GPU–Accelerated WENO Schemes for DNS of Compressible Turbulent Flows*

Youngdae Kimc,1, Debojyoti Ghoshb,∗, Emil M. Constantinescu*c, Ramesh Balakrishnan*a

aComputational Science Division, Argonne National Laboratory, 9700 S Cass Ave., Lemont, 60439, IL, United States
bCenter for Applied Scientific Computing, Lawrence Livermore National Laboratory, 7000 East Ave., Livermore, 94550, CA, United States
cMathematics and Computer Science Division, Argonne National Laboratory, 9700 S Cass Ave, Lemont, 60439, IL, United States

Abstract

This paper explores strategies to transform an existing CPU-based high-performance computational fluid dynamics (CFD) solver, HyPar [1], for compressible flow simulations on emerging exascale heterogeneous, CPU+GPU, computing platforms. The scientific motivation for developing a GPU enhanced version of HyPar is to simulate canonical flows, such as homogeneous isotropic turbulence (HIT) of compressible flow in a triply periodic box. We show that optimizing memory operations and thread blocks results in a code that is more than 200x faster on GPUs than on CPUs. Using multiple GPUs

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration and by the U.S. Department of Energy, Office of Science, under contract number DE-AC02-06CH11357. E. Constantinescu was partially supported by U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR). Part of this work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

∗Corresponding author

Email addresses: youngdaekim26@gmail.com (Youngdae Kim), ghosh5@llnl.gov (Debojyoti Ghosh), emconsta@anl.gov (Emil M. Constantinescu), bramesh@anl.gov (Ramesh Balakrishnan)

1Present address: ExxonMobil Technology and Engineering Company, Annandale, NJ, 08801, United States. This work was done while the author was at Argonne National Laboratory as Postdoctoral Appointee.
and MPI communication, we demonstrate both strong and weak scaling of our GPU-based HYPar implementation on the Summit supercomputer at Oak Ridge National Laboratory.

**Keywords:** Navier–Stokes equations, GPUs, WENO schemes, compressible flows, direct numerical simulation

**2010 MSC:** 76F65, 65Y05, 76F05, 35Q30, 65M06

## 1. Introduction

Turbulence is characterized by the seemingly chaotic, yet correlated, motion of fluid elements (in both the Eulerian and Lagrangian sense) over a range of spatial and temporal scales. A distinguishing feature of turbulence, however, is the lack of clear separation between the scales of motion (unlike in the kinetic theory of gases), the large number of degrees of freedom, and the large range of length and time scales. Hence, though it is accepted that the dynamics of turbulence is described by the Navier-Stokes equation, it is prohibitively expensive to simulate all the length and time scales of motion, and for many cases of interest practically impossible, to simulate turbulence without appropriate models to account for the effect of the small scales on the evolution of the turbulent flow field. As a result, various theoretical statistical models have been proposed to explain the underlying mechanisms in turbulent flow by decomposing the velocity $\vec{U}$, pressure $p$, and temperature $T$ fields into the average and fluctuating quantities, $A(\vec{r},t) = \bar{A}(\vec{r},t) + a(\vec{r},t)$, where $\bar{A}$ and $a$ denote the ensemble average $\langle A \rangle$ and fluctuating $a$ terms in the decomposition. Approaches to formulate statistical models of turbulence [2], such as direct interaction approximation (DIA) [3, 4] and eddy damped quasi-normal markovianization (EDQNM) [5] have proposed evolution equations for higher-order correlations that are obtained by taking moments of the Navier-Stokes equations (NSE). In these equations, the temporal evolution of correlations, on the left hand side of the NSE, calls for modeling higher-order moments on the right hand side of the NSE, where again, the strong spatio-temporal correlations between the velocity components $\langle u_i^m u_j^n \rangle$, and between other flow quantities, have precluded attempts to close the hierarchy of moment equations and devise a universal model for turbulent flows.

The availability of massively parallel computing platforms offers a route for direct numerical simulation (DNS) of the Navier-Stokes equations, for
canonical flows, on simple geometries and for increasing Reynolds numbers. One such canonical flow that continues to be simulated on newer parallel computing platforms is that of forced isotropic turbulence in a triply periodic box. Using innovative methods to stir the flow (to ensure that the turbulence does not decay), pseudo-spectral solvers for incompressible flows have been used to simulate HIT on boxes consisting of 12288^3 grid points to achieve a maximum Reynolds number $Re_\lambda = 1300$ (where $\lambda$ denotes the Taylor microscale)\[6\]. These DNS flow fields can then be used validate existing theories, and also inform the development of sub-grid models by exploring the general two-point, two-time, space-time velocity correlation, defined by

$$R(\vec{x}, t) = \langle u_i(\vec{x}, t)u_j(\vec{x} + \vec{r}, t + \tau) \rangle$$  \hspace{1cm} (1)

where, $u_i, u_j (i, j = 1, 2, 3)$ denotes the fluctuating velocity components, $\vec{x} + \vec{r} = (x_1 + \delta x_1, x_2 + \delta x_2, x_3 + \delta x_3)$ denotes the distance between two points in the flow, $\tau$ denotes the temporal window, and $\langle \cdot \rangle$ denotes the ensemble average. The flow is said to be decorrelated when the correlation decreases with increasing $|\vec{r}|$, and increasing $\tau$, and vanishes above a critical distance $|\vec{r}|_d$ and $\tau_d$ that denote the decorrelation length and time, respectively. Similar expressions can be defined to correlate other quantities, such as the pressure ($p$) and temperature ($T$) between two points, and at two different times.

While there exists a veritable body of literature for HIT simulations of incompressible flows, HIT simulations of compressible flows are not quite as extensive. DNS of compressible turbulence requires solving the energy equation, in addition to the momentum equations (as in incompressible flows). Another complication that arises in simulating compressible flows is the appearance of shocks, and shocklets in compressible HIT, where the flow properties change abruptly across the shocklets. Hence, numerical methods for compressible turbulent flows must capture shocks, and also resolve all the turbulent scales of motion with minimal dissipation and dispersion errors. Therefore, resolving the relevant turbulence structures in compressible flows calls for high order of numerical accuracy and together with the ability to capture unsteady shocklets/shock waves. Weighted essentially nonoscillatory (WENO) schemes \[7, 8, 9, 10\] are a family of methods that use solution-dependent interpolation to achieve high-order accuracy for smooth flows and yield nonoscillatory solution across shocks and other discontinuities. These methods are constructed as a weighted sum of lower order interpolation schemes, where the weights depend on the local smoothness of the solution. When the solution is smooth, the weights converge to their optimal values.
that result in a higher order scheme; at or near discontinuities, the weights approach zero to bias the overall interpolation away from the discontinuous feature and avoid numerical oscillations. In this paper, we consider the fifth-order WENO scheme (WENO5) [8] because it is especially popular due to its high accuracy, computational efficiency, and scalability on distributed memory, homogeneous (multi-core) machines.

Traditional WENO schemes do not have a high spectral resolution, and this limits their ability to resolve all scales of interest in turbulent flows. Several high-resolution alternatives have been proposed in the literature that are based on the WENO algorithm. Compact-WENO schemes, such as hybrid compact-WENO [11, 12, 13] and CRWENO [14, 15] schemes, combine the high-spectral resolution of spectral (Padé) schemes with the solution-dependent nonoscillatory nature of WENO schemes. Bandwidth-optimized and low dispersion WENO schemes [16] construct interpolations that use additional stencil points to yield a higher resolution instead of higher accuracy. Finally, there have been many efforts to optimize the computation of the WENO weights [17, 18, 19, 20] to improve their convergence to the optimal values when the flow is smooth but not well-resolved. In this paper, we consider the WENO5 scheme as implemented in [8]; the novelty rests on the fact that the WENO5 implementation here is among the earliest (if not the first) for simulating HIT in compressible flows on heterogeneous (i.e. CPU+GPU) platforms, such as Summit (OLCF). In subsequent research, we will consider compact-WENO schemes.

Explicit methods offer the highest level of parallelism because they require only local communication; however, they have strict time-step restrictions. Semi-implicit or IMEX methods and implicit time-stepping methods circumvent this restriction by treating the spatial components partially or completely implicitly [21]. These methods tend to be significantly more stable for larger time steps at a steep computational cost of solving linear or nonlinear systems. The tradeoff between having to take many smaller time steps in the explicit case and fewer but more expensive time steps in the IMEX or implicit methods is application dependent. In a previous study we explored porting semi-implicit time-stepped N-S to GPUs [22], which revealed several difficulties in implementing such methods on GPUs. In particular the linear solvers prove to be challenging. This was observed by others as well [23].

In this work, we explore strategies to efficiently accelerate existing high-performance CPU code-base HyPar [1] on GPUs. GPUs require a fundamentally different programming paradigm than CPUs. Some memory oper-
ations that are efficient on CPUs could cause a serious performance degradation on GPUs. Since efficient memory operations are crucial for fully utilizing the massive parallel computing capability of GPUs, our focus is on optimizing the memory access patterns of HYPAR on GPUs. In particular, we aim to avoid slow memory transactions and reduce as many wasted computational resources (such as thread blocks) and memory transactions as possible. Our optimization approach results in more than 200 times faster computation time on GPUs than on CPUs. Using multiple GPUs and MPI communication, we demonstrate the scalability of our GPU-based implementation on the Summit supercomputer at Oak Ridge National Laboratory. We evaluate strong and weak scaling and investigate the impact of communication cost on the overall computation time. For a grid with $256^3$ points, our current GPU-based implementation can perform 100 time steps in 2 seconds using 512 GPUs.

The rest of the paper is organized as follows. In Section 2, we introduce background on the governing equations for compressible Navier-Stokes equations, their numerical methods, and an isotropic turbulence decay example. Section 3 describes our kernel design principles for efficiently implementing the existing CPU code-base on GPUs, with a specific focus on optimizing its memory access patterns. In Section 4, we present the computational performance of our GPU-based implementation over the isotropic turbulence decay example. We perform numerical comparisons between CPU and GPU implementations and demonstrate the scalability of our GPU implementation. We conclude our paper in Section 5.

2. Background

In this section we briefly introduce governing equations for compressible Navier-Stokes equations, their numerical methods, and the isotropic turbulence decay example. The example will be used to evaluate the computational performance of our GPU-based implementation in Section 4.

2.1. Governing Equations

We consider the non-dimensional, compressible Navier–Stokes equations [24] that can be expressed as a system of hyperbolic–parabolic partial differential equations (PDEs) as:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} + \frac{\partial \mathbf{h}}{\partial z} = \frac{\partial \mathbf{f}^v}{\partial x} + \frac{\partial \mathbf{g}^v}{\partial y} + \frac{\partial \mathbf{h}^v}{\partial z},$$

(2)
where \( \mathbf{u} = [\rho, \rho u, \rho v, \rho w, e]^T \) is the vector of conserved variables. The convective fluxes are

\[
\mathbf{f} = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
(e + p) u
\end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
\rho vw \\
(e + p) v
\end{bmatrix}, \quad \mathbf{h} = \begin{bmatrix}
\rho w \\
\rho uw \\
\rho w^2 + p \\
\rho vw \\
(e + p) w
\end{bmatrix},
\]

where \( \rho \) is the density, \( u, v, w \) are the Cartesian components of the velocity, \( p \) is the pressure, and \( e \) is the internal energy given by

\[
e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho \left( u^2 + v^2 + w^2 \right),
\]

and \( \gamma = 1.4 \) is the heat coefficient ratio. The viscous fluxes are

\[
\mathbf{f}^v = \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{yx} \\
\tau_{zx} \\
\mathbf{v} \cdot \mathbf{\tau}_x - q_x
\end{bmatrix}, \quad \mathbf{g}^v = \begin{bmatrix}
0 \\
\tau_{xy} \\
\tau_{yy} \\
\tau_{zy} \\
\mathbf{v} \cdot \mathbf{\tau}_y - q_y
\end{bmatrix}, \quad \mathbf{h}^v = \begin{bmatrix}
0 \\
\tau_{xz} \\
\tau_{yz} \\
\tau_{zz} \\
\mathbf{v} \cdot \mathbf{\tau}_z - q_z
\end{bmatrix};
\]

the viscous stresses are given by

\[
\tau_{ij} = \mu \frac{M_{\infty}}{R e_{\infty}} \left[ \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right],
\]

where \( Re_{\infty} \) and \( M_{\infty} \) are the reference Reynolds and Mach numbers, respectively, \( \mu \) is the normalized coefficient of viscosity, \( \mathbf{v} \equiv (u, v, w) \) is the velocity vector, and

\[
\mathbf{\tau} = (\tau_x, \tau_y, \tau_z).
\]

The thermal conduction terms are

\[
q_i = -\frac{\mu}{(\gamma - 1) Pr} \frac{M_{\infty}}{Re_{\infty}} \frac{\partial T}{\partial x_i},
\]

where \( T = \gamma p/\rho \) is the temperature, and \( Pr = 0.72 \) is the Prandtl number.
2.2. Numerical Method

The physical domain is discretized using a three-dimensional grid with \( N \) points in each dimension. The convective terms on the left-hand-side (LHS) of (2) are discretized with the conservative finite-difference formulation \([9, 10]\) and the WENO5 scheme \([8]\). This section briefly describes the spatial discretization of the convective flux \( f \) along \( x \); this can be extended trivially to the convective terms along the other dimensions. The spatial derivatives in the viscous terms on the right-hand-side (RHS) are discretized using fourth-order central finite differences. We thus obtain an ordinary differential equation (ODE) in time; this is evolved using the fourth-order Runge-Kutta method. A more detailed description of the numerical methodology is available in prior publications \([14, 15, 25]\).

We describe the upwind discretization of the convective terms by considering an arbitrary grid line along \( x \) and ignoring the other dimensions. The derivative is computed at a grid point \( j \) as

\[
\frac{\partial f}{\partial x} \bigg|_j = \frac{1}{\Delta x} \left( \hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} \right) + O(\Delta x^p) \tag{9}
\]

where the locations \( j \pm 1/2 \) denote the cell interfaces (see Figure 1), and \( p \) is the order of the discretization scheme. The numerical flux at the cell interface, \( \hat{f}_{j+\frac{1}{2}} \), is computed using the Roe scheme \([26]\) with the Harten entropy fix \([27]\):

\[
\hat{f}_{j+\frac{1}{2}} = \frac{1}{2} \left( \hat{f}^L_{j+\frac{1}{2}} + \hat{f}^R_{j+\frac{1}{2}} \right) - \frac{1}{2} \left| A_{j+\frac{1}{2}} \right| \left( \hat{u}^R_{j+\frac{1}{2}} - \hat{u}^L_{j+\frac{1}{2}} \right), \tag{10}
\]

where the superscripts \( L, R \) denote left- and right-biased discretizations, respectively. The dissipation matrix, \( \left| A_{j+\frac{1}{2}} \right| \), is computed from the eigensystem.
evaluated at the Roe-averaged state at the cell interface \( j + \frac{1}{2} \) as

\[
\left| A_{j+\frac{1}{2}} \right| = X_{j+\frac{1}{2}} \left| \Lambda_{j+\frac{1}{2}} \right| X^{-1}_{j+\frac{1}{2}}, \tag{11}
\]

where \( X \) is the matrix with columns as the right eigenvectors, and \( \Lambda \) is a diagonal matrix with the eigenvalues as its entries.

Each scalar component of \( \hat{f}^{L,R}_{j+\frac{1}{2}} \) and \( \hat{u}^{L,R}_{j+\frac{1}{2}} \) is computed using the WENO5 scheme. We describe this method for a left-biased scalar variable, \( \hat{f}^{L}_{j+\frac{1}{2}} \); the procedure for a right-biased scalar variable, \( \hat{f}^{R}_{j+\frac{1}{2}} \), can be obtained by reflecting the expressions around the cell interface \( j + \frac{1}{2} \). We drop the superscript \( L \) in the text below.

WENO schemes use a solution-dependent interpolation stencil selection [7, 8] to achieve high-order accuracy where the solution is smooth and to avoid oscillations across discontinuities. The WENO5 scheme is constructed by identifying three third-order interpolation schemes at the cell interface; the final interpolation method is their weighted sum, where the weights depend on the smoothness of the stencils underlying the corresponding third-order interpolation. These weights approach optimal values for smooth solutions; consequently, the method achieves fifth order of accuracy. In the presence of discontinuities or sharp gradients, the weights corresponding to those stencils approach zero. The final method has a stencil biased away from the discontinuity thus avoiding numerical oscillations.

The three third-order interpolation schemes and their optimal weights at cell interface \( j + \frac{1}{2} \) are

\[
\hat{f}^{1}_{j+1/2} = \frac{1}{3} f_{j-2} - \frac{7}{6} f_{j-1} + \frac{11}{6} f_{j}, \quad c_1 = \frac{1}{10}, \tag{12}
\]
\[
\hat{f}^{2}_{j+1/2} = -\frac{1}{6} f_{j-1} + \frac{5}{6} f_{j} + \frac{1}{3} f_{j+1}, \quad c_2 = \frac{6}{10}, \tag{13}
\]
\[
\hat{f}^{3}_{j+1/2} = \frac{1}{3} f_{j} + \frac{5}{6} f_{j+1} - \frac{1}{6} f_{j+2}, \quad c_3 = \frac{3}{10}, \tag{14}
\]

The fifth-order interpolation scheme at \( j + 1/2 \) is obtained as

\[
\hat{f}_{j+1/2} = \sum_{k=1,2,3} c_k \hat{f}^{k}_{j+1/2} = \frac{1}{30} f_{j-2} - \frac{13}{60} f_{j-1} + \frac{47}{60} f_{j} + \frac{27}{60} f_{j+1} - \frac{1}{20} f_{j+2}. \tag{15}
\]
The solution-dependent weights are computed as
\[
\omega_k = \frac{\alpha_k}{\sum_k \alpha_k}; \quad \alpha_k = \frac{c_k}{(\epsilon + \beta_k)^p}; \quad k = 1, 2, 3,
\]  
(16)

where \(\epsilon = 10^{-6}\) is a small number to prevent division by zero and \(\beta_k\) are the smoothness indicators for the stencils:
\[
\beta_1 = \frac{13}{12}(f_{j-2} - 2f_{j-1} + f_j)^2 + \frac{1}{4}(f_{j-2} - 4f_{j-1} + 3f_j)^2,
\]  
(17)
\[
\beta_2 = \frac{13}{12}(f_{j-1} - 2f_j + f_{j+1})^2 + \frac{1}{4}(f_{j-1} - f_{j+1})^2,
\]  
(18)
\[
\beta_3 = \frac{13}{12}(f_j - 2f_{j+1} + f_{j+2})^2 + \frac{1}{4}(3f_j - 4f_{j+1} + f_{j+2})^2.
\]  
(19)

The WENO5 scheme is obtained by multiplying the third order interpolation schemes by the solution–dependent weights instead of the optimal weights:
\[
\hat{f}_{j+1/2} = \sum_{k=1,2,3} \omega_k \hat{f}_{j+1/2}^k
\]
\[
= \frac{\omega_1}{3} f_{j-2} - \frac{1}{6} (7\omega_1 + \omega_2) f_{j-1} + \frac{1}{6} (11\omega_1 + 5\omega_2 + 2\omega_3) f_j
\]
\[
+ \frac{1}{6} (2\omega_2 + 5\omega_3) f_{j+1} - \frac{\omega_3}{6} f_{j+2}.
\]  
(20)

If the solution is locally smooth, \(\omega_k \to c_k, k = 1, 2, 3\), and (20) is equivalent to (15).

2.3. Example: Isotropic Turbulence Decay

We simulate the decay of isotropic turbulence in a periodic domain; this is a canonical turbulent flow problem [28, 29] characterized by the transfer of energy from larger to smaller length scales. Our governing equations do not include a turbulence model; we thus conduct a direct numerical simulation (DNS) by resolving the Kolmogorov scale. The initial solution comprises a divergence-free velocity field with random isotropic fluctuations that satisfy the following kinetic energy spectrum:
\[
E(k) = 16 \sqrt{\frac{2}{\pi}} \frac{u_0^2}{k_0} \left(\frac{k}{k_0}\right)^4 \exp \left[-2 \left(\frac{k}{k_0}\right)^2\right],
\]  
(21)
(a) Density at $z = 0$ and $t/\tau = 3$.

(b) Vorticity magnitude at $z = 0$ and $t/\tau = 3$.

Figure 2: Direct numerical simulation of HIT in a triply-periodic domain discretized by a $128^3$ grid. The solution is obtained at a final time of $t/\tau = 3$, where $\tau$ is the turbulent time scale.

where $k$ is the wavenumber, $E$ is the kinetic energy, $u_0$ is the RMS turbulence intensity, and $k_0$ is the wavenumber corresponding to the maximum energy. The domain is a cube of length $2\pi$ with periodic boundaries. The initial density and pressure are constant ($\rho = 1$, $p = 1/\gamma$). We specify $u_0 = 0.3$ and $k_0 = 4$; this results in a smooth turbulent flow. The Taylor microscale-based Reynolds number, $Re_\lambda = \rho u_0 \lambda / \mu$, is specified as 50, where $\lambda$ is the Taylor microscale.

Figures 2(a) and 2(b) show the density and vorticity magnitude contours, respectively, on a two-dimensional plane at $z = 0$ for a solution obtained at $t/\tau = 3$, where $\tau = \lambda / u_0$ is the turbulent time scale. This solution is obtained on a grid with $128^3$ points and a time step $\Delta t = 0.025$ (CFL $\approx 1$). Figure 3 shows the initial and final energy spectra for the solution. As the flow evolves and the turbulence decays, we observe an energy transfer from the lower to higher wavenumbers, as expected. The $k^{-5/3}$ relationship is also plotted for reference. We use this example in our subsequent studies.

3. Implementation Principles on GPUs

In this section we present our kernel design principles to efficiently implement HyPar on GPUs, with a specific focus on optimizing its memory access patterns. Since many core operations of HyPar are memory-bound, it is crucial for computational performance to avoid slow memory transactions
and reduce as many wasted compute resources and memory transactions as possible. To achieve this, we introduce the following three design principles that target optimized computational performance on GPUs: i) lexicographic thread configuration; ii) removing data transfers between CPUs and GPUs during operation; iii) performing coalesced memory access. In the following subsections we introduce these principles one by one with numerical performance comparisons with those of alternative approaches. All of the numerical experiments in this section have been performed on a single Nvidia’s V100 using CUDA.

We note that we have also tried some number of user-defined caching approaches such as manually allocating dynamic shared memory (instead of relying on the underlying GPU’s automatic caching mechanism) to share function values in (17)–(19) between different grid points. However, we observed no gains or even worse performance than when we relied on the given automatic caching mechanism. Therefore, we did not employ manual shared memory management in our implementation. We believe that such a worse performance with shared memory is partly because of a significantly improved cache performance of the Volta architecture as described in [30, See
3.1. Lexicographic thread block configuration

By default, we have a one-to-one mapping from threads of a GPU kernel into the grid points of a discretization scheme so that each thread is assigned to a single grid point. One way to implement this mapping is to assign threads in the same lexicographic order of the coordinate values of the grid points. In this case, each thread block is one-dimensional, and the order of threads within a block follows the same lexicographic order of the corresponding grid points. An alternative way to implement the mapping is to use tiling. For example, if a grid is 64 × 64, we can generate thread blocks, each of which is of size 32 × 8 (256 threads per block). A total of 16 thread blocks are needed to cover the entire grid in this case.

The tiling approach is intuitive, however, it could cause many wasted threads when some dimension of the grid is not a multiple of the number of threads of a warp. For example, if a given grid is of size 65 × 64, the previous 32 × 8 thread block scheme will result in some thread blocks having many inactive threads. In this case, thread blocks covering grid points with 65 as its x-coordinate have only 8 active threads among 256 threads. Such an unfavorable grid naturally occurs when we perform computation using ghost points, which are added to the existing grid scheme.

Figure 4 compares the computation time between the tiling and lexicographic thread block configurations, obtained from a kernel computing the weights (16). The grid employed is of size 65 × 64 × 64, and the thread block configuration for the tiling approach is 32 × 8. As we see in the figure, the tiling approach shows a slower computation time than that of the lexicographic configuration. Similar results were obtained using different block configurations for tiling.

| Tiling | 0.48 (msecs) |
|--------|--------------|
| Lexicographic | 0.36 (msecs) |

Figure 4: Tiling vs lexicographic over weights computation (16)
3.2. No data transfers between CPUs and GPUs

When we solve the 3-dimensional Navier-Stokes equations (2) using the WENO5 scheme, our profiling results described in Figure 5 show that about 90% of the computation time has been spent in the five core operations. These are: 

- **WENO** – computing weights (16),
- **Interp** – calculation of the flux at cell interfaces (20),
- **Upwind** – computing the upwind flux using Roe's scheme (10),
- **Parabolic** – computing the viscous terms on the RHS of (2),
- **Derivative** – computing the derivatives in the viscous terms using fourth-order central finite differences.

Since these operations are defined for each grid point independently, they can be computed in parallel, providing an opportunity for acceleration on GPUs. Our initial implementation of computing weights (WENO) on GPUs shows about two orders of magnitude of faster computation time than on CPUs.

![Figure 5: Percentage of time spent on core operations](https://sourceware.org/binutils/docs/gprof)

However, if we include data transfer time to initiate the computation on the device and return the results back to the host, the overall computation time significantly degrades. In Figure 6, we present the computation times on CPUs and GPUs, respectively, and data transfer time for one function call of the WENO routine for $64 \times 64 \times 64$ grid. Although the computation time has improved by more than 400 times on GPUs, the time for data transfer dominates the overall computation time, making it even slower than on CPUs. The high data transfer time is attributed to the large memory size for storing weights, which is around 400 MB.

To avoid such significant degradation, we implement all operations that process data entirely on GPUs, except for the initial data read and return of a final solution. Since data required for each GPU kernel is processed only

---

2 We used gprof available at [https://sourceware.org/binutils/docs/gprof](https://sourceware.org/binutils/docs/gprof)
on GPUs, they can be readily found in GPU’s global memory. Therefore, we do not have to transfer any data between CPUs and GPUs during operation, removing one of the main performance bottlenecks. This allows us to recover the fast computation time on GPUs as shown in Figure 6. We note that we also used CUDA-aware MPI for MPI implementation to support multiple GPUs so that we do not have to communicate via staging through CPUs.

3.3. Coalesced memory access

In Figure 7(a) we describe the memory layout of our original CPU-based code, where we use double-precision for floating point computation. In the figure, each coordinate value of \((\bar{x}, \bar{y}, \bar{z})\) denotes the maximum grid coordinate value of the corresponding dimension, and the superscript/subscript on \(v\) represent the index of a grid point/variable, respectively. The five variables for each grid point are located one after the other in memory. Because grid points are allocated in memory in the lexicographic order and are accessed sequentially along with their five variables, memory accesses exhibit locality in this case, leading to fast memory operations through a high cache hit ratio.

However, this memory layout gives rise to 40-byte strided memory accesses on GPUs as shown in Figure 8(a) potentially incurring more memory transactions than needed. Unlike the CPU case, 32 threads in a warp are
executed in lockstep on GPUs. Since each grid point has five variables of size 8 bytes each (double-precision), a warp accessing the first variable of 32 grid points will result in 10 128-byte memory transactions\(^3\) assuming that the accessed data have not been found in cache. Bus utilization (the ratio of data actually read to fetched) is 20\% (\(= 256/1280 \times 100\)) in this case.

In contrast, if we allocate each variable of grid points one after the other as shown in Figure 7(b) we will need only 2 128-byte memory transactions with 100\% bus utilization (\(= 256/256 \times 100\)) as shown in Figure 8(b). Therefore, coalesced memory access provides more efficient memory transactions.

\[\begin{array}{c}
\text{0} & \cdots & \text{31} \\
\text{WARP} & & \\
\end{array}\]

\[\begin{array}{c}
\text{0} & \cdots & \text{31} \\
\text{WARP} & & \\
\end{array}\]

(a) 40-byte strided memory access for the old layout

(b) 8-byte strided memory access for the new layout

Figure 8: Different strides for different memory layouts

Although bus utilization is low in the former case, later accesses to other variables might be served via cache, resulting in similar overall memory access time to that of the latter case. However, this expectation depends on the lifetime of fetched data in cache. The amount of fetched data is proportional to the number of grid points. Since cache size is limited (128 KB for L1 cache on Nvidia’s Volta architecture), for larger number of grid points the likelihood of the eviction of data in cache becomes higher, reducing their lifetime in cache.

Figure 9 demonstrates the effect of the aforementioned two strided accesses on memory bandwidth with respect to varying grid sizes. In the figure, the \(x\)-label represents the size of each dimension, for example 16 repre-

\[^3\text{The granularity of L1 cache update is 128-byte.}\]
sents \(16 = |x| = |y| = |z|\). Since we have the same number of grid points along each dimension, the total number of grid points is \(16 \times 16 \times 16\) in this case. The memory bandwidth was measured on the kernel to compute the weights (16). We observe that the speedup of 8-byte strided access with respect to 40-byte strided access becomes larger as we increase the grid size. If data were frequently found in cache for 40-byte strided access, the bandwidth ratio between those two access methods would be similar and stay constant. However, the speedup is amplified as we increase the grid size, suggesting that there have been many more wasted memory transactions for 40-byte strided access than those of 8-byte strided access.

4. Experimental Results

In this section we present the computational performance of our GPU-based implementation on the isotropic turbulence decay example described in Section 2.3. In Section 4.2, we compare its computation time with that of the CPU-based implementation. We demonstrate the scalability of our implementation using multiple GPUs in Section 4.3.

4.1. Setting

We use the same parameters for the isotropic turbulence decay example as described in Section 2.3 except for time step which we set it to 0.002.
Since we are interested in mainly the speedup of the computation time of our GPU-based implementation, we perform 100 time steps and measure its wall time for all experiments in this section.

All experiments have been performed on the Summit supercomputer at Oak Ridge National Laboratory, where each compute node has 6 Nvidia’s Volta GPUs and 2 POWER9 CPU sockets each having 21 physical cores and 4 hardware threads on each physical core.

4.2. One GPU vs one CPU core

Figure 10 presents the wall times of one GPU and one CPU core, respectively, for executing 100 time steps over varying grid sizes. From the results, we make two observations. The first observation is that up until $64^3$ the grid size is not large enough to fully utilize the massive parallel computing capability of GPUs. Although the grid size becomes 8 times larger when we change its size from $32^3$ to $64^3$, the computation time on GPUs increases by just 4.46x. This behavior is in contrast to the proportional increase of wall times on CPUs as we increase the grid size. The disproportional increase of the computation time on GPUs between grids with $32^3$ and $64^3$ points implies that there are many number of idle computation units when we solve over grids with $32^3$ points or less.

Once we reach a grid with $64^3$ points, however, the computational resources on GPUs start to saturate. This is verified by checking the computation time between grids of sizes $64^3$ and $128^3$: the wall time increases exactly at the same rate as the increase of the grid size in this case. As shown in the figure, for grids having more than $64^3$ points this proportionality is maintained, implying that we are extensively making use of GPUs. In the case where multiple GPUs are employed as in Section 4.3, our observation provides a guideline for determining the appropriate number of grid points to be assigned to each GPU that prevents under utilization.

We note that a grid with $208^3$ points is the maximum size HYPar can run on one GPU because of the 32 GB memory limit on V100. For V100 with 16 GB of memory, the maximum size is around $160^3$. We also note that we did not measure the computation time on the CPU for the largest grid, since it is expected to be more than 5 hours based on its consistent increase in computation time as the grid size increases.

Our second observation is that the computation time on one GPU is
The speedup is largely attributed to the acceleration of the \texttt{WENO} routine: we achieved about 400 times faster computation time compared to that of the CPU-based code. Since it takes about 45\% of the total computation time on CPUs as described in Figure 5, the improved computation time of the \texttt{WENO} routine significantly affects the overall acceleration on GPU. However, not all routines showed such large gains. For the \texttt{Interp} and \texttt{Upwind} routines, the gains were about a factor of 100 and 250, respectively. This is because they are computationally less involving than the \texttt{WENO} routine.

We note that the accelerations for smaller grids are not as large as those for larger grids as shown in Figure 10, since they are not large enough to fully utilize GPUs as we have seen in the preceding observation.

---

\footnote{4}{Considering that each CPU on a node of the Summit supercomputers has 42 physical CPU cores, this speedup amounts to 5x speedup than that on a single CPU.}
Figure 11: Strong scaling over a grid with $256^3$ points

4.3. Multiple GPUs using MPI

We demonstrate scalability of HyPar by evaluating strong and weak scaling over varying number of GPUs and grid points. Communication between GPUs was performed via CUDA-aware MPI, which allowed us to directly communicate between memories of multiple GPUs on the same or different nodes without staging them through CPUs.

Figure 11 describes our strong scaling results. We fix the number of grid points to $256^3$ and compute the speedup over up to 512 GPUs. Since a grid with $256^3$ points cannot be loaded on a single GPU due to its memory limit, the $x$-axis starts from 8 GPUs so that each GPU is assigned to $128^3$ grid points. Table 1 presents the grid shape per GPU we used for decomposing $256^3$ grid for our strong scaling experiments.

From the result, we observe that our GPU implementation scales well with the number of GPUs. We were able to perform 100 time steps in 2 seconds using 512 GPUs for $256^3$ grid. However, we observe that the increase rate of the speedup diminishes as the number of GPUs increases. The reason for such decrease is because the MPI communication cost becomes a dominating factor to the overall cost.

The wall time for 8 GPUs was 24.62 secs, and it took about 3.14 secs for the MPI communication. In this case, the communication to computation percentage ratio was $12\% \left( = \frac{3.14}{24.62} \times 100 \right)$. However, for 64 GPUs the ratio became $45\% \left( = \frac{2.40}{5.24} \times 100 \right)$, and it was $58\% \left( = \frac{1.11}{1.90} \times 100 \right)$
Table 1: Grid shape per GPU for decomposing 256\(^3\) grid

| # GPUs | Grid shape per GPU |
|--------|--------------------|
| 8      | 128 × 128 × 128    |
| 16     | 64 × 128 × 128     |
| 32     | 64 × 64 × 128      |
| 64     | 64 × 64 × 64       |
| 128    | 32 × 64 × 64       |
| 256    | 32 × 32 × 64       |
| 512    | 32 × 32 × 32       |

For 512 GPUs. Since our implementation on GPUs is significantly faster than the CPU-based implementation, the impact of the communication cost quickly becomes substantial. We note that the diminishing rate seemed to be accelerated when we started to employ 32\(^3\) grids (for 128–512 GPUs). We think this is partly because GPUs were not fully utilized for such small grids, as we discussed in Section 4.2.

For weak scaling test, we used three different grid schemes per GPU, 64 × 64 × 64, 128 × 128 × 128 and 160 × 160 × 160. The size of the original grid increases proportionally to the number of GPUs: for 64 GPUs with 160 × 160 × 160 (128 × 128 × 128 and 64 × 64 × 64) grid per GPU, the shape of the original grid is 640 × 640 × 640 (512 × 512 × 512 and 256 × 256 × 256), hence 4 GPUs are assigned to each dimension.

Figure 12 presents our weak scaling results in terms of efficiency. A similar trend of diminishing efficiency for larger number of GPUs has been observed as with our strong scaling results. The diminishing rate largely depends on the communication to computation cost ratio. As we see in Figure 13, the ratio is higher for 64\(^3\) grid, 43% for 64 GPUs, than those for 128\(^3\) and 160\(^3\) grids, 27% and 23% for 64 GPUs, respectively. Therefore, 64\(^3\) grid showed a worse efficiency than those of 128\(^3\) and 168\(^3\) grids. In Figure 13, "Comp" denotes the pure computation time on each GPU. In all cases, the computation time on individual GPU was almost the same. We note that the original problem sizes of these schemes are different, hence faster wall time does not mean that it can solve the problem faster than the other scheme.
5. Conclusions

In this work, we explore the development of HYPar [1], a CPU-based high-performance code, to run efficiently on GPU based computing platforms. The naive use of the SIMD directives in an existing CPU code-base, by primarily targeting memory operations across the CPU-GPU bus, leads to severe performance degradation on GPUs. A bottom-up approach, that focused on forming the equations directly on GPUs, significantly reduces traffic between CPUs and GPUs, across the PCIe bus/NVLink, and improves the performance of the code quite significantly.

This work focuses on the three-dimensional compressible Navier-Stokes equations discretized in space by a nonlinear fifth-order WENO scheme and in time by an explicit Runge-Kutta method. This combination of numerical discretization schemes allows us to exploit high potential parallelism and scalability while maintaining high numerical accuracy and spectral resolution.

We demonstrate our results on a canonical turbulent flow problem, the decay of isotropic turbulence in a periodic domain characterized by the transfer of energy from larger to smaller length scales. To this end, we conduct DNS studies by resolving the Kolmogorov scale on a grid of size $512 \times 512 \times 512$. 

Figure 12: Weak scaling over up to 64 GPUs and $512^3$ grid
The WENO5 implementation in this paper is among the earliest (if not the first) for simulating HIT in compressible flows on heterogeneous platforms, such as Summit (OLCF). We carry out simulations on up to 512 GPUs with MPI communication across GPU containing nodes. Our results demonstrate that the optimizations proposed in this work can lead to more than 200x reduction in computation time on GPUs than on CPUs. The scalability of the GPU-accelerated code is evaluated by using strong and weak scaling, and we investigate the impact of communication cost on the overall computation time.

The results presented in this paper extend to low-dissipation, bandwidth-optimized WENO schemes that are better suited to DNS studies. In ongoing work, we are exploring compact-WENO schemes, such as the CRWENO or hybrid schemes, which have higher-spectral resolution and are more accurate. However, they require the solution of tridiagonal systems of equations; this presents additional challenges for GPUs.
References

[1] D. Ghosh, HyPar Repository, https://bitbucket.org/deboghosh/hypar (2015).

[2] J. M. Wallace, Space-time correlations in turbulent flow: A review, Theoretical and Applied Mechanics Letters 4 (2) (2014) 022003. doi:10.1063/2.1402203

[3] R. H. Kraichnan, The structure of isotropic turbulence at very high reynolds numbers, Journal of Fluid Mechanics 5 (4) (1959) 497–543. doi:10.1017/S0022112059000362

[4] R. H. Kraichnan, Kolmogorov’s hypotheses and eulerian turbulence theory, The Physics of Fluids 7 (1723) (1964). doi:10.1063/1.2746572

[5] M. Lesieur, S. Ossia, 3D isotropic turbulence at very high Reynolds numbers: EDQNM study, Journal of Turbulence 1 (1) (2000) 007.

[6] D. Buaria, A. Pumir, E. Bodenschatz, Self-attenuation of extreme events in navier-stokes turbulence, Nature communications 11 (1) (2020) 5852–5852.

[7] X.-D. Liu, S. Osher, T. Chan, Weighted essentially non-oscillatory schemes, Journal of Computational Physics 115 (1) (1994) 200–212. doi:10.1006/jcph.1994.1187

[8] G.-S. Jiang, C.-W. Shu, Efficient implementation of weighted ENO schemes, Journal of Computational Physics 126 (1) (1996) 202–228. doi:10.1006/jcph.1996.0130

[9] C.-W. Shu, S. Osher, Efficient implementation of essentially non-oscillatory shock-capturing schemes, Journal of Computational Physics 77 (2) (1988) 439–471. doi:10.1016/0021-9991(88)90177-5

[10] C.-W. Shu, S. Osher, Efficient implementation of essentially non-oscillatory shock-capturing schemes, II, Journal of Computational Physics 83 (1) (1989) 32–78. doi:10.1016/0021-9991(89)90222-2

[11] N. A. Adams, K. Shariff, A high-resolution hybrid compact-ENO scheme for shock-turbulence interaction problems, Journal of Computational Physics 127 (1) (1996) 27–51. doi:10.1006/jcph.1996.0156
[12] S. Pirozzoli, Conservative hybrid compact-WENO schemes for shock-turbulence interaction, Journal of Computational Physics 178 (1) (2002) 81–117. doi:10.1006/jcph.2002.7021.

[13] Y.-X. Ren, M. Liu, H. Zhang, A characteristic-wise hybrid compact-WENO scheme for solving hyperbolic conservation laws, Journal of Computational Physics 192 (2) (2003) 365–386. doi:10.1016/j.jcp.2003.07.006.

[14] D. Ghosh, J. D. Baeder, Compact reconstruction schemes with weighted ENO limiting for hyperbolic conservation laws, SIAM Journal on Scientific Computing 34 (3) (2012) A1678–A1706. doi:10.1137/110857659.

[15] D. Ghosh, J. D. Baeder, Weighted non-linear compact schemes for the direct numerical simulation of compressible, turbulent flows, Journal of Scientific Computing 61 (1) (2014) 61–89. doi:10.1007/s10915-014-9818-0.

[16] M. P. Martin, E. M. Taylor, M. Wu, V. G. Weirs, A bandwidth-optimized weno scheme for the effective direct numerical simulation of compressible turbulence, Journal of Computational Physics 220 (2006) 270–289.

[17] A. K. Henrick, T. D. Aslam, J. M. Powers, Mapped weighted essentially non-oscillatory schemes: Achieving optimal order near critical points, Journal of Computational Physics 207 (2) (2005) 542–567. doi:10.1016/j.jcp.2005.01.023.

[18] R. Borges, M. Carmona, B. Costa, W. S. Don, An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws, Journal of Computational Physics 227 (6) (2008) 3191–3211. doi:10.1016/j.jcp.2007.11.038.

[19] N. K. Yamaleev, M. H. Carpenter, Third-order energy stable WENO scheme, Journal of Computational Physics 228 (8) (2009) 3025–3047. doi:10.1016/j.jcp.2009.01.011.

[20] N. K. Yamaleev, M. H. Carpenter, A systematic methodology for constructing high-order energy stable WENO schemes, Journal of Computational Physics 228 (11) (2009) 4248–4272. doi:10.1016/j.jcp.2009.03.002.
[21] F. Giraldo, J. Kelly, E. Constantinescu, Implicit-explicit formulations of a three-dimensional nonhydrostatic unified model of the atmosphere (NUMA), SIAM Journal on Scientific Computing 35 (5) (2013) B1162–B1194. doi:10.1137/120876034.

[22] D. S. Abdi, F. X. Giraldo, E. M. Constantinescu, L. E. Carr, L. C. Wilcox, T. C. Warburton, Acceleration of the IMplicit–EXplicit non-hydrostatic unified model of the atmosphere on manycore processors, The International Journal of High Performance Computing Applications 33 (2) (2019) 242–267.

[23] S. Ha, D. You, A GPU-accelerated semi-implicit ADI method for incompressible and compressible Navier-Stokes equations, Bulletin of the American Physical Society 60 (2015).

[24] C. Hirsch, Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics: The Fundamentals of Computational Fluid Dynamics, Vol. 1 & 2, Elsevier Science, 2007.

[25] D. Ghosh, E. M. Constantinescu, J. Brown, Efficient implementation of nonlinear compact schemes on massively parallel platforms, SIAM Journal on Scientific Computing 37 (3) (2015) C354–C383. doi:10.1137/140989261.

[26] P. L. Roe, Approximate Riemann solvers, parameter vectors, and difference schemes, Journal of Computational Physics 43 (2) (1981) 357–372. doi:10.1016/0021-9991(81)90128-5.

[27] A. Harten, High resolution schemes for hyperbolic conservation laws, Journal of Computational Physics 49 (3) (1983) 357–393. doi:10.1016/0021-9991(83)90136-5.

[28] R. S. Rogallo, Numerical experiments in homogeneous turbulence, Tech. Rep. NASA-TM-81315, NASA Ames Research Center, Moffett Field, CA (September 1981).

[29] N. N. Mansour, A. A. Wray, Decay of isotropic turbulence at low Reynolds number, Physics of Fluids (1994-present) 6 (2) (1994) 808–814. doi:10.1063/1.868319.

[30] Nvidia, Nvidia Tesla v100 GPU architecture, Tech. rep. (2017).
