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Vacuum plume field reconstruction method for variable thrust engines based on deep learning

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Abstract. The vacuum plume field is crucial for analyzing the impact of spacecraft plume effects. It consists of continuous, transition, and free molecular flows, which complicate the resolution of macroscopic governing equations. The conventional method for calculating the vacuum plume field is the Direct Simulation Monte Carlo (DSMC) method, a computationally intensive microscopic simulation technique. Despite various efforts to enhance DSMC efficiency, recent advances in artificial intelligence (AI) offer the potential to accelerate computations by several orders of magnitude. This study introduces a deep learning (DL) surrogate model to reconstruct the vacuum plume flow field generated by a lunar lander engine. Previous studies typically focus on fixed input conditions, such as engines with constant thrust. In contrast, this study utilizes position, boundary conditions, and the free flow field of the engine at a given thrust as inputs for the convolutional neural network to predict the vacuum plume field for a variable-thrust engine at different altitudes. Additionally, the gradient-length local Knudsen number incorporated as a weighted factor in the loss function effectively improves the prediction accuracy of the shock wave region in the surrogate model. This research ensures accuracy while eliminating the repetitive calculations of DSMC, significantly enhancing efficiency.

Keywords: Vacuum plume; Deep learning; DSMC; Fluid mechanics; Knudsen number

1. Introduction

The vacuum plume emitted by spacecraft engines in space induces various effects, including aerodynamic forces, thermal loads, and contamination impacts, all of which significantly influence the success of space missions. The vacuum plume encompasses various distinct flow regimes: continuous flow, transition flow, and free molecular flow, typically simulated using the Direct Simulation Monte Carlo (DSMC) method initially proposed by Bird [1]. As a particle-based simulation technique, DSMC computes flow field characteristics through the statistical modeling of particle movement and collision processes, resulting in computationally intensive simulations.

Parallel computing architecture can significantly improve the efficiency of DSMC. For instance, J Li et al. [2] have explored hybrid parallel acceleration by leveraging both GPUs and CPUs, achieving notable acceleration in simulation speed. Additionally, R Jambunathan et al. [3] implemented an advanced MPI-CUDA hybrid parallelization strategy, achieving significant performance improvements in DSMC computations. Another approach to enhance computational efficiency involves reducing the number of

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simulated particles by adjusting the particle or cell weights within the computational domain while maintaining a relatively uniform distribution of particles per cell [4]. One such technique is the variable time step method [5]. However, these acceleration strategies typically yield speedup ratios limited to one order of magnitude, with multi-order magnitude acceleration remaining a challenging task.

Deep learning (DL) [6], as a branch of artificial intelligence, has demonstrated remarkable potential in fluid mechanics research. Guo et al. [7] proposed a data-driven flow field reconstruction framework utilizing convolutional neural networks (CNN) [8] to predict the flow field of automobiles. Fukami et al. [9] proposed a CNN-based super-resolution reconstruction methodology to convert low-resolution flow field data into high-resolution results, showcasing DL's capability in flow field resolution enhancement. In rarefied flow dynamics, Zhao et al. [10] introduced a data-driven nonlinear constitutive relationship (DNCR) through machine learning techniques. This approach modifies the heat flux and stress tensor in the Navier-Stokes (NS) equations using solutions derived from the unified gas kinetic scheme (UGKS) [11] solver, avoiding the calculation by DSMC. For vacuum plume, Cai et al. [12] proposed a CNN-DSMC framework to realize flow field reconstruction of a fixed thrust engine. Our previous research [13] extended this framework by investigating the influence of various impact surfaces and training methodologies on DL surrogate model accuracy.

However, these studies are limited to the reconstruction of the vacuum plume of the engine with fixed thrust and lack the feature representation across varying thrusts or engines. To address this limitation, this study introduces a novel approach by incorporating variable thrust engine vacuum plume field features into the DL surrogate model's inputs, enabling the trained model to accurately predict vacuum plume fields across varying thrust conditions. Furthermore, to optimize model performance, the gradient length Knudsen number is added to the loss function as a weight factor, thereby improving prediction accuracy.

2. Methodology

The simulation object of this study is the external vacuum plume field of a single variable thrust engine during lunar landing and the goal of the flow field reconstruction is to obtain a surrogate model with real-time prediction of the conserved quantity U of the vacuum plume field, which contains mass density, momentum density, and energy density and can be expressed as

$$U = \left[\rho, \rho u, \rho v, \varepsilon\right]^T \tag{1}$$

where ρ is the density of the plume, u and v are the axial and radial velocities, respectively, and ε is the total energy.

The whole flow field reconstruction process is divided into two phases: data preprocessing and training process, as shown in Figure 1.

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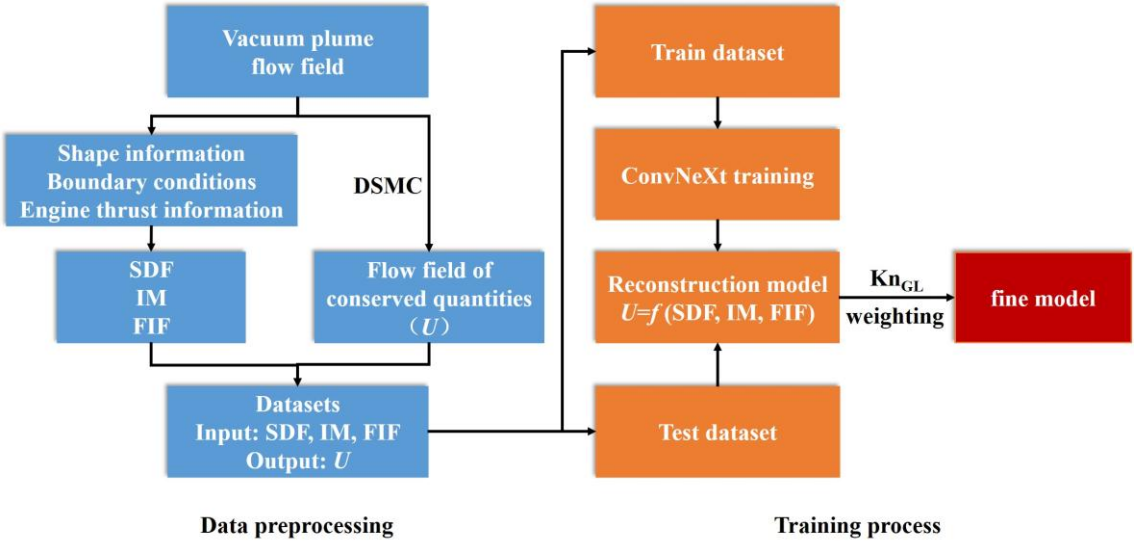

Figure 1. Vacuum plume flow field reconstruction process.

In data preprocessing, shape information, boundary conditions, and engine thrust information in the computing domain are used as input features in the training process. These inputs are systematically paired with high-fidelity DSMC simulation outputs generated by the plume work station (PWS) [14], which serve as ground truth labels. The ConvNeXt [15] structure neural network, one of the strongest CNNs, is employed during training.

For flow field computations, a hybrid CFD-DSMC coupling methodology is implemented, combining computational fluid dynamics (CFD) simulation for the internal nozzle flow with the DSMC method for the external. In the DSMC simulation, the 10 m×5 m space is discretized into a 512×256 Cartesian grid. The variables of the field are normalized by standardization or taking the logarithm. In this study, the engine thrust information is abstracted into the free initial field (FIF) of the engine under the corresponding thrust. FIF extracts the plume core area of the engine in free space. After comparative tests, the parameters of FIF are selected as $\widetilde{\rho u}$, $\widetilde{\rho v}$ and $\tilde{p}$, where $\tilde{p} = 0.1\lg(p + 1\text{e-}10[\text{Pa}])$.

In the training process, the surrogate model is trained based on the ConvNeXt structured CNN with the obtained datasets. The neural network mainly consists of an encoder and a decoder, which are responsible for extracting multilevel features and restoring resolution, respectively. The downsample layer in the encoder extracts local spatial features by conventional convolution operation and improves training stability by layer normalization. AdamW optimizer [16] is used in the optimization process and the loss function is expressed as

$$Loss_{data} = \sum_{m=1}^{N}\left[\left(\rho_m^P - \rho_m^T\right)^2 + \left|\rho u_m^P - \rho u_m^T\right| + \left|\rho v_m^P - \rho v_m^T\right| + \left(\varepsilon_m^P - \varepsilon_m^T\right)^2\right] \tag{2}$$

where N is the batch size, the subscript m represents summing the m-th data in the batch, and the superscripts P and T represent the predicted and ground truth values, respectively.

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After training a model with minimum test loss for certain epochs, the gradient length Knudsen number (Kn_{GL}) is added as a weighting factor in the loss function to further improve the accuracy

$$\mathrm{Kn}_{GL}^{Q} = \frac{\lambda}{Q}|\nabla Q| \tag{3}$$

where λ is the mean free path of plume molecules in the VHS model, Q represents a flow variable which is $\tilde{\rho}$ in this study.

3. Results

To verify whether the surrogate model can predict the flow field of different engine thrusts, the accuracy and efficiency of the trained surrogate model are evaluated through the test dataset in this section. A comparative analysis of training methodologies further elucidates the functional role of the Gradient Length Knudsen (Kn_{GL}) parameter in model optimization.

Figure 2(a)-(d) demonstrates the flow fields of normalized conserved variables with a height of 3.8 m and 7500 N thrust. The left half of each subgraph is the prediction result of the CNN surrogate model, and the right half is the DSMC result. The prediction results of the CNN model are consistent with the DSMC simulation results, and the overall shape of the plume, the position of the compression and the shock wave are predicted accurately. The absolute error between prediction and DSMC results is given in Figure 3(a)-(d). The whole flow field can be divided into four regions with large errors: the backflow region, the region around the lander, the compression wave, and the shock wave near the lunar surface. The statistical fluctuation of DSMC is large when the number of simulation particles is small, and the result has obvious numerical noise. The error in the backflow region is mainly determined by the characteristics of DSMC, and the results in this region can show that the surrogate model has the ability to anti-noise. The remaining three areas with large errors are mainly related to the large gradient of flow field parameters. The overall prediction error remains within an acceptable range.

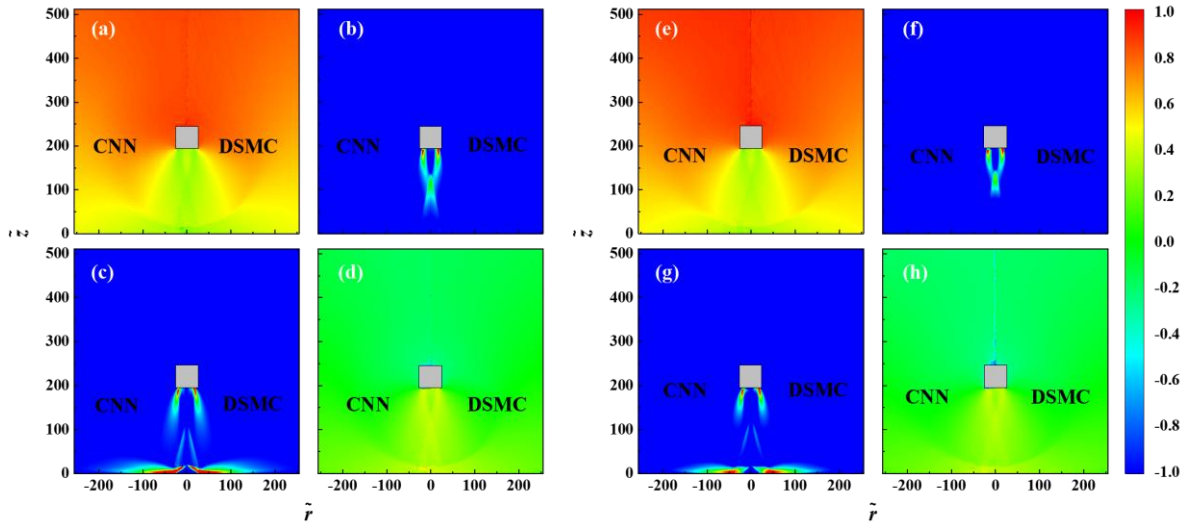

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Figure 2. The prediction and DSMC results of (a) $\tilde{\rho}$, (b) $\widetilde{\rho u}$, (c) $\widetilde{\rho v}$, and (d) $\tilde{\varepsilon}$ with a height of 3.8 m and 7500 N thrust and (e) $\tilde{\rho}$, (f) $\widetilde{\rho u}$, (g) $\widetilde{\rho v}$, and (h) $\tilde{\varepsilon}$ with a height of 3.8 m and 4000 N thrust.

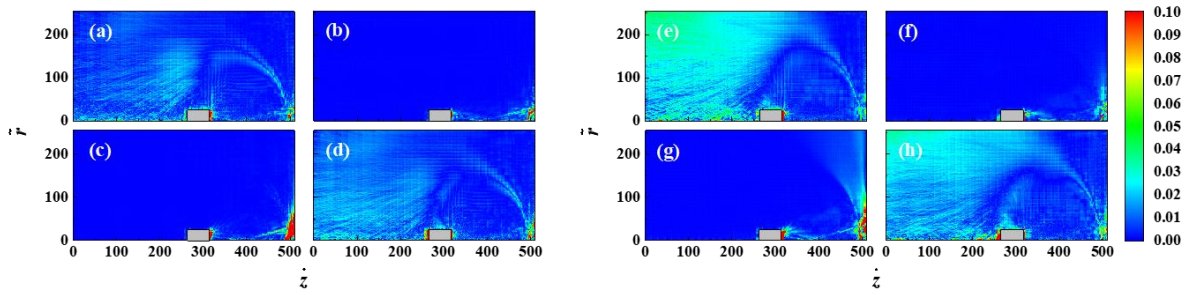

Figure 3. The absolute error between prediction and DSMC results of (a) $\tilde{\rho}$, (b) $\widetilde{\rho u}$, (c) $\widetilde{\rho v}$, and (d) $\tilde{\varepsilon}$ with a height of 3.8 m and 7500 N thrust and (e) $\tilde{\rho}$, (f) $\widetilde{\rho u}$, (g) $\widetilde{\rho v}$, and (h) $\tilde{\varepsilon}$ with a height of 3.8 m and 4000 N thrust.

Considering the thrust variable, Figure 2(e)-(h) and Figure 3(e)-(h) demonstrate the result and error with a height of 3.8 m and 4000 N thrust. The prediction results are amazingly consistent with those calculated by DSMC. The characteristics of compression wave thickness, decay distance of $\widetilde{\rho u}$, and the shape of the flow field near the lunar surface are predicted accurately. In terms of error, the prediction error distribution under 4000 N thrust is similar to that under higher thrust, except that the error in the backflow region increases. This is because as the engine thrust decreases, the number of simulated particles deployed in the same DSMC configuration decreases, resulting in greater numerical noise in the backflow region. This shows that it is feasible to abstract the engine thrust information into FIF as the input feature since FIF provides the initial conditions for the neural network to recognize the flow field structure under different thrusts.

Figure 4 shows the average absolute error of conserved quantities predicted by the model before (original model) and after (Kn_{GL} model) Kn_{GL} weighted training. In Figure 4(a), compared with the original model, the accuracy of the prediction results after weighted training is improved, but relatively small, while in Figure 4(b), the accuracy of the Kn_{GL} model is greatly improved, reaching 11.73%. This shows that in the weighted training process, the neural network focuses on the downward flow region, especially the error in the region with large gradients of flow parameters. While the accuracy of the area of concern is greatly improved, the accuracy of the prediction results of the Kn_{GL} model is still improved in the whole flow field, indicating that the weighted training has little loss on the accuracy of the backflow region, and is suitable for improving the accuracy of the surrogate model.

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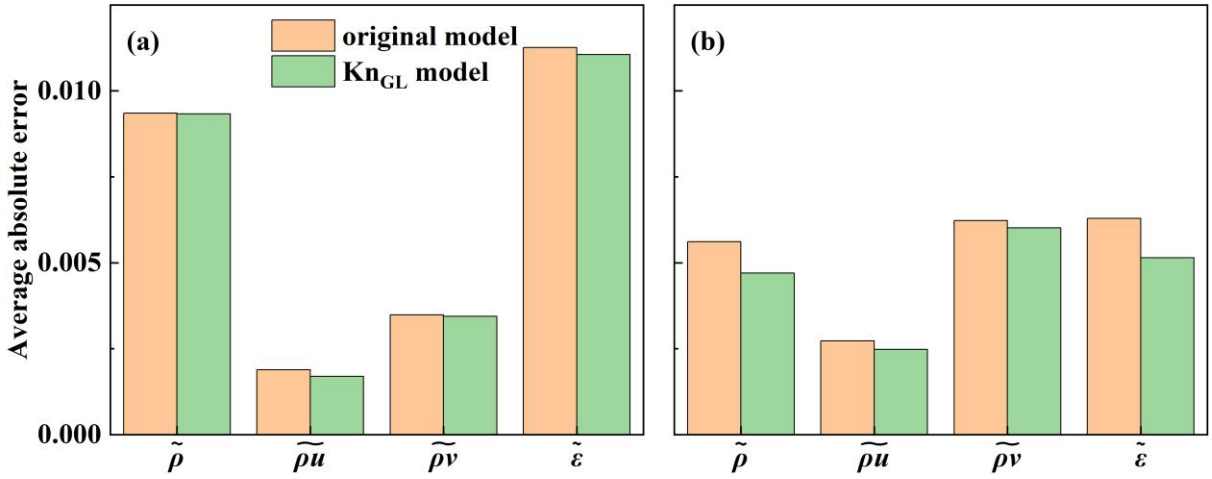

Figure 4. The average absolute error of conserved quantities between the original and Kn_{GL} model prediction results in (a) the whole flow field and (b) the flow field except the backflow region.

Finally, the calculation time of different simulation methods for the vacuum plume field is compared. The efficiency test is performed on four cases in the test dataset, utilizing a 24-thread CPU to run the DSMC program in parallel, and the surrogate model training process was performed on an Nvidia Quadro RTX-A100. For each surrogate model, the time used to compare efficiency is the time to load the model and output the result file, because the training time can be regarded as the time to build the DSMC code or configure the cases. Compared with the original surrogate model, the Kn_{GL} model only needs a small amount of extra training time, and the speedup of both reaches 4 orders of magnitude compared with the DSMC program, which shows the superior performance of the flow field reconstruction model based on deep learning.

4. Conclusion

A deep learning-based vacuum plume field prediction method for variable thrust engines is constructed in this study. A novel thrust characterization approach is implemented through the abstraction of engine thrust into free initial flow field (FIF) representations, enabling parametric encapsulation of thrust-specific plume field. At the same time, to improve the prediction accuracy of the model in shock waves and other large error regions, the gradient length Knudsen number (Kn_{GL}) is calculated and the loss function is weighted based on the trained model. The flow field reconstruction method based on deep learning proposed in this study can predict the vacuum plume flow field of variable thrust engines with high accuracy and efficiency, and the accuracy can be further improved by improving the training method, which expands the application of artificial intelligence technology in the field of vacuum plume.

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