = \log_{10} p, T^* = \log_{10} T \tag{3}$$

Furthermore, considering the symmetry of the shear stress components in the y and z directions with respect to flow parameters, a local coordinate system is established, as depicted in Figure 1(b). The extracted I_p serve as the input for the neural networks. The fundamental architecture of the neural network is illustrated in Figure 2(a). A trainable weighted subnetwork is introduced to assign weight coefficients to each input channel based on the provided input conditions, enabling the neural network output to be expressed as:

$$output = M\left(\left(1 + W\left(I_p\right)\right) I_p\right) \tag{4}$$

where W represents the weighting subnetwork, and M denotes an MLP, in this study, both of them are implemented as fully connected neural networks, achieving an optimal training accuracy.

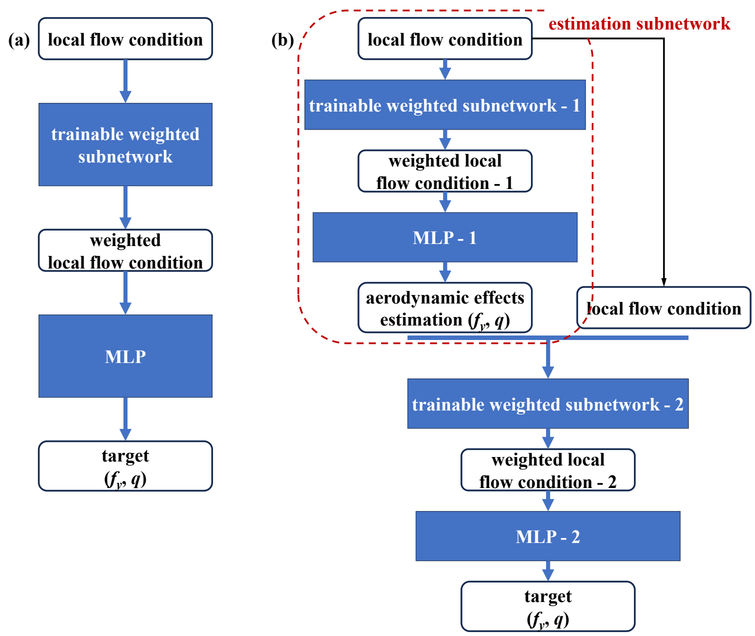

Figure 2 neural network structures: a. the trainable weighted subnetwork enhanced (TWSE) model, b. the model using a cascading structure

Additionally, recognizing that wall-bounded aerodynamic effects directly reflect the near-wall flow state, a serial output structure is designed, as illustrated in Figure 2(b). The predictions of the first-stage network for wall aerodynamic effects are incorporated into the second-stage model as updated input variables I_p':

$$I_p' = \left\{U_i^*, \rho^*, p^*, T^*, Ma, \left(\frac{\partial U_i^*}{\partial x_i}\right), \left(\frac{\partial \rho^*}{\partial x_i}\right), \left(\frac{\partial p^*}{\partial x_i}\right), \left(\frac{\partial T^*}{\partial x_i}\right), \left(\frac{\partial Ma}{\partial x_i}\right), \left(\frac{\partial \left(U_i^*\right)^2}{\partial x_i}\right), output\right\} \tag{5}$$

Two separate deep learning models are constructed to predict the wall shear stress components f_y and heat flux density q, respectively. The role of the two subnetworks is further analysed. The loss function used for training is the mean squared error (MSE). To mitigate overfitting and assess the model's generalization capability for unseen conditions, the dataset is partitioned into training, validation, and test sets according to the corresponding flow conditions.

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Results

In this study, the three models were each trained for 10,000 steps on a GPU. The training, validation, and test datasets encompass flow states near the plate, covering continuum, transitional, and rarefied flow regimes. Taking the test case shown in Figure 3 as an example, the region of maximum heat flux density is primarily aligned with the engine nozzle and exhibits continuum flow characteristics. As the engine jets expand into the vacuum and interact, the flow transitions into a regime with a Knudsen number approaching 1, eventually diffusing outward into a rarefied flow state.

Figure 3 presents the model predictions for a representative test case, demonstrating strong agreement between the deep learning model and the DSMC computational results for both shear stress components and heat flux density. The error distribution of the shear stress components is relatively uniform, with larger errors concentrated in regions where multiple engine jets interact. Table 1 summarizes the prediction errors across the entire test dataset, revealing that the three models exhibit similar average errors in shear force predictions. This may be attributed to the increased complexity of the flow conditions in jet interaction regions compared to regions dominated by a single nozzle, suggesting that higher-resolution grids or enhanced neural network input features may be required to improve accuracy.

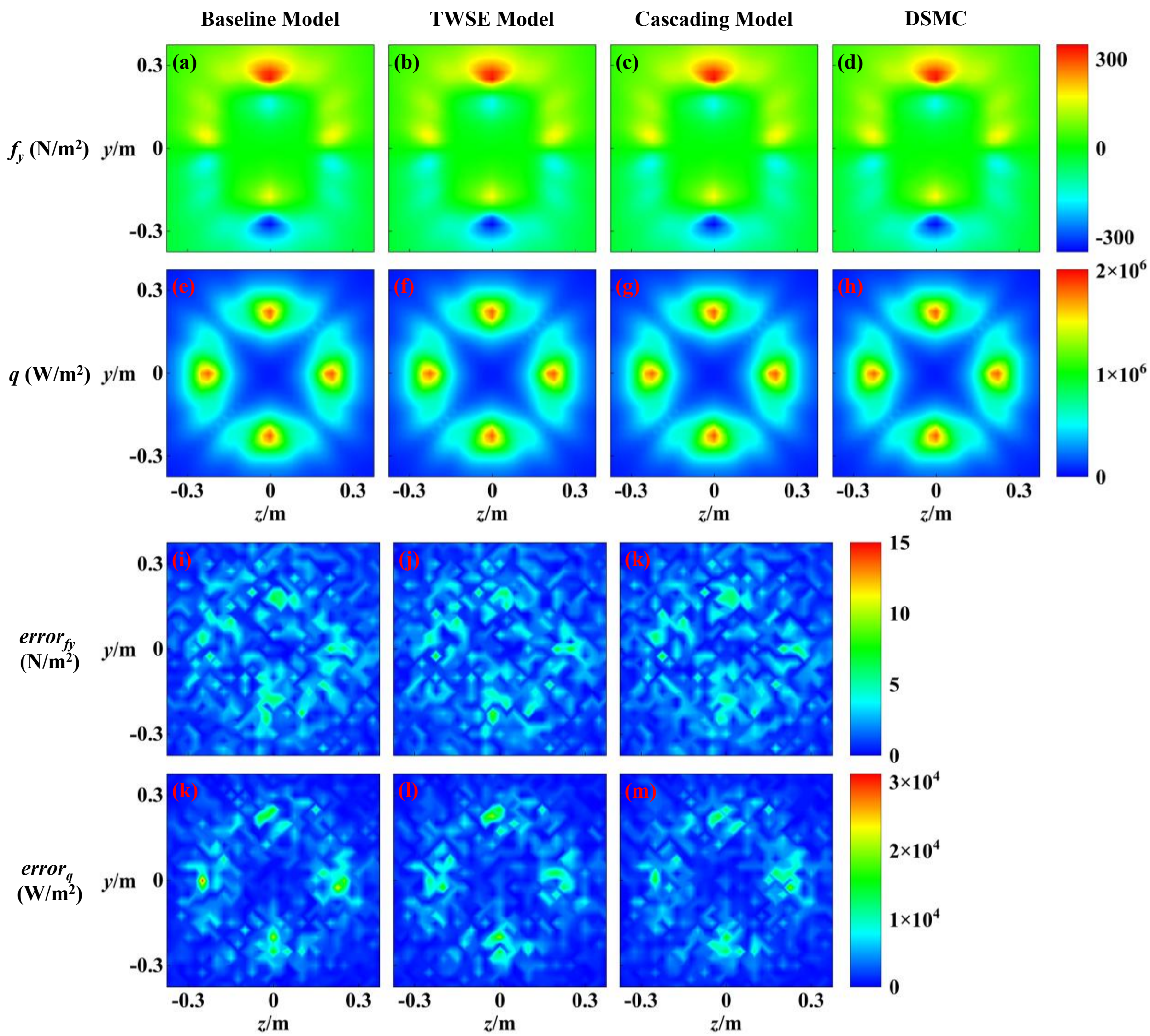

Figure 3 prediction results for aerodynamics and thermal effects: a-d. results for f_y, e-h. results for q, i-k. absolute error for f_y prediction, k-m. absolute error for q prediction

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In contrast, the prediction errors for heat flux density are primarily concentrated at peak values, as illustrated in Figure 3. A clear distinction in predictive accuracy is observed among the three models, with the serial-structured model achieving the highest accuracy, while the baseline model performs the worst. The results in Table 1 further validate this observation, demonstrating that both enhanced model architectures enable a more precise representation of local flow conditions. Given the relatively small proportion of continuum-flow nodes in the test dataset, these findings suggest that the proposed improvements enhance the model's ability to capture variations in flow states.

Table 1 prediction performances for aerodynamics and thermal effects

	DSMC	Baseline model	Model with weighted subnetwork	Model with serial structure
f_y error (N/m^2)	—	1.63	1.61	1.59
q error (W/m^2)	—	2518	2459	2445

For the serial-structured model, additional validation of its f_y predictions is provided in Figure 4(a), which presents results along the $z = 0$ and $y = 0$ axes. Considering the symmetry of the heat flux distribution observed in Figure 3, only the $z = 0$ axis is used for comparison in Figure 4(b). The results indicate that the model successfully captures both peak values and lower-magnitude variations for f_y and q, further demonstrating the effectiveness of the proposed deep learning approach.

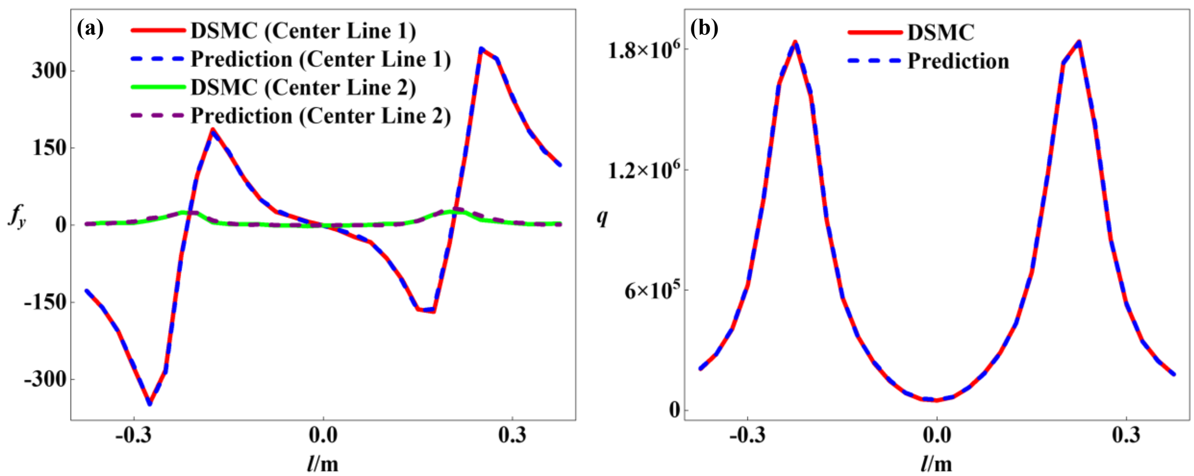

Figure 4 prediction of aerodynamics and thermal effects along $z = 0$ and $y = 0$ axes

Conclusion

This study investigates the potential of deep learning methods for computing surface-distributed aerodynamic and thermal effects. A deep learning-based surrogate model is developed, incorporating local nondimensionalization and structural enhancements to predict aerodynamic and thermal effects based on local flow field characteristics. The model's predictions on the test dataset show strong agreement with DSMC results, demonstrating its ability to accurately capture key local flow features and validating the feasibility of using deep learning for local aerodynamic effects prediction. The results for local heat flux prediction indicate that the proposed weighted subnetwork and serial model structure enhance the model's ability to identify and adapt to local flow conditions. However, these improvements have a limited impact on the accuracy of shear stress predictions, suggesting that higher-resolution computational data or further refinements in the model's learning capabilities may be required to improve prediction accuracy in complex flow regimes. These findings provide valuable insights for future advancements in deep learning-based aerodynamic and thermal modeling.

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