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6. AUTHOR(S)
David Gottlieb
C.W. Shu
P.F. Fischer
W.S. Don

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Division of Applied Mathematics
Brown University
Providence, RI 02912

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Final Report

High Order Accuracy Computational Methods In Aerodynamics Using Parallel Architectures

AFOSR 95-1-0074

David Gottlieb, Chi-Wang Shu, P.f. Fischer and W.S. Don
Division of Applied Mathematics, Brown University

The main theme of this research is the application of high order accurate schemes to complicated flow problems. The advantage of using high order schemes for long time simulations is widely recognized by now. Also for problems where fine details of the flow field have to be captured accurately the use of high accuracy schemes is mandatory. These two classes of problems encompass many of the current problems in scientific computing.

1. Spectral shock capturing techniques

The problem in applying spectral methods to shock wave problems is their sensitivity to discontinuities. The presence of shock wave creates theoretical as well as practical difficulties.

Two major theoretical breakthroughs that occured in the last period, may clear the way to the successful implementation of spectral methods in simulating complicated shock waves interactions.

The first development involved the solution of the Gibbs phenomenon. The Gibbs phenomenon is related to the well known fact that the rate of convergence of the sequence of partial sums of the Fourier series representation of a function deteriorates rapidly when the function has discontinuities. In essence the new result says that the first N Fourier coefficients of a piecewise analytic function (a finite number of bounded jump discontinuities is permitted) carries much more information than can be revealed by forming the N th order Fourier partial sum. In fact it has been shown that these N coefficients contain enough information so that one can constructively form an approximation to the unknown piecewise analytic function which is exponentially accurate in N. This result had been extended too any polynomial method, such as the commonly used Chebyshev method.

The second development concerns the convergence of spectral methods for non-linear hyperbolic equations. It has been shown that with a suitable addition of (spectrally amall) artificial dissipation the method converges. Moreover it has been shown that the usual filtering technique can be cast in terms of the above analized artficial dissipation.

While the above results create a breakthrough that indicate that high order methods are useful for shock wave calculations, a lot of work has still to be done in making the process efficient. Stabilizing the scheme in an optimal way, and extracting the information in an efficient way have to be further studied.

2. High order ENO schemes

We have been continuing our investigation of ENO schemes using point-flux and TVD Runge-Kutta time discretization formulations in the following directions:

(1) Towards the convergence issues, we have investigated entropy consistency for high order Hermite type finite difference and discontinuous Galerkin methods as a first step. We have been able to obtain a cell entropy inequality for the square entropy, for such high order schemes (no restriction on order of accuracy) without resorting to the help of nonlinear limiters. The result is

valid for multi space dimensions with arbitrary triangulations and for any fluxes (no restriction on convexity). This is a significant improvement in obtaining cell entropy inequalities since all the previous work in this direction must either resort to modifications to existing limiters or resort to complicated global analysis, and be restricted to second order accuracy. We plan to continue the investigation towards full convergence proofs;

(2) Application of ENO schemes to combustion problems. The first test case is shock interaction with hydrogen bubbles. Different configuration of bubbles is studied to see the effect of shock interaction. High order accuracy is crucial in this problem due to the detailed structures of the solution behind the shock. This project is on going. Stiff source terms must be treated adequately for future tests;

(3) Comparison of two different formulation of ENO schemes: finite volume vs finite difference. The comparison is performed on problems related to curved boundary, inflow outflow boundary conditions, shocks oblique to the grids, and CPU time. It is found out that finite difference version of ENO scheme (the one based on point values and numerical fluxes of Shu and Osher) is much cheaper to run, and can obtain results comparable to finite volume ENO in most of the test cases.

(4) ENO schemes based on rational function building blocks are being investigated. As a first step we are investigating approximation results. The potential here is that in most rapid transition regions, rational functions approximate the true solution better than polynomials. This project is on going.

The results of comparing the two formulations of ENO schemes (the cell-averaged version and the point value version indicate that for most test cases, the two formulations of ENO schemes yields the same accuracy whereas the point value ENO scheme is much faster.

3. Parallel computing for high order schemes

(a) Spectral Elements for incompressible flows

The research objective here is to develop parallel algorithms for computational fluid dynamics (CFD) which will permit solution of incompressible flows with the accuracy and resolution demanded by large eddy simulations (LES) of turbulent flows in complex geometries. The work is subdivided into three principal areas: high-order flexible discretizations, fast multi-level iterative solvers, and implementation of LES modeling technology. *All of this work is being developed within the computational framework of distributed memory architectures which provide a favorable price/performance ratio for this class of problems.*

Our numerical approach is based upon the spectral element method, which retains many of the essential features of global spectral discretizations, namely, rapid (exponential) convergence, minimal numerical dissipation and dispersion per degree-of-freedom, and efficient tensor product factorization of spatial derivative operators. The computational domain is subdivided into large macro-elements and the solution, data, and geometry within each element are expressed in terms of high-order polynomials. The use of a weighted-residual procedure permits a reduction in inter-element continuity requirements from C^1 to C^0, which in turn leads to a reduction in inter-processor communication. The locally-structured/globally-unstructured, approach of the spectral element discretization is ideally suited to the two-level memory hierarchy associated with distributed memory parallel computers.

The performance of general geometry incompressible codes is largely tied to the speed of the elliptic solver for the pressure; development of fast multi-level iterative solvers is a major focus of our current efforts. Presently, we employ a two-level conjugate gradient based solver which uses deflation to project out the coarse grid modes, thereby reducing the condition number of the underlying iteration matrix. The system is preconditioned by local finite-element based operators which are significantly less expensive to invert than their high-order counterparts. In effect, one can obtain high-order accuracy at low-order cost. We have addressed all of the parallel issues associated with this approach, including the use of an efficient parallel coarse-grid solve, and are able to compute Navier-Stokes solutions at a resolution of 3 million gridpoints on the 512 node Intel Delta at the rate of 4 minutes per time step (6.5 GFLOPS). To improve upon this result, we are currently developing a preconditioner based upon a Schur-complement formulation for the interface variables. This approach leads not only to better conditioning, but also to reduced degrees-of-freedom, which in turn permits the use of projection techniques in which very good initial guesses can be generated by projecting the residual onto results from previous time steps.

Accurate numerical simulation of many high Reynolds number engineering flows will continue to be limited by resolution requirements for the foreseeable future. However, progress is being made to the point where the combination of high-resolution ($> 10^6$ gridpoints) and advanced large-eddy simulation (LES) models will be able to conquer many important problems in the near future. Our goal is to couple the latest LES technology developed within the turbulence community with a general geometry Navier-Stokes code capable of solving these demanding problems.

Because of the large number of degrees-of-freedom involved, effective use of high-performance distributed memory parallel architectures is essential to economic resolution of these problems. Principal parallel issues to be addressed include: development of coarse-grid solve strategies which will remain competitive as the number of processors and dimension of the coarse-grid system continue to increase; and development of optimal communication strategies for the complex subdomain interfaces arising from nonconforming discretizations.

(b) Spectral methods for compressible flows.

Spectral methods involve the approximation of the unknown solution in terms of global polynomials. This fact make them difficult to implement on parallel computers. A popular method to overcome the limitations of spectral methods is to use multidomain techniques, in which a complex domain is decomposed into several simpler subdomains. This method has been applied successfully to incompressible flows (the Specral-Element technique) or to problems in structural mechanics (the h-p method).

Multidomain spectral methods are suitable for coarse grain parallel computing, each domain is assigned to a different processor.

The main question is: Are multidomain methods efficient? This question has not been yet answered for those methods applied to hyperbolic equations. If we denote by $W(p,N)$ the work involved in approximating k waves using p sub domains (and N points in each domain) to obtain an error of at most $e^{-\epsilon}$, then $W(p,N)$ is minimized if

$$p \sim \frac{\pi k}{\epsilon} \tag{1}$$

Thus the optimal number of subdomain *increases* with the complexity of the problem (or number of waves) but *decreases* if the required accuracy increases. This result may serve as a guideline to the optimal number of subdomain. The formula above can be suitably modified for parallel computers.

A key issue in the application of multidomain spectral methods to the numerical solution of hyperbolic equations is the interface boundary conditions. This leads to the question of the imposition of boundary conditions, both analytic and numerical, in the numerical solutions of *systems* of hyperbolic equations. For truly time dependent problems stability in the classical sense (Lax and G-K-S stability) is not enough. Even stable schemes may exhibit a non-physical growth in time. From a practical point of view, in order to achieve reasonable accuracy for large time, meshes much too fine for the computers available in the foreseeable future are required.

We have found a systematic procedure for designing time-stable, as well as G-K-S stable schemes of high-order accuracy. The new schemes are guaranteed to be time-stable for any hyperbolic system (as long as the system has a bounded energy). We have extended this methodology to Navier Stokes equations in three space dimensions. We have showed that the SAT boundary condition assures the correct behavior as the Reynolds number tends to infinity.

(c) Parallel implementation of ENO schemes on CM-5

The main cost in ENO schemes is in its logic step in choosing local stencils by comparing divided difference tables of the function. Although great effort has been spent on efficiently vectorizing this part for CRAY supercomputers, due to the inevitable gathering-scattering process, ENO schemes still do not run very fast on CRAY computers. Recently we have been exploring the structure of the ENO algorithm to suit the parallel structure of CM-5. The algorithm has been slightly re-formulated (in a mathematically equivalent way) to reduce communications and to eliminate communications between other than next neighbors, at the price of a slightly increased operation count. Our CM-5 two dimensional ENO code for compressible Euler and Navier-Stokes equations is a magnitude faster than our ENO code on CRAY for a 400x400 grid. Three dimensional code also shows a speed up, although it has not been optimized yet (for three dimensions, storage is a big restriction, and the structure of the program must be modified accordingly). Currently we are trying to improve the CM-5 code and applying it to reactive flows. .

4. Fuel air mixing enhanced by shock induced vortices

In designing supersonic combuster for the next generation of supersonic transport, we look for an efficient combuster such that :

- allow better load to weight ratio by carrying less fuel,
- reduce chemical product that contribute to pollution due to incomplete burning of fuel.

One of the technique currently under study in enhancing mixing of a hydrogen jet (fuel) and air (oxidizer) is to allow the existing shock inside the combustion chamber to interact with the hydrogen jet . By doing so, vorticity are generated according to the vorticity equation of the Navier Stokes equation, The pressure gradient of the shock and the density gradient between the air and hydrogen provides an efficient mechanism for vorticity generation along the surface of the hydrogen jet. The vorticity forced the jet to curl up and stressed. The increased surface area allows greater mixing of air and hydrogen where combustion can take place. Even though the problem is three dimensional steady state, it had been argued that the three dimensional steady flow can be directly associated with a corresponding two dimensional unsteady calculation in this particular physical setting.

Numerical simulations are a necessary part of this investigation. For these type of problem, it is important to capture the complex physics with high accuracy. Finite difference scheme , with their inherent dissipative nature for stability reason, can only yields a quantitative result of the flow fields. Often, for long time integration, the loss of accuracy in the earlier stage affect the development of the flow in later time.

We had applied two codes for simulating the above problem. A spectral shock capturing code and a finite difference ENO code. We have employed all the theoretical techniques developed in order to run succesfully the codes.

we computed the solution of these problem with various configuration of multiple jets placement. Our results found that different initial placement of the jets yields distinct final configurations (Moreover, the spectral code is fully capable of capturing the fine scale structure of the interactions, including some that had not been seen in finite difference code. One distinct feature of this calculation is the penetration of an air stream (heavy fluid) into the hydrogen (light fluid) causing instability that exhibit a mushroom shape structure This study can be used to guided researcher in develop fuel jet configuration for the scramjet engine with greater confident. Our goal in this research is to extend this problem to a three dimensional steady and/or unsteady simulation with full chemistry model.

5. Multiscale Computing

Many relevant physical phenomena involve infinite number of scales. In nonlinear problems it is desirable to find a way to take into account the effect of the scales which are neglected on those which are taken into account.

Two approaches have been investigated for this type of problems: *Nonlinear Galerkin Methods* and *Wavelet based Schemes.*

We have studied the implementation of the Nonlinear Galerkin in the context of collocation discretizations. We have found interesting characterizations, in the physical space, of a small scale function and a large scale function.

Using the above we have presented an efficient pseudospecral NLG scheme for the periodic Burgers equation, The case of Chebyshev approximations to nonperiodic problems, in which the concept of large and small scales have to be redefined is currently under investigation.

In a thesis by L. Jameson and in a subsequent paper , the Daubechies wavelet based differentiation matrix was constructed. The relationship between this matrix and finite difference methods was clarified. This serves as a basis for current work by Bruce Bauer a doctoral student on wavelet optimized finite difference methods.

Jameson also analyzed the differentiation matrix based on the compactly supported Daubechies wavelets. He showed that in this case there is a loss of the superconvergence. The same result holds for the finite element schemes.