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Final Report

**Theoretical and Experimental
Studies of Reacting Compressible
Flow**

AASERT Grant No. F49620-93-1-0532

Dr. Arje Nachman, Program Manager
Physical Mathematics and Applied Analysis
Directorate of Mathematical and Computer Sciences
United States Air Force Office of Scientific Research
Bolling, AFB, D. C.

Parent Award
F086300-91-K-0057

9/1/93 - 2/28/97

D. S. Stewart
University of Illinois at Urbana-Champaign
Principal Investigator

Abstract

This proposal for this grant requested funds to support travel expenses for graduate students to participate in summer workshop programs and experimental research at the facilities of the Armament Directorate of Wright Laboratories at Eglin AFB. Funds were also requested to support a Graduate Research Assistant (GRA) to support related, theoretical research. The area of the research supported by the grant was multi-dimensional, time-dependent, reacting compressible flows. The AASERT grant was an extension of a pre-existing research program at the University of Illinois, "Studies of Reactive Flow for the Design of Explosive Systems", funded by the Armament Directorate of Wright Laboratory, Eglin AFB, the parent award F086300-91-K-0057.

The research of the parent award was directed at the engineering design of explosive systems, specifically condensed phase explosives and the use of related numerical technologies. The funds from the AASERT grant allowed students to visit shock physics experimental and range facilities and engineers at Eglin AFB in a way that would not have been possible and was not supported by any other grant. The travel funds allowed greater coordination with a parallel experimental efforts at Los Alamos National Laboratory, also funded by WL/Eglin AFB. Students were able to travel and be resident with the PI (D. S. Stewart) during extended summer stays at Eglin AFB and participate in planned workshop activities. Theoretical efforts addressed detonation wave tracking strategies, some important previously unresolved issues in stability of non planar detonation flows and have had a direct impact on the research in the parent award, particularly the numerical technology and basic understanding. Six major archival papers are listed that directly used AASERT funding. Three Ph.D. dissertations were directly benefited by AASERT funding. Finally, two computer codes, AXS and DKAPPA3D, partly funded by AASERT, were developed. These codes have been transferred to Eglin AFB.

Introduction

This document is a final report for an Augmentation Award for Science and Research Training (AASERT) funded by the Air Force Office of Scientific Research, Physical Mathematics and Applied Analysis, Dr. Arje Nachman, program manager. The work was carried out by D. Scott Stewart, Principal Investigator (PI) in the Department of Theoretical and Applied Mechanics (TAM) at the University of Illinois at Urbana-Champaign (UIUC). Herein the PI's group will be referred to as UIUC. The report is split into sections as follows.

Section 1. is a brief summary of the stated goals and objectives as represented in the original proposal and their relation to the parent award F08630-91-0057, which was funded by Wright Laboratories, Armament Directorate, Eglin AFB, (Dave Wagon initial program manger, Michael Nixon, program manager, and Dr. Foster, technical contact, Eglin, AFB).

Section 2. summarizes the main research accomplishments, for which AASERT funding played an important role. Here we note that the effect of this support has enabled the publication of a significant number of archival publications (6 are listed), with novel research findings and the writing two major research codes, DKAPPA3D and AXS.

Section 3. is an accounting of the use of the AASERT funds for i) student support and ii) student travel.

Section 4. is a listing of AASERT supported archival papers and Ph.D. theses.

Section 1. Summary of goals and objectives in the original proposal

Parent Award: Studies of Reactive Flow for the Design of Explosive Systems F08630-91-K-0057

The research of the parent award (F08630-91-K-0057) was concerned with developing more accurate ways to calculate detonation wave interactions that arise in the design of explosive systems with multiple points of initiation and with confinement from inert materials. The research was concerned principally with the development of new asymptotic results from detonation theory to develop detonation shock evolution equations, and the numerical solution of those evolution equations.

Visits to Eglin AFB

Specific and representative experimental explosive design configurations were chosen so as to constrain both the theory and the numerics for explosive system design. The activity and pattern of research practiced by the PI, (D. Scott Stewart) and the Wright Lab engineers, (Dr. Joe Foster, Michael Nixon, later Dr. Dave Belk, for example) during the course of this work involved extended stays at Eglin AFB in the summer period, and occasionally shorter visits during the academic year. During visits to Eglin, the PI and students were able to visit remote sites, the Advanced Warhead Experimentation Facility (AWEF) and the high pressure combustion facility on Okaloosa Island, in particular as well as computational facilities at the main base.

Extended visits with and exposure to WL/MNM personnel was deemed critical in helping to keep the research focused on real engineering systems, despite the advanced analytical character of the work carried out at UIUC. The students (Tariq Aslam, Michael Blossom and David Ford, Jin Yao, Gregory Ruderman and Shaojie Xu, all U.S. domestic students) were supported either directly by AASERT graduate research funds, or their travel to Eglin was covered or both. In the PI's opinion, the main training goals exposure to USAF organization and laboratory facilities and the development of long-term relationships of the students with the Air Force, was achieved, quite independently of the substantial success achieved in the various research activities identified by the ASSERT proposal.

Goals of the ASSERT proposal

The stated goals of the ASSERT proposal were as follows:

- For students to accompany the PI to Eglin, AFB during summers, (in particular) to participate in research activities and summer workshops.
- For students to participate (be exposed to) experiments at Eglin AFB. (An extended goal was to work with Eglin engineering personnel at Eglin.)
- To support advanced analytical and numerical work on detonation theory at Illinois. In particular there was to be a focus on stability theory and confirmation by direct numerical simulation.

Section 2. Summary of main research accomplishments

The most significant research accomplishments using AASERT funds include:

- Level-Set Implementation of Detonation Shock Dynamics (see papers No. 1 and No. 3 in Section 3)
- Advances in the theory of multi-dimensional detonation theory (see papers No. 2 and No. 4 in Section 3)
- Development of a high resolution reactive Euler equation direct solver (see papers No. 5 in Section 3)

Two computer codes were written, DKAPPA3D (a detonation wave tracker) and AXS (a direct reactive Euler equation solver were written)

In addition, some work on stochastic theory and turbulent combustion (see paper No. 6 in Section 3.) and the ignition of energetic material was supported.

Impact of Dr. Nachman and the 2nd Wright Laboratory/AFOSR Workshop

Our program manager Dr. Arje Nachman's technical suggestions and input had an early and notable impact on our work during the time of this grant. In particular, Dr. Nachman, suggested to the PI (Scott Stewart) that he look at the numerical work of Prof. Osher and his colleagues from the UCLA school of numerical algorithms. In particular, Nachman's suggestion influenced our group to look at the level-set technique as a means to write a three-dimensional wave tracker, which was a goal of the parent grant. This later led to the invitation of Osher to an AF workshop held at Eglin, July 1994. UIUC found that we could adapt the level-set ideas of Osher and Sethian, (Journal of Comp. Phys. 79, 12-49 (1988)) to our needs to develop the wave tracker (DKAPPA3D and papers No. 3 and No. 5), whose development was one of our pre-identified goals.

Code Development

The wave tracker work led to the development of a proto-type code,

- DKAPPA3D

written at Illinois by T. Aslam and D. S. Stewart. This code calculates the motion of a 3-D detonation shock surface according to a normal velocity curvature propagation rule for the motion of the detonation shock. (The latter rule is taken from the theory of Detonation Shock Dynamics). A copy of this code has been delivered to personnel at WL/MNM, (Michael Nixon).

The work on development of a direct numerical solver, led to the later development of the hydro-code

- AXS.

The code AXS was written by T. Aslam, S. Xu and D. Scott Stewart is a code based on high resolution solver technology. One of its implementations is a solver that uses a 3rd

order Runge-Kutta time-integration and a fourth and fifth order weighted ENO scheme of Osher and Enquist. The AXS code can be used to solve ideal and non-ideal detonation equation of state, the latter is suitable for detonation modeling of condensed phase explosive. A copy of this code is available on request from the PI.

The Second Wright Laboratory/AFOSR Workshop on Integrated Theory and Numerics for Design Applications, July 1994

A collaboration between the PI, Dr. Arje Nachman AFSOR/NM, Dr. Marc Jacobs and Dr. Joseph Foster, WLMNMW and the PI, led to the Second Wright Laboratory/AFOSR Workshop on Integrated Theory and Numerics for Design Applications, which was held at Eglin AFB, in July 1994. Approximately 70 participants attended from academia, national laboratories and industry. In particular, the PI's students (Aslam, Blossom, Ford, Yao and Xu) were able to attend. Prof. Osher was in attendance and the interactions at the workshop between UIUC and Prof. Osher, heavily influenced our decision to use the numerical methods that were later implemented in AXS and DKAPPA3D, in particular.

Hypersonic Combustion

During the grant hypersonic combustion was a focus. Michael Blossom was the first AASERT fellow and his early efforts included visits with the Eglin AF personnel at Okaloosa Island facility during Spring and Summers 1994 and 1995. Blossom carried out a literature search on the RAM accelerator configuration and blunt body projectiles fired into explosive atmosphere. Later the bow shock stability problem was formulated. (In a related problem, part of Yao's thesis examined the problem of stability of curved near-CJ detonations, which is work recorded in Yao's thesis, but is not published.) Later the PI identified that Blossom should work on developing a modern stability code. At about this time the Eglin program on the RAM accelerator was hit with two catastrophes. One was the appearance of Hurricane Opal in October of 1995, which hit the Island facility and caused major disruption. Also the funding for the RAM accelerator program at Eglin was eliminated and the program was closed. Despite that, we had fully intended that Blossom continue his work on this project. Indeed, as a consequence, one of the test configurations for the code AXS, developed by Aslam, Xu and Stewart was that of shock diffraction past a cylinder and the code was designed by our group to have the capability for the direct numerical simulation needs of Blossom.

However, Blossom resigned in the Spring of 1996, having completed a course work Master degree in TAM and subsequently took a job with Ford Motor Company in Detroit, Michigan. Finally, Brett Okhuysen was partly funded in the Fall of 1996, (by means of a no-cost extension of the ASSERT grant). His assignment was to set up AXS to carry out DNS of the blunt body configuration. Also Brett, in collaboration with Prof. Mark Short (funded by a current AFOSR grant) ported AMARITA to UIUC's computers (a code written by James Quirk of Cal. Tech) for the purposes of conducting similar numerical experiments. Okhuysen's efforts (carried out in the period of the 6 - month no cost extension 9/1/96 to 2/28/97) still reside within the group and represents an ongoing and active project, although no research publications have yet resulted.

Stochastic Theory and Turbulent Combustion

The original premise of David Ford's thesis was to use stochastic and probabilistic methods to average microstructure of reacting flows. One of the ultimate aims is to develop methodology for computing the "effective" relationship between the detonation normal velocity (D) and curvature (κ), when the upstream properties of the explosive has a well-described microstructure with random variations. This problem fundamentally is a

study in stochastic PDEs since the underlying D-kappa relation in a laminar flow, is a nonlinear heat equation, which limits to a Burger's equation, for nearly flat, nearly steady waves. Also we know from our conversations with Eglin personnel that there is an ongoing interest in turbulent flame propagation and prediction in the context of weapon efficacy.

Our work started with a detailed investigations of work by G. Shivashinsky on the prediction of the stationary turbulent flame speed in a turbulent flow field. In that paper Shivashinsky mentioned the use of renormalization group ideas. We were then led to carefully read about the RNG in the turbulence literature, and quickly realized that we needed to understand the fundamental premise of this work in the context of the turbulence literature, where it has been principally been developed for PDEs. Ford has been engaged in examination of the fundamental of RNG-type methodology, but from a probabilistic viewpoint of conditional averaging. His work has now led to a systematic, probabilistic measure theoretic treatment of Navier-Stokes turbulence. A model for conditionally averaged flow fields is developed, which leads to models that are analogous to models for Large Eddy Simulation. A paper by Ford, with D. S. Stewart and R. Moser, entitled "Conditionally averaged projections of the Navier-Stokes turbulence as low wave number projections" had been written and will be submitted to Journal of Fluid Mechanics, (see paper No. 6). Ford will be supported in this summer of 1997, by a different grant to finish a second problem that similarly averages the PDE associated with the randomized Burger's equation that is associated with the $D_n - \kappa$ relation for condensed explosives. This work will represent the completion of this effort. Ford will receive his Ph.D. in August 1997.

Modeling of the ignition of energetic materials

During the summer of 1995, ASSERT funds were used to support the travel of Greg Ruderman (U.S. Air Force Palace Knight Fellow) to Eglin AFB, for a two-week visit. While at Eglin we visited the AWEF site, where the engineers of WL/MNMW reside. Work on Ruderman's thesis topic, modeling of the mechanical ignition of energetic materials was started and the basic premise of his work was formulated. The status of the mechanical modeling currently being used by Eglin personnel and contractors was assessed. Subsequently the equation of state for solid HMX explosive that included the kinetics of melting and gasification to reacted products was formulated as a first step in the creation of a quantitatively accurate and analytically tractable model for mechanical ignition.

Section 3. Use of AASERT funds

Graduate Research Associates

During the grant the following student received AASERT funding for all or part of their graduate student research assistantships in various semesters. Tariq Aslam, Michael Blossom, and David Ford, and Brett Okhuysen, all U. S. citizens.

Student funded travel

During the grant students received AASERT support of their travel expenses while being supported on the ASSERT grant, the parent award, or a grant from the Department of Energy/Los Alamos National Laboratory. Many of these stays were extensive and had duration of two weeks or more at Eglin AFB. Students that made extended stays at Eglin include: Tariq Aslam, Michael Blossom, Dave Ford and Gregory Ruderman. In addition some ASSERT funds were used to fund graduate student travel to the 2nd WL/AFOSR

workshop held in July 94, and included: Aslam, Blossom, Ford, Yao and Xu, the latter two U. S. permanent residents. Finally AASERT funding was used to wholly or partly support student travel to national research conferences, such as American Physical Society, (Aslam and Xu), International Colloquium on Dynamics of Explosive and Reactive Systems (Aslam and Yao) and Gordon Research Conference on Energetic Materials (Aslam and Ruderman).

Section 4. Archival papers and Ph.D. theses

Archival papers citing AASERT funding with abstracts

Below we list important papers written (in chronological order) that cite AASERT funding. The abstract of each paper is reproduced here below the paper entry to summarize the research findings.

1. Stewart, D. S., Aslam, T., Yao, J. and Bdzil, J. "Level-set techniques applied to unsteady detonation propagation", *Modeling in Combustion Science*, J. Buckmaster and T. Takeno, eds. *Lecture Notes in Physics*, 449, 352-369, Springer Verlag, (1995).

"Here we are concerned with describing the dynamics of multi-dimensional detonation as a self-propagating surface. The detonation shock has been shown under certain circumstances to be governed by an intrinsic relation between the normal shock velocity and the local curvature, obtaining $D_n - \kappa$ relation. Once the initial shock position is given, the subsequent motion of the shock can be determined by solving a scalar partial differential equation (PDE) for the shock position. The ingredients for the prediction of the motion of the shock, include the $D_n - \kappa$ relation determined from theory or experiment, the initial configuration of the shock and confinement boundary conditions. Thus we are also concerned about efficient numerical solution of the scalar PDE in three-dimensions, in cases that include multiply-connected and disjoint shock surfaces. This has led us to consider the level-set techniques of Osher and Sethian [1] which are naturally suited to these problems."

2. Yao, J. and Stewart D. S., "On the dynamics of multi-dimensional detonation", *Journal of Fluid Mechanics*, 309, 225-2275 (1996).

"We present an asymptotic theory for the dynamics of the detonation when the radius of curvature of the detonation shock is large compared to the one-dimensional, steady, Chapman-Jouguet (CJ) detonation reaction-zone thickness. The analysis considers additional time-dependence in the slowly varying reaction zone to that considered in previous works. The detonation is assumed to have a sonic point in the reaction-zone structure behind the shock, and is referred to as an *eigenvalue* detonation. A new, iterative method is used to calculate the eigenvalue relation, which ultimately is expressed as an intrinsic partial differential equation (PDE) for the motion of the shock surface. Two cases are considered for an ideal equation of state. The first corresponds to a model of a condensed-phase explosive, with modest relation rate sensitivity, and the intrinsic shock surface PDE is a relation between the normal detonation shock velocity, D_n , the first normal time derivative of the normal shock velocity, \dot{D}_n , and the shock curvature, κ . The second case corresponds to a gaseous explosive mixture, with the

large reaction rate sensitivity of Arrhenius kinetics, and the intrinsic shock surface PDE is a relation between the normal shock velocity, D_n , its first and second normal time derivatives of the normal shock velocity, \dot{D}_n , \ddot{D}_n , and the shock curvature K and its first normal time derivative of the curvature, \dot{K} . For the second case, one obtains a one-dimensional theory of pulsations of plane CJ detonation and a theory that predicts the evolution of self-sustained cellular detonation. Versions of the theory include the limits of near-CJ detonation, and when the normal detonation velocity is significantly below its CJ value. The curvature of the detonation can also be of either sign, corresponding to both diverging and converging geometries.

3. Aslam, T., Bdzil, B. and Stewart, D. S., "Level-set methods applied to modeling detonation shock dynamics", *Journal of Computational Physics*, 126, 390-409 (1996)

We give an extension of the level-set formulation of Osher and Sethian, which describes the dynamics of surfaces that propagate under the influence of their own curvature. We consider an extension of their original algorithms for finite domains that includes boundary conditions. We discuss this extension in the context of a specific application that comes from the theory of Detonation Shock Dynamics (DSD). We give an outline of the theory of DSD which includes the formulation of the boundary conditions that comprise the engineering model. We give the formulation of the level-set method, as applied to our application with finite boundary conditions. We develop a numerical method to implement arbitrarily complex 2-D boundary condition, and give a few representative calculations. We also discuss the dynamics of level curve motion and point out restrictions that arise when applying boundary conditions.

4. Stewart, D. S., Aslam, T. and Yao, J. "On the evolution of cellular detonation", *Proceedings of the 26th International Symposium on Combustion*, pp. 2981-2989, The Combustion Institute, (1996).

A detonation shock-evolution equation that predicts both pulsating and cellular detonation has been derived in the limit of near-Chapman-Jouguet detonation, weak curvature, slow temporal variation, and large activation energy with a newly applied technique of successive approximation. The evolution equation describes a wave hierarchy that is consistent with the linear stability theory of the evolution equation. We define the parameter regime for which the equation applies. The transverse wave instability, as indicated from analysis, leads to cellular detonation. Triple-point tracks correspond to shock-shock intersections of the dynamic solutions of smooth portions of the front. The dynamics of the cellular detonation are consistent with the notion that the power of the detonation front is derived from the normal reaction zone and the triple points are generated as the interaction of the independently propagating fronts and the consequent shock-shock intersections, not as the centers of blast waves. Explicit criteria from prediction of cell widths and cell aspect ratios are given.

5. Xu, Shaojie, Aslam, T. and Stewart, D. S., "High resolution simulation of ideal and non-ideal compressible reaction flow with embedded internal boundaries", *Combustion Theory and Modeling*, 1, No. 1, 113-142 (1997).

The paper explains the methodology use to develop a high-resolution, multi-dimensional Euler solver that is capable of handling non-ideal equation of state and stiff chemical source terms. We have developed a pointwise implementation that has computational advantages for our intended applications, as opposed to a finite volume implementation. Our solver allows for the placement of internal reflective boundaries and the standard inflow and outflow and reflective boundaries at the edge of the domain. We discuss the spatial discretization and the temporal integration schemes, upwinding and flux splitting and the combined use of the Lax-Friedrichs and Roe scheme to solve for the required fluxes. A complete description of the pointwise internal boundary method is given. An overall summary of a representative code structure is given. We provide details on the verification of our integrated set of algorithms that resulting in an application code. We demonstrated the order of convergence for test problems. Two example application from measurement of detonation shocked dynamics and deflagration to detonation transition in porous energetic materials are presented.

6. Ford, David, K., Stewart, D. Scott and Moser, R. D., "Conditionally averaged projections of Navier-Stokes turbulence as low wave number representations", to be submitted to *Journal of Fluid Mechanics*

The formal Fourier transform of the Navier-Stokes equations on an unbounded domain leads to a nonlinear algebraic relation between square integrable random variables (the amplitudes and phases of the various Fourier modes). The goal of this work is to reduce the number of degrees of freedom of the system by projecting both sides of the nonlinear algebraic relation onto a subspace of the underlying Hilbert space. This is accomplished by simply taking conditional averages. Implicit in the projection operator then is a probability measure. The form of the projections depends heavily on the choice of measure. As this measure describes a mechanical system, namely a turbulent field, it is somewhat constrained by standard applications of invariance arguments and dimensional analysis. Unfortunately, but not surprisingly, the reduced set of physically admissible measures is still large (the "closure difficulty"). In this paper a particular choice of measures is made using the physically based theory of high field sensitivity. The projection associated with this measure is carried out and an eddy viscosity is calculated.

Ph.D. Thesis competed supported by AASERT funding (with abstracts)

Tariq D. Aslam, May 1996, Ph. D.

Thesis Title: Investigations on Detonation Shock Dynamics

Abstract: A detonation is a combustion-driven shock wave. ... Of particular interest in detonation problems is the motion of the detonation shock. changes to the reaction zone may cause large variations in the strength and speed of the detonation front, so it can not be ignored in modeling detonations. For typical explosives, the reaction zone may be thousands of times smaller than the engineering scale. This multi-scaled nature of detonate can pose problems when trying to predict the motion of the detonation front.

Detonation shock dynamics is an asymptotic theory whose key results is an intrinsic partial differential equation for the dynamics of the detonation shock front. It will be demonstrated that the theory can predict several aspects of unsteady multi-dimensional detonation accurately. Three intrinsic relations will be examined and compared with direct numerical simulations. Their relevance to modeling detonation dynamics will also be given. Numerical methods, based on level-set ideas, will be given for propagating multi-dimensional detonation fronts in arbitrarily complex geometries.

Shaojie Xu, May 1996, Ph. D.

Thesis Title: Modeling and Numerical Simulation of Deflagration to Detonation Transition in Porous Energetic Materials

Abstract: An understanding of deflagration to detonation transition (DDT) in porous energetic material is important to various engineering applications. ... Two topics related to multi-dimensional simulation of DDT in energetic materials are presented in this work.

The objective of the first part is to develop a model that has a relatively simple mathematical structure. ... Three simplified DDT models, named Bdzil-Kapila-Stewart (BKS), solid-void-gas (SVG) and gas-interpolated-Stewart-Prasad-Asay (GISPA), are considered in the study, among them SVG and GISPA are newly developed. ...

The second part of the study is devoted to a high-quality numerical method, suitable for multi-dimensional direct numerical simulation of DDT with nonlinear material on a complex geometry. The method is developed through an integration of contemporary shock-capturing methods. The new finite-difference scheme adopts the method-of-lines approach, which allows for independent temporal and spatial discretization. The temporal integration uses a third order Runge-Kutta method with the property of total variation diminishing (TVD), while the spatial integration employs a fourth-order essentially non-oscillatory (ENO) scheme. In order to implement the scheme for nonlinear material, a Roe's-linearized Riemann solver is developed in two dimensions for an equation of state that describes an HMX material. To fulfill the needs of engineering applications, an internal boundary method is developed on a structured grid. The internal boundary algorithm also a two-dimensional non-deformable body of arbitrary shape to be inserted in a flow field. A second-order reflective boundary condition is implemented along the internal boundary. ...

JinYao, May 1996, Ph. D.

Thesis Title: The Dynamics of Multi-dimensional detonation

Abstract: See abstract of archival paper No. 2.