Large-Scale Investigation of 3D Discontinuous-Galerkin-Hancock Method for Hyperbolic Balance Laws with Stiff Local Sources

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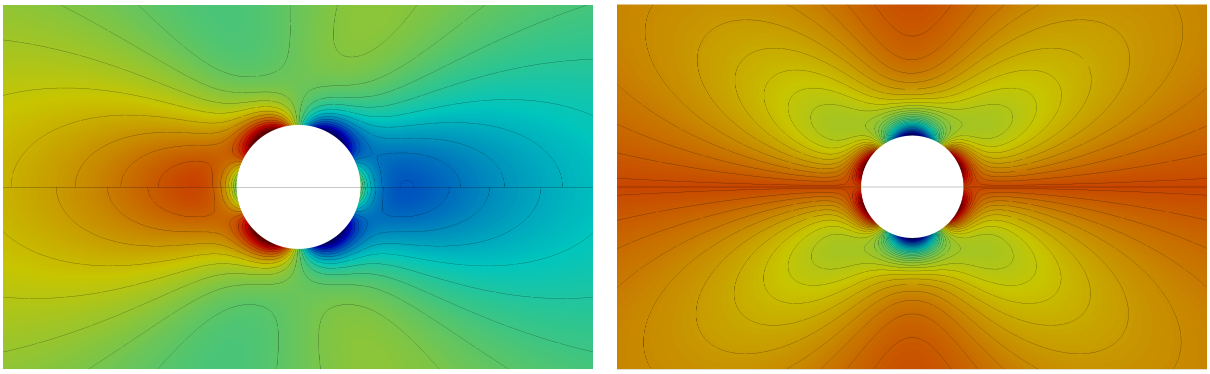
Abstract: A previously proposed third-order accurate, coupled space-time discontinuous-Galerkin Hancock (DGH) method is presented in a multi-dimensional, massively parallel, large-scale computational framework for the first time. The DGH method is shown to achieve third-order solution accuracy for hyperbolic equations with stiff sources using only linear basis functions. The scheme achieves high-parallel efficiency on distributed-memory architectures with 100,000's of compute cores.

Keywords: Numerical Algorithms, Discontinuous Galerkin, High-Order Schemes, Coupled Space-Time Methods, Large-Scale Parallel Scalability.

1 Scope of Work

Efficient approaches for the solution of first-order hyperbolic balance laws are important for a variety of physically complex flows such as multiphase, reacting, and non-equilibrium flows. The governing partial differential equations (PDEs) for such flows often include stiff local source terms, which may require special numerical treatments. The use of high-order numerical schemes (i.e., higher than second-order accuracy) in conjunction with scalable and efficient parallel implementations provides a viable solution for mitigating the computational cost of large-scale simulations of such physically complex flows.

The current study investigates the capabilities of a particular member of the discontinuous-Galerkin (DG) family of schemes for a range of problems described by first-order hyperbolic PDEs with stiff local source terms. Specifically, the coupled space-time discontinuous-Galerkin Hancock (DGH) method, originally proposed by Suzuki [1] for the efficient solutions of hyperbolic balance laws resulting from non-equilibrium extended hydrodynamics is considered. For the present work, the scheme has been implemented in a massively parallel, multi-dimensional framework for practical computations—this marks the first time it has been presented as such. The current paper describes the evaluation of the scheme at large computational scale for various PDEs. Although only linear basis functions are used, the DGH scheme is shown to achieve third-order accuracy in coupled space time on skewed hexahedral elements (results to be provided in the final paper), and it has been proven to be highly efficient on large-scale, distributed-memory architectures.



(a) The deviatoric x-direction pressure, $P_{xx} - p$. (b) The shear pressure, P_{xy}.

Figure 1: DGH prediction (top half) and exact solution (bottom half) of Stokes flow.

2 Sample Results

To demonstrate the convergence accuracy of the third-order DGH scheme, Table 1 shows the error norms and convergence order achieved with the linear convection-relaxation equation on a series of 3D grids. Furthermore, in a strong-scaling study, the DGH scheme was shown (Fig. 2) to achieve a parallel efficiency of about $E_p = 0.96$ on up to 262,144 computational cores of Intel "Knights Landing" 7230 on the Theta KNL system located at the Argonne National Laboratory.

Table 1: ℓ^2 error norms and solution accuracy order obtained for the linear convection-relaxation equation on a series of 3D Cartesian grids.

# of Elements	ℓ^2 Error	Order
$80 \times 80 \times 80$	9.030×10^{-4}	——
$160 \times 160 \times 160$	1.231×10^{-4}	2.87
$200 \times 200 \times 200$	6.376×10^{-5}	2.95
$300 \times 300 \times 300$	1.911×10^{-5}	2.97
$350 \times 350 \times 350$	1.207×10^{-5}	2.98

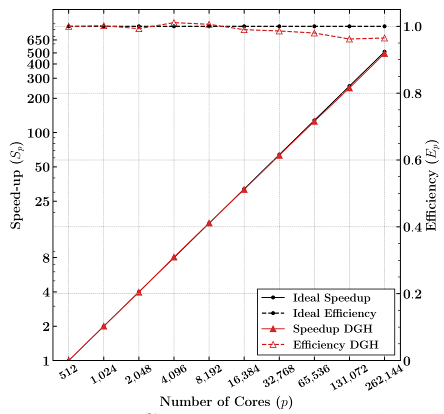


Figure 2: Strong scaling analysis.

One of the main motivations for the development of the current code is the large-scale efficient solution of moment-closure models from the kinetic theory of gases. Such models offer hyperbolic-relaxation models that can be used as an alternative to the compressible Navier-Stokes equations for continuum flows, while also remaining valid for significant departures from local thermodynamic equilibrium. As a demonstration of such a hyperbolic model's ability to accurately describe traditional viscous flows, Fig. 1 compares a moment-closure solution for low-Reynolds-number flow past a circular cylinder to the classical analytic Navier-Stokes solution. Despite the fact that the flow Mach number is only Ma $= 0.0018$, the compressible Gaussian moment-closure solution is accurate without the need for low-Mach-number preconditioning.

The final paper will provide a detailed formulation of the DGH method for arbitrary multi-dimensional elements. Additional numerical results are shown to demonstrate the capabilities of the large-scale implementation of the scheme.

References

[1] Y. Suzuki. PhD thesis, University of Michigan, 2008.