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13. ABSTRACT (Maximum 200 words)

This project is about the algorithm development, analysis, implementation and application aspects of high order finite difference weighted essentially non-oscillatory (WENO) schemes, finite volume WENO schemes, discontinuous Galerkin finite element methods and spectral methods for solving convection dominated problems requiring long time integration and small dissipation/dispersion with discontinuous or high gradient solutions. Algorithm development and analysis, investigation about efficient implementation including parallel implementations, and applications in computational fluid dynamics, computational semiconductor device simulation and other areas, are performed. The achievement strengthens our objective to obtain powerful and reliable high order numerical algorithms and use them to solve convection dominated problems, especially those of army interest.

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Final Report of ARO Grant DAAD19-00-1-0405

High Order Numerical Methods for Convection Dominated Problems

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July 1, 2000 to July 30, 2004

1. Foreword

This project is about the algorithm development, analysis, implementation and application aspects of high order finite difference weighted essentially non-oscillatory (WENO) schemes, finite volume WENO schemes, discontinuous Galerkin finite element methods and spectral methods for solving convection dominated problems requiring long time integration and small dissipation/dispersion with discontinuous or high gradient solutions. Algorithm development and analysis, investigation about efficient implementation including parallel implementations, and applications in computational fluid dynamics, computational semiconductor device simulation and other areas, are performed. The achievement strengthens our objective to obtain powerful and reliable high order numerical algorithms and use them to solve convection dominated problems, especially those of army interest.

4. Statement of the Problem Studied

The problems studied in this project involve numerical solutions of convection dominated partial differential equations. These problems typically have solutions which are either discontinuous, or with discontinuous derivatives, or containing sharp gradient regions which are difficult to be completely resolved on today's computers. Our objective is to develop, analyze and apply numerical methods which "capture" the discontinuities or sharp gradient regions, without fully resolving them, while maintaining nonlinearly stable transitions for these discontinuities or sharp gradients and high order accuracy in the smooth part of the domain. 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 study of efficient and high order finite difference WENO schemes on multiple domains with overlaps, which will be useful for general problems of overlaying domains and is of interest to 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.

5. Summary of the Most Important 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 54 publications (among them 32 appeared in refereed journals, 6 appeared in conference proceedings and book chapters, 9 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, 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, [a1] (all the numbering of references are according to that of Section 6). 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. A survey of the SSP time discretizations is also given in [b1].

Discontinuous Galerkin (DG) method has been extensively developed, analyzed and applied during this period. In [a4], Cockburn and Shu have given an extensive review of the state of the art of this method. In [a6,a7,a30,a31] and [d12,d14], Yan and Shu, Levy, Shu and Yan, and Xu and Shu developed and analyzed nonlinearly stable local discontinuous Galerkin (LDG) methods for partial differential equations containing third and higher spatial derivatives, including the KdV equations, time dependent bi-harmonic equations, $K(m,n)$ equations with compacton solutions, KdV-Burgers type equations, the general fifth-order KdV type equations and the fully nonlinear $K(n,n,n)$ equations, the Kuramoto-Sivashinsky equations and the Ito-type coupled KdV equations, one and two dimensional generalized nonlinear Schrödinger equation and the coupled nonlinear Schrödinger equation, and the two dimensional Kadomtsev-Petviashvili equation and Zakharov-Kuznetsov equation. These LDG methods satisfy cell entropy inequalities and are nonlinearly stable in L^2 or other norms for quite general nonlinear cases, and are flexible in h-p adaptivity and efficient for parallel implementation. In [a12,a25] and [d5], Cockburn, Luskin, Shu and Suli, Ryan and Shu, and Ryan, Shu and Atkins have explored the higher order convergence rates in negative norms for discontinuous Galerkin methods applied to linear hyperbolic problems, and an efficient, local post-processing technique which can recover $(2k+1)$-th order of accuracy, instead of the usual $(k+1)$-th order, in L^2 norm, for DG solutions to linear hyperbolic problems including those with variable and discontinuous coefficients. This technique can also recover derivatives of the numerical solution with enhanced order of accuracy. Such methods are expected to be extremely useful for adaptive computations and this will be explored in the future. In [a18,d2], Zhang and Shu explored a method to analyze the convergence and rate of convergence for discontinuous Galerkin methods and related spectral finite volume method (which is a Petrov-Galerkin method), and used it to analyze three different formulations of the discontinuous Galerkin method for solving diffusion problems, as well as to compare discontinuous Galerkin method with the spectral finite volume method. In [a23] and [d6,d7], Qiu and Shu developed a new approach using weighted essentially non-oscillatory (WENO) reconstructions as limiters for the discontinuous Galerkin methods solving hyperbolic problems containing strong discontinuities, thus allowing the method to be both high order accurate and non-oscillatory for strong discontinuities. A Hermite WENO reconstruction procedure, which relies on a more compact stencil in the reconstruction to achieve high order accuracy, is also developed. In [a28], [b6] and [d1], Cockburn, Li and Shu, and Li and Shu developed the locally divergence-free discontinuous Galerkin method for solving the Maxwell equations and the MHD equations. In [a29], Zhang and Shu have given an error estimate for the fully discrete Runge-Kutta discontinuous Galerkin method applied to nonlinear scalar hyperbolic conservation laws with smooth solutions. In [d16], a heterogeneous multiscale method based on the discontinuous Galerkin method is developed by Chen, E and Shu. This paper demonstrates the good potential of discontinuous Galerlin method in multiscale calculations.

WENO (weighted essentially non-oscillatory) finite difference and finite volume methods have been extensively developed and applied during this period. In [a3], these methods are compared with the discontinuous Galerkin method and a guideline is given as to when each method has its unique advantage. In [a5], a technique is introduced to treat the appearance of negative linear weights in WENO reconstructions while maintaining the stability of the approach. In [a8,a15,a24] and [b2], WENO methods are developed to solve models in semiconductor device simulations, including the direct numerical simulation via the Boltzmann-Poisson equations, which is very difficult because of the high dimensions (a two dimensional simulation would involve 2 space dimensions, 3 phase dimensions plus time, i.e. 5+1 dimensions). In [a10], high order central WENO schemes are developed and analyzed. A comprehensive survey of WENO schemes and DG methods is given in [a11]. In [a14], a high order WENO method is developed for solving the Hamilton-Jacobi equations on arbitrary triangulations. In [a17], a multi-domain finite difference WENO method, which can be used on quite general geometry and yet is much less expensive than finite volume WENO method, is developed and applied to computational fluid dynamics problems. In [a19,a22] and [b5], the resolution properties of high order WENO schemes when used on problems with both shocks and complicates smooth structures are explored, and it is concluded that higher order WENO schemes still have advantages in obtaining a comparable resolution with smaller CPU cost. In [a20], a Lax-Wendroff type time discretization procedure is developed for finite difference WENO schemes, which could be more efficient than the traditional Runge-Kutta time discretization under certain circumstances. In [a21], a WENO solver is developed for a multi-class MWR traffic model. In [a26], a WENO scheme is developed for a particle-fluid two phase problem. In [a32], a WENO scheme is developed for cosmological hydrodynamic problem in astrophysics. In [d11,d15], well balanced, high order finite difference WENO schemes are developed which can maintain exactly certain steady state solutions and at the same time are genuinely high order accurate for general solutions of the shallow water equations and the hyperbolic model of chemosensitive movements.

In spectral methods, Carpenter, Gottlieb and Shu [a13] proved conservation and convergence of a class of global schemes including the spectral methods and compact methods.

6. List of All Publications and Technical Reports Supported under This Grant

(a) Papers published in peer-reviewed journals

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

2. T. Zhou, Y. Guo and C.-W. Shu, *Numerical study on Landau damping*, Physica D, v157 (2001), pp.322-333.
3. T. Zhou, Y. Li and C.-W. Shu, *Numerical comparison of WENO finite volume and Runge-Kutta discontinuous Galerkin methods*, Journal of Scientific Computing, v16 (2001), pp.145-171.
4. B. Cockburn and C.-W. Shu, *Runge-Kutta Discontinuous Galerkin methods for convection-dominated problems*, Journal of Scientific Computing, v16 (2001), pp.173-261.
5. J. Shi, C. Hu and C.-W. Shu, *A technique of treating negative weights in WENO schemes*, Journal of Computational Physics, v175 (2002), pp.108-127.
6. J. Yan and C.-W. Shu, *A local discontinuous Galerkin method for KdV type equations*, SIAM Journal on Numerical Analysis, v40 (2002), pp.769-791.
7. J. Yan and C.-W. Shu, *Local discontinuous Galerkin methods for partial differential equations with higher order derivatives*, Journal of Scientific Computing, v17 (2002), pp.27-47.
8. J. Carrillo, I. Gamba, A. Majorana and C.-W. Shu, *A WENO-solver for the 1D non-stationary Boltzmann-Poisson system for semiconductor devices*, Journal of Computational Electronics, v1 (2002), pp.365-370.
9. P. Lin and C.-W. Shu, *Numerical solution of a virtual internal bond model for material fracture*, Physica D, v167 (2002), pp.101-121.
10. J. Qiu and C.-W. Shu, *On the construction, comparison, and local characteristic decomposition for high order central WENO schemes*, Journal of Computational Physics, v183 (2002), pp.187-209.
11. C.-W. Shu, *High order finite difference and finite volume WENO schemes and discontinuous Galerkin methods for CFD*, International Journal of Computational Fluid Dynamics, v17 (2003), pp.107-118.
12. B. Cockburn, M. Luskin, C.-W. Shu and E. Süli, *Enhanced accuracy by post-processing for finite element methods for hyperbolic equations*, Mathematics of Computation, v72 (2003), pp.577-606.
13. M. Carpenter, D. Gottlieb and C.-W. Shu, *On the conservation and convergence to weak solutions of global schemes*, Journal of Scientific Computing, v18 (2003), pp.111-132.
14. Y.-T. Zhang and C.-W. Shu, *High order WENO schemes for Hamilton-Jacobi equations on triangular meshes*, SIAM Journal on Scientific Computing, v24 (2003), pp.1005-1030.

15. J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *A WENO-solver for the transients of Boltzmann–Poisson system for semiconductor devices. Performance and comparisons with Monte Carlo methods*, Journal of Computational Physics, v184 (2003), pp.498-525.

16. R. Fedkiw, G. Sapiro and C.-W. Shu, *Shock capturing, level sets and PDE based methods in computer vision and image processing: a review of Osher's contributions*, Journal of Computational Physics, v185 (2003), pp.309-628.

17. K. Sebastian and C.-W. Shu, *Multi domain WENO finite difference method with interpolation at sub-domain interfaces*, Journal of Scientific Computing, v19 (2003), pp.405-438.

18. M. Zhang and C.-W. Shu, *An analysis of three different formulations of the discontinuous Galerkin method for diffusion equations*, Mathematical Models and Methods in Applied Sciences (M^3AS), v13 (2003), pp.395-413.

19. J. Shi, Y.-T. Zhang and C.-W. Shu, *Resolution of high order WENO schemes for complicated flow structures*, Journal of Computational Physics, v186 (2003), pp.690-696.

20. J. Qiu and C.-W. Shu, *Finite difference WENO schemes with Lax-Wendroff type time discretization*, SIAM Journal on Scientific Computing, v24 (2003), pp.2185-2198.

21. M. Zhang, C.-W. Shu, G.C.K. Wong and S.C. Wong, *A weighted essentially non-oscillatory numerical scheme for a multi-class Lighthill-Whitham-Richards traffic flow model*, Journal of Computational Physics, v191 (2003), pp.639-659.

22. Y.-T. Zhang, J. Shi, C.-W. Shu and Y. Zhou, *Numerical viscosity and resolution of high-order weighted essentially nonoscillatory schemes for compressible flows with high Reynolds numbers*, Physical Review E, v68 (2003), article number 046709, pp.1-16.

23. J. Qiu and C.-W. Shu, *Hermite WENO schemes and their application as limiters for Runge-Kutta discontinuous Galerkin method: one dimensional case*, Journal of Computational Physics, v193 (2003), pp.115-135.

24. J. Carrillo, I. Gamba, A. Majorana and C.-W. Shu, *A direct solver for 2D non-stationary Boltzmann-Poisson systems for semiconductor devices: a MESFET simulation by WENO-Boltzmann schemes*, Journal of Computational Electronics, v2 (2003), pp.375-380.

25. J. Ryan and C.-W. Shu, *On a one-sided post-processing technique for the discontinuous Galerkin methods*, Methods and Applications of Analysis, v10 (2003), pp.295-307.

26. Q. Zhang, M. Zhang, G. Jin, D. Liu and C.-W. Shu, *Modeling, numerical methods and simulation for particle-fluid two phase flow problems*, Computers and Mathematics with Applications, v47 (2004), pp.1437-1462.

27. Y. Guo, C.-W. Shu and T. Zhou, *The dynamics of a plane diode*, SIAM Journal on Mathematical Analysis, v35 (2004), pp.1617-1635.

28. B. Cockburn, F. Li and C.-W. Shu, *Locally divergence-free discontinuous Galerkin methods for the Maxwell equations*, Journal of Computational Physics, v194 (2004), pp.588-610.

29. Q. Zhang and C.-W. Shu, *Error estimates to smooth solutions of Runge-Kutta discontinuous Galerkin methods for scalar conservation laws*, SIAM Journal on Numerical Analysis, v42 (2004), pp.641-666.

30. D. Levy, C.-W. Shu and J. Yan, *Local discontinuous Galerkin methods for nonlinear dispersive equations*, Journal of Computational Physics, v196 (2004), pp.751-772.

31. Y. Xu and C.-W. Shu, *Local discontinuous Galerkin methods for three classes of nonlinear wave equations*, Journal of Computational Mathematics, v22 (2004), pp.250-274.

32. L.-L. Feng, C.-W. Shu and M. Zhang, *A hybrid cosmological hydrodynamic/N-body code based on a weighted essentially non-oscillatory scheme*, Astrophysical Journal, v612 (2004), pp.1-13.

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

1. C.-W. Shu, *A survey of strong stability preserving high order time discretizations*, in *Collected Lectures on the Preservation of Stability under Discretization*, D. Estep and S. Tavener, editors, SIAM, 2002, pp.51-65.

2. J.A. Carrillo, I. Gamba, O. Muscato and C.-W. Shu, *Comparison of Monte Carlo and deterministic simulations of a silicon diode*, in *Transport in Transition Regimes*, N.B. Ben Abdallah, A. Arnold, P. Degond, I. Gamba, R. Glassey, C. Levermore and C. Ringhofer, editors, IMA Volumes in Mathematics and Its Applications, v135, Springer-Verlag, New York, 2003, pp.75-84.

3. C.-W. Shu, *An overview on high order numerical methods for convection dominated PDEs*, in *Hyperbolic Problems: Theory, Numerics, Applications*, T.Y. Hou and E. Tadmor, editors, Springer-Verlag, Berlin, 2003, pp.79-88.

4. Y.-T. Zhang and C.-W. Shu, *Third and fourth order weighted ENO schemes for Hamilton-Jacobi equations on 2D unstructured meshes*, in *Hyperbolic Problems: Theory, Numerics, Applications*, T.Y. Hou and E. Tadmor, editors, Springer-Verlag, Berlin, 2003, pp.941-950.
5. Y.-T. Zhang, J. Shi, C.-W. Shu and Y. Zhou, *Resolution of high order WENO schemes and Navier-Stokes simulation of the Rayleigh-Taylor instability problem*, in Computational Fluid and Solid Mechanics 2003, K.J. Bathe, Editor, the Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics, June 17-20, 2003, volume 1, pp.1216-1218, Elsevier Science.
6. B. Cockburn, F. Li and C.-W. Shu, *Discontinuous Galerkin methods for equations with divergence-free solutions: preliminary results*, in Computational Fluid and Solid Mechanics 2003, K.J. Bathe, Editor, the Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics, June 17-20, 2003, volume 2, pp.1900-1902, Elsevier Science.

(d) Manuscripts submitted, but not published

1. F. Li and C.-W. Shu, *Locally divergence-free discontinuous Galerkin methods for MHD equations*, Journal of Scientific Computing, to appear.
2. M. Zhang and C.-W. Shu, *An analysis of and a comparison between the discontinuous Galerkin and the spectral finite volume methods*, Computers and Fluids, to appear.
3. Y. Ha, C. Gardner, A. Gelb and C.-W. Shu, *Numerical simulation of high Mach number astrophysical jets with radiative cooling*, Journal of Scientific Computing, to appear.
4. W.-S. Don, D. Gottlieb, C.-W. Shu, O. Schilling and L. Jameson, *Numerical convergence study of nearly-incompressible, inviscid Taylor-Green vortex flow*, Journal of Scientific Computing, to appear.
5. J. Ryan, C.-W. Shu and H. Atkins, *Extension of a post-processing technique for the discontinuous Galerkin method for hyperbolic equations with application to an aeroacoustic problem*, SIAM Journal on Scientific Computing, to appear.
6. J. Qiu and C.-W. Shu, *Runge-Kutta discontinuous Galerkin method using WENO limiters*, SIAM Journal on Scientific Computing, to appear.
7. J. Qiu and C.-W. Shu, *Hermite WENO schemes and their application as limiters for Runge-Kutta discontinuous Galerkin method II: two dimensional case*, Computers and Fluids, to appear.

8. J. Qiu and C.-W. Shu, *Hermite WENO schemes for Hamilton-Jacobi equations*, Journal of Computational Physics, to appear.
9. F. Li and C.-W. Shu, *Reinterpretation and simplified implementation of a discontinuous Galerkin method for Hamilton-Jacobi equations*, Applied Mathematics Letters, to appear.
10. J. Qiu, M. Dumbser and C.-W. Shu, *The discontinuous Galerkin method with Lax-Wendroff type time discretizations*, submitted to Computer Methods in Applied Mechanics and Engineering.
11. F. Filbet and C.-W. Shu, *Approximation of hyperbolic models for chemosensitive movement*, submitted to SIAM Journal on Scientific Computing.
12. Y. Xu and C.-W. Shu, *Local discontinuous Galerkin methods for the Kuramoto-Sivashinsky equations and the Ito-type coupled KdV equations*, submitted to Computer Methods in Applied Mechanics and Engineering.
13. D. Levy, S. Nayak, C.-W. Shu and Y.-T. Zhang, *Central WENO schemes for Hamilton-Jacobi equations on triangular meshes*, submitted to SIAM Journal on Scientific Computing.
14. Y. Xu and C.-W. Shu, *Local discontinuous Galerkin methods for nonlinear Schrodinger equations*, submitted to Journal of Computational Physics.
15. Y. Xing and C.-W. Shu, *High order finite difference WENO schemes with the exact conservation property for the shallow water equations*, submitted to Journal of Computational Physics.
16. S. Chen, W. E and C.-W. Shu, *The heterogeneous multi-scale method based on the discontinuous Galerkin method for hyperbolic and parabolic problems*, submitted to Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal.

7. List of Participating Scientific Personnel

1. Chi-Wang Shu, Professor, Principle Investigator.
2. Jing Shi, graduate student, partial RA. Ph.D. degree in 2001.
3. Jennifer Ryan, graduate student, partial support. Ph.D. degree in 2003.
4. Yong-Tao Zhang, graduate student, partial RA. Ph.D. degree in 2003.
5. Zhengfu Xu, partial RA. Ph.D. degree expected in 2005.