

Neural Network Enhanced Shock-Capturing Schemes for Compressible Flows

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In this research, machine learning techniques will be applied to shock-capturing schemes to further enhance the numerical methods' accuracy on unsteady turbulent compressible flow problems. The main purpose of this research is to find a more computationally efficient method for evaluating fluxes through artificial neural networks. To reduce the cost of the data-driven method, the neural network has to be compact, physics-informed, and intrinsically numerical accurate. In the current stage of this research, the target shock-capturing method is the fifth-order weighted essentially non-oscillatory (WENO) method. The smoothness indicators, nonlinear weights, and flux evaluation coefficient will be replaced by neural networks and trained by several compressible flow data set. The possible testing problems are inviscid Burgers' equation, the Shu-Osher problem, and the 2D double Mach reflection test. These problems are highly turbulent and consists discontinuous shock interfaces where traditional WENO methods would introduce too much numerical diffusion.

I. INTRODUCTION

High-order CFD methods are one of the most popular research topics in the CFD research community. The methods are potentially more computationally efficient than the low-order methods by using fewer computational grid points to achieve the same degree of accuracy [1]. However, due to the Gibbs phenomenon, conventional high-order approximations will suffer numerical instability in the vicinity of the discontinuous interfaces and eventually lead to failed simulations. This causes high-order methods very hard to apply to complex application problems, especially for flow fields that are highly turbulent or contain shock waves. In the field of supersonic and hypersonic simulation, shock-fitting and shock-capturing methods are the two common approaches to address problems involved with strong shock waves.

The shock-fitting method is introduced by Moretti and Abbett [2] for simulating the supersonic flow around blunt objects. The method treats the shock front as one of the boundary conditions and the inflow states are computed through the Rankine-Hugoniot jump condition [3]. To track the location of the shock front, the shock movement can be computed through the time derivative of the Rankine-Hugoniot conditions with a characteristic relation [4], the time derivative of the Rankine-Hugoniot conditions with a momentum equation [5], or the shock velocity evaluated through Riemann invariants [2, 6]. Since the fluid states behind the shock front usually are relatively smooth compared with the solution around the shock, this allows conventional high-order approaches can be applied to the problem with strong shock when combined with shock-fitting techniques [7]. However, shock-fitting requires posteriori knowledge of the flow field to specify the shock front location in the computational domain. This makes shock-fitting methods are hard to ap-

ply on problems with multiple shock interactions or flow field with shock bubbles.

On the other hand, shock capturing methods use more robust flux evaluation schemes and thus require no empirical understanding of the flow field. Hence shock-capturing methods are more popular in both academic research and industrial applications for the past few decades [7]. To address the numerical instability due to the strong shock, several shock-capturing frameworks have been proposed, such as the total variation diminishing (TVD) approach from Harten [8], Monotonic Upstream-centered Schemes for Conservation Laws (MUSCL) from Van Leer [9], and the essentially non-oscillatory (ENO) family from Harten [10]. In the ENO family, the weighted essentially non-oscillatory (WENO) [11–13] methods gain more popularity among other shock-capturing methods due to the adaptive stencil selection process with nonlinear weights. Even though WENO methods have shown their capability in hypersonic flow simulations [14–16], the methods introduce excess amounts of numerical diffusion around discontinuous interfaces [17, 18]. To further improve the accuracy and efficiency of the WENO methods, several WENO variant schemes are proposed and tested on different PDE problems [19].

In recent years, data-driven modeling and analysis have become popular research topics in the field of fluid mechanics [20, 21]. The underlying physics can be extracted from analyzing the data of large-scale simulation or experimental measurement and helps researchers to understand fluid behavior in different ways. Data-driven techniques have been applied to PDE solving for accelerating simulations or improving solution accuracy. One of the common approaches is implementing an artificial neural network into the simulation routing and using the output from the network to estimate numerical coefficients or variables. To ensure the conservation laws of fluid, most of the data-driven models are physics-informed. One of the application is applying neural network on turbulence modeling for evaluating the

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anisotropic Reynolds stress [22], LES wall shear stress [23], or subgrid-scale eddy viscosity [24].

This research focuses on applying neural network on the shock-capturing scheme, or more specific, the WENO methods from Jiang and Shu [12]. Similar works have been done by literatures [25–27].

II. OBJECTIVES

The goal of this research is to improve the 5th-order WENO method with neural networks in terms of computational efficiency. The idea is to construct a physics-informed model for the compressible flow problems. The ultimate goal is to establish a framework for effectively designing neural networks which can be applied to various nonlinear PDE simulations, to accelerate the simulation of compressible flow, and to discover undiscovered numerical properties for CFD.

III. APPROACH

A. Weighted Essentially Non-Oscillatory Scheme

The one-dimensional scalar conservation law can be expressed as follow:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0 \quad (1)$$

u is the state variable and f is the flux for the corresponding state. For the essentially non-oscillatory (ENO) family, the methods consider the solution on the grids are cell average of the state \bar{u} . The conservation law of cell average can be obtained through volume integrating equation 1 with a given domain $\Omega = \{(x, t) : x_{j-1/2} \leq x \leq x_{j+1/2}, t_i \leq t \leq t_{i+1}\}$ and apply Green's theorem:

$$\int_{x_{j-1/2}}^{x_{j+1/2}} (u^{i+1} - u^i) dx + \int_{t_i}^{t_{i+1}} (f_{j+1/2} - f_{j-1/2}) dt = 0 \quad (2)$$

note the cell average:

$$\bar{u}_j = \int_{x_{j-1/2}}^{x_{j+1/2}} u dx \quad (3)$$

with an infinitesimally small time step and the grid size h , the time derivative of the cell average:

$$\frac{\partial \bar{u}}{\partial t} + \frac{1}{h} (f_{j+1/2} - f_{j-1/2}) = 0 \quad (4)$$

The above equation provides the framework of the ENO family approach. The equation is similar to the finite volume method but also can be used in finite difference method.

The challenge of cell average representation is to estimate the flux of the actual state on the cell edge from

cell averages. The flux can utilize the neighboring cell averages and be estimated by the reconstruction via deconvolution [10] or the reconstruction via primitive function [11] process. For instance, the possible formulations of third-order ($r = 3$) flux reconstruction on a cell edge can be:

$$\begin{aligned} \hat{f}_{j+1/2}^{(1)} &= \frac{1}{3} \bar{f}_{j-2} - \frac{7}{6} \bar{f}_{j-1} + \frac{11}{6} \bar{f}_j \\ \hat{f}_{j+1/2}^{(2)} &= -\frac{1}{6} \bar{f}_{j-1} + \frac{5}{6} \bar{f}_j + \frac{1}{3} \bar{f}_{j+1} \\ \hat{f}_{j+1/2}^{(3)} &= \frac{1}{3} \bar{f}_j + \frac{5}{6} \bar{f}_{j+1} - \frac{1}{6} \bar{f}_{j+2} \end{aligned} \quad (5)$$

where \bar{f} is the flux based on cell average on the grid.

One of the novelties in the ENO family schemes is the algorithm adaptively selecting stencils depending on the total variation. In Harten approach [8], they measure the total variation of candidate stencils recursively in L^1 -norm and select the smoothest stencil. Shu and Osher [11] measure the total variation in L^2 -norm which the measurement coefficients can be precomputed and the recursive stencil searching process is not required. Liu et al. [28] introduced the first weighted essentially non-oscillatory (WENO) scheme in the literature which uses nonlinear weights ω to linearly combine the candidate stencils together. In other words, the WENO method approximates the reconstructed flux on cell edges by a summation of the candidate stencils ($r = 3$):

$$f_{j+1/2} \approx \hat{f}_{j+1/2} = \omega_1 \hat{f}_{j+1/2}^{(1)} + \omega_2 \hat{f}_{j+1/2}^{(2)} + \omega_3 \hat{f}_{j+1/2}^{(3)} \quad (6)$$

where

$$\omega_i = \frac{\sigma_i}{\sum_{k=1}^r \sigma_k} \quad (7)$$

and

$$\sigma_i = \frac{\gamma_i}{(\epsilon^* + \beta_i)^2} \quad (8)$$

$\epsilon^* = 10^{-6}$ and γ is the optimal coefficients of the scheme. For $r = 3$ case, the optimal coefficients are:

$$\gamma_1 = \frac{1}{10}, \quad \gamma_2 = \frac{3}{5}, \quad \gamma_3 = \frac{3}{10} \quad (9)$$

When the smooth indicators β are all identical or small enough, the nonlinear weights ω will reduce to the optimal coefficients γ which make the flux reconstruction process $2r - 1$ th order accurate. Hence, the WENO method with $r = 3$ is also known as WENO5. Jiang and Shu [12] suggested the smooth indicator β should be computed as follow to guarantee the $2r - 1$ th order accuracy in smooth region:

$$\beta_i = \sum_{l=1}^{r-1} h^{2l-1} \int_{x_{j-1/2}}^{x_{j+1/2}} \left(\frac{\partial^l \hat{f}^{(i)}}{\partial \xi^l} \right)^2 d\xi \quad (10)$$

For $r = 3$ case, the above integration yields:

$$\begin{aligned}\beta_1 &= \frac{13}{12}(\bar{f}_{j-2} - 2\bar{f}_{j-1} + \bar{f}_j)^2 + \frac{1}{4}(\bar{f}_{j-2} - 4\bar{f}_{j-1} + 3\bar{f}_j)^2 \\ \beta_2 &= \frac{13}{12}(\bar{f}_{j-1} - 2\bar{f}_j + \bar{f}_{j+1})^2 + \frac{1}{4}(\bar{f}_{j-1} - \bar{f}_{j+1})^2 \\ \beta_3 &= \frac{13}{12}(\bar{f}_j - 2\bar{f}_{j+1} + \bar{f}_{j+2})^2 + \frac{1}{4}(3\bar{f}_j - 4\bar{f}_{j+1} + \bar{f}_{j+2})^2\end{aligned}\quad (11)$$

This study will focus on the WENO method ($r = 3$) implemented by Jiang and Shu [12] and the scheme will be referred to WENO5-JS. The following neural network enhanced shock-capturing schemes will base on the WENO5-JS.

B. Stevens and Colonius Approach

In Stevens and Colonius research [25], they proposed a methodology to enhance WENO5-JS and potentially other shock-capturing schemes. The idea of this approach is to utilize the coefficients from a known shock-capturing method, in this case, WENO5-JS, and improve the coefficient for evaluating the flux on cell edge through a neural network. They expressed equation 6 in terms of coefficients of cell average fluxes:

$$\hat{f}_{j+1/2} = c_{-2}\bar{f}_{j-2} + c_{-1}\bar{f}_{j-1} + c_0\bar{f}_j + c_1\bar{f}_{j+1} + c_2\bar{f}_{j+2}\quad (12)$$

The first step of obtaining the neural network enhanced coefficients, c_i , is computing the corresponding coefficients from WENO5-JS, \tilde{c}_i :

$$\begin{aligned}\tilde{c}_{-2} &= \frac{1}{3}\omega_1 \\ \tilde{c}_{-1} &= -\frac{7}{6}\omega_1 - \frac{1}{6}\omega_2 \\ \tilde{c}_0 &= \frac{11}{6}\omega_1 + \frac{5}{6}\omega_2 + \frac{1}{3}\omega_3 \\ \tilde{c}_1 &= \frac{1}{3}\omega_2 + \frac{5}{6}\omega_3 \\ \tilde{c}_2 &= -\frac{1}{6}\omega_3\end{aligned}\quad (13)$$

Then these five WENO5-JS coefficient are the input to the neural network which returns the change to each coefficient, $\Delta\tilde{c}_i$. The network has three hidden layers with three perceptrons in each layer. The study of neural network structure selection will be discussed in the later section. After the change of the coefficients, $\Delta\tilde{c}_i$, have been decided, the value will be added to the WENO5-JS coefficients, \tilde{c}_i , to get the preliminary coefficients, \hat{c}_i . To ensure the conservative property of the interpolation process, the sum of \hat{c}_i should be unity. This can be achieved by convert the problem to a problem that minimizing the

change of coefficient in terms of L^2 -norm:

$$\begin{aligned}\min_{c \in \mathbb{R}^5} \sum_{i=-2}^2 (c_i - \hat{c}_i) \\ \text{s.t. } \sum c_i = 1\end{aligned}\quad (14)$$

where c is the finalized machine learning coefficients. The above affine transformation can analytically computed by:

$$\Delta c_i = \frac{1 - \sum \hat{c}_i}{5}\quad (15)$$

where

$$c_i = \hat{c}_i + \Delta c_i\quad (16)$$

The neural network predicted flux will be computed by an inner product of the cell average flux with the finalized coefficients c_i . Fig. 1 is the resulting schematic of the entire prediction process. In the literature, Stevens and Colonius referred to this procedure as WENO-NN. The detailed properties and training data used for the networks will be revealed in the following sections.

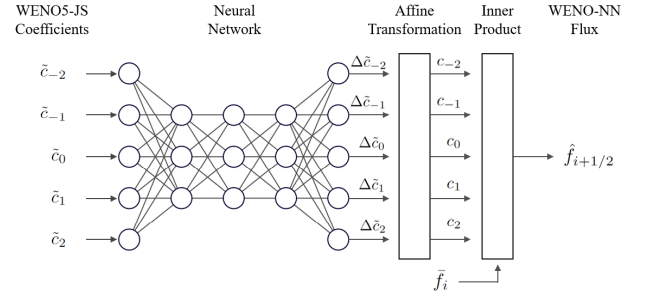


FIG. 1. Schematic of the neural network enhanced shock-capturing procedure by Stevens and Colonius [25]

IV. DATA SET

A. WENO-NN

The training data for WENO-NN is from a set of analytic functions. The input cell average data can be obtained through the spatial integration from equation 3 and output of the flux on cell edge will also be stored. The candidate functions are step functions, sawtooth waves, hyperbolic tangent functions, sinusoids, polynomials, and sums of the above. To prevent duplicate information in the data set, newly imported data will be checked if any similar data is already existed in L^2 norm sense. The expected amount of data entries is around 70,000.

V. NUMERICAL IMPLEMENTATIONS

A. WENO5-JS Solver

The WENO5-JS solver is the base solver for all of the data-driven approaches and coded in C++. The solver establishes the fundamental framework for implementing machine learning shock-capturing schemes and provides baseline solutions for evaluating computational efficiency between different methods. For the flux splitting, the solver uses the local Lax-Friedrichs method [4] for low computation time and an acceptable amount of numerical diffusion:

$$f_{LF}^{\pm}(u) = \frac{1}{2} [f(u) + \pm \alpha u] \quad (17)$$

$$\alpha = \max \left| \frac{\partial f}{\partial u} \right|$$

where α is the maximum eigenvalue from the system Jacobian matrix. The third-order SSP Runge-Kutta scheme [29] is used for time integration for the temporal total variation diminishing property and the low storage character. The time-stepping procedure can be expressed as:

$$\begin{aligned} u^{(1)} &= u^{(n)} + \Delta t L(u^{(n)}) \\ u^{(2)} &= \frac{3}{4}u^{(n)} + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}) \\ u^{(n+1)} &= \frac{1}{3}u^{(n)} + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}) \end{aligned} \quad (18)$$

The validity of the WENO5-JS solver has been verified by the Shu-Osher problem. Shu-Osher problem is a classic test case for shock-capturing due to the problem contains both shock wave and turbulent behavior. Fig. 2 shows the density distribution from both Shu and Osher [11] and the implemented WENO5-JS solver. The exact solution is computed from 10,000 uniform grid points in x-direction with CFL number $\nu = 0.8$. The numerical results are based on 200 grid points. The literature and the WENO5-JS are consistent with each other. Both low-resolution results are smeared right behind the shock due to the excess amounts of numerical error in the ENO family. The consistency of the two figures provides reliability to the WENO5-JS solver.

B. WENO-NN

WENO-NN uses both Keras [30] and TensorFlow [31] package in Python for the network training. The network weights are searched through the Adam optimizer [32]. Adam optimizer uses stochastic gradient descent to prevent neural network traps into local minimum and

records the descending direction to simulating the momentum of gradient drop. To make the training process parallelizable, patch training is used for the training process. The data is split into batches with around 100 data points in each batches. The training process requires around 10 epochs to complete and the weights of the network are randomly initialized. Sigmoid function is selected for the hidden layer activation function and the output activation function is a linear function. $\lambda = 0.1$ is used for L^2 regularization to prevent network over-fitting and the data is split into a training set of 80% of the data and a validation set of the other 20%. Mean squared error (MSE) is used for the training loss:

$$MSE = \frac{\sum_i^N (y_i - y_i^*)^2}{N} \quad (19)$$

The details of training procedure and parameter study will be revealed later.

VI. UPCOMING WORK

The upcoming work for this study is to start training the neural network with the data set from the analytical functions. After the training stage complete, the WENO-NN will be implemented in the current C++ codes and the methods will be evaluated and compared with WENO5-JS.

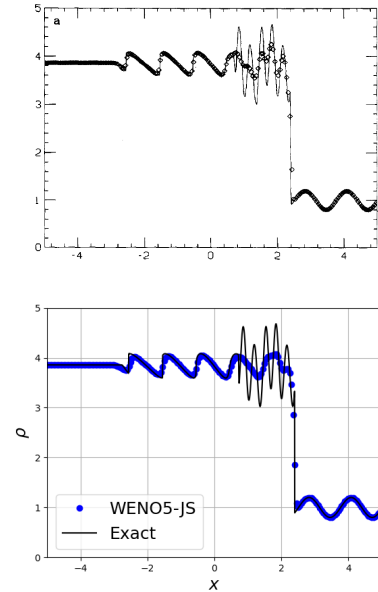


FIG. 2. Density distribution of Shu-Osher problem from Shu and Osher [11] (top) and the implemented WENO5-JS solver (bottom)

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