# FINAL PROGRESS REPORT

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## ANALYSIS OF MULTI-SCALE PHENOMENA AN TRANSIENTS IN EXPLOSIVES AND COMPLEX ENERGETIC SYSTEMS

### AFOSR Grant # FA9550-06-1-0044

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For the period January 2006 – June 2009

## Overview

**Year 1** Activity in the first year of the grant was spent developing solutions for unit cell problems for detonation in condensed explosive diffracting past dense inert metal particles, for applications to dense, inert, metal-filled explosives. The models solve the motion of a detonation shock past a sphere, where the detonation shock obeys an evolution law obtained from detonation shock dynamics. Two invited review papers on detonation theory were completed in the first year. One was a review of detonation stability with propulsion applications, [1] for the *Journal of Propulsion and Power*, (with former student Aslan Kasimov). The other was on the dynamics of detonation in explosive systems [2], (with John Bdzil) for the prestigious, *Annual Review of Fluid Mechanics, (published January 2007).* Both were comprehensive reviews and describe the mathematical basis for detonation stability and the nonlinear dynamics of detonation.

**Year 2** Activity in the second year of the grant was spent on: 1) Continued development of analytical and numerical solutions for detonation diffraction past an inert spheres embedded in condensed explosives. 2) Careful numerical modeling of deflagration to detonation transition in porous energetic solids, and comparison with experiments carried out with the explosive powder. 3) Identifying organizing concepts from statistical mechanics to develop an analogy for the multi-scale statistical design of high energy density materials (explosives and propellants). 4) A study of nonlinear mode selection of initially linear detonation instability to nonlinear instability was carried out in the shock-attached formulation, both analytically and numerically.

**Year 3** During most of the third year of the grant, D. S. Stewart was on sabbatical at Eglin Air Force Base (AFB) under the auspices of a National Academy Senior Research Fellowship, (administered by the National Research Council) and was resident and physically located in Niceville Florida to work at the Air Force Research Laboratory Munitions Directorate located on Eglin AFB, Florida. During year 3, grant activities focused on: 1) Detonation shock dynamics for complex and nonideal explosives, including new descriptions for detonation shock dynamic

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**14. ABSTRACT** This report summarizes the activities of a 3-year grant and 6 month extension supported by the Air Force Office of Scientific Research. The main topics covered by our investigations, are described succinctly as: 1) Complexity and meso-scale investigations of condensed explosive and reactive materials that include dynamical interaction of reactive flow at the scale of the microstructure of the material. We developed concepts related to the multi-scale statistical design of high energy density materials and specific modeling approaches required to described metal loaded, condensed phase explosives, with a reduced detonation theories. 2) Theory and simulation for porous energetic explosives and multiphase reactive materials. This included asymptotic derivation of a theory of detonation shock dynamics for a porous energetic materials, and the development of entirely new models that can be used to describe non-classical detonation phenomena observed in reactive materials (sometime referred to as 'solid state detonation'.) 3) Linear and nonlinear theory for stability of detonations, formulated in the shock attached frame. The grant also supported the completion of two comprehensive review articles on detonation stability theory and detonation shock dynamics.

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behaviors for explosive that have both porosity and exothermic energy release.  2) Modeling of insensitive munitions and blast. 3) Extensions of geometrical shock dynamics for integrated explosive system design (where we developed new extensions to geometrical shock dynamics for non-ideal inerts to propagate lead shock waves by solution of front equations for the shock). 4) Modeling complexity in the ignition process: Initial, mesoscopic simulations of embedded explosive particles in an inert matrix material. Specifically, we identified new "jetting" phenomena and other energy localization phenomena from simulation (in collaboration with Dr. Foster). 5) Mesoscopic simulation tools development. 6) Progress on various chapters of a monograph, "Detonation Dynamics", was made.

Unfortunately, the completion of our first archival papers on the detonation shock dynamics descriptions for unit cell problems was delayed due in part to unsatisfactory student progress, which ultimately led to a project switch within our group, with when Brandon Lieberthal replacing Steve Holman, who was then assigned to work on a different project. Liberthal has been working on completing the calculations started earlier with Stewart and John Bdzil, and is doing a very good job. A full-length paper will be completed soon.

Stewart also helped the AFRL Munitions Directorate establish a new Directorate/University Consortium (Institute) on nano-energetic materials, called the "Florida Institute for Research into Energetics", (FIRE).

**6 Month Extension of the 3 Year Grant** During the 6 month extension period, Dr. John Bdzil (retired Senior Staff Member and Fellow, Los Alamos National Laboratory) and new Theoretical and Applied Mechanics student Brandon Lieberthal, who was hired as a Graduate Research Assistant, worked on the problem of shock diffraction past spheres and unit cell problems, with Stewart and Bdzil.

## _Research Highlights by Area_

In the following sections we give a brief summary of the research supported by this grant, organized by area.

## Complexity, Meso-scale investigations

**Multi-scale statistical design of high energy density materials (Foster/Stewart/ Thomas), [6]** Concepts from statistical mechanics were used to develop an analogy that can address statistical uncertainties of the engineering specifications of explosive system and their impact on the performance properties of those systems, as described by us in [6].  We used this study the work to help us organize our modeling approach that we used in the later years of this grant, especially as applied to novel and nanoenergetic materials. It is important to have general well-organized approaches that embrace to intrinsic complexity associated with the manufacture real energetic materials. In particular, one can envision for a simple explosive system like a manufactured heterogeneous condensed explosive, that manufacturing properties like the explosive compound grain sizes and their size distributions are a set of design specification that can be chosen. The macroscopic Chapman-Jouguet velocity of the composite is the output of the system and is the performance property of that design. The engineering design of new energetic materials is then represented by a hierarchy of specifications on materials and processes that apply to the physical function of the component; the formalism can provide a well-posed basis

for the interpretation of design/ function relationships and fluctuations in behavior. The statistical mechanics analogy is to be used by us to suggest way to formulate and understand the relationships between the inputs to the unit cell problems (engineering specifications) and the output of the macroscopic system (performance quantities like average detonation speed). We expect to illustrate this approach using variations of the unit cell problem discussed above and its impact on average detonation speed of the explosive.

**Modeling unit cell interaction for the microstructure of a hetergenous explosive: Detonation diffraction past an inert (D. S. Stewart, J. B. Bdzil, B. Lieberthal, J. W. Walter, and T. Aida) [9,15]** We developed an approach to model multi-phase (metal loaded) blast explosive, which is primarily condensed explosive by volume with inert embedded particles. The asymptotic theory of detonation shock dynamics governs the detonation shock propagation in the explosive. The detonation shock moves at a normal speed that depends on the shock curvature. The shock angle with the particle boundary is also prescribed. We describe theory to predict the behavior of a collection of such detonation shock/particle interactions in the larger aggregate. A unit cell problem, of a detonation shock diffracting over a sphere, is analyzed by analytical and numerical means. The properties of an ensemble of such unit cell problems are discussed with implications for the macroscopic limiting behavior of the heterogeneous explosive. In particular we demonstrated that the there is an effective media limit that is associated with detonation shock dynamics models propagating over both linear and cylindrical arrays of particles, with significant reduction of the effective detonation speed.

**Studies of meso-structural influences on energetic material response to thermo mechanical loading, with application to condensed explosives, (Joseph C. Foster, D. S. Stewart, and Sunhee Yoo) [8]** The engineering design of high energy density material [HEDM] is often application specific. In order to analyze the functional relationship between design and application we adopted the position that the design is defined by the suite of specifications and processes used to fabricate the component, [6]. And this idea lead us to investigation meso-scale based energy localization mechanisms associated with an designed initial configuration, and subsequent reactive flow dynamics. This leads to the identification of family of physical configurations allowed by the design specification. In particular we identified novel mechanisms that have probably been overlooked that lead to huge local (and thus non-equilibrium) fluctuations associated with jetting and collapse of cavities in the interstices of regular arrays, and even nominal modulated limit cycle behavior.

## Porous and Multiphase theory, Reactive materials

**Modeling deflagration-to-detonation transition in granular explosive pentaerythritol tetranitrate (PETN) (Saenz/Stewart) [7]** A modeling study on deflagration to detonation transition in granular explosive was completed and published in [1] with student Juan Saenz. The model used a continuum mixture theory model with reactants, products and porosity treated essentially as separate phases. The model represents a macroscopic limit of a corresponding mesoscopic model of the same material, where the response of individual particles are modeled and averages of the collections of particles are recorded. One of the most important conclusions is that the microstructure of the explosive must be included to describe an individual transition to detonation event since the distance to detonation found both

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from experiment and from the macroscopic continuum theory limit is on the order of the grain-scale of the energetic explosive powder. In particular, the model was based on an approach suggested by Stewart *et al.* Phys. Fluids 6, 2515 199, and we did a very detailed comparison of all model prediction with *all* of the available experimental data. We demonstrate the model's ability to capture DDT in PETN powders by matching transients typically observed in experiments through simulation. We show that for flows calculated using nonideal EOSs and complex reaction kinetics such as those formulated in our model, it is possible to define a separatrix, i.e., the *C+* characteristic that separates the *C+* characteristics that evolve into the detonation front from those that evolve away from it. This work provides a macroscopic limit of deflagration to detonation transition in granular explosives, that is in turn a limiting behavior for the mesoscopic models under development.

**Asymptotic studies of detonation shock dynamics for 0orous explosives and energetic materials (Saenz/Stewart) [10]** One of the consequences of the study published in [7], was that it became clear one could carry out an asymptotic theory for detonation shock dynamics of weakly curved detonation when there were two competing processes in addition to the losses due to curvature, namely exothermic reaction and endothermic porous compaction. The energy that drives compaction is absorbed by the material as the microstructure changes and the specific internal energy of the solid-void mixture increases due to the increase in density as voids become occupied by solids. These changes affect the reactive properties of the material and the mechanics and dynamics of detonation waves in explosive powders. The effects of explosive powder compaction on detonation wave dynamics have not been well characterized. We use the theory of Detonation Shock Dynamics (DSD) to analyze the effects of compaction on the dynamics and geometry of detonation waves in explosive powders, and developed results from the numerical solution of the DSD theory equations as well as from asymptotic DSD theory. This work will soon appear in its complete form in Juan Saenz PhD thesis, and longer archival papers.

**Modeling solid state detonation and detonation with designed microstructure (Yoo/Stewart/Lambert) [11,14]** Solid state detonation (SSD) refers to non-classical supersonic reactive wave phenomena in energetic materials that are not typically considered explosives. Reactive energetic materials include both metal/metal oxide and metal oxide/polymer systems with thermitic reactions. Like conventional solid explosives, reactive materials are manufactured composites with a well-defined microstructure. Ingredients include nano-engineered energetic materials with novel surface and reaction properties. The manufactured materials can still be described by a continuum limit informed by the microstructural properties. The SSD is a reactive wave in the energetic material that nominally runs at pressures much lower than what is observed in "ideal" explosives.

To establish base-line descriptions we developed a simple model for the phenomenological study of SSD in the porous mixtures of meso- scale aluminum/oxidizer. An AL/Teflon mixture was chose to inform the base line model, because because there is a significant amount of data and experiments for this material. Calculations of the ambient sound speed of AL/Teflon were found to be in the range between 1.14 *km/sec* and 5.23 *km/sec* depending on the reactants mass ratio. However from estimates obtained from Cheetah 5.0 thermo-equilibrium software provided by L. Fried and the Lawrence Livermore National Laboratory, we found that the typical (sonic) CJ

wave speed was as low as 1.42 *km/sec,* which is in fact subsonic relative to the initial ambient reactants (whose the ambient mixture sound speed was 2.33 *km/sec).* The resolution is that the lead front ahead of the reaction zone was processed by a compaction wave first, followed by an energy releasing reaction that terminates on a sonic state or CJ state. We developed an analytic solution with the assumption that a pure compaction wave is followed by a reaction wave. Then we developed another analytic solution with the assumption that the reaction and compaction processes occur simultaneously. Finally we carried out a direct simulation of the reverse impact and show clearly that a stable quasi-steady structure is obtained via the compaction and reaction processes that terminate at the CJ state estimated by Cheetah.

# Stability

**Mode selection in weakly unstable two-dimensional detonations (Taylor/Kasimov/Stewart) [12]** With student Brian D. Taylor and former student A. R. Kasimov, we developed a formulation of the reactive Euler equations in the shock-attached frame to study the two-dimensional instability of weakly unstable detonation through direct numerical simulation. The results are shown to agree with the predictions of linear stability analysis. Comparisons are made with linear perturbation growth rates and oscillation frequencies as a function of transverse disturbance wavelength. The perturbation eigenfunctions predicted by linear stability analysis are directly validated through numerical simulation. Three regimes of unstable behavior - linear, weakly non-linear, and fully non-linear are explored and characterized in terms of the power spectrum of the normal shock velocity for a Chapman-Jouguet detonation with weak heat release.

**"On the State of Detonation Stability Theory and Its Application to Propulsion",** (**Stewart/Kasimov) [1]** The theory of detonation stability was reviewed in a comprehensive fashion and some comments on its usefulness for application to propulsion was provided by us.

# Other

**The Dynamics of Detonation in Explosive Systems (Bdzil/Stewart) [2]** The modern theory of detonation shock dynamics was described (in an abbreviated form) for the *Annual Review of Fluid Mechanics.*

**Integrated experiment and modeling of insensitive high explosives, (D. Scott Stewart, David E. Lambert, Sunhee Yoo, Mark Lieber, and Steven Holman) [13]** New design paradigms for insensitive high explosives are being sought for use in munitions applications that require enhanced safety, reliability and performance. We developed an integrated approach to develop predictive models, guided by experiments. Insensitive explosive can have relatively longer detonation reaction zones and slower reaction rates than their sensitive counterparts. Specifically we used detonation shcok dynamics (DSD) to pose candidate predictive models. We discussed the variation of the pressure dependent reaction rate exponent and reaction order on the length of the supporting reaction zone, the detonation velocity curvature relation, the computed critical energy required for initiation, the relation between the diameter effect curve and the corresponding normal detonation velocity curvature relation. These metrics are the ones used by experimentalists.

## Archival publications (published) during reporting period directly supported or related to grant research

[1.] Stewart, D. S., and A. R. Kasimov, "On the State of Detonation Stability Theory and Its Application to Propulsion," *Journal of Propulsion and Power, Vol. 22, No. 6. ,*2006, 1230-1244. (INVITED REVIEW)

[2.] Bdzil J. B. and Stewart D. S., "The Dynamics of Detonation in Explosive Systems," *Annual Review of Fluid Mechanics*, 39:263-92, 2007. (INVITED REVIEW)

[3.] Stewart, D. S., K. A. Thomas, S. Clarke, H. Mallett, E. Martin, M. Martinez, A. Munger, and J. Saenz, "On the Initiation Mechanism in Exploding Bridgewire and Laser Detonators," *Shock Compression of Condensed Matter*, Baltimore, Michael D. Furnish, Mark L. Elert, Thomas P. Russell, and Carter T. White, eds., AIP Press, 2006, 471-474.

[4.] Martin, E. S., K. A. Thomas, S. A. Clarke, J. E. Kennedy, and D. S. Stewart, "Measurements of the DDT Process in Exploding Bridgewire Detonators," *Shock Compression of Condensed Matter*, Baltimore, Michael D. Furnish, Mark L. Elert, Thomas P. Russell, and Carter T. White, eds., AIP Press, 2006, 1093-1096.

[5.] D. S. Stewart, J.A. Sáenz, G. Rodriguez, A. R. Valenzuela, S. A. Clarke, A. A. Akinci, K. Thomas , "The initiation mechanism of direct optical initiation (DOI) detonators," to appear in the *Proceedings of the 13th(International)  Detonation Symposium*, 2006, Norfolk Va.

[6.] Multi-scale statistical design of high energy density materials, Joseph C. Foster, Jr., D. Scott Stewart, and Keith Thomas, *Shock Compression of Condensed Matter - 2007*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 995, pp. 369-373, December 2007

[7.] "Modeling deflagration-to-detonation transition in granular explosive pentaerythritol tetranitrate", Juan A. Sáenz and D. Scott Stewart, *Journal of Applied Physics*. 104, 043519 (2008)

[8.] "Meso-structural influence on energetic material response to thermal mechanical loading", Joseph C. Foster, Jr.,  D. S. Stewart,  and Sunhee Yoo, *Shock Compression of Condensed Matter - 2009*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 1195, pp. 45-48, December 2009

[9.] "Modeling unit cell interaction for the microstructure of a heterogeneous explosive: Detonation diffraction past an inert sphere", D. S. Stewart, J. B. Bdzil, J. W. Walter, and T. Aida, *Shock Compression of Condensed Matter - 2009*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 1195, pp. 117-120, December 2009

[10] "Detonation shock dynamics for porous explosives and energetic materials", Juan A. Saenz

and D. Scott Stewart, *Shock Compression of Condensed Matter - 2009*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 1195, pp. 99-102, December 2009

[11] "Modelling solid state detonation and detonation with designed microstructure", Sunhee Yoo, D. Scott Stewart, and David E. Lambert, *Shock Compression of Condensed Matter - 2009*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 1195, pp. 87-90, December 2009

[12] Taylor B, Kasimov A. R., and , Stewart D. S., "Mode selection in unstable two-dimensional detonations", Combustion Theory and Modelling, vol. 13, issue 6, pp. 973-992, 2009

[13] "Integrated experiment and modeling of insensitive high explosives", D. Scott Stewart, David E. Lambert, Sunhee Yoo, Mark Lieber, and Steven Holman, *Shock Compression of Condensed Matter - 2009*: Proceedings of the American Physical Society Topical Group on Shock Compression of Condensed Matter; AIP Conf. Proc., Volume 1195, pp. 91-94, December 2009

[14] "Modeling solid state detonation and reactive materials", Sunhee Yoo, D. Scott Stewart, David E. Lambert, Mark A. Lieber and Matthew J. Szuck, submitted to the *Proceedings of the 14th International Detonation Symposium*, April 2010.

[15] "Mesoscale modeling of metal-loaded high explosives", John B. Bdzil, Brandon Lieberthal and D. Scott Stewart, submitted to the *Proceedings of the 14th International Detonation Symposium,* April 2010.

# Personnel Supported by This Grant

| | |
|---|---|
| D. Scott Stewart | PI, Professor, University of Illinois Urbana-Champaign |
| Joseph C. Foster | Visiting Research Professor, Illinois |
| John B. Bdzil | Visiting Research Professor, Illinois |
| Steven Holman | Graduate Student, Illinois |
| Juan Saenz | Graduate student, Illinois |
| Brian Taylor | Graduate student, Illinois |
| Brandon Liberthal | Graduate student, Illinois |

# Honors & Awards Received  (D. S. Stewart)

Shao Lee Soo, Professor of Mechanical Science and Engineering, University of Illinois, 2008
National Academy Fellow, Senior Research Award, 2007, (highest ranking)
Who's Who in America, 2007
Associate Fellow, AIAA, 2004
Phi Kappa Phi, 2004
Fellow Institute of Physics, 1999
Fellow, American Physical Society, Division of Fluid Dynamics, 1998

## Prestigious Invited Lectures/Presentations During the Grant

Invited Lecture, Gordon Research Conference on Energetic Materials, Tilton School, Tilton, NH, June 16th, 2008

Invited Colloquium Speaker, Mechanical Engineering, University of Pittsburgh (Peyman Givi Host), February 2008

Engineering and Applied Science, Harvard, University (Mahadaven, Hutchison Hosts), April 2008

Keynote Lecturer, 2nd ECCOMAS Conference on Computational Combustion, TU-Delft, July 2007

## Other Notable

Organizer and Chair, 12th International Conference on Numerical Combustion, SIAM, Monterey CA, March 2008

Technical Director, Florida Institute for Research in Energetics (FIRE), Jan. 2008 – to date

## AFRL Points of Contact

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