



**AFRL-OSR-VA-TR-2012-1411**

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## High-Order Particle-Mesh Algorithms for Computation of Particle-Laden Shocked Flows

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**5-31-2012**

**Final Report**

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AF Office Of Scientific Research (AFOSR)/RTB1  
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Air Force Materiel Command

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) 5-31-2012		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 4-30-2009-11-30-2012	
4. TITLE AND SUBTITLE HIGH-ORDER PARTICLE-MESH ALGORITHMS FOR COMPUTATION OF PARTICLE-LADEN SHOCKED FLOWS				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER F9550-09-1-0097	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Gustaaf B. Jacobs				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Aerospace Engineering, San Diego State University, 5500 Campanile Drive, San Diego, CA, 92182				8. PERFORMING ORGANIZATION REPORT NUMBER 55776A-P3666	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 4015 Wilson Blvd., Rm 713 Arlington, VA 22203-1954				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT UU (Unclassified, Unlimited) DISTRIBUTION A: Distribution approved for public release.					
13. SUPPLEMENTARY NOTES					
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15. SUBJECT TERMS Higher-Order Flow Solvers, Eulerian-Lagrangian, Shocks, Particle-Laden Flow, Turbulence					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT  UU (Unclassified, unlimited)	18. NUMBER OF PAGES  5	19a. NAME OF RESPONSIBLE PERSON Gustaaf B. Jacobs
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER (include area code) 619-594-4046

Standard Form 298 (Rev. 8/98)  
Prescribed by ANSI Std. Z39.18

Final Report on

# **High-Order Particle-Mesh Algorithms for Computation of Particle-Laden Shocked Flows**

AFOSR GRANT NO. F9550-09-1-0097

April 1, 2009- November 30, 2011

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## **Objectives**

The objective of this project was to develop an efficient and accurate Eulerian-Lagrangian (EL) method based on a Hybrid high-order WENO-Spectral and WENO-Central Difference Navier-Stokes solver that combines an excellent shock capturing and accurate solution of small scale flow features and particle physics with computational efficiency. Another aim was to validate the method against published cases of a shock-particle cloud interaction.

## **Approach**

Algorithm development concentrates on the high-order coupling of the Lagrangian particle solver to the Eulerian Hybrid WENO-spectral element and WENO-Finite Difference scheme and the development of a parallel, particle Navier-Stokes solver. The Hybridization of high-order WENO methods, Spectral and Finite Difference Methods ensures that shocks and small scales are captured in a non-oscillatory manner by WENO, while Spectral and Finite Difference methods improve accuracy and computational efficiency in non-shocked regions. The high-order and stable interpolation between the particles and the flow ensures that the favorable characteristics of the Euler solver are preserved in the high-order Eulerian-Lagrangian solver. The performance of the method is assessed through published benchmark cases.

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## Results

### 1. Hybrid WENO-Finite Difference, Navier-Stokes Solver

We have developed and assessed the performance of a parallel Hybrid WENO-Finite Difference Navier-Stokes solver [1]. Depending on the ratio of WENO usage versus Finite Difference usage in a computational domain, the Hybrid improved computational efficiency by sever factors. With an increasing order of the scheme, the capturing of growth of small scale instability improves (Fig. 1). Effectively, a lesser grid resolution is required with an increased order of approximation that improves computational efficiency further by several factors depending on the problem.

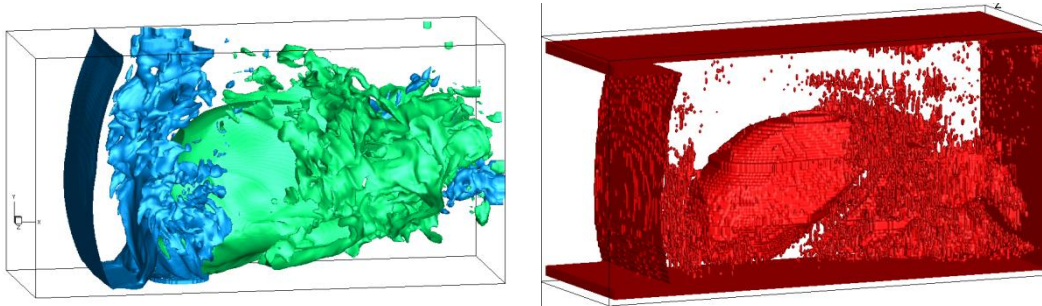


Figure 1. Left figure: Iso-surfaces of the number in a Hybrid computation of a sonic air injection in supersonic cross stream visualizing both shocks and small scale structures. Right Figure: Based on a Multiresolution analysis, a WENO-Z scheme is used in the red surface areas where sharp gradients occur including shocks and sharp shear layers, while a Finite Difference scheme is used in other areas with small scale turbulent structures.

The performance of the Hybrid was assessed for a benchmark sonic injector in supersonic cross stream (Fig. 2).

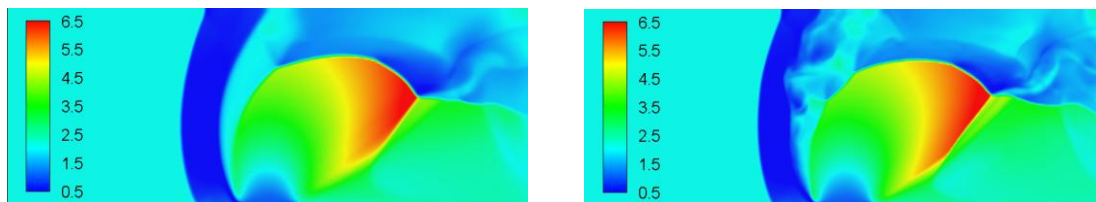


Figure 2. A Mach contour slice visualization along the center surface of a 3D computation of sonic air injection in supersonic cross stream. A seventh order computation (right figure) captures instabilities in the shear layer emanating from the base of the sonic injector while a lower-order computation on the same grid (left figure) dissipates the instability entirely.

## 2. Higher-Order Eulerian-Lagrangian Hybrid WENO-Z-Finite Difference based method

A higher-order Hybrid WENO-Z-Finite Difference based Eulerian-Lagrangian method was developed [2]. A higher-order ENO method determines the stencil of interpolation based on a smoothness determination through divided differences on the Eulerian grid (Fig. 3). The ENO interpolation prevented spurious Gibbs oscillations that were shown to yield inaccurate and/or unstable results if Central Interpolation was employed. High-order B-Spline functions (Fig. 3) weight the particle forcings to neighbouring Eulerian grid points ensuring smooth sources in the Eulerian conservation equations that account for the coupling from the Lagrangian to the Eulerian grid.

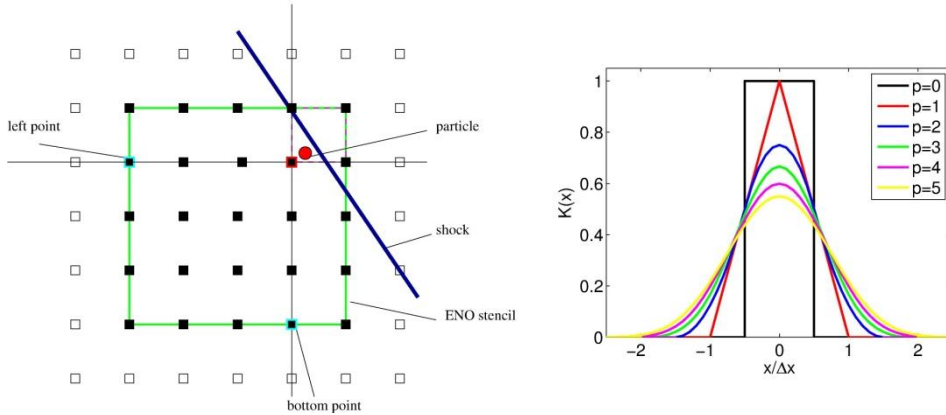


Figure 3. The particle solver was coupled to the higher-order Hybrid Euler solver in a higher-order manner that prevent spurious Gibbs oscillations through an ENO interpolation (left figure) and a higher B-Spline function (right figure).

The performance of the Eulerian-Lagrangian method was assessed against a published experiment of the interaction of a cloud of bronze particles with a moving shock (Fig. 4) in 1D [2], 2D [2,3,7] and 3D [4]. With increasing order of the scheme, small structures were captured more accurately. Hybridization of Central and ENO interpolation based on the Multi-Resolution coefficient reduced computational cost by several factors.

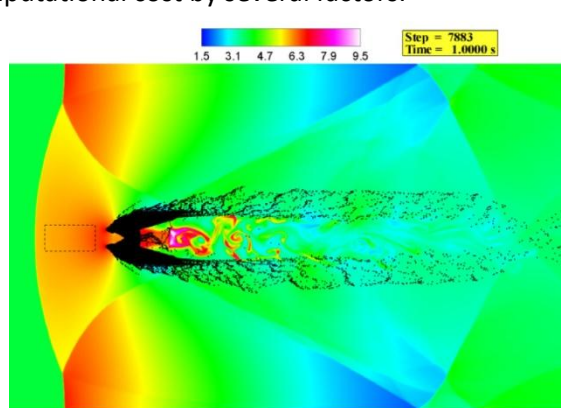


Figure 4. Higher-Order Eulerian-Lagrangian computation of the interaction between the accelerated flow behind a moving shock and a cloud of bronze particles show that the higher Eulerian-Lagrangina method sharply captures shock while resolving small scale phenomena in the particle and gas phase.

The code was extended and validated to include the two-way coupled effects of evaporation between a liquid particle and the gas phase [6].

### 3. Higher-Order Eulerian-Lagrangian Spectral based method

Higher-order interpolation methods were developed to couple Eulerian Spectral methods with Lagrangian particle methods [9,10]. An interpolation based on the spectral basis ensured that high-order accuracy of the spectral solver is preserved in the particle tracer [9]. Combined with weighting methods based on B-Spline projections onto a spectral grid, the Spectral based Eulerian-Lagrangian algorithm spectrally converges to analytical solutions. A weighting function was developed that is based on a mixed polynomial approximation to a delta function projected onto a spectral basis [10]. This weighting function ensured an accurate capturing of singular interfaces between particle clouds and gasses, while providing higher-order convergence to exact solutions away from the interface (Fig. 5).

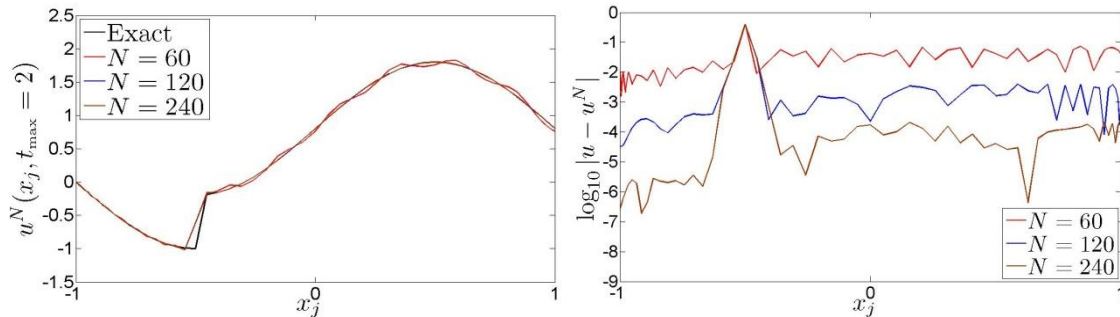


Figure 5. The sharp interface induced in an Eulerian solver by a singular particle (left figure) is captured accurately if a the weighting function is approximated by a mixed polynomial representation of a delta function, while higher-order convergence is achieved away from the interface with increasing degrees of freedom, N (right figure).

### 4. Parallelization

The Eulerian and Eulerian-Lagrangian solvers were both parallelized based on spatial domain decomposition and partitioning with an acceptable scale-up. Expensive subroutines in the Hybrid solver were ported to GPU and show moderate acceleration. A high degree of fragmentation of the data with WENO coverage for certain type of shocked flows (Fig. 1), reduced the vectorization efficiency and increased cache misses and the frequency of memory dumps. An active area of research is to scale-up the Hybrid.

#### Personnel Supported

Sean Davis	Ph.D. student, SDSU
Jean-Piero Suarez	Ph.D. student, SDSU
Hesam Abasi	Ph.D. student, University of Illinois at Chicago
Juan Rueda	International M.Sc. student, University of Valladolid
Alfredo de Gregorio	International M.Sc. student, University of Valladolid
Antonio de Gregorio	International M.Sc. student, University of Valladolid

Justin Meijerink	Visiting Researcher, University of Twente, The Netherlands
Ron Caplan	Researcher, Computational Science Research Center, SDSU
Thomas Dittmann	M.S student, SDSU
Wai-Sun Don	Professor, Hong Kong Baptist University, Hong Kong
Gustaaf B. Jacobs	Associate Professor, San Diego State University

### **Publications resulting from this award**

1. Don, W.S., De Gregorio, A., Suarez, JP., Jacobs, G.B., "Assessing the Performance of a Three Dimensional Hybrid Central/WENO Finite Difference Scheme with Computation of a Sonic Injector in Supersonic Cross Flow", submitted to Advances in Applied Mathematics and Mechanics, 2012.
2. Jacobs, G.B., Don, W.S., "A High Order WENO-Z Finite Difference-Based Particle-Source-in-Cell Method for Computation of Particle-Laden Flows with Shocks", J. Comp. Phys., 228 (5), 2009.
3. Jacobs, G.B., Don, W.S., Dittmann, T., "High-Order Resolution Eulerian-Lagrangian Simulations of Particle Dispersion in the Accelerated Flow behind a Moving Shock", Theoretical and Computational Fluid Dynamics, 26 (37-50) 2012.
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5. Dittmann, T.B., Jacobs, G.B., and Don, W.S. "Dispersion of a Cloud of Particles by a Moving Shock: Effects of Shape, Angle of Incidence and Aspect Ratio", AIAA-2011-411, 2011.
6. Meijerink, J. and Jacobs, G.B. "A WENO-Z Based Eulerian- Lagrangian Code for Simulation of Shocked Flows Laden with Evaporating Droplets", AIAA-2010-1553, 2010.
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10. Suarez, JP and Jacobs, G.B., "Hybrid High-order Eulerian-Lagrangian methods for simulations of particle-laden flow with shocks ", CSRC Research Reports, CSRC-2012-1.
11. De Gregorio, Antonio, "Assesing the Performance of a Three-Dimensional Hybrid Central/WENO Finite Difference Scheme with Computation of a Sonic Injector in Supersonic Cross Flow", M.S. Thesis, SDSU and University of Valladolid, 2011.
12. Dittmann, Thomas, "Computation of a normal shock wave propagating through a particle cloud of varying shape", M.S. thesis, SDSU, 2011.
13. Rueda, Juan. "Lagrangian coherent structures in a supersonic jet stream", M.S. thesis, SDSU and U. of Valladolid, 2011.
14. De Gregorio, Alfredo, "Numerical Investigation of Air and Ethylene Injection into Supersonic Cross Flow", M.S. thesis, SDSU and U. of Valladolid, 2010.

### **AFRL Points of Contact**

Douglas Davis and Mark Hagenmaier, AFRL/RZ, WPAFB, OH.

### **Transitions**

WENO-Z based Particle-Mesh Solver was transitioned to AFRL/RZ