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13. ABSTRACT *(Maximum 200 words)*

This project is about the design, analysis and application of high order accurate and nonlinearly stable finite difference (including finite volume), finite element and spectral algorithms for computing solutions of partial differential equations which are either discontinuous or with sharp gradients. Algorithm development, theoretical study about stability and convergence of the algorithms, investigation about efficient implementation including parallel implementations, and applications in compressible and incompressible gas dynamics and in semiconductor device simulations, are performed. The achievement strengthens our objective to obtain powerful and reliable high order numerical algorithms and use them to solve problems containing discontinuous solutions, especially those of army interest.

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Final Report of ARO Grant DAAH04-94-G-0205

High Order Numerical Methods for Discontinuous or High Gradient Problems

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May 15, 1994 to January 15, 1998

1. Abstract

This project is about the design, analysis and application of high order accurate and nonlinearly stable finite difference (including finite volume), finite element and spectral algorithms for computing solutions of partial differential equations which are either discontinuous or with sharp gradients. Algorithm development, theoretical study about stability and convergence of the algorithms, investigation about efficient implementation including parallel implementations, and applications in compressible and incompressible gas dynamics and in semiconductor device simulations, are performed. The achievement strengthens our objective to obtain powerful and reliable high order numerical algorithms and use them to solve problems containing discontinuous solutions, especially those of army interest.

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.

Our approach is to explore the robustness and efficiency of high order numerical algorithms for nonsmooth problems both through theoretical guidance, often obtained with rigorous proofs on simplified model problems, and through numerical experiments on real application problems. We do not try to modify algorithms just for the purpose of convergence proofs, if such modifications are not justified by numerical experiments. For finite difference schemes, we are exploring the very efficient ENO schemes of Shu and Osher based on point values, numerical fluxes, and nonlinearly stable high order Runge-Kutta time discretizations, and the recently developed WENO (Weighted ENO) schemes. For finite element methods, we are exploring the Runge-Kutta discontinuous Galerkin methods of Cockburn and Shu, which combine the advantage of finite elements (weak formulation, automatic energy stability, easy handling of complicated geometry and boundary conditions) with features of high resolution finite difference schemes (approximate Riemann solvers, limiters). Effective ways to handle viscous terms are being investigated. For spectral methods, we are exploring reconstruction techniques of Gottlieb and Shu to apply spectral approximations to discontinuous functions and still obtain uniform spectral accuracy.

We have been cooperating with Dr. Rupak Biswas of RIACS and Dr. Roger Strawn of US Army AFDD, at NASA Ames Research Center, on the investigation of developing high order high resolution numerical methods for the simulation of helicopter rotor blade motion. This is a very demanding simulation since the vortex motion after interaction with shocks should be sustained for long time/distance, and only high order methods with low dissipation can achieve this. We have already performed simulations for a model problem, namely a moving vortex in a uniform flow which is an exact solution of the Euler equations. Both 2D and 3D simulations are performed, with vortex moving in different directions and with both uniform and nonuniform (but smooth) Cartesian grids. The results clearly show the advantage of using high order methods for this model problem. We are currently in the process of combining the WENO scheme (as the background solver) and the existing inner solver near the blade which is of finite volume type.

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 28 publications (among them 22 in refereed journals) resulting from this project, see Section 4 for a list of them.

About high order essentially non-oscillatory (ENO) finite difference schemes, jointly with Yanni Zeng, we have applied ENO method to the viscoelastic model with fading memory [15] (all the numbering of references are according to that of Section 4). The memory term is treated by introducing new variables and rewrite the system by adding more differential equations but without explicit memory terms. The appearance of the memory terms regularizes the solution somewhat, and in many cases it is still a theoretically open question whether shocks will develop from smooth initial data. We have performed theoretical analysis about the linearized system for large time, and have applied ENO scheme to study the nonlinear system for both local time and large time. The high order accuracy and sharp, non-oscillatory shock transition allow us to obtain fine resolution for tens of thousands of time steps, and to study the shock interactions after the formation of shocks.

In [4], which results from an invited talk in the Third International Colloquium of Numerical Analysis, we have compared ENO finite difference, finite volume and discontinuous Galerkin finite element methods, in terms of their shock resolution, grid orientation effects, cost, and ability to handle complicated geometry and boundary conditions.

Also on finite difference, Harabetian, Osher and Shu have investigated a novel Eulerian approach for simulating vortex motion using a level set regularization procedure [12]. Our approach uses a decomposition of the vorticity of the form $\xi = P(\varphi)\eta$, in which both φ (the level set function) and η (the vorticity strength vector) are smooth. We derive coupled equations for φ and η which give a regularization of the problem. The regularization is topological and is automatically accomplished through the use of numerical schemes whose viscosity shrinks to zero with grid size. There is no need for explicit filtering, even when singularities appear in the front. The method also has the advantage of automatically allowing topological changes such as merging of surfaces. Numerical examples including two and three dimensional vortex sheets, two dimensional vortex dipole sheets and point vortices, are given. To our knowledge, this is the first three dimensional vortex sheet calculation in which the sheet evolution feeds back to the calculation of the fluid velocity.

Application of ENO scheme to the study of shock longitudinal vortex interaction problem is carried out, jointly with Erlebacher and Hussaini [16]. We have studied the shock/longitudinal vortex interaction problem in axisymmetric geometry. Linear analysis, shock fitting code, and shock capturing ENO are used in different parameter range, to study various cases of nearly linear regime, weakly nonlinear regime, and strong nonlinear regime. Vortex breakdown as a function of Mach number ranging from 1.3 to 10 is studied, extending the range of existing results. For vortex strengths above a critical value, a triple point forms on the shock, leading to a Mach disk. This leads to a strong recirculating region downstream of the shock. It is found out that a secondary shock forms, to provide the necessary deceleration so that the fluid velocity can adjust to downstream conditions at the shock.

The important issue of maintaining positivity of density and pressure for high order calculations of Euler equations of compressible gas dynamics is considered in [11].

As an important development about the high order essentially non-oscillatory (ENO) finite difference schemes, Jiang and Shu have been investigating WENO (weighted ENO) schemes [13]. WENO is a modification and improvement of ENO schemes. Instead of using only one of the many candidate stencils based on local smoothness as in ENO, WENO uses a linear combination of the contribution from all candidate stencils, each with suitable nonlinear weight. The weights are chosen so that in smooth regions, they are close to an optimal linear weight which gives the highest possible order of accuracy of an upwind-biased linearly stable scheme. Near shocks, however, those stencils which contain the shock are assigned weights which are essentially zero. Thus WENO resembles a linear high order upwind biased scheme in smooth regions, and ENO near shocks, with a smooth numerical flux function. Another advantage of WENO, due to its smoothness of fluxes, is that convergence for smooth solutions can be proven. Also, convergence towards steady states is easier than ENO. Numerical experiments, including shock vortex interaction problems relevant to the joint work of the PI and ARO scientists Drs. Rupak and Strawn on the simulation of helicopter rotor blade motion, have been performed with very good results.

In [26], jointly with Siddiqi and Kimia, we have developed a geometric shock capturing ENO methodology suitable for subpixel interpolation (subcell resolution). The method gives excellent result for curve evolution and representation on a fixed, coarse grid.

In the lecture note [27], we describe the construction, analysis, and application of ENO (Essentially Non-Oscillatory) and WENO (Weighted Essentially Non-Oscillatory) schemes for hyperbolic conservation laws and related Hamilton-Jacobi equations. ENO and WENO schemes are high order accurate finite difference schemes designed for problems with piecewise smooth solutions containing discontinuities. The key idea lies at the approximation level, where a nonlinear adaptive procedure is used to automatically choose the locally smoothest stencil, hence avoiding crossing discontinuities in the interpolation procedure as much as possible. ENO and WENO schemes have been quite successful in applications, especially for problems containing both shocks and complicated smooth solution structures, such as compressible turbulence simulations and aeroacoustics. This lecture note is basically self-contained. It is our hope that with this note and with the help of the quoted references, the reader can understand the algorithms and code them up for applications. Sample codes are also available from the author.

About the discontinuous Galerkin methods, Atkins and Shu have developed a discontinuous Galerkin formulation that avoids the use of discrete quadrature formulas [21]. The application is carried out for one and two dimensional linear and nonlinear test problems. This approach requires less computational time and storage than conventional implementations but preserves the compactness and robustness inherent in the discontinuous Galerkin method.

In [22], jointly with Cockburn, we study the Local Discontinuous Galerkin methods for nonlinear, time-dependent convection-diffusion systems. These methods are an extension of the Runge-Kutta Discontinuous Galerkin methods for purely hyperbolic systems to convection-diffusion systems and share with those methods their high parallelizability, their high-order formal accuracy, and their easy handling of complicated geometries, for convection dominated problems. It is proven that for scalar equations, the Local Discontinuous Galerkin methods are L^2-stable in the nonlinear case. Moreover, in the linear case, it is shown that if polynomials of degree k are used, the methods are k-th order accurate for general triangulations; although this order of convergence is suboptimal, it is sharp for the LDG methods. Preliminary numerical examples displaying the performance of the method are shown.

In [25], again jointly with Cockburn, we extend the Runge-Kutta discontinuous Galerkin method to multidimensional nonlinear systems of conservation laws. The algorithms are described and discussed, including algorithm formulation and practical implementation issues such as the numerical fluxes, quadrature rules, degrees of freedom, and the slope limiters, both in the triangular and the rectangular element cases. Numerical experiments for two dimensional Euler equations of compressible gas dynamics are presented that show the effect of the (formal) order of accuracy and the use of triangles or rectangles, on the quality of the approximation.

Jointly with Hu, we present a discontinuous Galerkin finite element method for solving the nonlinear Hamilton-Jacobi equations [28]. This method is based on the Runge-Kutta discontinuous Galerkin finite element method for solving conservation laws. The method has the flexibility of treating complicated geometry by using arbitrary triangulation, can achieve high order accuracy with a local, compact stencil, and are suited for efficient parallel implementation. One and two dimensional numerical examples are given to illustrate the capability of the method.

For spectral methods, jointly with David Gottlieb, we have been continuing on our investigation of overcoming Gibbs phenomenon, i.e., to recover exponential accuracy from a spectral partial sum of a piecewise analytic function. We have investigated the problem of recovering exponential accuracy in a sub-interval, with the assumption that the function is analytic in this sub-interval but may have discontinuities at one or both boundary. The Fourier and Legendre Galerkin cases are considered in [10]. The general Gegenbauer Galerkin case is considered in [1]. The collocation case is considered in [2]. We review the history of the Gibbs phenomenon as well as efforts for its resolution in [17]. Also, jointly with Peter Wong, we have performed a detailed numerical study about numerical accuracy when spectral method is applied to a nonlinear conservation law with discontinuous solutions [5], [14]. We assess the accuracy of Fourier Galerkin and collocation method applied to Burgers equation with smooth initial condition but with a shock developed in finite time. We find that, unlike in the linear PDE case, the moments with respect to analytic functions, in particular the first few Fourier coefficients, are no longer very accurate. However the numerical solution does contain accurate information which can be extracted by a post-processing based on Gegenbauer polynomials.

Jointly with S. Gottlieb, we have further explored a class of high order TVD (total variation diminishing) Runge-Kutta time discretization initialized by Shu and Osher, suitable for solving hyperbolic conservation laws with stable spatial discretizations [18]. We illustrate with numerical examples that non-TVD but linearly stable Runge-Kutta time discretization can generate oscillations even for TVD (total variation diminishing) spatial discretization, verifying the claim that TVD Runge-Kutta methods are important for such applications. We then explore the issue of optimal TVD Runge-Kutta methods for second, third and fourth order, and for low storage Runge-Kutta methods.

We have been continuing our investigation on adapting shock capturing algorithms for semiconductor device simulations. Jointly with Jerome [3], we have studied the effect of the common practice of neglecting the convective terms (inertial approximation) in the hydrodynamic model in device simulations. We find out that this inertial approximation, though very convenient for the application of exponential fitting type methods, is nevertheless not valid near the diode junctions, resulting in significant error in the result. We have also studied the characteristic modes of some modified hydrodynamic models and energy transport models, the purpose being to make sure that such modifications do not change the mathematical properties of the models dramatically. Jointly with Chen, Cockburn and Jerome, we have extended the discontinuous Galerkin method to the hydrodynamic model of semiconductor device simulations [6]. Jointly with Jerome, we have studied the response of the hydrodynamic model to heat conduction, mobility, and relaxation expressions [7]. Also jointly with Jerome, we have performed analysis and simulation for the energy transport models for semiconductors [9].

Jointly with G. Chen, J. Jerome and D. Wong of Northwestern University, we have introduced a novel two carrier (electro) hydrodynamic model for semiconductor device simulations, which incorporates higher dimensional geometric effects into a one dimensional model[19], [20]. A rigorous mathematical analysis is carried out for the evolution system in the case of piezotropic flow, including realistic carrier coupling. The proofs are constructive in nature, making use of generalized Godunov schemes with a novel fractional step, steady-state component, and compensated compactness. Two important applications are studied. We simulate: (1) the GaAs device in the notched oscillator circuit; and, (2) a MESFET channel, and its steady-state symmetries. The first of these applications is the well known Gunn oscillator, and we are able to replicate Monte-Carlo simulations, based upon the Boltzmann equation. For the second application, we observe the effect of a symmetry breaking parameter, the potential bias on the drain. In high order essentially non-oscillatory (ENO) finite difference schemes,

Jointly with Cercignani, Gamba and Jerome, we have been investigating a new high field model for the semiconductor devices [23], [24]. It is our hope that this new model, coupled with a domain decomposition technique, will give more accurate description of the small devices currently being used with relatively small computational effort.

Jointly with Chen, Eisenberg and Jerome, we have explored a hydrodynamic model of temperature change in open ionic channels [8]. This is an important problem in computational biology.

4. List of All Publications Supported by This Grant

1. D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon IV: recovering exponential accuracy in a subinterval from a Gegenbauer partial sum of a piecewise analytic function*, Mathematics of Computation, v64 (1995), pp.1081-1095.

2. 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, v71 (1995), pp.511-526.

3. 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 of Integrated Circuits and Systems, v14 (1995), pp.917-923.

4. 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.

5. C.-W. Shu and P. Wong, *A note on the accuracy of spectral method applied to nonlinear conservation laws*, Journal of Scientific Computing, v10 (1995), pp.357-369.

6. Z. Chen, B. Cockburn, J. Jerome and C.-W. Shu, *Mixed-RKDG Finite element methods for the 2-D hydrodynamic model for semiconductor device simulation*, VLSI Design, v3 (1995), pp.145-158.

7. J. Jerome and C.-W. Shu, *The response of the hydrodynamic model to heat conduction, mobility, and relaxation expressions*, VLSI Design, v3 (1995), pp.131-143.

8. D.P. Chen, R. Eisenberg, J. Jerome and C.-W. Shu, *A hydrodynamic model of temperature change in open ionic channels*, Biophysical Journal, v69 (1995), pp.2304-2322.

9. J. Jerome and C.-W. Shu, *Energy transport systems for semiconductors: Analysis and simulation*, in World Congress of Nonlinear Analysts '92, V. Lakshmikantham, Editor, Walter de Gruyter, Berlin and New York, 1996, pp. 3835-3846.

10. 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, v33 (1996), pp.280-290.

11. B. Perthame and C.-W. Shu, *On positivity preserving finite volume schemes for Euler equations*, Numerische Mathematik, v73 (1996), pp.119-130.

12. E. Harabetian, S. Osher and C.-W. Shu, *An Eulerian approach for vortex motion using a level set regularization procedure*, Journal of Computational Physics, v127 (1996), pp.15-26.

13. G. Jiang and C.-W. Shu, *Efficient implementation of weighted ENO schemes*, Journal of Computational Physics, v126 (1996), pp.202-228.

14. C.-W. Shu and P. Wong, *A numerical study on the accuracy of Fourier spectral methods applied to the nonlinear Burgers equation*, in Proceedings of the Third International Conference on Spectral and High Order Methods, A.V. Ilin and L.R. Scott, Editors, Houston Journal of Mathematics, 1996, pp. 131-138.

15. C.-W. Shu and Y. Zeng, *High order essentially non-oscillatory scheme for viscoelasticity with fading memory*, Quarterly of Applied Mathematics, v55 (1997), pp.459-484.

16. G. Erlebacher, M.Y. Hussaini and C.-W. Shu, *Interaction of a shock with a longitudinal vortex*, Journal of Fluid Mechanics, v337 (1997), pp.129-153.

17. D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon and its resolution*, SIAM Review, v30 (1997), pp.644-668.

18. S. Gottlieb and C.-W. Shu, *Total variation diminishing Runge-Kutta schemes*, Mathematics of Computation, v67 (1998), pp.73-85.

19. G.-Q. Chen, J. Jerome and C.-W. Shu, *Analysis and simulation of extended hydrodynamic models: the multi-valley Gunn oscillator and MESFET symmetries*, VLSI Design, to appear.

20. G.-Q. Chen, J. Jerome, C.-W. Shu and D. Wang, *Two carrier semiconductor device models with geometric structure*, to appear in Modeling and Computation for Applications in Mathematics, Science, and Engineering, J. Jerome, editor, Oxford University Press.

21. H. Atkins and C.-W. Shu, *Quadrature-free implementation of the discontinuous Galerkin method for hyperbolic equations*, AIAA Paper 96-1683, 1996. AIAA Journal, to appear.

22. B. Cockburn and C.-W. Shu, *The local discontinuous Galerkin method for time-dependent convection-diffusion systems*, SIAM Journal on Numerical Analysis, to appear.

23. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *Applicability of the high field model: an analytical study via asymptotic parameters defining domain decomposition*, VLSI Design, to appear.

24. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *Applicability of the high field model: a preliminary numerical study*, VLSI Design, to appear.

25. B. Cockburn and C.-W. Shu, *The Runge-Kutta discontinuous Galerkin method for conservation laws V: multidimensional systems*, Journal of Computational Physics, to appear.

26. K. Siddiqi, B. Kimia and C.-W. Shu, *Geometric shock-capturing ENO schemes for subpixel interpolation, computation and curve evolution*, Computer Vision Graphics and Image Processing: Graphical Models and Image Processing (CVGIP:GMIP), to appear.

27. C.-W. Shu, *Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws*, in *Advanced Numerical Approximation of Nonlinear Hyperbolic Equations*, A. Quarteroni, Editor, Lecture Notes in Mathematics, CIME subseries, Springer-Verlag, to appear.

28. C. Hu and C.-W. Shu, *A discontinuous Galerkin finite element method for Hamilton-Jacobi equations*, Submitted to Journal of Computational Physics.

4. List of Participating Scientific Personnel

1. Chi-Wang Shu, Professor, Principle Investigator.
2. Carl Quillen, graduate student, partial RA. Ph. D. degree in 1995.
3. Guangshan Jiang, graduate student, partial RA. Ph. D. degree in 1995.
4. Sigal Gottlieb, graduate student, partial RA. Ph. D. degree expected in 1998.
5. Changqing Hu, partial RA. Ph. D. degree expected in 1999.