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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) WENO schemes, finite element discontinuous Galerkin methods, 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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weighted essentially non-oscillatory schemes, discontinuous Galerkin methods, norm-preserving Runge-Kutta methods, Euler equations, semiconductor device simulations

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Enclosure 3

Final Report of ARO Grant DAAG55-97-1-0318

High Order Numerical Methods for Long Time Solutions with Discontinuities

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June 1, 1997 to May 31, 2001

1. Foreword

This project is about the design, analysis and application of high order accurate and nonlinearly stable finite difference (including finite volume) WENO schemes, finite element discontinuous Galerkin methods, 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.

4. 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 and finite volume WENO schemes, finite element discontinuous Galerkin methods, 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 WENO schemes based on point values, numerical fluxes, and nonlinearly stable high order Runge-Kutta time discretizations. 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 and higher derivative 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 continuing on the cooperation 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 and in general the problems of overlaying domains.

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 44 publications (among them 17 appeared in refereed journals, 12 appeared in conference proceedings and book chapters, 8 accepted and to appear in refereed journals, and 7 preprints submitted for publications) resulting from this project, see Section 6 for a list of them.

S. Gottlieb and C.-W. Shu 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 [a1] (all the numbering of references are according to that of Section 6). 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. Also, S. Gottlieb, C.-W. Shu and E. Tadmor have reviewed and further developed a class of strong stability preserving (SSP) high order time discretizations for semi-discrete method of lines approximations of partial differential equations, [a17]. Termed TVD (total variation diminishing) time discretizations before, these high order time discretization methods preserve the strong stability properties of first order Euler time stepping and has proved very useful especially in solving hyperbolic partial differential equations. The new developments include the construction of optimal explicit SSP linear Runge-Kutta methods, their application to the strong stability of coercive approximations, a systematic study of explicit SSP multi-step methods for nonlinear problems, and the study of the strong stability preserving property of implicit Runge-Kutta and multi-step methods.

B. Cockburn and C.-W. Shu have extended the Runge-Kutta discontinuous Galerkin method to multidimensional nonlinear systems of conservation laws, [a2]. 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.

H. Atkins and C.-W. Shu have developed a discontinuous Galerkin formulation that avoids the use of discrete quadrature formulas, [a3]. 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.

G. Chen, J. Jerome and C.-W. Shu have introduced a novel two carrier (electro) hydrodynamic model for semiconductor device simulations, which incorporates higher dimensional geometric effects into a one dimensional model, [a4]. 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.

C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu have been investigating a new high field model for the semiconductor devices [a4,a5]. 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. Preliminary investigations strongly demonstrate this potential.

B. Cockburn and C.-W. Shu have studied the Local Discontinuous Galerkin methods for nonlinear, time-dependent convection-diffusion systems, [a7]. 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.

P. Montarnal and C.-W. Shu have used a recently developed energy relaxation theory by Coquel and Perthame and high order weighted essentially non-oscillatory (WENO) schemes to simulate the Euler equations of real gas [a8]. The main idea is an energy decomposition under the form $\varepsilon = \varepsilon_1 + \varepsilon_2$, where ε_1 is associated with a simpler pressure law (γ-law in this paper) and the nonlinear deviation ε_2 is convected with the flow. A relaxation process is performed for each time step to ensure that the original pressure law is satisfied. The necessary characteristic decomposition for the high order WENO schemes is performed on the characteristic fields based on the ε_1 γ-law. The algorithm only calls for the original pressure law once per grid point per time step, without the need to compute its derivatives or any Riemann solvers. Both one and two dimensional numerical examples are shown to illustrate the effectiveness of this approach.

C. Hu and C.-W. Shu have constructed third and fourth order WENO schemes on two dimensional unstructured meshes (triangles) in the finite volume formulation, [a9]. The third order schemes are based on a combination of linear polynomials with nonlinear weights, and the fourth order schemes are based on combination of quadratic polynomials with nonlinear weights. We have addressed several difficult issues associated with high order WENO schemes on unstructured mesh, including the choice of linear and nonlinear weights, what to do with negative weights, etc. Numerical examples are shown to demonstrate the accuracies and robustness of the methods for shock calculations.

C. Hu and C.-W. Shu have presented a discontinuous Galerkin finite element method for solving the nonlinear Hamilton-Jacobi equations [a10]. 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. Also, O. Lepsky, C. Hu and C.-W. Shu have further investigated this method from theoretical and computational points of view, [a11]. This method handles the complicated geometry by using arbitrary triangulation, achieves the high order accuracy in smooth regions and the high resolution of the derivatives discontinuities. Theoretical results on accuracy and stability properties of the method are proven for certain cases and related numerical examples are presented.

C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu have described benchmark comparisons for a GaAs $n^+ - n - n^+$ diode in [a12]. A global kinetic model is simulated, using fifth order WENO schemes, and compared with various realizations of the hydrodynamic model, depending on mobility calibration. Finally, the channel region alone is simulated, with interior boundary conditions derived from the kinetic model, by use of the high-field (augmented drift-diffusion) model.

D. Balsara and C.-W. Shu have developed a class of higher order (from 7th to 13th) WENO schemes in [a13]. Numerical tests are given in assessing the accuracy and non-oscillatory properties of such schemes. These schemes might be useful in situations when really high order accuracy is needed.

J.-G. Liu and C.-W. Shu have introduced a high order discontinuous Galerkin method for two dimensional incompressible flow in the vorticity stream-function formulation, [a14]. The momentum equation is treated explicitly, utilizing the efficiency of the discontinuous Galerkin method. The stream-function is obtained by a standard Poisson solver using continuous finite elements. There is a natural matching between these two finite element spaces, since the normal component of the velocity field is *continuous* across element boundaries. This allows for a correct upwinding gluing in the discontinuous Galerkin framework, while still maintaining total energy conservation with no numerical dissipation and total enstrophy stability. The method is efficient for inviscid or high Reynolds number flows. Optimal error estimates are proven and verified by numerical experiments.

C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu have developed a domain decomposition method for silicon devices in [a15], in which we use different models in different parts of the domain to achieve the effect of correct modeling and efficient numerical computations.

J. Carrillo, I. Gamba and C.-W. Shu have performed computational macroscopic approximations to the 1-D relaxation-time kinetic system for semiconductors in [a16]. The main contribution is the development of a new hydrodynamic model which is valid in the ballistic limit, as verified by analysis and numerical experiments.

In the submitted manuscripts (some of them already accepted for publications), we have made progress in techniques of treating negative weights in WENO schemes, enhanced accuracy by post-processing for the discontinuous Galerkin method applied to hyperbolic problems, a local discontinuous Galerkin method for KdV type equations, and high order central WENO schemes.

6. List of All Publications Supported by This Grant

(a) Papers published in peer-reviewed journals

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

2. B. Cockburn and C.-W. Shu, *The Runge-Kutta discontinuous Galerkin method for conservation laws V: multidimensional systems*, Journal of Computational Physics, v141 (1998), pp.199-224.

3. H. Atkins and C.-W. Shu, *Quadrature-free implementation of the discontinuous Galerkin method for hyperbolic equations*, AIAA Journal, v36 (1998), pp.775-782.

4. 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, v6 (1998), pp.277-282.

5. 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, v8 (1998), pp.135-141.

6. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *Applicability of the high field model: a preliminary numerical study*, VLSI Design, v8 (1998), pp.275-282.

7. B. Cockburn and C.-W. Shu, *The local discontinuous Galerkin method for time-dependent convection-diffusion systems*, SIAM Journal on Numerical Analysis, v35 (1998), pp.2440-2463.

8. P. Montarnal and C.-W. Shu, *Real gas computation using an energy relaxation method and high order WENO schemes*, Journal of Computational Physics, v148 (1999), pp.59-80.

9. C. Hu and C.-W. Shu, *Weighted essentially non-oscillatory schemes on triangular meshes*, Journal of Computational Physics, v150 (1999), pp.97-127.

10. C. Hu and C.-W. Shu, *A discontinuous Galerkin finite element method for Hamilton-Jacobi equations*, SIAM Journal on Scientific Computing, v21 (1999), pp.666-690.

11. O. Lepsky, C. Hu and C.-W. Shu, *Analysis of the discontinuous Galerkin method for Hamilton-Jacobi equations*, Applied Numerical Mathematics, v33 (2000), pp.423-434.

12. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *Device benchmark comparisons via kinetic, hydrodynamic, and high-field models*, Computer Methods in Applied Mechanics and Engineering, v181 (2000), pp.381-392.

13. D. Balsara and C.-W. Shu, *Monotonicity preserving weighted essentially non-oscillatory schemes with increasingly high order of accuracy*, Journal of Computational Physics, v160 (2000), pp.405-452.

14. J.-G. Liu and C.-W. Shu, *A high order discontinuous Galerkin method for 2D incompressible flows*, Journal of Computational Physics, v160 (2000), pp.577-596.

15. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *A domain decomposition method for silicon devices*, Transport Theory and Statistical Physics, v29 (2000), pp.525-536.

16. J.A. Carrillo, I. Gamba and C.-W. Shu, *Computational macroscopic approximations to the 1-D relaxation-time kinetic system for semiconductors*, Physica D, v146 (2000), pp.289-306.

17. S. Gottlieb, C.-W. Shu and E. Tadmor, *Strong stability preserving high order time discretization methods*, SIAM Review, v43 (2001), pp.89-112.

(b) Papers published in non-peer-reviewed journals or in conference proceedings

1. C. Hu and C.-W. Shu, *High order weighted ENO schemes for unstructured meshes: preliminary results*, Computational Fluid Dynamics 98, Invited Lectures, Minisymposia and Special Technological Sessions of the Fourth European Computational Fluid Dynamics Conference, K. Papailiou, D. Tsahalis, J. Periaux and D. Knorzer, Editors, John Wiley and Sons, v2, September 1998, pp.356-362.

2. C. Cercignani, I. Gamba, J. Jerome and C.-W. Shu, *A domain decomposition method: a simulation study*, in Proceedings of 1998 Sixth International Workshop on Computational Electronics (IWCE-6), Osaka University, Japan, October 19-21, 1998, IEEE Catalog Number 98EX116, pp.174-177.

3. C.-W. Shu, *Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws*, in *Advanced Numerical Approximation of Nonlinear Hyperbolic Equations*, B. Cockburn, C. Johnson, C.-W. Shu and E. Tadmor (Editor: A. Quarteroni), Lecture Notes in Mathematics, volume 1697, Springer, 1998, pp.325-432.

4. G.-Q. Chen, J. Jerome, C.-W. Shu and D. Wang, *Two carrier semiconductor device models with geometric structure*, Modeling and Computation for Applications in Mathematics, Science, and Engineering, J. Jerome, editor, Oxford University Press, 1998, pp.103-140.

5. D. Gottlieb and C.-W. Shu, *A general theory for the resolution of the Gibbs phenomenon*, in Atti Dei Convegni Lincei, v147, Tricomi's Ideas and Contemporary Applied Mathematics, Academia Nazionale dei Lincei, 1998, pp.39-48.

6. C.-W. Shu, *High order ENO and WENO schemes for computational fluid dynamics*, in *High-Order Methods for Computational Physics*, T.J. Barth and H. Deconinck, editors, Lecture Notes in Computational Science and Engineering, volume 9, Springer, 1999, pp.439-582.

7. B. Cockburn, G. Karniadakis and C.-W. Shu, *The development of discontinuous Galerkin methods*, in *Discontinuous Galerkin Methods: Theory, Computation and Applications*, B. Cockburn, G. Karniadakis and C.-W. Shu, editors, Lecture Notes in Computational Science and Engineering, volume 11, Springer, 2000, Part I: Overview, pp.3-50.

8. B. Cockburn, J. Jerome and C.-W. Shu, *The utility of modeling and simulation in determining transport performance properties of semiconductors*, in *Discontinuous Galerkin Methods: Theory, Computation and Applications*, B. Cockburn, G. Karniadakis and C.-W. Shu, editors, Lecture Notes in Computational Science and Engineering, volume 11, Springer, 2000, Part II: Invited Papers, pp.147-156.

9. B. Cockburn, M. Luskin, C.-W. Shu and E. Suli, *Post-processing of Galerkin methods for hyperbolic problems*, in *Discontinuous Galerkin Methods: Theory, Computation and Applications*, B. Cockburn, G. Karniadakis and C.-W. Shu, editors, Lecture Notes in Computational Science and Engineering, volume 11, Springer, 2000, Part III: Contributed Papers, pp.291-300.

10. C. Hu, O. Lepsky and C.-W. Shu, *The effect of least square procedure for discontinuous Galerkin methods for Hamilton-Jacobi equations*, in *Discontinuous Galerkin Methods: Theory, Computation and Applications*, B. Cockburn, G. Karniadakis and C.-W. Shu, editors, Lecture Notes in Computational Science and Engineering, volume 11, Springer, 2000, Part III: Contributed Papers, pp.343-348.

11. J.-G. Liu and C.-W. Shu, *A numerical example on the performance of high order discontinuous Galerkin method for 2D incompressible flows*, in *Discontinuous Galerkin Methods: Theory, Computation and Applications*, B. Cockburn, G. Karniadakis and C.-W. Shu, editors, Lecture Notes in Computational Science and Engineering, volume 11, Springer, 2000, Part III: Contributed Papers, pp.369-374.

12. C.-W. Shu, *Different formulations of the discontinuous Galerkin method for the viscous terms*, in *Advances in Scientific Computing*, Z.-C. Shi, M. Mu, W. Xue and J. Zou, editors, Science Press, 2001, pp.144-155.

(d) Manuscripts submitted, but not published

1. M. Anile, J. Carrillo, I. Gamba and C.-W. Shu, *Approximation of the BTE by a relaxation-time operator: simulations for a 50nm-channel Si diode*, VLSI Design, to appear.
2. K. Banoo, J.-H. Rhew, M. Lundstrom, C.-W. Shu and J. Jerome, *Simulating quasi-ballistic transport in Si nanotransistors*, VLSI Design, to appear.
3. T. Zhou, Y. Guo and C.-W. Shu, *Numerical study on Landau damping*, Physica D, to appear.
4. A. Arnold, J.A. Carrillo, I. Gamba and C.-W. Shu, *Low and high field scaling limits for the Vlasov and Wigner-Poisson-Fokker-Planck systems*, Transport Theory and Statistical Physics, to appear.
5. T. Zhou, Y. Li and C.-W. Shu, *Numerical comparison of WENO finite volume and Runge-Kutta discontinuous Galerkin methods*, Journal of Scientific Computing, to appear.
6. C.-W. Shu, *High order finite difference and finite volume WENO schemes and discontinuous Galerkin methods for CFD*, International Journal of Computational Fluid Dynamics, to appear.
7. J. Shi, C. Hu and C.-W. Shu, *A technique of treating negative weights in WENO schemes*, Journal of Computational Physics, to appear.
8. B. Cockburn and C.-W. Shu, *Runge-Kutta Discontinuous Galerkin methods for convection-dominated problems*, Journal of Scientific Computing, to appear.
9. B. Cockburn, M. Luskin, C.-W. Shu and E. Süli, *Enhanced accuracy by post-processing for finite element methods for hyperbolic equations*, submitted to Mathematics of Computation.
10. J.A. Carrillo, I. Gamba, O. Muscato and C.-W. Shu, *Comparison of Monte Carlo and deterministic simulations of a silicon diode*, to appear in IMA Volumes in Mathematics and Its Applications, Springer-Verlag.
11. J. Yan and C.-W. Shu, *A local discontinuous Galerkin method for KdV type equations*, submitted to SIAM Journal on Numerical Analysis.
12. J. Qiu and C.-W. Shu, *On the construction, comparison, and local characteristic decomposition for high order central WENO schemes*, submitted to Journal of Computational Physics.

13. C.-W. Shu, *Recent development and applications of WENO schemes*, to appear in the Proceedings of the Third AFOSR International Conference on DNS/LES (TAICDL), 2001.

14. C.-W. Shu, *Development and applications of WENO schemes in continuum physics*, to appear in the Proceedings of the International Workshop on Computational Methods for Continuum Physics and Their Applications (IWCCPA), 2001.

15. P. Lin and C.-W. Shu, *Numerical solution of a virtual internal bond model for material fracture*, submitted to Physica D.

7. List of Participating Scientific Personnel

1. Chi-Wang Shu, Professor, Principle Investigator.

2. Sigal Gottlieb, graduate student, partial RA and postdoctoral research associate. Ph.D. degree in 1998.

3. Changqing Hu, graduate student, partial RA. Ph.D. degree in 1999.

4. Jing Shi, graduate student, partial RA. Ph.D. degree in 2001.

5. Jue Yan, partial RA. Ph.D. degree expected in 2002.