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Form Approved
OMB No 0704-0188

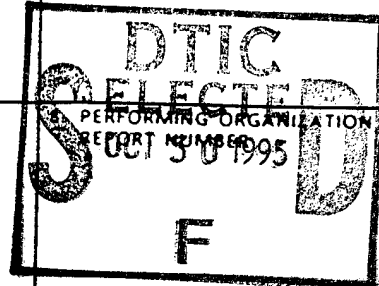
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1. AGENCY USE ONLY (Leave blank) 2. REPORT DATE: June 26, 1995 3. REPORT TYPE AND DATES COVERED: Final Report, 5/1/91 - 4/30/95

4. TITLE AND SUBTITLE: Multi-Dimensional High Order Non-Oscillatory Numerical Methods for Discontinuous Problems in Parallel Structure 5. FUNDING NUMBERS: DAAL03-91-G-0123

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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES): U.S. Army Research Office, P. O. Box 12211, Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

ARO 28716.10-MA

11. SUPPLEMENTARY NOTES: The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

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12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

In this project we have studied high order finite difference, finite element, and spectral methods for the numerical solution of discontinuous or high gradient solutions. Theoretical study of algorithm development, stability, accuracy and convergence analysis, as well as applications of the algorithms to computational fluid dynamics (both compressible and incompressible) and semiconductor device simulation are performed. Parallel implementation issues of these high order methods are also studied.

19951026 036

DTIC QUALITY INSPECTED 8

14. SUBJECT TERMS

15. NUMBER OF PAGES: 8

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT: UNCLASSIFIED

18. SECURITY CLASSIFICATION OF THIS PAGE: UNCLASSIFIED

19. SECURITY CLASSIFICATION OF ABSTRACT: UNCLASSIFIED

20. LIMITATION OF ABSTRACT: UL

Final Report of ARO Grant DAAL03-91-G-0123
Multi-Dimensional High Order Non-Oscillatory Numerical
Methods for Discontinuous Problems in Parallel Structure

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May 1, 1991 to April 30, 1995

1. Abstract

In this project we have studied high order finite difference, finite element, and spectral methods for the numerical solution of discontinuous or high gradient solutions. Theoretical study of algorithm development, stability, accuracy and convergence analysis, as well as applications of the algorithms to computational fluid dynamics (both compressible and incompressible) and semiconductor device simulation are performed. Parallel implementation issues of these high order methods are also studied.

2. Statement of the Problem Studied

The problems studied in this project involve numerical solutions of partial differential equations, mainly hyperbolic type or convection dominated parabolic type equations, with solutions which are either discontinuous, or with discontinuous derivatives, or containing sharp gradient regions which are difficult to be completely resolved on today's computer. The methods we investigate fall into the category of "shock capturing" schemes, which means that these methods try to capture shocks or other types of discontinuities and/or sharp gradient regions with a relatively coarse grid, rather than completely resolving them. These methods are useful when it is either impossible or too costly to completely resolve certain solution structure. High order accurate finite difference, finite element and spectral methods have all been considered. Parallel implementation issues of these high order methods are also studied.

Applications of the algorithms developed and analyzed in this project have been carried out to compressible and incompressible flow calculations, and semiconductor device simulations. We have been using the Connection Machine CM-5 at the Army High Performance Computing Research Center at the University of Minnesota to develop highly efficient two and three dimensional flow solvers using high order difference (ENO) methods. Collaborations have also been pursued with Dr. Nisheeth Patel of

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Ballistic Research Lab and Professor Bernardo Cockburn of University of Minnesota, about joint efforts of parallel implementation and application of the discontinuous finite element method for 3D Navier-Stokes equations.

3. Summary of Research Results

Research has been performed in all areas listed in the original proposal, and progress and results consistent with the original objectives have been obtained. There are 27 publications (among them 19 in refereed journals) resulting from this project, see Section 4 for a list of them.

The main class of finite difference methods we have been investigating is the ENO (Essentially Non-Oscillatory) high order methods using fluxes and point values, first developed by Shu and Osher in 1988, using the adaptive adaptive interpolation procedure in the original ENO schemes of Harten, Osher, Engquist and Chakravarthy. The advantage of the version of ENO schemes based on point values and nonlinearly stable Runge-Kutta time discretizations, designed by Shu and Osher, is that the resulting scheme is cost efficient for two and three dimensional problems. A comparison of the efficiency of the two types of ENO schemes is performed in [13] (all the numbering of references are according to that of Section 4). In this same paper we have explored the boundary treatment for high order ENO schemes in two dimensional problems with a non-rectangular domain. Both wall and inflow/outflow boundaries are considered. It is found out that careful treatment of different boundary conditions is essential for the realization of high order accuracy and stability for such problems. We have also found out that the grid orientation effect, which is present because of the dimension by dimension feature of the algorithm, is actually diminished with the increase of order of accuracy and is, for the test problems we have computed, negligible for fourth order schemes.

In [11], E and Shu adapted ENO methodology to solve incompressible flows and investigated several resolution issues. This is a generalization of the second order Godunov type methods used by Bell, Colella and Glaz. The main difference from the compressible flow is the presence of the incompressibility condition, which is a global condition and, if not treated carefully, may affect local approximation performance. Although the work in [11] is still preliminary (only periodic boundary conditions were considered, for which the incompressibility condition can be easily enforced with Fourier transform using the projection method), it does provide the key evidence that the high order ENO methodology can be applied to incompressible flow and has good resolution power for certain important physical quantities.

As to the practical issue of parallel implementation of ENO algorithm, we have successfully developed two and three dimensional ENO code for the Connection Machine CM-5 at the Army High Performance Computing Research Center located at University of Minnesota. We have used the fact that communication is costly and

other than next neighbor communication should be minimized, to modify the implementation of the algorithm (without changing the mathematical content) so that communication is reduced and other than next neighbor communication is basically eliminated, at the cost of a slightly increased operation count and, in the two dimensional case, increased storage space [3]. The resulting CM-5 code using 128 nodes, for a two dimensional grid size of 400^2 , is almost a magnitude faster than our CRAY YMP code. Application of ENO schemes to the problem of two dimensional shock interaction with a hydrogen bubble, which is a prototype of hypersonic mixing problem, is also carried out in [3].

Adaptation and application of ENO schemes to semiconductor device simulation has been actively pursued. There are various models in device simulation. Most of them are incomplete parabolic type equations, with source terms coupled to a potential equation, and with a significant hyperbolic part. This significant hyperbolic part, and the fact that solutions can typically vary by several magnitudes over a short region covered by a only a few grid points, warrants the application of high order shock capturing methods. Jointly with Professor Joseph Jerome of Northwestern University who is an applied mathematician, Professor Umberto Ravaioli of University of Illinois who is a device engineer, and their collaborators, we have investigated two dimensional energy models (both the hydrodynamic model and the energy transport model) of device simulation from both a modeling and a computational point of view. My main concern in this project is to understand the mathematical structure of the various models, the corresponding solution behavior (especially those related to high gradient regions similar to compressible gas flow), then trying to resolve issues related to the adaptation and application of high order numerical schemes (both ENO and finite element techniques). As a result of several years' research, the algorithm based on ENO methodology has been developed into a robust and reliable tool for device simulation using various models. In [1] a new energy transport model is discussed and tested to show its improvement upon spurious velocity overshoot at the right junction for a standard $n+-n-n+$ channel; in [4], [7] and [8] the hydrodynamic model and the energy transport model are analyzed, and algorithm based on ENO methodology is designed and tested on two dimensional problems. This algorithm is used to compare the two different models for their accuracy in describing the physical phenomena in the device; [18] concerns the algorithm development using discontinuous Galerkin method and mixed finite element method for the hydrodynamic model in two dimensions, and a numerical test using a 2D MESFET device; [6] studies shock formation and shock width in small devices; [19] explores the response of the hydrodynamic model to heat conduction, mobility and relaxation expressions, [15] and [24] study the crucial issue of whether transport effect is important or not in one and two dimensional devices, the result is positive and indicates the importance of using the full hydrodynamic models and hyperbolic based algorithms.

Also among finite difference techniques for flow calculations is the class of compact schemes. Compact schemes usually can be designed to have high (spectral like)

resolution for various waves and are particularly suitable for long time calculation such as direct numerical simulation of turbulence. In [9], Cockburn and Shu provided a framework to apply compact schemes for shocked or high gradient problems. TVB compact schemes in 1D and L_∞ stable schemes in two and higher dimensions are discussed and tested. The basic idea of compact schemes (using rational functions rather than polynomials to form the approximation) can also be combined with ENO ideas to obtain another type of ENO schemes, which is currently under investigation.

The combination of applied analysis and direct numerical simulation to study physics of fluids phenomena, is carried out jointly with Professor Weinan E of Courant Institute. We have studied the effective equations and the inverse cascade of energy for the two dimensional Kolmogorov flow in [5], and the small scale structure in Boussinesq convection in [12]. Typically, analysis (formal as well as rigorous asymptotic analysis) is carried out as far as possible, while carefully designed numerical simulation (often with the aid of partial result from analysis) is carried out to continue the attack.

The important issue of maintaining positivity of pressure and density in high order finite volume type compressible flow calculations in multidimensional arbitrary triangulations is analyzed in [20]. Adaptation of ENO schemes to solve the viscoelasticity equation with fading memory, and related theoretical study of shock formation and long time behavior, are performed in [26]. Application of ENO ideas to computer vision problems is performed in [27].

We have been investigating the possibility of applying spectral method to shocked problems. Two approaches are considered: The first is of non-oscillatory type: either to add into the spectral basis some discontinuous functions to make the approximation non-oscillatory (Cai, Gottlieb and Shu), or to use some conservative, high order hybridizing between spectral and ENO fluxes (Cai and Shu). This approach has the advantage that essentially no oscillations will appear in the process of numerical simulation, hence one can obtain results similar to those obtained by high resolution finite difference schemes. Another approach is to use some mild high frequency filtering just to stabilize the solution, which is still oscillatory, then to post-process the solution to obtain accurate, non-oscillatory output. This approach is based upon the philosophy that, although the numerical solution itself may be oscillatory, its moments (i.e., its integration against smooth functions) are spectrally accurate. This can be proven for linear problems and is also believed to be true in some sense for nonlinear problems. In order to perform this post-processing, an adequate reconstruction procedure, which can recover spectrally accurate point values everywhere, including at the discontinuity itself, from the oscillatory spectral partial sum, must be developed. Recently, we obtained a breakthrough result in this direction [2], [10], [21], [22], [23], which established the theoretical foundation of this approach and opened the road for practical computations. The recovering of exponentially accurate points everywhere including at the discontinuities themselves, is rigorously proven and successfully implemented even for small to moderate N (the number of modes or grid points), for

both Fourier and polynomial methods, and for both Galerkin and collocation. The crucial issue of assessing information content of using a spectral method to solve a nonlinear conservation law is studied in [25], using the reconstruction procedure described before.

Another quite successful technique for hyperbolic conservation laws is the discontinuous Galerkin finite element method. In this method the partial differential equation is multiplied by a test function, integrated over a cell, and formally integrated by parts to obtain a weak formulation. A solution is sought among discontinuous (across cell interface) piecewise polynomials of r -th degree for a $(r + 1)$ -th order method. Because of the discontinuity at cell interface, this method can accommodate successful finite difference methodology (approximate Riemann solvers and limiters) into a finite element framework (Cockburn and Shu). Theoretical results similar to finite difference methods, such as total variation stability for 1D and maximum norm stability for 2D and 3D, can be proved for this class of discontinuous Galerkin methods of arbitrary order of accuracy and for (almost) arbitrary triangulations. An essential difference between this class of finite element method and the finite volume method (which can also be defined on an arbitrary triangulation) is that the latter has only one independent degree of freedom (the cell average) over each cell, while the former has many (for example, it has three degrees of freedom for the piecewise linear case in 2D). This fact renders the scheme more local (no wide stencil reconstruction is needed to compute the flux at cell interface), hence more suitable for parallel computing, and provides a different setting for theoretical justification of stability and convergence of the algorithm. For example, the recent result of Jiang and Shu [14], [16] proves a cell entropy inequality for the square entropy, which implies L_2 stability in general and convergence in some special cases, for arbitrary triangulations in any space dimension and arbitrary order of accuracy, without even using nonlinear limiters. This result is much stronger than the corresponding results for finite volume or finite difference schemes, which typically require one space dimension, a convex physical flux and no more than second order accuracy to prove the same entropy inequality. In practice, finite element methods can handle complicated geometry and boundary conditions more easily.

4. List of All Publications Supported by This Grant

1. D. Chen, E. Kan, U. Ravaioli, C.-W. Shu and W. Dutton, *An improved energy transport model including nonparabolicity and non-Maxwellian distribution effects*, IEEE Electron Device Letters, v13 (1992), pp.26-28.
2. D. Gottlieb, C.-W. Shu, A. Solomonoff and H. Vandeven, *Journal of Computational On the Gibbs phenomenon I: recovering exponential accuracy from the Fourier partial sum of a non-periodic analytic function*, Journal of Computational and Applied Mathematics, v43 (1992), pp.81-98.

3. C. Quillen and C.-W. Shu, *Parallel implementation and application of high order ENO schemes*, in Modeling and Simulation Volume 23, Part 5, Proceedings of the 23rd Annual Pittsburgh Conference on Modeling and Simulation, W. Vogt and M. Mickle, editors, University of Pittsburgh, 1992. pp.2739-2746.
4. J. Jerome and C.-W. Shu, *Essentially Non-Oscillatory methods for two-dimensional hydrodynamic models*, in Proceedings of the International Workshop on Computational Electronics, Beckman Institute, University of Illinois, May 1992, pp.83-86.
5. W. E and C.-W. Shu, *Effective equations and the inverse cascade theory for Kolmogorov flows*, Physics of Fluids A, v5 (1993), pp.998-1010.
6. C. Gardner, J. Jerome and C.-W. Shu, *The ENO method for the hydrodynamic model for semiconductor devices*, in High Performance Computing, 1993: Grand Challenges in Computer Simulation, Adrian Tentner, editor, the Society for Computer Simulation, San Diego, 1993. pp.96-101.
7. J. Jerome and C.-W. Shu, *Energy transport systems for semiconductors: Analysis and simulation*, in the Proceedings of the World Congress of Nonlinear Analysis, Tampa, 1992.
8. J. Jerome and C.-W. Shu, *Energy models for one-carrier transport in semiconductor devices*, in IMA Volumes in Mathematics and Its Applications, v59, W. Coughran, J. Cole, P. Lloyd and J. White, editors, Springer-Verlag, 1994, pp.185-207.
9. B. Cockburn and C.-W. Shu, *Nonlinearly stable compact schemes for shock calculations*, SIAM Journal on Numerical Analysis, v31 (1994), pp.607-627.
10. D. Gottlieb and C.-W. Shu, *Resolution properties of the Fourier method for discontinuous waves*, Computer Methods in Applied Mechanics and Engineering, v116 (1994), pp.27-37.
11. W. E and C.-W. Shu, *A numerical resolution study of high order essentially non-oscillatory schemes applied to incompressible flow*, Journal of Computational Physics, v110 (1994), pp.39-46.
12. W. E and C.-W. Shu, *Numerical study of the small scale structures in Boussinesq convection*, Physics of Fluids A, v6 (1994), pp.49-58.
13. J. Casper, C.-W. Shu and H.L. Atkins, *A comparison of two formulations for high-order accurate essentially non-oscillatory schemes*. AIAA Journal, v32 (1994), pp.1970-1977.
14. G. Jiang and C.-W. Shu, *On cell entropy inequality for discontinuous Galerkin methods*, Mathematics of Computation, v62 (1994), pp.531-538.

15. J. Jerome and C.-W. Shu, *Transport effect, hyperbolicity, and shock capturing algorithms for device simulations*, in Proceedings of the Third International Workshop on Computational Electronics, Portland, Oregon, May 18-20, 1994, pp.252-255.
16. G. Jiang and C.-W. Shu, *Stability of discontinuous Galerkin methods for general triangulations*, in Developments in Theoretical and Applied Mechanics, Volume XVII, edited by I.C. Jong and F.A. Akl, Louisiana Tech University and University of Arkansas, 1994, pp.227-234.
17. C.-W. Shu, *Essentially non-oscillatory finite difference, finite volume and discontinuous Galerkin finite element methods for conservation laws*, in Proceedings of the Third International Colloquium on Numerical Analysis, Plovdiv, Bulgaria, August 1994. D. Bainov and V. Covachev, editors, VSP International Science Publishers, the Netherlands, 1995, pp.171-180.
18. Z. Chen, B. Cockburn, J. Jerome and C.-W. Shu, *Finite element computation of the hydrodynamic model of semiconductor devices*, VLSI Design, to appear.
19. J. Jerome and C.-W. Shu, *The response of the hydrodynamic model to heat conduction, mobility, and relaxation expressions*, VLSI Design, to appear.
20. B. Perthame and C.-W. Shu, *On positive preserving finite volume schemes for compressible Euler equations*, Numerische Mathematik, to appear.
21. D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon III: recovering exponential accuracy in a sub-interval from a spectral partial sum of a piecewise analytic function*, SIAM Journal on Numerical Analysis, to appear.
22. D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon IV: recovering exponential accuracy in a sub-interval from a Gegenbauer partial sum of a piecewise analytic function*, Mathematics of Computation, to appear.
23. D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon V: recovering exponential accuracy from collocation point values of a piecewise analytic function*, Numerische Mathematik, to appear.
24. J. Jerome and C.-W. Shu, *Transport effects and characteristic modes in the modeling and simulation of submicron devices*, IEEE Transactions on Computer-Aided Design, to appear.
25. P. Wong and C.-W. Shu, *A note on the accuracy of spectral method applied to nonlinear conservation laws*, Journal of Scientific Computing, to appear.
26. C.-W. Shu and Y. Zeng, *High order essentially non-oscillatory scheme for viscoelasticity with fading memory*, Quarterly of Applied Mathematics, to appear.

27. P. Stoll, C.-W. Shu and B. Kimia, *Shock capturing numerical methods for viscosity solutions of certain PDEs in computer vision: the Godunov, Osher-Sethian and ENO schemes*, LEMS preprint 132, Division of Engineering, Brown University, 1994.

4. List of Participating Scientific Personnel

1. Chi-Wang Shu, Associate Professor, Principle Investigator.
2. Denise Chen, graduate student, summer RA. Master's degree in 1992.
3. Carl Quillen, graduate student, RA. Ph. D. degree in 1995.
4. Guangshan Jiang, graduate student, RA. Ph. D. degree in 1995.