GPU-Accelerated Discontinuous Galerkin Methods: 30x Speedup on 345 Billion Unknowns

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Abstract—A discontinuous Galerkin method for the discretization of the compressible Euler equations, the governing equations of inviscid fluid dynamics, on Cartesian meshes is developed for use of Graphical Processing Units via OCCA, a unified approach to performance portability on multi-threaded hardware architectures. A 30x speedup over CPU-only implementations using non-CUDA-Aware MPI communications is demonstrated up to 1,536 NVIDIA V100 GPUs and parallel strong scalability is shown up to 6,144 NVIDIA V100 GPUs for a problem containing 345 billion unknowns. A comparison of CUDA-Aware MPI communication to non-GPU-direct communication is performed demonstrating an additional 24% speedup on eight nodes composed of 32 NVIDIA V100 GPUs.

Index Terms—Computational Fluid Dynamics, Discontinuous Galerkin Methods, OCCA, GPU Computing

I. INTRODUCTION

A transformation in computing architectures has emerged over the past decade in the quest to keep Moore’s Law alive, leading to significant advancements in Artificial Intelligence and Machine Learning techniques [1], [2]. The success of Machine Learning has caused a role reversal, now becoming a primary driver in the development of massively-parallel thread-based hardware indicative of future exascale-era architectures [3]. Traditional Computational Science applications such as Computational Fluid Dynamics (CFD) has eschewed the use of Graphical Processing Units (GPU) due to their programming complexity to achieve high performance. However, in this ever-changing computing landscape, algorithms suitable for these platforms are now forefront in the advancement

Low-order discretizations such as the finite volume method [4], [5] have been the industrial standard in CFD for the last 40 years. However, these algorithms suffer from low arithmetic intensity [1] making them ill-suited for GPUs. To leverage these new architectures and enable higher-fidelity simulations, an insurgence of algorithmic advancement for high-order methods, such as the discontinuous Galerkin method [6] and the flux-reconstruction method [7], has bustled within the Computational Science community. These high-order methods have higher-algorithmic intensity reflecting the increased compute to communication ratios as needed for GPUs.

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1Arithmetic intensity is the ratio of floating-point operations performed to the amount of memory used in the calculation.

This work develops a discontinuous Galerkin method to discretize the governing equations of fluid dynamics concerning aerospace and atmospheric applications suitable for the use of GPUs in a distributed computing environment. Within this work, we make simplifications such as conforming to Cartesian meshes to establish a performance ceiling for future algorithmic developments. We employ an abstraction thread-programming model known as OCCA [8], an open-source library, enabling the use of GPUs, CPUs, and FPGAs, to achieve performance portability. The performance of the method is analyzed and comparisons of network communications via CUDA-Aware MPI are performed. Lastly, we demonstrate the parallel scalability of the implementation up to 6,144 NVIDIA V100 GPUs.

II. DISCONTINUOUS GALERKIN METHOD

A. Governing Equations

The governing equations utilized in this work are the three-dimensional compressible inviscid Euler equations, which are written in conservative form:

\[
\frac{\partial Q(x,t)}{\partial t} + \nabla \cdot F(Q(x,t)) = 0
\]  

(1)

representing the conservation of mass, momentum, and energy for a fluid. The solution vector \(Q\) represents the conservative flow variables and the matrix \(F\) represents the Cartesian flux components. \(Q\) and \(F\) are defined as follows:

\[
Q = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho E
\end{bmatrix}, \quad 
F = \begin{bmatrix}
F^1 \\
F^2 \\
F^3
\end{bmatrix} = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho u w \\
\rho u H \\
\rho v \\
\rho v^2 + p \\
\rho v w \\
\rho v H \\
\rho w \\
\rho w^2 + p \\
\rho w H
\end{bmatrix}
\]  

(2)

where \(\rho\) is density, \(u, v, w\) are velocity components in each spatial coordinate direction, \(p\) is pressure, \(E\) is total internal energy, and \(H = E + \frac{p}{\gamma - 1}\) is total enthalpy. These equations are closed using the ideal gas equation of state:

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

(3)

where \(\gamma = 1.4\) is the ratio of specific heats.
B. Discretization

This work constrains the computational domain to Cartesian meshes. Under these assumptions, arithmetic simplifications are performed to increase computational performance. Within this setting, the governing equations are discretized via the discontinuous Galerkin (DG) method [9] assuming a weighted residual formulation. A weak-formulation is established by multiplying each governing equation by a set of test functions, $\psi_s$, and integrating over the Cartesian element volume $\Omega_k$:

$$
\int_{\Omega_k} \left( \frac{\partial Q}{\partial t} + \nabla \cdot F \right) \psi(x) \, dx = 0
$$

Integrating by parts, the weak-form residual $R_{\text{Weak}}$ is defined as:

$$
R_{\text{Weak}} = \int_{\Omega_k} \frac{\partial Q}{\partial t} \psi(x) \, dx - \int_{\Omega_k} (F \cdot \nabla) \psi(x) \, dx + \int_{\Gamma_k} (F^* \cdot \nu) \psi(x|\Gamma_k) \, d\Gamma_k = 0
$$

The discrete residual contains integrals over mesh element boundaries $\Gamma$ where special treatment is needed for the fluxes. The advective fluxes $F^*$ are calculated using an approximate Riemann solver, namely, the Lax-Friedrichs method [10]. To complete the spatial discretization, the solution is approximated as follows:

$$
Q(x, t) = \sum_{s=1}^{N} \hat{Q}_s(t) \phi_s(x)
$$

where $\phi_s(x)$ are chosen to be the same as the test functions $\psi_s(x)$. A collocation approach is chosen for computational efficiency by choosing the basis and test functions to be Lagrange interpolation polynomials

$$
\ell_s(x) = \prod_{i=1, i \neq s}^{N} \frac{x - \xi_i}{\xi_s - \xi_i}, \quad s = 1, \ldots, N
$$

where $N = p + 1$: $p$ is the user-chosen polynomial degree, and numerical integration via Gauss-Legendre quadrature is used. Lastly, we implement a low-storage explicit Runge-Kutta method to discretize the temporal component of (4).

III. CPU Implementation

This work serves within the larger computational framework known as the Wyoming Wind and Aerospace Applications Komputation Environment (WAKE3D) [11]–[13]. WAKE3D has been demonstrated on various aerodynamics problems [14] and wind energy applications [15]–[18]. The framework is composed of multiple software components, namely, NSU3D [19], DG4EST [16], [20], and TIOGA [21], [22]. Figure 1 illustrates the simulation of a Siemens SWT-2.3-93 wind turbine using WAKE3D.

The computational kernel within the DG4EST component, known as CartDG [23]–[25], is the primary focus of this work. CartDG is a discontinuous Galerkin method designed for computational efficiency on Cartesian meshes utilizing tensor-product collocation-based basis functions. The CPU implementation has achieved over 10% sustained peak of theoretical compute performance [26] using the viscous formulation as shown in Figure 2. CartDG utilizes the Message Passing Interface (MPI) for distributed-memory computation and enables computation-communication overlap to hide communication latency. It has been demonstrated to scale to over one million MPI ranks [11] on ALCF Mira Supercomputer.

![Fig. 2. Sustained peak performance of CartDG on Intel Xeon E5-2697V2 processors for various solution orders.](image-url)
Discontinuous Galerkin methods exhibit multiple levels of parallelism: coarse-grain parallelism via mesh decomposition and fine-grain parallelism via single instruction, multiple data within a mesh element. In this work, the MPI programming model is employed for coarse-grain parallelism and OCCA [8] is utilized for fine-grain parallelism. We select the CUDA-backend within OCCA to execute the kernels on NVIDIA V100 GPUs. OCCA provides a kernel language known as OKL, a simple extension of the C-language, enabling explicit architecture-independent fine-grain parallelized code. The sample code shown below illustrates the spatial residual volume kernel (second term) from [4] using OKL.

Listing 1. OCCA Volume Flux Kernel Example

Discontinuous Galerkin method discretizes mesh elements into multiple solution modes per variable which depend on the solution polynomial degree established a priori by the user. For example, in three-dimensional space, suppose the polynomial degree $p = 6$, then the number of modes per conservative variable within an element is $(p+1)^3 = 343$. To map the discretization to the hardware, we assign one hardware thread per mode, which is seen in the code sample indicated by the `cubeThreads` definition. The `@inner` attribute assigns a thread to each index $(i,j,k)$ mode.

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**Table I**

| GPU | ON | OFF | Speedup |
|-----|----|-----|---------|
| 4   | 17.94 | 23.22 | 1.29x |
| 8   | 10.60 | 13.22 | 1.25x |
| 16  | 6.34  | 7.87  | 1.24x |
| 32  | 3.73  | 4.62  | 1.24x |

**V. PERFORMANCE RESULTS: MIT SATORI**

The GPU implementation of CartDG is tested on the MIT Satori supercomputer. Satori is composed of 64 IBM Power9 processors. For example, in three-dimensional space, suppose the polynomial degree $p = 6$, then the number of modes per conservative variable within an element is $(p+1)^3 = 343$. To map the discretization to the hardware, we assign one hardware thread per mode, which is seen in the code sample indicated by the `cubeThreads` definition. The `@inner` attribute assigns a thread to each index $(i,j,k)$ mode.

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**Fig. 3.** Parallel strong scalability of CartDG on MIT Satori using up to 64 GPUs. A 29% speedup is achieved at 4 GPUs contained in a single node and a 24% speedup is achieved at 32 GPUs when using GPU Direct-enabled CUDA-Aware MPI compared to standard MPI.
VI. PERFORMANCE RESULTS: ORNL SUMMIT

We test the same implementation on ORNL Summit. Summit has nearly the same architecture as MIT Satori but contains 6 NVIDIA V100 GPUs and 2 IBM AC-922 22-core processors per node. Summit contains 4,608 nodes totaling 27,648 GPUs and 202,752 CPU cores and has achieved 148.6 PetaFLOPS in the LINPACK benchmark [27], [28].

A. Strong Scalability

We perform a second parallel strong-scalability test on ORNL Summit using a 512 × 512 × 768 mesh composed of p = 6, seventh-order accurate elements, totaling 69,055,021,056 degrees-of-freedom (345,275,105,280 unknowns). This problem size is chosen to give approximately 11 million degrees-of-freedom per GPU when using all GPUs on 1,024 nodes. The strong-scaling test measures the wall-clock time to solve 100 Low-Storage Explicit Runge-Kutta 5-stage 4th-order (LSERK45) time steps. The benchmark used 128, 256, 512, 920, and 1024 nodes. Figure 4 displays the scaling results. We note that these results do not utilize CUDA-Aware MPI; the information required by neighboring cores is first transferred to the host CPU, exchanged via MPI, then transferred to the GPU. Table IV tabulates the wall-clock times at various node counts for the CPU and GPU implementations.

![Figure 4. Parallel strong scalability of CartDG on ORNL Summit using up to 1,024 nodes (6,144 GPUs/45,056 CPU cores).](image)

| ORNL Summit: GPU Performance | Kernel   | Time (sec) | PetaFlops | Achieved Theoretical Peak |
|------------------------------|----------|------------|-----------|---------------------------|
| Volume                       | 1.77     | 4.84       | 22.5%     |
| Surface                      | 2.15     | 2.45       | 11.4%     |
| Update-Project               | 6.00     | 0.49       | 2.3%      |
| Communication                | 10.18    | –          | –         |
| Overall                      | 20.45    | 0.82       | 3.8%      |

TABLE III

CUDA-AWARE MPI COMPARISON TO REGULAR MPI ON ONE NODE USING SIX NVIDIA V100 GPUs DEMONSTRATING A 40% SPEEDUP.

| ORNL Summit: CUDA-Aware MPI |
|-----------------------------|
| Problem Size: 21,337,344 DOF. |

| Kernel   | Single Node Time (sec) | On | Off |
|----------|------------------------|----|-----|
| Volume   | 1.67                   | 1.68 |
| Surface  | 2.04                   | 2.04 |
| Update-Project | 5.70 | 5.70 |
| Communication | 10.65 | 5.13 |
| Overall   | 10.37                  | 14.55 |

B. GPU Performance

As demonstrated in the strong-scaling figure, the performance improvement is approximately 30x when using all six GPUs compared to using both CPUs per node only (using 44 cores per node). Table II demonstrates the computational kernel breakdown of the GPU simulation on 512 nodes. The volume kernel corresponding to the code sample achieved nearly 5 PetaFLOPs of performance on 512 nodes. Additionally, the communication overhead is large in comparison to the computational time. This is due to not utilizing the CUDA-Aware MPI on Summit, which allows for faster GPU-GPU communication on a node and overlap of computation and communication.

A communication benchmark is conducted using a single node with six GPUs interconnected with NVLink for a problem containing 21,337,344 DOFs. As shown in Table III, CartDG achieves an 8x speedup in communication time using the GPUDirect CUDA-Aware MPI on one node corresponding to a 40% overall speedup in time to solution. This result corroborates the results achieved on MIT Satori and illustrates a significant communication improvement when using GPUDirect CUDA-Aware MPI. This contrasts the result found by [29] which tested a similar high-order solver on ORNL Summit indicating a slow-down in performance when using CUDA-Aware MPI.

VII. CONCLUSION

This work developed a high-order discontinuous Galerkin method on Cartesian meshes for the use of heterogeneous architectures including GPUs. Performance benchmarks on MIT Satori and ORNL Summit demonstrated significant speedups achieved including a 30x time to solution over the CPU-only implementation. Further, the benefits of utilizing GPUDirect were shown, improving the overall performance by 24% across multiple nodes and an 8x improvement in communication time within one node. If the CUDA-Aware MPI performance improvement holds at scale, as indicated by the results performed on MIT Satori, a GPU to CPU performance improvement of 40-50x is expected.

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