Advanced Scientific Computing Research
FY 2006 Accomplishment

Mathematical Modeling and Adaptive Methods for Multi-Material Reactive Flow in Complex Geometries

William Henshaw [*], Lawrence Livermore National Laboratory
Donald Schwendeman, Rensselaer Polytechnic Institute
Jeffrey Banks, Sandia National Laboratory

Summary

Mathematical analysis of models for multi-material reactive flow and the development of adaptive numerical methods for their solution are rich areas of active research. Current work is aimed at models of heterogeneous explosives. The objective is to understand the behavior of the models and to develop extensions, where appropriate, to provide improved predictive capabilities.

Multi-material flows arise in many areas of science and engineering. The geometry of such flows can be comparatively simple as in the case of an isolated bubble suspended in a flow, or complex as in the case of heterogeneous high-energy explosives. The aim of our research is two-fold. We are interested in both the development and behavior of mathematical models for multi-material reactive flow and the development of adaptive high-resolution numerical methods for the accurate solution of the mathematical models that arise.

Our current focus is on transient behavior of high-speed reactive flows, whose mathematical description is governed by nonlinear hyperbolic partial differential equations representing balance laws for mass, momentum, energy, and material species. Such equations are difficult to solve numerically because they possess shock waves and contact discontinuities where the components of the solution (such as its pressure and velocity) change abruptly, as well as thin layers in time and space where reaction is important. In addition, interfaces separating pure components of the multi-material flow may exist and their accurate description is an important requirement of the numerical approach. As a result, solution adaptive methods and the ability to handle flows in complex domains are essential, and even then an accurate numerical description is a difficult task.

One application of our work involves the mathematical study of models for heterogeneous high-energy explosives. Such materials are morphologically, mechanically and chemically complex, and the development and study of mathematical models is an active area of research. Continuum descriptions of these heterogeneous materials can be more or less complex depending on the extent to which averaging and homogenization has been brought to bear (implicitly or explicitly) on the modeling process. One model, called ignition and growth, treats the explosive as a homogeneous mixture of two distinct constituents, the unreacted explosive and the products of reaction. To each constituent is

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[*] Center for Applied Scientific Computing: (925) 423-2697, henshaw1@llnl.gov, UCRL-ABS-223120

assigned an equation of state, and a multi-stage reaction-rate law is prescribed for the conversion of the explosive to products. It is assumed that the two constituents are always in pressure and temperature equilibrium.

While the ignition-and-growth model is often employed to interpret experimental results, its mathematical behavior is not fully understood. For example, Figure 1 shows the diffraction of a planar detonation by a 90-degree corner. Of particular interest is the behavior of the solution behind the weakened diffracted shock, and whether sustained pockets of unreacted material, or "dead zones," appear. Experimental evidence suggests that such zones exist, but our calculations show that they are not predicted in the present ignition-and-growth model.

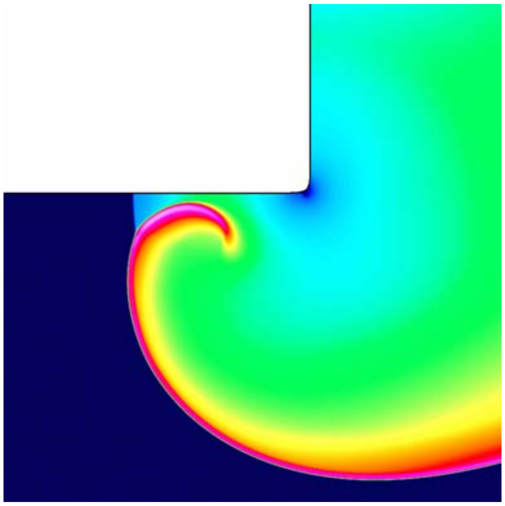

Figure 1. Detonation diffraction by a 90-degree rigid corner. Shaded contours of pressure. The detonation appears in red. It forms a sharply curved front that propagates upwards to consume the unreacted material behind the weaken shock.

The results shown in Figure 1 are obtained for a rigid confinement of the explosive. Compliant confinement, representing its own computational challenges, alters the results somewhat as shown in Figure 2. Here, the detonation is turned less severely by the corner, but the outcome is similar. While the reaction zone separates from the weakened diffracted shock, the unreacted material behind is later consumed by a laterally propagating detonation.

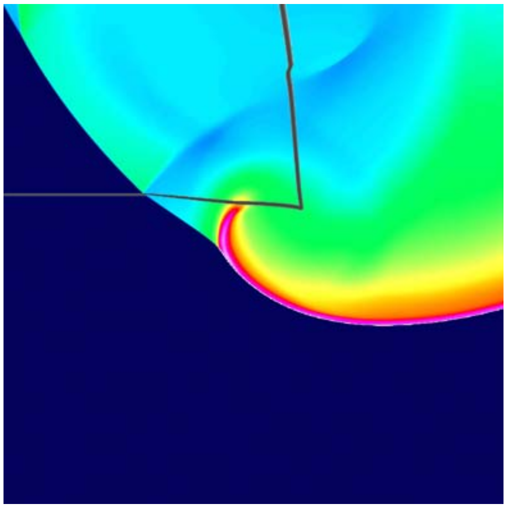

Figure 2. Detonation diffraction by a 90-degree compliant corner. Shaded contours of pressure. The detonation forms a sharply curved front that propagates leftwards to consume the unreacted material behind the weaken shock. The grey curve indicates the material interface.

An extension of the ignition-and-growth model, which includes a model of desensitization of the heterogeneous explosive due to exposure to weak shocks is under current development and study. Such an extension will enable higher fidelity in modeling detonation behavior and will provide a better tool for interpreting experimental results.

For further information on this subject contact:
Dr. Anil Deane, Program Manager
Mathematical, Information, and Computational
Sciences Division
Office of Advanced Scientific Computing Research
Phone: (301) 903-1465
deane@er.doe.gov