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14. ABSTRACT
We have performed research on the design of new algorithms and improvement of existing algorithms for high order accurate finite difference and finite volume weighted essentially non-oscillatory (WENO) schemes and discontinuous Galerkin finite element methods, for solving partial differential equations with discontinuous, rapidly changing, or multiscale solutions. Applications to computational fluid dynamics, astrophysical problems, and pedestrian flows are addressed. The objective of improving the range of applicability, efficiency, robustness, and

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Report Title

Final Report: High Order Accurate Algorithms for Shocks, Rapidly Changing Solutions and Multiscale Problems

ABSTRACT

We have performed research on the design of new algorithms and improvement of existing algorithms for high order accurate finite difference and finite volume weighted essentially non-oscillatory (WENO) schemes and discontinuous Galerkin finite element methods, for solving partial differential equations with discontinuous, rapidly changing, or multiscale solutions. Applications to computational fluid dynamics, astrophysical problems, and pedestrian flows are addressed. The objective of improving the range of applicability, efficiency, robustness, and scalability in massive parallel environment of the proposed methods for various physical problems has been achieved. Particular attention has been paid to army related applications including the pedestrian flow problems.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/07/2013	9.00	Chi-Wang Shu, Yingjie Liu, Zhiliang Xu. Hierarchical reconstruction with up to second degree remainder for solving nonlinear conservation laws, Nonlilnearity, (12 2009): 0. doi: 10.1088/0951-7715/22/12/001
01/07/2013	18.00	Juan Cheng, Chi-Wang Shu, Qinghong Zeng. A Conservative Lagrangian Scheme for Solving Compressible Fluid Flows with Multiple Internal Energy Equations, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (11 2012): 1307. doi: 10.4208/cicp.150311.090112a
01/07/2013	17.00	Juan Cheng, Chi-Wang Shu. Improvement on Spherical Symmetry in Two-Dimensional Cylindrical Coordinates for a Class of Control Volume Lagrangian Schemes, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (04 2012): 1114. doi: 10.4208/cicp.030710.131210s
01/07/2013	16.00	Tao Xiong, Mengping Zhang, Chi-Wang Shu, S.C. Wong, Peng Zhang. High-Order Computational Scheme for a Dynamic Continuum Model for Bi-Directional Pedestrian Flows, Computer Aided Civil and Infratructure Engineering, (05 2011): 298. doi: 10.1111/j.1467-8667.2010.00688.x
01/07/2013	15.00	Rui Zhang, Mengping Zhang, Chi-Wang Shu. On the Order of Accuracy and Numerical Performance of Two Classes of Finite Volume WENO Schemes, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (03 2010): 807. doi: 10.4208/cicp.291109.080410s
01/07/2013	14.00	Juan Cheng, Chi-Wang Shu. A cell-centered Lagrangian scheme with the preservation of symmetry and conservation properties for compressible fluid flows in two-dimensional cylindrical geometry, Journal of Computational Physics, (09 2010): 7191. doi: 10.1016/j.jcp.2010.06.007
01/07/2013	13.00	YunXian Liu, Chi-Wang Shu. Error analysis of the semi-discrete local discontinuous Galerkin method for semiconductor device simulation models, Science China Mathematics, (08 2010): 3255. doi: 10.1007/s11425-010-4075-7
01/07/2013	12.00	Ishani Roy, Chi-Wang Shu, Li-Zhi Fang. RESONANT SCATTERING AND Ly? RADIATION EMERGENT FROM NEUTRAL HYDROGEN HALOS, The Astrophysical Journal, (06 2010): 604. doi: 10.1088/0004-637X/716/1/604
01/07/2013	11.00	Yinhua Xia, Yan Xu, Chi-Wang Shu. Local discontinuous Galerkin methods for the generalized Zakharov system, Journal of Computational Physics, (02 2010): 1238. doi: 10.1016/j.jcp.2009.10.029
01/07/2013	10.00	Y. Xu, C. W. Shu. Dissipative Numerical Methods For the Hunter-Saxton Equation, Journal of Computational Mathematics, (10 2010): 606. doi: 10.4208/jcm.1003-m0003
02/22/2012	2.00	Wei Liu Liu, Li Yuan, Chi-Wang Shu. A Conservative Modification to the Ghost Fluid Method for Compressible Multiphase Flows, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (10 2011): 0. doi: 10.4208/cicp.201209.161010a
02/22/2012	3.00	Olivier Bokanowski, Yingda Cheng, Chi-Wang Shu. A Discontinuous Galerkin Solver for Front Propagation, SIAM Journal on Scientific Computing, (08 2011): 0. doi: 10.1137/090771909
02/22/2012	4.00	Yuanyuan Liu, Chi-Wang Shu, Mengping Zhang. High Order Finite Difference WENO Schemes for Nonlinear Degenerate Parabolic Equations, SIAM Journal on Scientific Computing, (08 2011): 0. doi: 10.1137/100791002
02/22/2012	5.00	Rui Zhang, Mengping Zhang, Chi-Wang Shu. High order positivity-preserving finite volume WENO schemes for a hierarchical size-structured population model, Journal of Computational and Applied Mathematics, (10 2011): 0. doi: 10.1016/j.cam.2011.05.007

02/22/2012	6.00	Zhiliang Xu, Yingjie Liu, Huijing Du, Guang Lin, Chi-Wang Shu. Point-wise hierarchical reconstruction for discontinuous Galerkin and finite volume methods for solving conservation laws, Journal of Computational Physics, (07 2011): 0. doi: 10.1016/j.jcp.2011.05.014
02/22/2012	1.00	Yan Xu, Chi-Wang Shu. Local Discontinuous Galerkin Methods for the Degasperis-Procesi Equation, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (04 2011): 0. doi: 10.4208/cicp.300410.300710a
02/22/2012	7.00	Yang Yang, Ishani Roy, Chi-Wang Shu, Li-Zhi Fang. EFFECT OF DUST ON Ly? PHOTON TRANSFER IN AN OPTICALLY THICK HALO, The Astrophysical Journal, (10 2011): 0. doi: 10.1088/0004-637X/739/2/91
02/22/2012	8.00	Tao Xiong, Peng Zhang, S. C. Wong, Chi-Wang Shu, Meng-Ping Zhang. A Macroscopic Approach to the Lane Formation Phenomenon in Pedestrian Counterflow, Chinese Physics Letters, (10 2011): 0. doi: 10.1088/0256-307X/28/10/108901

TOTAL: **18**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received   Paper

TOTAL:

Number of Manuscripts:

Books

Received   Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Fellow (inaugural class), American Mathematical Society (AMS), November 2012.

Fellow (inaugural class), Society for Industrial and Applied Mathematics (SIAM), May 2009.

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Ishani Roy	0.50	
Yang Yang	0.50	
FTE Equivalent:	**1.00**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Chi-Wang Shu	0.10	
FTE Equivalent:	**0.10**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:......	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):......	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:......	0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Ishani Roy
Total Number: **1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

We have performed research on the design of new algorithms and improvement of existing algorithms for high order accurate finite difference and finite volume weighted essentially non-oscillatory (WENO) schemes and discontinuous Galerkin finite element methods, for solving partial differential equations with discontinuous, rapidly changing, or multiscale solutions. Applications to computational fluid dynamics, astrophysical problems, and pedestrian flows are addressed. The objective of improving the range of applicability, efficiency, robustness, and scalability in massive parallel environment of the proposed methods for various physical problems has been achieved. Particular attention has been paid to army related applications including the pedestrian flow problems. There are 18 refereed journal papers published which have quoted partial support from this ARO grant.

We explicitly construct the entropy solutions for the Lighthill-Whitham-Richards (LWR) traffic flow model with a flow-density relationship which is piecewise quadratic, concave, but not continuous at the junction points where two quadratic polynomials meet, and with piecewise linear initial condition and piecewise constant boundary conditions. The existence and uniqueness of entropy solutions for such conservation laws with discontinuous fluxes are not known mathematically. We have used the approach of explicitly constructing the entropy solutions to a sequence of approximate problems in which the flow-density relationship is continuous but tends to the discontinuous flux when a small parameter in this sequence tends to zero. The limit of the entropy solutions for this sequence is explicitly constructed and is considered to be the entropy solution associated with the discontinuous flux. We apply this entropy solution construction procedure to solve four representative traffic flow cases, compare them with numerical solutions obtained by a high order weighted essentially non-oscillatory (WENO) scheme, and discuss the results from traffic flow perspectives.

High order accurate weighted essentially non-oscillatory (WENO) schemes have been used extensively in numerical solutions of hyperbolic partial differential equations and other convection dominated problems. However the WENO procedure can not be applied directly to obtain a stable scheme when negative linear weights are present. We have performed a detailed study on the positivity of linear weights in a few typical WENO procedures, including WENO interpolation, WENO reconstruction and WENO approximation to first and second derivatives, and WENO integration. Explicit formulae for the linear weights are also given for these WENO procedures. These results should be useful for future design of WENO schemes involving interpolation, reconstruction, approximation to first and second derivatives, and integration procedures.

The interaction between a shock wave and two counter rotating vortices is simulated systematically through solving the two dimensional, unsteady compressible Navier-Stokes equations using a fifth order weighted essentially nonoscillatory (WENO) finite difference scheme. The main purpose of this study is to reveal the mechanism of sound generation in the interaction between a shock wave and two counter rotating vortices. It is found that there are two regimes of sound generation in this interaction. The first regime corresponds to the shock interaction with two isolated vortices, in which the sound wave generated by the interaction between the shock wave and two counter rotating vortices equals to the linear combination of the sound waves generated by the interactions between the same shock wave and each vortex. The second regime corresponds to the shock interaction with a coupled vortex pair, in which the sound wave comes from two processes. One is the vortex coupling, and the second is the interaction between the shock wave and the coupled vortex pair.

We have developed a macroscopic model for pedestrian flow using the dynamic continuum modeling approach. We consider a two-dimensional walking facility that is represented as a continuum within which pedestrians can move freely in any direction. A pedestrian chooses a route based on his or her memory of the shortest path to the desired destination when the facility is empty, and at the same time tries to avoid high densities. In this model, pedestrian flow is governed by a two-dimensional conservation law, and a general speed-flow-density relationship is considered. The model equation is solved numerically using the discontinuous Galerkin method, and a numerical example is employed to demonstrate both the model and the effectiveness of the numerical method.

We have presented further development of the local discontinuous Galerkin (LDG) method designed earlier by us and a new dissipative discontinuous Galerkin (DG) method for the Hunter-Saxton equation. The numerical fluxes for the LDG and DG methods are based on the upwinding principle. The resulting schemes provide additional energy dissipation and better control of numerical oscillations near derivative singularities. Stability and convergence of the schemes are proved theoretically, and numerical simulation results are provided to compare with the earlier schemes.

Using a combination of critical point theory of ordinary differential equations and numerical simulation for the three-dimensional unsteady Navier-Stokes equations, we study possible flow structures of the vortical flow, especially the unsteady vortex breakdown in the interaction between a normal shock wave and a longitudinal vortex. The topological structure contains two parts. One is the sectional streamline pattern in the cross-section perpendicular to the vortex axis. The other is the sectional streamline pattern in the symmetrical plane. In the cross-section perpendicular to the vortex axis, the sectional streamlines have spiral or center patterns depending on a specific function. Depending on the sign of a parameter in this function, the sectional streamlines spiral either inward or outward in the near region of the center, or form a nonlinear center. If this parameter changes its sign along the vortex axis, one or more limit cycles appear in the sectional streamlines in the cross-section perpendicular to the vortex axis. Numerical simulation for two typical cases of shock induced vortex breakdown is performed. The onset and time evolution of the vortex breakdown are studied. It is found that there are more limit cycles for the sectional streamlines in the cross-section perpendicular to the vortex axis. In addition, we find that there are quadru-helix structures in the tail of the vortex breakdown.

The 21 cm emission and absorption from gaseous halos around the first generation of stars substantially depend on the Wouthuysen-Field (W-F) coupling, which relates the spin temperature with the kinetic temperature of hydrogen gas via the resonant scattering between Lyα photons and neutral hydrogen. Therefore, the existence of Lyα photons in the 21 cm region is essential. Although the center object generally is a strong source of Lyα photons, the transfer of Lyα photons in the 21 cm region is very inefficient, as the optical depth of Lyα photons is very large. Consequently, the Lyα photons ν_0 from the source may not be able to transfer to the entire 21 cm region timely to provide the W-F coupling. This problem is especially important considering that the lifetime of first stars generally is short. We investigate this problem with the numerical solution of the integrodifferential equation, which describes the kinetics of Lyα resonant photons in both physical and frequency spaces. We show that the photon transfer process in the physical space is actually coupled to that in the
frequency space. First, the diffusion in the frequency space provides a shortcut for the diffusion in the physical space. It makes the mean time for the escape of resonant photon in optical depth τ media roughly proportional to the optical depth τ, not τ^2. Second and more importantly, the resonant scattering is effective in bouncing photons with frequency $\nu\neq \nu_0$ back to ν_0. This process can quickly restore ν_0 photons and establish the local Boltzmann distribution of the photon spectrum around ν_0. Therefore, the mechanism of ``escape via shortcut'' plus ``bounce back'' enables the W-F coupling to be properly realized in the 21 cm region around first stars. This mechanism also works for photons injected into the 21 cm region by redshift.

For high order shock capturing numerical methods, we have introduced a new technique to work with the hierarchical reconstruction (HR) idea of Liu, Shu, Tadmor and Zhang, to effectively reduce spurious oscillations without local characteristic decomposition for numerical capturing of discontinuous solutions. The new technique uses HR on partial neighboring cells, which lowers the order of the remainder while maintaining the theoretical order of accuracy, essentially eliminates overshoots/undershoots for the fourth and fifth order cases (in one dimensional numerical examples) and reduces the numerical cost.

We have developed a local discontinuous Galerkin (LDG) method for the generalized Zakharov system. Two energy conservations of the LDG scheme are proved for the generalized Zakharov system. Numerical experiments for the Zakharov system are presented to illustrate the accuracy and capability of the methods, including accuracy tests, plane waves, soliton-soliton collisions of the standard and generalized Zakharov system and a two-dimensional problem.

We have considered two commonly used classes of finite volume weighted essentially non-oscillatory (WENO) schemes in two dimensional Cartesian meshes. We compare them in terms of accuracy, performance for smooth and shocked solutions, and efficiency in CPU timing. For linear systems both schemes are high order accurate, however for nonlinear systems, analysis and numerical simulation results verify that one of them (Class A) is only second
order accurate, while the other (Class B) is high order accurate. The WENO scheme in Class A is easier to implement and costs less than that in Class B. Numerical experiments indicate that the resolution for shocked problems is
often comparable for schemes in both classes for the same building blocks and meshes, despite of the difference in their formal order of accuracy. The results in this work may give some guidance in the application of high order finite volume schemes for simulating shocked flows.

With a state-of-the-art numerical method for solving the integral-differential equation of radiative transfer, we investigate the flux of the Lyα photon ν_0 emergent from an optically thick halo containing a central light source. Our focus is on the time-dependent effects of the resonant scattering. We first show that the frequency distribution of photons in the halo are quickly
approaching to a locally thermalized state around the resonant frequency, even when the mean intensity of the radiation is highly time-dependent.

We have continued our earlier effort in developing local discontinuous Galerkin (LDG) finite element methods to discretize moment models in semiconductor device simulations. We consider drift-diffusion (DD) and high-field (HF) models of one dimensional devices, which involve not only first derivative convection terms but also second derivative diffusion terms, as well as a coupled Poisson potential equation. Error estimates are obtained for both models with smooth
solutions. The main technical difficulties in the analysis include the treatment of the inter-element jump terms which arise from the discontinuous nature of the numerical method, the nonlinearity, and the coupling of the models. A simulation is also performed to validate the analysis.

We have developed a new cell-centered control volume Lagrangian scheme for solving Euler equations of compressible gas dynamics in cylindrical coordinates. The scheme is designed to be able to preserve one-dimensional spherical symmetry in a two-dimensional cylindrical geometry when computed on an equal-angle-zoned initial grid. Unlike many previous area weighted schemes that possess the spherical symmetry property, our scheme is discretized on the true volume and it can preserve the conservation property for all the conserved variables including density, momentum and total energy. Several two dimensional numerical examples in cylindrical coordinates are presented to demonstrate the performance of the scheme in terms of symmetry, accuracy and non-oscillatory properties.

We have presented a high-order weighted essentially non-oscillatory (WENO) scheme, coupled with a high-order fast sweeping method, for solving a dynamic continuum model for bi-directional pedestrian flows. The dynamic continuum model for bi-directional pedestrian flows is composed of a coupled system of
a conservation law and an Eikonal equation. We present the first-order
Lax-Friedrichs difference scheme with first order Euler forward time discretization, the third order WENO scheme with third order total variation diminishing (TVD) Runge-Kutta time discretization, and the fast sweeping method, and demonstrate how to apply them to the model under study. We present a comparison of the numerical results of the model from the first order and high-order methods, and conclude that the high-order methods are more efficient than the first order one, and they both converge to the same solution of the physical model.

Technology Transfer