# Boundary Condition-based Machine Learning Algorithm for Fast Prediction of Supersonic Flows

Rachakonda Naga Sai Prakash∗ Indian Institute of Technology Guwahati Guwahati-781039, Assam, India. r.naga@iitg.ac.in

Tapan K. Mankodi Department of Mechanical Engineering Indian Institute of Technology Guwahati

Niranjan Sahoo Department of Mechanical Engineering Indian Institute of Technology Guwahati

#### Abstract

A new neural network-based machine learning algorithm is presented for predicting the flow field around a bluff body in supersonic conditions. The gas flow field generally depends on the geometry, inlet (ICs) and boundary conditions (BCs). In the conventional approach, the compressible Naiver-Stokes-Fourier (NSF) equations are solved on a discretized computational domain with appropriate initial and boundary conditions using either Riemann or Boltzmann approach to obtain the solution, which is a computationally time-consuming task. The proposed approach is our first attempt to predict the flow field without explicitly solving the NSF equations using deep neural networks. Further, the proposed "boundary condition-based machine learning algorithm (BCML)" falls under the category of physics-guided neural network. The training data is generated using in-house Riemann flux solver-based NSF code and converted into a BCML-compatible format. After optimization, the BCML DNN model captured shock structures and other related wave patterns for flow around an arbitrarily shaped bluff body with an arbitrary choice of initial and boundary conditions. The new BCML model has the potential to become a generic ML model that can be used to accelerate CFD solutions for a wide range of problems.

#### 1 Boundary Condition-based Machine Learning Model

Generally, the ML models designed to predict flow fields apply to a specific problem and are not extendable to a class of flows Sekar et al. [2019]. The overall objective of the proposed boundary condition-based machine learning (BCML) algorithm is to construct a physics-guided general-purpose algorithm that can assist the current CFD algorithms in the fast prediction of the flow field for steadystate compressible gas flows. The preliminary work here focuses on supersonic external flows containing wave features, such as shock structures and rarefaction patterns.

Boundary conditions are inherent to solving partial differential equations and directly influence the solution, which, in the present case, is the flow field in the domain. In the present work, the influence of various surrounding boundaries on the solution at a point is modelled by angular discretization. This results in the concept of generators, which are lines originating from this point that eventually end at a boundary. The proposed algorithm predicts the flow field at any point in the domain using the relative distance of this point along the generators with the various boundaries and the corresponding boundary conditions. A distance function and boundary conditions for the various generators form the input side of the DNN model, and the non-conservative variables such as pressure, temperature and

<sup>∗</sup>Corresponding author: Rachakonda Naga Sai Prakash

<sup>1</sup>st Conference on Applied AI and Scientific Machine Learning (CASML 2024).

velocity constitute the model's output. The boundary condition for each generator consisted of four values (one each for pressure, temperature and normal and tangential components of velocity along the direction of a generator) for modelling either Dirichlet or von Neumann boundary conditions. Depending upon the choice of boundary type, the set of four values will either be zero or non-zero. A total of 9 input variables are modelled for each of the generators. A range of distance functions were employed to account for the influence of a boundary on a point, and it was found that an exponential function of decaying nature was appropriate:

$$
f(x) = exp\left(-2x^{0.5}\right) \tag{1}
$$

where  $x$  is the length of a generator from the point to the end of the boundary.

### 2 Training and Testing of BCML model for supersonic flows

Supersonic airflow around a square bluff body in a two-dimensional domain in frozen condition serves as the training data for the BCML model. Ambient gas conditions correspond to that at an altitude range of  $40 - 60$  km Olynick et al. [1999] with the Mach number ranging from Mach 2 to Mach 8. Flow field data was generated using in-house finite volume method code solving the Navier-Stokes-Fourier equations for a wide range of angle of attack (AOA) and surface temperatures on the bluff body. The data generated from the NSF solver was modied into BCML-compatible data format by calculating the distances of various generators from the cell centres to the boundaries using the ray-tracing algorithm. The architecture of the DNN model was optimized using the training data, and an accuracy of 94.23% was obtained for a 16-generator BCML model.



Figure 1: Contour plot of pressure obtained using CFD solver (left) and BCML algorithm (right).

The new 16-generator BCML model was used to predict the flow field around a square bluff body with an angle of attack and ambient and boundary conditions that are not part of the training data. Figure 1 shows the comparison of the pressure contour plot obtained from the FVM solver (left) and the BCML (right) model. The new model captures the features and flow field qualitatively. The overall error was less than 5%. It must be added that the results improve with increasing the number of generators, and this analysis is still in progress.

### 3 Future Work

The BCML model can quickly predict a rough flow field for supersonic external flows. The computational cost of the FVM solver for estimating steady-state solution, as shown in Figure 1, was around 144 CPU hours. In contrast, the BCML model predicts the flow-field solution in 21 seconds. Currently, efforts are being made to improve the overall accuracy and generality of the model for a wide range of simulation conditions. Further, the BCML model can potentially assist traditional CFD algorithms in decreasing computational costs. The flow field estimation from the BCML model can help to construct an optimum mesh and sub-domain for parallelization for the FVM solver. Further, the BCML flow field data can serve as an initial guess value for the CFD solvers, accelerating convergence and thus significantly reducing runtime. The final work will include an in-depth evaluation of the BCML model from an accuracy and efficiency point of view.

## References

- David Olynick, Y-K Chen, and Michael E Tauber. Aerothermodynamics of the stardust sample return capsule. *Journal of Spacecraft and Rockets*, 36(3):442–462, 1999.
- Vinothkumar Sekar, Qinghua Jiang, Chang Shu, and Boo Cheong Khoo. Fast flow field prediction over airfoils using deep learning approach. *Physics of Fluids*, 31(5), 2019.