Final report for DOE Contract DE-FG02-98ER25346 entitled

Parallel High Order Accuracy Methods Applied to Non-Linear Hyperbolic Equations and to Problems in Materials Sciences.

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Note: This grant was originally awarded to Professor David Gottlieb and the majority of the work envisioned reflects his original ideas. However, when Prof Gottlieb passed away in December 2008, Professor Hesthaven took over as PI to ensure proper mentoring of students and postdoctoral researchers already involved in the project. This unusual circumstance has naturally impacted the project and its timeline. However, as the report reflects, the planned work has been accomplished and some activities beyond the original scope have been pursued with success.

Project overview and main results

The effort in this project focuses on the development of high order accurate computational methods for the solution of hyperbolic equations with application to problems with strong shocks. While the methods are general, emphasis is on applications to gas dynamics with strong shocks.

In the following we shall discuss a number of efforts and main results in some detail and refer to the references for more details.

Hybrid schemes for turbulent mixing

In the past we showed that high order methods are beneficial for turbulent mixing problems that require high resolution for the faithful representation of the fine scale structures. We have continued to play particular attention to the important problems associated with the Ritchmyer-Meshkov instability that develops when perturbations on an interface separating gases with different properties grow following the passage of a shock.

The Richtmyer-Meshkov instability is a fundamental fluid instability that develops when perturbations on an interface separating gases with different properties grow following the passage of a shock. This instability is typically studied in shock tube experiments, in which an incident shock passes through an initially perturbed interface separating the gases. Following the passage of the shock, the interface is set in motion along the direction of shock propagation and a transmitted shock enters the second gas. The misalignment of the density and pressure gradients cause a deposition of vorticity $\omega \equiv \nabla \times u$ on the interface through baroclinic vorticity production. The vorticity deposited by the shock on the interface drives the instability, which results in interpenetrating bubbles and spikes. At later times, complex roll-up structures form on the spike and the vorticity forms strong cores. The transmitted shock reflects from the end wall of the shock tube and interacts with the evolving interface during the reshock phase, further contributing to the development of complex interacting fluid and wave structures.

In the past we showed that high order methods are beneficial for this class of problem that requires high resolution for the faithful representation of the fine scale structures. In our previous research, the formally high-order accurate weighted essentially non-oscillatory (WENO) shock-capturing method using a third-order total-variation diminishing (TVD) Runge-Kutta time-evolution scheme is applied to the two-dimensional single-mode Richtmyer-Meshkov instability with reshock for long evolution times. The initial conditions and computational domain for the simulations are modeled after the single-mode, Mach 1.21 air(acetone)/SF_6 shock tube experiment of Collins and Jacobs.

In our research, the formally high-order accurate weighted essentially non-oscillatory (WENO) shock-capturing method coupled with the high order central finite difference scheme along with the switch based on the high order multi-resolution analysis (Hybrid) using a third-order total-variation diminishing (TVD) Runge-Kutta time-evolution scheme is applied to the two-dimensional single-mode Richtmyer-Meshkov instability with reshock for long evolution times.

Among the numerous advances completed during this work, the highlights are

- We have improved the classical WENO scheme (WENO-Z) scheme, which yields the high formal order of accuracy and is less dissipative.

- The original algorithm based on the classical WENO scheme is extended to the high order hybrid WENO/Central finite difference scheme (Hybrid). The switching of the spatial algorithm is based on the high order multi-resolution algorithm by Harten. The resulting Hybrid scheme has an improved speedup and accuracy due to the removal of the ex- pensive characteristic forward projection and backward projection after reconstruction of the multi-dimensional Euler flux in the characteristic based WENO scheme for the Euler equations.

- The Euler solver is extended to the full Navier-Stokes solver with physical relevant viscosity and conductivity based on the binary mixing relations.

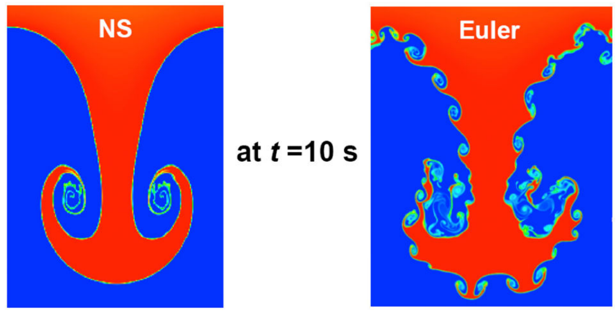
- The two dimensional solvers of the Euler equations and the Navier-Stokes equations are ex- tended to full three dimensions to take in account of the three dimensional effects, realistic geometries and membrane configurations for physical relevant simulations of Richtmyer-Meshkov instability.

- We systematically and self-consistently explore and quantify a broad array of quantities characterizing two-dimensional single-mode Richtmyer-Meshkov instability-induced mixing based on the latest improvements made to the high order hybrid WENO/Central finite difference scheme for the Navier-Stokes equations.

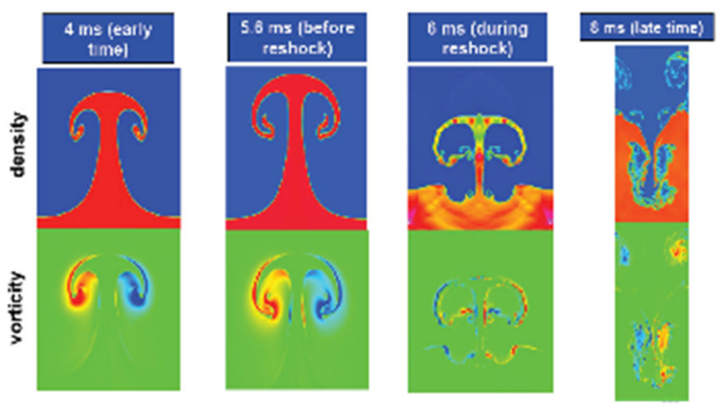
- We demonstrated the capability of the hybrid scheme for three-dimensional RMI with a noisy two-modes perturbed material interface.

- The density, vorticity, simulated density Schlieren and baroclinic vorticity production fields are qualitatively compared from the simulations. Also modeled quantitatively are the mixing layer widths, circulation, mixing profiles, chemical products and mixing fractions, energy spectra, statistics and probability distribution functions.

The high order shock capturing algorithm provides a robust MPI parallel framework for the multi-dimensional high order numerical simulation of the fully-nonlinear evolution of hydrodynamic instabilities and late-time mixing generated by single- or multi-mode Richtmyer-Meshkov, Rayleigh-Taylor and Kelvin-Helmholtz instabilities. The nonlinear system of hyperbolic partial differential equations can be solved in one, two or three spatial dimensions.



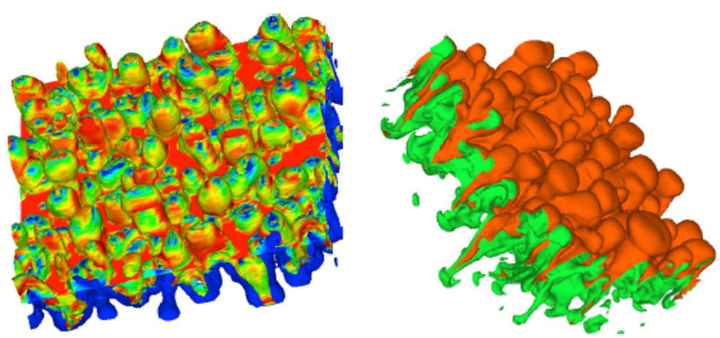
Raleigh-Taylor instability illustrating the important and qualitative differences between a simulation based on Navier-Stokes (left) and the Euler (right) equations.



The density and vorticity fields of the simulation by the hybrid method for the Navier-Stokes equations at the early time, before, and after the reshock.

All simulations are performed on the parallel supercomputers at the Lawrence Livermore National Laboratory (LLNL) of Department of Energy. The research is the result of an extensive long-term (9+ years) collaborative effort with Dr. Oleg Schilling who is a Theoretical, Computational and Applied Physicist in the AX Division of Lawrence Livermore National Laboratory, Department of Energy. The high order codes developed by the co-PI (Don) are used by Dr. Schilling in aid of his turbulence modeling effort of the Initial Confinement Fusion (IFC) Program for the National Ignition Facility Programs (NIF), at LLNL.

We have demonstrated the simulating of three dimensional Rayleigh-Taylor instability using the hybrid high order WENO-Central finite difference scheme with a multimode interfacial perturbation fit to Gaussian spectrum with specified RMS amplitude, bandwidth and diffusion width. The hydrostatic pressure p0 = 1000dyn/cm2 is selected for simulating near incompressible fluid. Below, we show the isosurface of the density at the early and late time evolution of the flow where the color of the left figure indicates the vorticity magnitude.



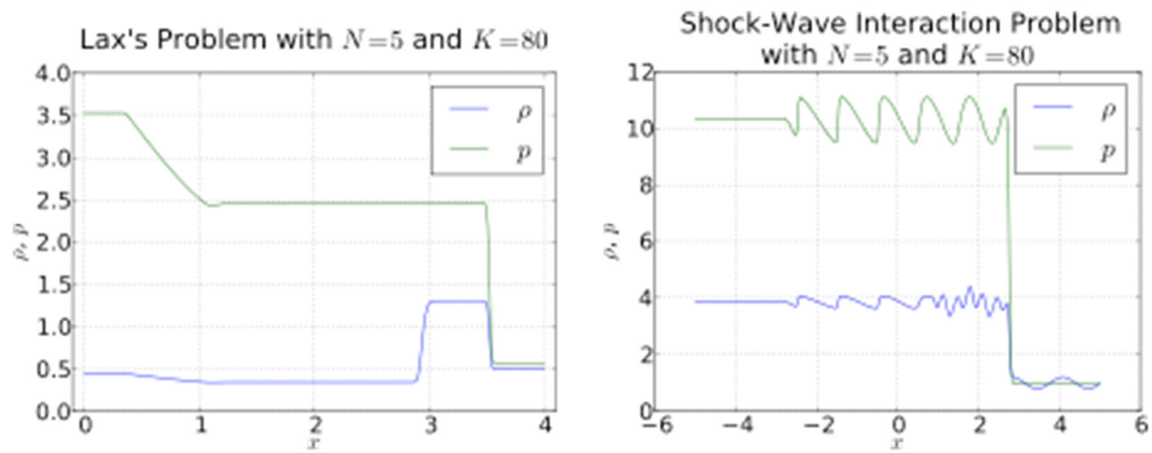
The isosurface of the density and vorticity in the three dimensional simulation of Rayleigh– Taylor instability based on the Navier-Stokes equations at the (Left) early and (Right) late time.

In summary, the high order shock capturing algorithm provides a robust MPI parallel framework for the multi-dimensional high order numerical simulation of the fully-nonlinear evolution of hydrodynamic instabilities and late-time mixing generated by single- or multi-mode Richtmyer-Meshkov, Rayleigh-Taylor and Kelvin-Helmholtz instabilities. The nonlinear sys- tem of hyperbolic partial differential equations can be solved in one, two or three spatial dimensions. The second order terms of the Navier-Stokes equations are discretized via the high order central difference scheme. The hybridization between these two schemes are accomplished via the high order multi-resolution analysis. All simulations are performed on the parallel supercomputers at the Lawrence Livermore National Laboratory (LLNL) of Department of Energy.

Nonlinear artificial viscosity techniques for Discontinuous Galerkin Methods
We have developed a novel, cell-local, GPU-suited shock detector for use with discontinuous Galerkin (DG) methods. The output of this detector is a reliably scaled, element-wise smoothness estimate, which is suited as a control input to a shock capture mechanism. Using an artificial viscosity in the latter role, we have obtained a DG scheme for the numerical solution of nonlinear systems of

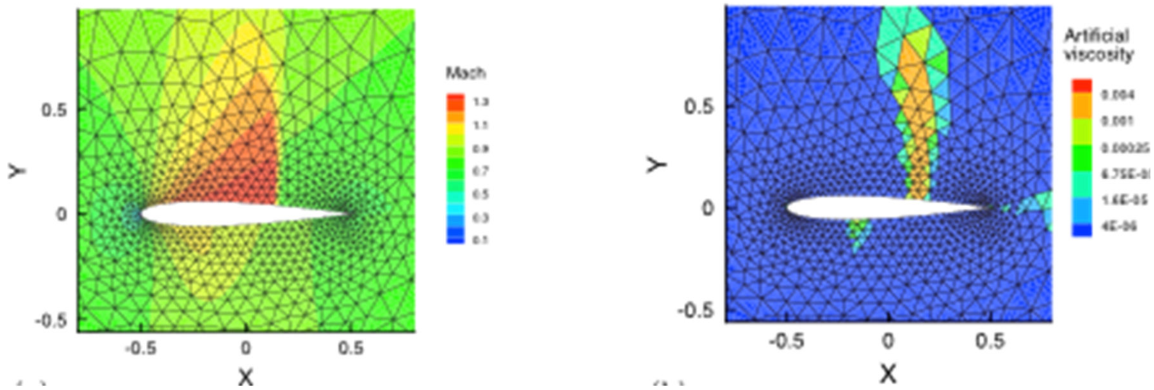
conservation laws.

The motivation for the construction of the detector lies in the marked gains in execution speed of DG possible through the use of graphics processors (GPUs) that we have recently demonstrated. Building on previous work we have thoroughly justified the design of the scheme and analyzed its performance on a number of synthetic and real-world benchmarks.



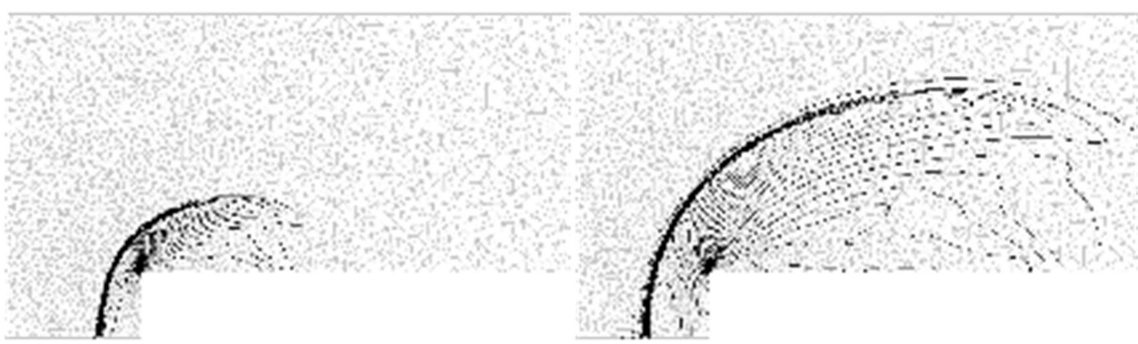
Approximate solution of classic shock-tube problems using a high-order discontinuous Galerkin methods with the new nonlinear artificial viscosity. Note the lack of Gibbs oscillations even at 5th order accuracy.

Diffusion coefficients are selected based on the local smoothness of the solution. In smooth region of the solution, the coefficient must be negligibly small whereas in discontinuous region the coefficient must be sufficiently large to smooth the solution. It is found previously that this technique has a potential of delivering sub-cell shock capturing. We have confirmed this by solving the Euler system on the NACA0012 airfoil configuration with farfield Mach number of M = 0.8 and 1.25 degrees incidence. Mach contours and artificial viscosity are shown below, respectively, for approximation order N = 3 and an isotropic triangular mesh with E = 1822 elements. From the figures, it is seen that the discontinuity is resolved within an array of elements with a single element width and the artificial viscosity is primarily large in the neighborhood of elements containing the shock. Convergence of the surface pressure coefficient is not uniform as approximation order increases. We attribute this to the failure of accurately estimating the required amount of diffusion for a given flow and geometry on one hand and the mesh and approximation order on the other hand. Search for finding a reliable method to estimate a proper amount of diffusion coefficient is ongoing work.



Mach contours for M=0.85 and 1.25 degrees incidence farfield low over NACA0012 airfoil for a mesh with E = 1822 triangles and approximation order N = 3; (b) artificial viscosity for the same problem. The underlying mesh with E = 1822 triangles are also shown.

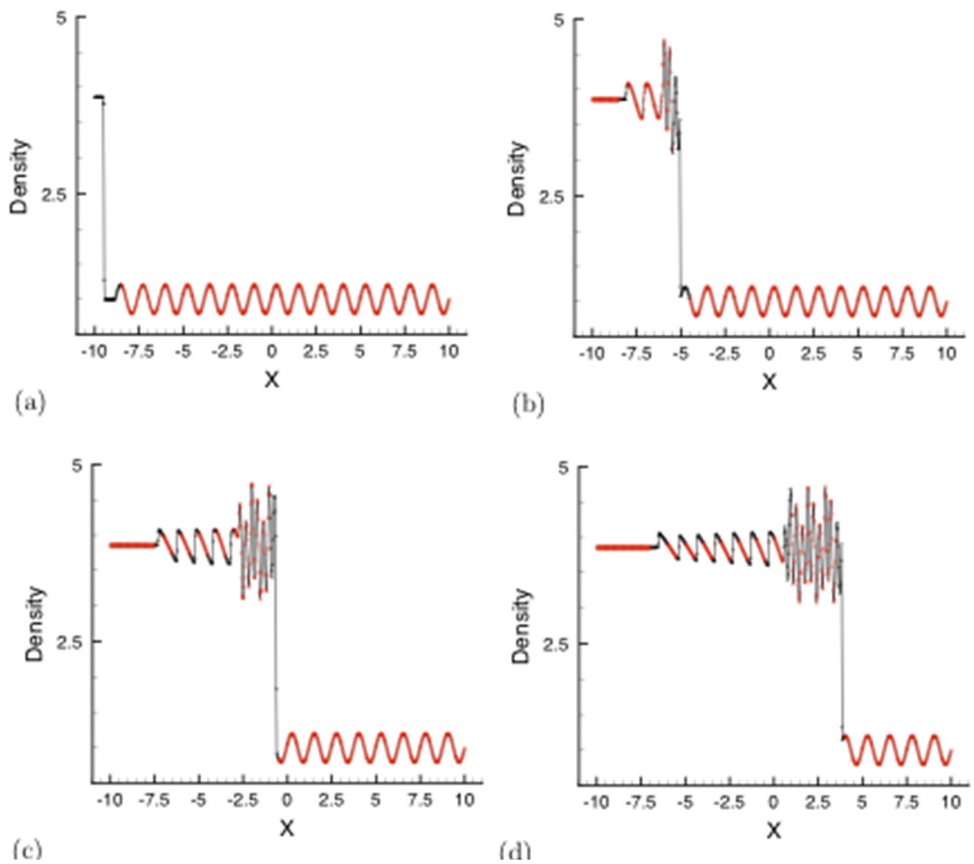
To illustrate the versatility and robustness of the general approach, we also show results for the forward facing step as classic benchmark case. At least visually, the results are in agreement with previously published results.



Two-dimensional backward facing step test for nonlinear artificial viscosity model at Mach 3.

Hybrid Fourier Continuation-WENO scheme for Euler equations.
We have developed a multi-domain Fourier-Continuation/WENO hybrid method (FC-WENO) that enables high-order and non-oscillatory solution of systems of nonlinear conservation laws, and which enjoys essentially dispersionless, spectral character away from shocks, as well as mild CFL constraints. The hybrid scheme employs the expensive, shock-capturing WENO method in small regions containing discontinuities and the efficient Fourier continuation method in the rest of the computational domain, to yield a highly effective overall scheme for applications with a mix of discontinuities and complex smooth structures. The accuracy, stability and efficiency of the new FC-based method for conservation laws has been investigated for both problems in which solutions are smooth and problems for

which solutions contain shock discontinuities; in particular, in the latter case we have compared the efficiency of the hybrid FC-WENO method to that of a purely WENO-based approach and shown our new methods to be superior.

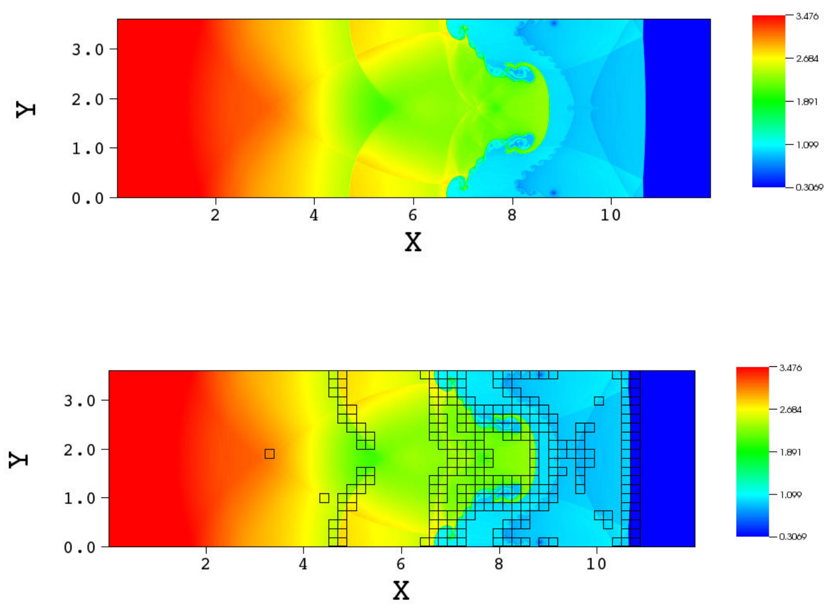


Density profiles for classic shock-entropy problem at T=0.0013 (a), T=1.25 (b), T=2.5 (c), T=3.75 (d). Black marks WENO regions and red marks Fourier regions.

A major advance in this work over our past hybrid schemes are the ability to use a Fourier method in the smooth regions, resulting in a fast and accurate approach. The requirement for periodicity is addressed by continuation that effectively overcomes this at minimal additional cost. The equidistant grid in both the Fourier region and the WENO region makes the interfacing straightforward and the switching is accomplished through a multi-resolution analysis of the local solution.

In a variety of examples, including Euler problems that govern the interaction of a strong shock with a very small entropy wave, we have demonstrated that the hybrid strategy is several times faster than the pure WENO solver for a comparable level of accuracy.

Most recent results include the extension of this approach to the multi-dimensional case. As a proof of concept in multiple dimensions, we also developed a two-dimensional version of the multi-domain FC-WENO point-wise hybrid solver for Euler equations and the single component (constant γ) case. The framework has been implemented and tested with success on parallel processors using the massage passing interface (MPI) as well as on many core graphic processing units (GPUs). The performance of the hybrid solver in simulating early stages of a Richtmyer-Meshkov instability problem have been investigated.

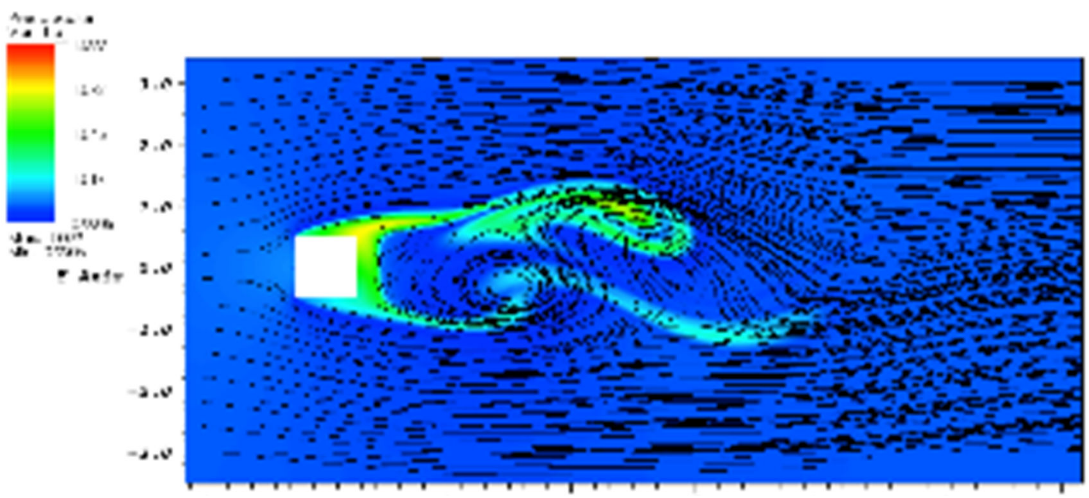


(Top) Density contours for a Richtmyer-Meshkov instability at physical time of 128μs in which a shock wave with Mach of 4.46 interacting with a single-mode disturbed interface of Xenon and Argon gases; (Bottom) WENO domains are also shown using the square symbols.

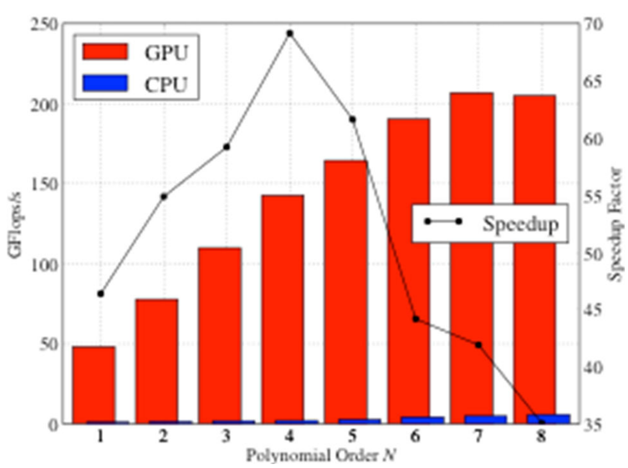
As an illustration of these initial developments, consider a Mach 4.46 shock interacting with material interface of two gases Xenon and Argon in a spatial domain of [12, 3.6] similar to that in [10]. Figure 2 (a) depict the density at physical time of ≈ 128μs for resolutions of a (64 × 20) array of sub-domains and the number of points per domain of NP = 322. Figure 2 (b) also shows the sub-domains discretized using the WENO solver. Clearly, the use of WENO scheme is restricted to regions containing discontinuous solutions, hence decreasing the overall computational cost.

The hybrid solver also displays great parallel performance, 96% or higher efficiency, crucial for the three-dimensional computations

GPU acceleration of Euler and Navier-Stokes DG solvers.
In this effort, the GPU implementation of discontinuous Galerkin solvers for the Euler and compressible Navier-Stokes equations has been developed. This DG ethod parallelizes very well because the solution of a grid cell only depends on the solutions of its direct neighbors. Graphics processors can perform thousands of operations in parallel, i.e. at the same time, and therefore reach higher computation speeds than CPUs if used in the right way. However, the implementation of GPU's is nontrival and has required substantial attention to algorithm reformulations and careful implementations. The potential for substantial speed up of complex simulations is, however, clear, in particular at high order and for large-scale applications with a demonstrated acceleration exceeding a factor of 50.



Instant streamlines for flow around a square cylinder.



Performance for three-dimensional Navier-Stokes solver on GPU's at different order of approximation. This demonstrates a potential for acceleration over a CPU based approach exceeding 50 for general DG schemes on unstructured grids

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