Analytic and computational studies on micro-propulsion and micro-detonics

January 2003-December 2005. Final report. Dr. Arje Nachman, AFOSR/NM

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1. Objectives

The PIs were funded by the AFOSR to conduct several theoretical investigations on aspects of micro-propulsion and micro-detonics technology. These included: (i) An examination of unsteady inert and reactive flows in rectangular and cylindrical channels with side- and end-wall mass injection intended as a model of micro-size rocket thrusters. (ii) An investigation of two issues associated with developing small-scale pulsed detonation wave engines. These concern the dynamics and criticality of ignition in slender two-dimensional channels, and the derivation of better models that describe the failure of detonations to propagate in thin channels. (iii) Several theoretical studies on problems associated with micro-detonics (miniaturized explosive systems). Topics to be studied include detonation propagation, diffraction and extinction in micro-detonic systems, including investigations and fundamental modeling of bridgewire and explosive foil initiators.

(a) *Personnel supported*

- Dr. Mark Short, Associate Professor.
- Prof. D. Scott Stewart, Professor.
- Dr. Aslan Kasimov, PostDoctoral Research Associate (Stewart), May 2004-June 2005.
- Mr. Aslan Kasimov, Graduate Student (Stewart).
  - "Theory of Instability and Nonlinear Evolution of Self-Sustained Detonation Waves". Ph.D., Spring 2004.
- Mr. Dave Kessler, Graduate Student (Short). Supported by AFOSR and DOE ASCI.
  - "Edge-flames and Combustion at the Microscale". Ph.D. Spring 2006.
- Ms. Iana Anguelova, Graduate Student (Short). (Dept. of Mathematics), UIUC. Supported by AFOSR and NSF Math.
  - "Quantization of Vertex Algebras". Ph.D. (Dept. of Mathematics) Spring 2006.
- Mr. Charles B. Kiyanda, Graduate Student (Short). Dept. of Theoretical and Applied Mechanics.

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14. ABSTRACT
Several theoretical investigations of micro-detonics and micro-propulsion model systems have been undertaken. These include new asymptotic theories of the nonlinear evolution and failure of self-sustained detonations based on the concept of limiting characteristic surfaces, detonation stability formulations for arbitrary (condensed-phase) equations of state and multi-step reaction mechanisms, and direct detonation initiation in both gaseous and condensed-phase systems. Several experimental and theoretical studies have also been conducted on combustion limits and fluid flow inside micro-combustors and micro-propulsion devices.

15. SUBJECT TERMS
micro-detonics, micro-propulsion, ignition, failure, self-sustained detonations, stability

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(*b*) *Recognitions*

• John Bdzil (LANL) & Stewart completed an invited review article for "Annual Review of Fluid Mechanics" entitled "The Dynamics of Detonation in Explosive Systems" to appear in the 2007 volume.
• Short gave an invited lecture: *Theory & Modeling of Detonation Wave Stability: A Brief Look at the Past and Toward the Future.* Special Session on "Detonation - Past and Future" in honor of A.K. Oppenheim's 90th Birthday, at the 20th International Colloquium on the Dynamics of Explosions and Reactive Systems, Montreal, Canada, Jul 31st-Aug 5th.
• Short was promoted to Associate Professor with tenure at UIUC in August 2003.
• Stewart was elected Associate Fellow of AIAA, January 2005.

(*c*) *Transitions*

• Dr. Kasimov took a position as an Instructor in the Department of Mathematics at the Massachusetts Institute of Technology in Fall 2005.
• Dr. Kessler was awarded a National Research Council Research Associateship Fellowship, administered by the National Academies. He'll be taking up his award at the Naval Research Laboratories in August 2006.
• Dr. Anguelova was awarded a Canadian PostDoctural Research Fellowship and is currently at the Centre Interuniversitarie en Calcul Mathematique Algebrique.
• Mr. Kiyanda will become a GRA at Los Alamos National Laboratory, with Short continuing as his Ph.D. advisor.

2. Research completed with AFOSR support

(*a*) *Reseach summary: Prof. D.S. Stewart*

(1) *A.R. Kasimov and D.S. Stewart* 2004 *On the dynamics of self-sustained one-dimensional detonations: A numerical study in the shock-attached frame* Phys. Fluids. 16, 3566-3578.
Abstract: In this work we investigate the dynamics of self-sustained detonation waves that have an embedded information boundary such that the dynamics is influenced only by a finite region adjacent to the lead shock. We introduce the boundary of such a domain, which is shown to be the separatrix of the forward characteristic lines, as a generalization of the concept of a sonic locus to unsteady detonations. The concept plays a fundamental role both in steady detonations and in theories of much more frequently observed unsteady detonations. The definition has a precise mathematical form from which its relationship to known theories of detonation stability and nonlinear dynamics can be clearly identified. With a new numerical algorithm for integration of reactive Euler equations in a shock-attached frame, that we have also developed, we demonstrate the main properties of the unsteady sonic locus, such as its role as an information boundary. In addition, we introduce the so-called "nonreflecting" boundary condition at the far end of the computational domain in order to minimize the influence of the spurious reflected waves.
(2) *A.R. Kasimov and D.S. Stewart* 2005 *Asymptotic theory of evolution and failure of self-sustained detonations* J. Fluid Mech. 525, 161-192.

Abstract: Based on a general theory of detonation waves with an embedded sonic locus that we have previously developed, we carry out asymptotic analysis of weakly curved slowly varying detonation waves and show that the theory predicts the phenomenon of detonation ignition and failure. The analysis is not restricted to near Chapman- Jouguet detonation speeds and is capable of predicting quasi-steady, normal detonation shock speed versus curvature ($D - \kappa$) curves with multiple turning points. An evolution equation that retains the shock acceleration, $\dot{D}$, namely a $\dot{D} - D - \kappa$ relation is rationally derived which describes the dynamics of pre-existing detonation waves. The solutions of the equation for spherical detonation are shown to reproduce the ignition/failure phenomenon observed in both numerical simulations of blast wave initiation and in experiments. A single-step chemical reaction described by one progress variable is employed, but the kinetics is sufficiently general and is not restricted to Arrhenius form, although most specific calculations are performed for Arrhenius kinetics. As an example, we calculate critical energies of direct initiation for hydrogen- oxygen mixtures and find close agreement with available experimental data.
(3) *D.S. Stewart & A.R. Kasimov* 2006 *Theory of detonation with an embedded sonic locus.* SIAM J. Appl. Math. 66, 384-407.
Abstract: A steady planar self-sustained detonation has a sonic surface in the reaction zone that resides behind the lead shock. In this work we address the problem of generalizing sonic conditions for a three-dimensional unsteady self-sustained detonation wave. The conditions are proposed to be the characteristic compatibility conditions on the exceptional surface of the governing hyperbolic system of reactive Euler equations. Two equations are derived that are necessary to determine the motion of both the lead shock and the sonic surface. Detonation with an embedded sonic locus is thus treated as a two-front phenomenon: a reaction zone whose domain of influence is bounded by two surfaces, the lead shock surface and the trailing characteristic surface. The geometry of the two surfaces plays an important role in the underlying dynamics. We also discuss how the sonic conditions of detonation stability theory and detonation shock dynamics can be obtained as special cases of the general sonic conditions.
(4) *A.R. Kasimov and D.S. Stewart* 2005 *Theory of direct initiation of gaseous detonations and comparison with experiment* TAM Report No. 1043 UILU ENG-2004-6004 ISSN 0073-5264
Abstract: In this work we discuss the application of an evolution equation that we have developed for the dynamics of a slowly evolving weakly-curved detonation to a problem of direct detonation initiation. Despite the relative simplicity of the theory, it successfully explains basic features of the initiation process which are observed in experiments and numerical simulations. Moreover, the theory allows one to calculate initiation energies based on the explosive chemical and thermodynamic properties only, without having to invoke significant modeling assumptions. The evolution equation exhibits the competing effects of the exothermic heat release, curvature, and shock acceleration. The detonation dynamics during the initiation depends on the relative strength of the heat release and flow divergence, resulting in successful initiation of self-sustained detonation if the heat release is sufficiently stronger than divergence or in failure if otherwise. Using global kinetic data from Caltech detonation database, which are derived from detailed chemical calculations, we have calculated critical initiation energies of

spherical detonation for hydrogen-oxygen, hydrogen-air, and ethylene-air mixtures at various equivalence ratios and found a very good agreement with recent experimental data.

(5) A. R. Kasimov 2004 *Theory of Instability and Nonlinear Evolution of Self-sustained Detonation Wave.* Ph.D. thesis, Theoretical and Applied Mechanics, May 2004.

Abstract: Linear stability properties and nonlinear dynamics of self-sustained detonations is investigated by means of asymptotic analysis and numerical simulations. The normal-mode linear stability analysis is carried out for gaseous detonations propagating in cylindrical tubes. By comparison of the stability predictions with experiments, it is shown that the instability plays a fundamental role in the onset of spin detonation. We derive far-field closure conditions for unsteady and multi-dimensional detonation waves in arbitrary explosive media as intrinsic properties of the reactive Euler equations in the embedded sonic surface, which is a characteristic surface. The conditions generalize previously known sonic conditions for self-sustained detonations. We investigate the nature of the sonic conditions numerically with a new numerical technique for solving the Euler equations and demonstrate that the sonic locus is a characteristic surface and an information boundary that isolates the reaction zone from the far-field flow.
Starting with the general formulation, we derive an asymptotic evolution equation for self-sustained detonations in the limits of slow-time variation and weak curvature and find that the equation predicts ignition and failure of detonations. Based on the evolution equation, we formulate a theory of direct initiation of gaseous detonation that can predict critical conditions from first principles; we show that the theoretically predicted critical energies are in close agreement with experiment. The ignition theory is also extended to explosives with arbitrary equation of state. With the general conditions at the sonic locus available, we formulate the stability problem for high-explosive detonations described by non-ideal equation of state and calculate stability characteristics of detonation in PBX-9502 and nitromethane.

(*b*) *Reseach summary: M. Short*

(1) *M. Short, J.B. Bdzil & I. I. Anguelova Stability of Chapman?Jouguet detonations for a stiffened-gas model of condensed-phase explosives.* J. Fluid Mech. 2006, 552, pp. 299-309.

Abstract: The analysis of the linear stability of a planar Chapman-Jouguet detonation wave is reformulated for an arbitrary caloric (incomplete) equation of state in an attempt to better represent the stability properties of detonations in condensed-phase explosives. Calculations are performed on a "stiffened-gas" equation of state which allows us to prescribe a finite detonation Mach number while simultaneously allowing for a detonation shock pressure that is substantially larger than the ambient pressure. We show that the effect of increasing the ambient sound speed in the material, for a given detonation speed, has a stabilizing effect on the detonation. We also show that the presence of the slow reaction stage, a feature of detonations in certain types of energetic materials, where the detonation structure is characterized by a fast reaction stage behind the detonation shock followed by a slow reaction stage, tends to have a destabilizing effect.

(2) *C. Miesse, R.I. Masel, M. Short & M.A. Shannon Experimental observations of methane-oxygen diffusion flame structure in a sub-millimetre microburner* Combust. Theory and Modell. 9, 2005, 77-92
Abstract: We examine the structure of confined, laminar methane-oxygen diffusion flames in an alumina microburner with a sub-millimetre dimension. To minimize termination of gas-phase combustion via surface radical quenching, the reactor walls are chemically treated and annealed. We show, through chemiluminescent images, that gas-phase methane-oxygen diffusion flames exist in the microburner without the need for catalytic reaction. However, their structure differs from the continuous laminar diffusion flame profiles that we would expect in a similar burner configuration on a macroscopic scale. Instead, we observe a sequence of isolated reaction zones structures (flame cells) that form along the length of the microburner combustion channel aligned in the direction of the gas flow. This form of cellular diffusion flame instability appears to be unique to wall-confined combustion in microscale devices. The number of flame cells observed depends on the inlet gas velocities and initial mixture strengths.
(3) *D.A. Kessler, M. Short, J. Buckmaster Edge-flames and cellular structures in oscillatory premixed counterflows.* Proc. Combust. Instit. 30 (2005) 331-337
Abstract: We examine edge-flames in the context of symmetric counterflows of fresh mixture, and examine their dynamics when the rate of strain is varied periodically in time. For a Lewis number of 1, extinction boundaries and zero (in the mean) edge propagation speed boundaries are constructed in the forcing amplitude? Damkohler number plane. Forcing can turn advancing edges into retreating edges. For a Lewis number of 0.3, the fundamental distinction is between flames that display cellular structures and flames that do not. Forcing can convert a non-cellular flame into one with cells; and it can strongly affect the dynamics of cellular structures that exist in the absence of forcing.
(4) *Craig Miesse, R.I. Masel, M. Short, M.A. Shannon Diffusion flame instabilities in a 0.75mm non-premixed microburner* Proc. Combust. Instit. 30 (2005) 2499-2507.
Abstract: We examine the cellular instabilities of laminar non-premixed diffusion flames that arise in a polycrystalline alumina microburner with a channel wall gap of dimension 0.75mm. Changes in the flame structure are observed as a function of the fuel type (H2, CH4, and C3H8) and diluent. The oxidizer is O2/inert. In contrast to previous observations on laminar diffusion flame instabilities, the current instabilities occur in the direction of flow above the splitter plate, and only occur for the heavier fuel types. They are not observed in a H2/O2 mixture, which will only support a continuous laminar flame inside our burner, regardless of the initial mixture strength and whether or not the flame is in near-quenching conditions. The only exception is when helium is added to the H2/O2 mixture, raising the effective Lewis numbers of both components.
(5) *M. Short & Y. Liu Edge-flame structure and oscillations for unit Lewis numbers in a non-premixed counterflow.* Combust. Theory Modell. 8 (2004) 425-447
Abstract: We examine the structure and oscillatory instability of low Peclet number, nonpremixed edge-flames in a fixed rectangular channel, closed at one end, with constant side-wall mass injection, one surface supplying fuel, the other oxidizer. Both reactant components have unit Lewis numbers. This study is motivated by issues regarding the nature of combustion that may occur in a propellant crack formed at the interface between the fuel-binder and oxidizer in a hetero-

geneous propellant. Flux conditions are imposed on the fuel and oxidizer at the injection walls, while the temperature on the boundary walls is held constant. For situations in which steady burning occurs, the flame has two components: an edge that faces towards the closed end of the channel and a trailing one-dimensional diffusion flame. A large Damkohler number study of the trailing, planar, strained diffusion flame structure is conducted and a new solvability condition uncovered in this limit, whereby the flame may not exist if the supply mixture strength is sufficiently far from stoichiometric. Numerical calculations also reveal that axial oscillations of the edge-flame in the channel may occur, but for a finite range of mixture strengths sufficiently far from stoichiometric values. The importance of mixture strength, heat losses to the relevant injection surface and the channel end-wall, and the role of the injection surface reactant flux conditions in inducing the oscillations are emphasized. Finally we explore the effect on the combustion structure of varying Peclet number and of different injection velocity magnitudes on the side-wall surfaces.

(6) *G.J. Sharpe & M. Short Shock-induced ignition of thermally sensitive explosives* IMA Journal of Applied Mathematics (2004) 69, 493-520

Abstract: The process of planar detonation ignition, induced by a constant-velocity piston or equivalently by a shock reflected from a stationary wall, is investigated using high resolution one-dimensional numerical simulations. The standard one-step model with Arrhenius kinetics, which models thermally sensitive explosives, is employed. Emphasis is on comparing and contrasting the results of the finite activation temperature simulations with high activation temperature asymptotic predictions and previous simulations. During the induction phase, it is shown that the asymptotic results give qualitatively good predictions. However, for parameters representative of gaseous explosives, subsequent to thermal runaway at the piston and the formation of a reaction wave, the high activation temperature asymptotic theory is qualitatively incorrect for moderately high activation temperatures. It is shown that the results are very sensitive to the value of the activation temperature, especially the distance from the piston at which a secondary shock forms and the degree of unsteadiness in the reaction wave which moves away from the piston. The dependence of the ignition evolution on the other parameters (initial shock Mach number, heat of reaction and polytropic index) is also investigated. It is shown that qualitative predictions regarding the dependence of the ignition evolution on each of the parameters can be elucidated from finite activation temperature homogeneous explosion calculations together with the high activation temperature asymptotic shock ignition results. It is found that for sufficiently strong initiating shocks the ignition evolution is qualitatively different from cases studied previously in that no secondary shock forms. For a high polytropic index, corresponding to a simple equation of state model for condensed phase explosives, the results are in much better qualitative agreement with the asymptotic theory.

(7) *P.A. Blythe, A.K. Kapila & M. Short Homogeneous ignition for a three-step chain-branching reaction model* J. Eng. Math. 2006, to appear. *Abstract:* Spatially homogeneous thermal explosions governed by a three-step chain-branching kinetic model are described in the asymptotic limit of large activation energy for a range of chain-branching cross-over temperatures. The model consists of a sequence of chain-initiation, chain-branching and chain-termination steps. Temperature sensitive Arrhenius kinetics is employed for the initiation and branching

steps, while the termination step has a temperature-independent rate. Marked distinctions in structure arise as the magnitude of the chain-branching crossover temperature is increased relative to the initial system temperature. Attention is focused on the regime where the chain-branching cross-over temperature is close to the initial system temperature. Results are also obtained for the fast and slow explosion limits where the two temperatures are not close.

(8) M. Short, I.I. Anguelova, T.D. Aslam, J.B. Bdzil, A. Henrick & G.J. Sharpe 2006 *Detonation stability for a pressure-sensitive reaction model with a variable reaction order.* J. Fluid Mech., to appear.

Abstract: The linear and nonlinear stability of Chapman-Jouguet (CJ) and overdriven detonations of Zeldovich-von Neumann-Döring (ZND) type are examined in the context of the idealized condensed phase (liquid or solid) detonation model. This model includes a two-component mixture (fuel and product), with a one-step irreversible reaction possessing a rate that is pressure-sensitive (p^n) and has a variable reaction order (ν). It also assumes a constant-γ caloric equation of state for an ideal fluid, in which the adiabatic exponent $\gamma = 3$, and invokes the strong shock limit. A linear stability analysis of the steady, planar, idealized condensed-phase ZND detonation wave is conducted using a normal-mode approach. An asymptotic analysis of the perturbation variable structure at the end of the reaction zone is conducted, and boundedness (or closure) conditions derived, whose precise form depends on the detonation overdrive (f) and reaction order. Boundedness conditions must be imposed in the cases where $f = 1$, $1/2 \leq \nu \leq 1$, and $f > 1$, $\nu = 1$, while an acoustic radiation condition, which imposes zero signal amplitude on the forward-going characteristic at the end of the reaction zone, is required in the cases where $f > 1$, $1/2 \leq \nu < 1$, for which no boundedness condition exists. We also find that while the boundedness or radiation conditions can have a similar structural form for CJ and overdriven waves, they have a different physical interpretation. The results of the linear stability analysis are presented for one- and two-dimensional perturbations, and several differences are highlighted with the known linear stability characteristics of ZND detonations governed by the idealized gas-phase detonation model. The long-time nonlinear behavior of one-dimensional pulsating, idealized condensed-phase detonations are also examined, and show the prominence of a 'beating' instability. These calculations are conducted using a new, high-order, algorithm that employs a shock-fitting strategy, an approach that has significant advantages over standard shock-capturing methods for calculating unstable detonations with pressure-sensitive reaction rate laws.

(9) V. Gorchkov, C.B. Kiyanda, M. Short & J.J. Quirk. *A detonation stability formulation for arbitrary equations of state and multi-step reaction mechanisms.* Proc. Combust. Instit., 2006, to appear.

Abstract: A general normal-mode linear stability formulation of steady planar detonation waves is presented that is valid both for an arbitrary equation of state and for multi-step, multi-species chemical kinetics. The general formulation can be used for many purposes, including an examination of gaseous detonation stability with complex reaction kinetics, in which the individual reacting species have variable thermochemical properties. In the present paper, we consider two cases that could not be obtained by previous one-step chemistry, polytropic gas formulations: the first concerns the effect of a difference in heat capacities between product and fuel species, as well as a possible mole change, in a single-step

irreversible reaction. The second examines the effects of exothermic or endothermic heat release/absorption in the chain-initiation stage of a model three-step reaction.

(10) *V. Gorchkov & M. Short* 2006 *The evolution of fast deflagration waves as a consequence of detonation failure* Combust. Theory Modelling, submitted.

Abstract: When irregular cellular detonations are transmitted through a section of a shock tube lined with porous walls, it has been observed experimentally that sufficient attenuation of the transverse shock waves causes the detonation to fail, manifested by a decoupling between the shock and reaction zone structures. The resulting reaction structure consists of a weaken, near steady one-dimensional shock wave that trails a near steady fast deflagration wave which runs at approximately 40% of the original Chapman-Jouguet detonation velocity. We propose that the failure of the detonation in these circumstances is due to a one-dimensional instability. We analyse the mechanism of one-dimensional Chapman-Jouguet detonation failure and the resulting reaction structure in a model with a three-step chain-branching model. Failure arises due to a sufficiently large-amplitude instability which causes the shock temperature to drop below the chain-branching cross-over temperature. The resulting structure is similar to that observed in the porous tube wall experiments, with a fast deflagration running at approximately 50% of the original Chapman-Jouguet detonation velocity.

(11) In addition to the articles that have appeared or are scheduled to appear, Short has two articles in preparation related to the work on microthruster fluid flow analysis. These are:

- D.A. Kessler & M. Short 2006 *Flows in microchannels with injection. Asymptotic and numerical solutions.*
- D.A. Kessler & M. Short 2006 *Reactive flows in microchannels with injection.*

3. Interactions & Code Development

(*a*) *Lab Interactions/Transactions*

Short and Stewart have had extensive links on-going research at Eglin AFB (Dr. Dave Lambert), and with Los National National Laboratory (Dr. Keith Thomas, Dr. Jim Kennedy, Dr. John Bdzil, Dr. Larry Hill, Dr. Steve Son).

(*b*) *Principal Air Force Contacts and Collaborations of D. Scott Stewart, MIE, UIUC*

D. Scott Stewart had numerous interactions with the following AF personnel, on AF-related research.

AFRL/MNMW

Dr. David Lambert, Dr. Joel House, Donald Cunard

These interaction were mainly concerned with reactive flow problems associated with AFRL/MNMW explosive systems. In particular Stewart's group wrote a paper on experimental validation of detonation shock dynamics accepted for publication,

5. Lambert, D. E. , Stewart, D. Scott, Yoo, Sunhee and Wescott, Bradley L., "Ex-

perimental Validation of Detonation Shock Dynamics in Condensed Explosives," 2005 J. Fluid Mech 546, 227-253.

We believe the excellent agreement of theory, multi-material simulation and experiment represents a breakthrough in explosive modeling.

AFRL/MNAC

Dr. Kirk Vanden, Dr. Yen Tu

These interactions were mainly concerned with the transfer of Illinois codes, like DSD-Program burn into AFRL/MNAC target production hydrocodes like, CTH (A Sandia National Laboratory code). We hosted Dr. Yen Tu at Illinois to implement the transfer of Illinois' level set code into CTH.

A complete account of Stewart's acitivities supported by AFRL/MN can be found in the final report

6. "Tools for Design of Advanced Explosive Systems and Other Investigations on Ignition and Transient Detonation" A Grant from the U. S. Air Force Research Laboratory, Munitions Directorate to the University of Illinois, F08630-00-1-0002, Final Report: Period of Performance 2/2000 to 2/2005.

This report cites support from AFOSR/NM as making essential contributions to the overall effort of Stewart?s research group at Illinois.

A new five year renewal grant was awarded to Stewart by AFRL/MN, "Tool for Understanding Transients in Explosive and Energetic Systems", from 3/2005 to 2/2010. This work will continue to look at specific aspects of Munition Directorate explosive systems and will uses advanced theory and numerics to carry enable quantitative prediction of explosive systems and define critical experiments.

AFRL/PRS Dr. Gregory Ruderman

Stewart had discussions with Dr. Ruderman about using Level set methodology to carry out solid propellant grain burn back for three dimensional solid rocket motor design.

(*c*) *Principal National Laboratory Contacts and Collaborations of D. Scott Stewart, MIE, UIUC*

The research carried in Stewart's group benefited from numerous collaborations and interactions with colleagues at the National Laboratories

Dr. John Bdzil, (Fellow) Los Alamos National Laboratory (LANL)

Dr. William C. Davis (Fellow), LANL

Dr. R. Gustavsen, LANL

Dr. Larry Hill, LANL

Dr. Keith Thomas, LANL

(*d*) *INDEX OF ILLINOIS CODES*

Here we list an index of Illinois codes developed in Stewart's group that were either used for the research described here or written during the period of grant performance. These codes have been and are available to MN/MNW and MN/MNAC personnel. In particular this software is the result of development of the asymptotic theory of DSD and the use of level-sets and advanced numerics, both supported by AFOSR/NM grants to Stewart's group. Since these codes embody physical modeling advances, theoretical (and asymptotic) analysis and implementation of advanced numerics; these codes demonstrate technology transfer. Many of these codes have been transferred to AF-lab personnel and workers at other universities.

DSDTOOLS: This refers to a package implementation of a collection of program that are linked together in a C/C++ framework. DSDTOOLS has a GUI interface and runs on Windows at this time. One can select different explosives and inerts and can compute basic properties of ZND detonations, and specific DSD quantities, like the D-kappa relation.

NONIDK: This is a Fortran code that computes the D-kappa relation for a general equation of state. A C-version of this code exists and is installed in the DSDTOOLS package.

WAVETRACKER: There is a 2DWAVETRACKER and a 3DWAVETRACKER. Both maintain and propagate level sets representations of surfaces, that can either be a detonation shock or a material interface. This is written in a C/C++ framework. The WAVETRACKER software is fully incorporated into WT/MULTIMAT

AXS: Is a standalone, high order TVD, reactive Euler solver that can used to calculate reactive flow dynamics in 2D domains with arbitrary shapes. The initial shape is prescribed by a level set. The code can accept nonideal equations of state. It can be run in a 1D mode. It is used for simpler investigation and teaching. It is written in Fortran.

WT/ MULTIMAT: This code is a multi-material Euler solver with materials boundary represented by level sets, maintained by the WAVETRACKER software.

DSDPB: Refers to a collection of subroutines that have been developed to implement the Program burn algorithm in legacy hydrocodes. Program burn requires the computation of TOA for the explosive and includes a target code specific algorithm to release the heat of detonation in the target code. Program burn has previously been implemented in EPIC, various LANL codes (MESA, and others) by Dr. John Bdzil and colleagues at LANL, and is currently being implemented into Sandia-based CTH in collaboration with Dr. Yen Tu MN/MNAC. The DSDPB were co-developed with J. Bdzil LANL.

EOSPKG: Is part of DSDTOOLS - and is a standalone package that defines the EOS subroutines needed to implement the "wide-ranging" EOS and rate laws, and has been transferred to collaborators at LANL and RPI, CalTech and others.

Acknowledgment/Disclaimer

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