Multidimensional Detonation Solutions from Reactive Navier-Stokes Equations [1]

Sandeep Singh [2], Joseph M. Powers[3], and Samuel Paolucci[4]

Department of Aerospace and Mechanical Engineering
University of Notre Dame
Notre Dame, Indiana 46556-5637
USA
219-631-5978 (phone)
219-631-8341 (fax)

This study will describe multi-dimensional detonation wave solutions of the compressible reactive Navier-Stokes equations. As discussed in detail by Fickett and Davis [1], a steady one-dimensional detonation with a spatially resolved reaction zone structure is known as ZND wave, named after Zeldovich, von Neumann, and Döring. In experiments [2] and calculations with simplified models [3], [4], [5], [6], it has been observed and predicted that these ZND waves are unstable. In the experiments, detonation in a tube with walls coated with a thin layer of soot etches detailed regular patterns on the tube walls, indicating the existence of cellular detonation wave structure. Linear analysis [3] demonstrates the fundamental instability of the one-dimensional ZND structure. This is extended by analysis of the full one-dimensional unsteady Euler equations to describe galloping detonations [4]. In two-dimensional calculations [5] it is found that complex cellular structures and transverse waves evolve from the original one-dimensional, steady detonation, for cases in which the steady one-dimensional structure is unstable. Grismer and Powers [6] have shown numerically that detonations which are guaranteed stable in one dimension can be unstable when the geometry is relaxed to include two-dimensional effects. Most calculations are done with compressible reactive Euler equations, and two-dimensional cell size is often predicted to be dependent on grid resolution, which indicates numerical viscosity is playing a determining role in predicting the physics. To remedy this, we reintroduce in this study the usually-neglected physical mechanisms of mass, momentum, and energy diffusion to the conservation equations. In this abstract, we give results of our initial calculations which are very similar to those of Lindström [7]. The full paper will extend these results to consider the effects of diffusion on one-dimensional structure, wall boundary layer effects, and the corrections for diffusion coefficients with dependency on thermodynamic properties. If feasible, the full paper will also present some three-dimensional results.

The model equations are as follows, employing essentially the same non-dimensionalization as that of Ref. [5], with extensions made to account for the diffusion coefficients:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + P - \boldsymbol{\tau}) = 0, \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}\right)\right) + \nabla \cdot \left(\rho \mathbf{u}\left(e + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}\right) + P\mathbf{u} - \boldsymbol{\tau}\cdot\mathbf{u} + \mathbf{q}\right) = 0, \tag{3}$$

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[2] Graduate Research Assistant, ssingh@nd.edu.

[3] Associate Professor, powers@nd.edu.

[4] Associate Professor, paolucci@chaos.ame.nd.edu.

$$\frac{\partial}{\partial t}(\rho\lambda) + \nabla\cdot(\rho\mathbf{u}\lambda + \mathbf{j}) = \omega. \quad (4)$$

Equations (1-4) are evolution equations for mass, momentum, energy, and reaction progress, respectively. The independent variables are time t, and position coordinates, which do not appear explicitly with the vector notation used. The dependent variables ρ, $\mathbf{u}$, P, $\boldsymbol{\tau}$, e, $\mathbf{q}$, λ, $\mathbf{j}$, and ω are the density, velocity vector, pressure, viscous stress tensor, internal energy per unit mass, heat flux vector, reaction progress variable, diffusive mass flux, and reaction source term, respectively. We develop appropriate initial and boundary conditions which will be given in detail in the full paper.

To form a complete system of equations, we specify the following constitutive equations:

$$\boldsymbol{\tau} = \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T - \frac{2}{3}(\nabla\cdot\mathbf{u})\,\mathbf{I}\right), \quad (5)$$

$$\mathbf{q} = -k\nabla T, \quad (6)$$

$$\mathbf{j} = -\rho\mathcal{D}\nabla\lambda, \quad (7)$$

$$e = \frac{1}{\gamma-1}\frac{P}{\rho} - \lambda q_o, \quad (8)$$

$$P = \rho T, \quad (9)$$

$$\omega = a\rho(1-\lambda)\,e^{-E/T}. \quad (10)$$

In Eq. (5), we take the viscous stress to be a linear function of the strain rate for an isotropic material which obeys Stokes' assumption. In Eqs. (6-7), the heat and mass diffusion flux vectors are specified by Fourier's and Fick's Laws, The gas is taken to be an ideal gas with constant specific heat in Eqs. (8-9). respectively. The reaction kinetics are for a material which reacts irreversibly in a one step Arrhenius fashion to form products with identical properties as the reactants. Parameters in Eq. (5-9), μ, k, $\mathcal{D}$, a, E, q_o, γ, are dimensionless coefficients for viscosity, heat conduction and species diffusion, reaction kinetics constant, activation energy, chemical heat release, and ratio of specific heats, respectively. The diffusion coefficients μ, k, and $\mathcal{D}$ can also be formulated to account for temperature dependency, not shown here. So as to minimize the size of the computational domain, we study solutions of Eqs. (1-9) in a frame which is stationary with respect to the steady wave speed predicted by steady inviscid analysis.

The numerical method used to solve Eq. (1-9) uses a simple finite difference scheme with second order central differences to model spatial gradients. Because of the inclusion of physical diffusive terms, there is no need to take extraordinary measures, such as embodied in Roe or FCT schemes, in performing spatial discretization. Because of the simplicity of the spatial discretization, it is then possible to develop an efficient method to advance the solution in time. We use an implicit method based on a trapezoidal scheme which is second order accurate in time. The implicit time stepping technique allows use of much larger time steps relative to typical explicit schemes, which have limitations due to convection, diffusion, and reaction. Use of larger time steps comes at the expense of a matrix inversion, necessary at every time step. For general systems, this can be prohibitively expensive; however, we develop a method which allows fully three dimensional systems to be inverted by inverting a series of block tridiagonal matrices. The block tridiagonal systems can be solved much more efficiently than general systems.

We next describe a sample two-dimensional result. A grid with dimensions of 561×401 in the x and y directions, respectively, is used. The domain lengths are such that $\Delta x = \Delta y = 1/400$. All calculations were performed on a UltraSparc1 workstation. The computational time for the reported simulation was roughly six hours.

Two-dimensional calculations are performed for a viscous detonation wave propagating in a rectangular channel with parallel rigid walls. The boundary layers at the wall distort the plane

detonation front and are the source of transverse waves. The initial profile used for one set of calculations is an inviscid steady traveling ZND wave, which is a one-dimensional solution of reactive Euler equations. Another set of calculations is done for a perturbed initial profile, similar to what Bourlioux and Majda [5] have done. In this case periodic boundary conditions are used at the upper and lower boundaries, which are determined by the wavelength of the periodic disturbance induced.

Fig. 1 shows lines of constant density which form a a cellular structure which has evolved in a two-dimensional flow solution of reactive Navier-Stokes equation with periodic boundary conditions at the upper and lower boundaries. Parameter values utilized are listed in the figure caption and are

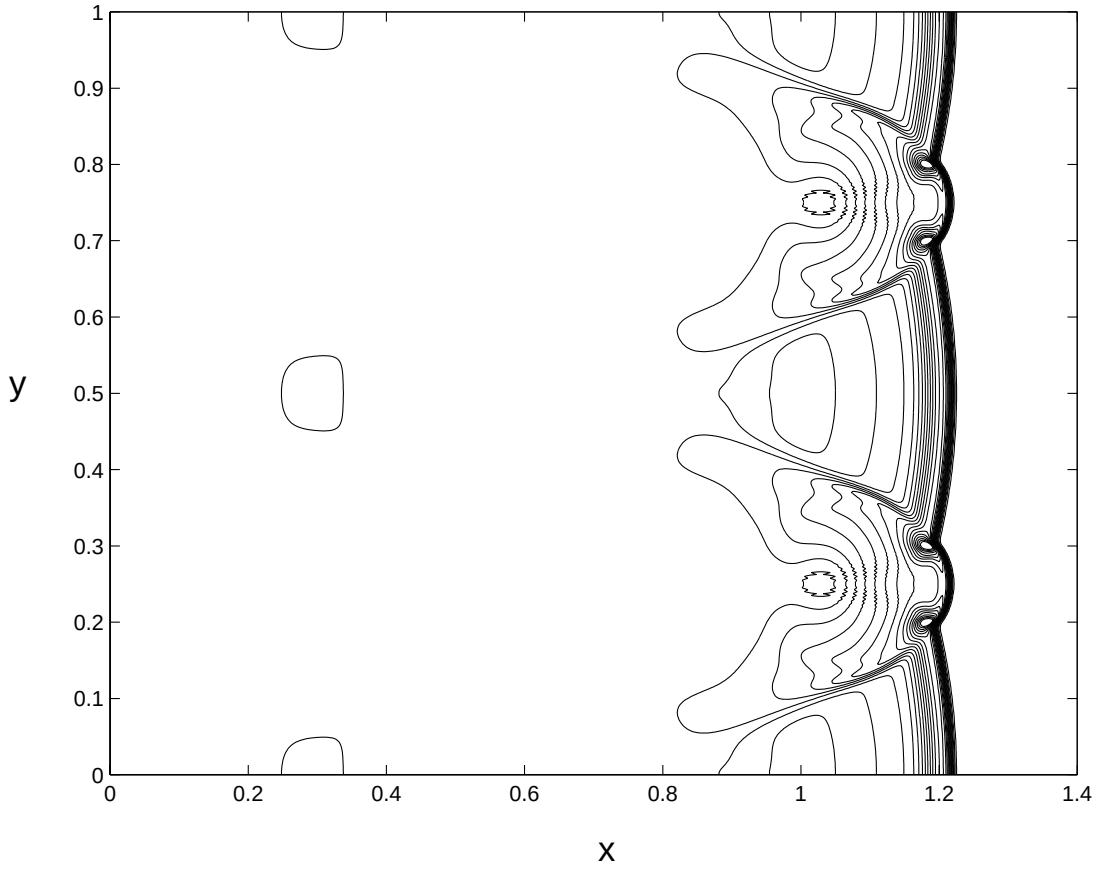

Figure 1: Isochoric contours from numerical solution of reactive Navier-Stokes equations at dimensionless time $t = 0.125$ for grid resolution of $\Delta x = \Delta y = 1/400$. The initial profile is a one-dimensional steady ZND wave. Parameters are $\mu = k = \mathcal{D} = 0.01$, $q_\circ = 50$, $E = 50$, $\gamma = 1.2$ and $a = 10^4$.

identical to those used in Ref. [7], and the viscous analog of those commonly used in inviscid studies. It remains to be demonstrated whether all diffusive and reactive scales are fully resolved, but this will be addressed in the full paper. It is noted that the structure obtained bears strong similarity to those predicted by inviscid calculations. Similar calculations will be done for the channel flow where the boundary layer at the walls initiates the transverse wave structure. The convergence of the numerical method with reduction in grid size will be studied in order to determine the grid density

for which the viscous length scales are resolved. The unstable cell formation at the detonation front for different physical parameters will be studied.

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