# Discrete approximations of detonation flows with structured detonation reaction zones by discontinuous front models: A program burn algorithm based on Detonation Shock Dynamics

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**Abstract**

In the design of explosive systems the generic problem that one must consider is the propagation of a well-developed detonation wave sweeping through an explosive charge with a complex shape. At a given instant of time the lead detonation shock is a surface that occupies a region of the explosive and has a dimension that is characteristic of the explosive device, typically on the scale of meters. The detonation shock is powered by a detonation reaction zone, sitting immediately behind the shock, which is on the scale of 1 millimeter or less. Thus, the ratio of the reaction zone thickness to the device dimension is of the order of 1/1000 or less. This scale disparity can lead to great difficulties in computing three-dimensional detonation dynamics. An attack on the dilemma for the computation of detonation systems has lead to the invention of sub-scale models for a propagating detonation front that we refer to herein as program burn models. The program burn model seeks not to resolve the fine scale of the reaction zone in the sense of a DNS simulation. The goal of a program burn simulation is to resolve the hydrodynamics in the inert product gases on a grid much coarser than that required to resolve a physical reaction zone. We first show that traditional program burn algorithms for detonation hydrocodes used for explosive design are inconsistent and yield incorrect shock dynamic behavior. To overcome these inconsistencies, we are developing a new class of program burn models based on detonation shock dynamic (DSD) theory. It is hoped that this new class will yield a consistent and robust algorithm which reflects the correct shock dynamic behavior.

## Introduction

In the design of explosive systems one must consider the propagation of a well-developed detonation wave sweeping through an explosive charge with a complex shape. At a given instant the lead detonation shock is a surface that occupies a region of the explosive and has a dimension that is characteristic of the explosive device, typically on the scale of meters. The detonation shock is powered by a detonation reaction zone sitting immediately behind the shock, which is on the scale of 1 millimeter or less. Then the ratio of the reaction zone thickness to the device dimension is of the order of 1/1000 or less. This scale disparity can lead to great difficulties in computing three-dimensional (3D) detonation dynamics.

Assume (as we do for the rest of the abstract) that the physical problem of modeling the dynamic propagation of the detonation and the motion of the reacted products in the following flow is completely and satisfactorily described by a solution to the compressible Euler equations for a reactive flow with a specified equation of state for the explosive and reaction rate of the form

$$e = e(p, v, \lambda), \qquad r = r(p, v, \lambda)\,,$$

where $p, v, \lambda$ are the pressure, specific volume and the progress variable of chemical reaction. Note that $\lambda = 0$ corresponds to unreacted explosive and $\lambda = 1$ corresponds to completely reacted explosive. Then the prediction of the detonation dynamics can be achieved in principle by a direct numerical solution (DNS) of the Euler equations. In order to get a high quality solution to the reactive Euler equations, it is essential to have enough points in the reaction zone. Unfortunately, even with modern algorithms, as many as 50 cells in the shock normal direction may be required to resolve the detonation reaction zone so as to compute the detonation speed with sufficient accuracy [1] . When one considers the consequences of such a fine scale for the reaction zone, combined with the requirement for global temporal and spatial accuracy in the meter sized domain of the engineering device, huge computational resources are required

(even with today's TeraFlop parallel computing resources) for a DNS of a detonation wave sweeping through a system. [1]

The computational barrier to 3D design of explosive systems through direct simulation of the reactive Euler equations is not newly discovered, and dates back to systematic use of computer to design explosive systems that started shortly after WWII. A dilemma presents itself when one needs to make predictions in engineering systems. One would like to throw away the fine scale of the reaction zone, but one needs to resolve it to accurately calculate the flow. A similar dilemma occurs for the direct simulation of turbulence up to large engineering scales and its resolution has led to the invention of classes of sub-scale models and most recently large eddy simulations.

For detonation propagation an attack on the problem has similarly lead to the invention of sub-scale models for the detonation fronts that we refer to herein as Program Burn (PB) models. The program burn model seeks not to resolve the fine scale of the reaction zone in the sense of a DNS simulation but rather to deposit a prescribed amount of energy (and more generally mass and momentum) into a very few number of computational cells behind a pre-calculated shock front. The effective reaction zone in a program burn is always constrained to be a finite number of cells thick (between one and four say) and in the limit that the cell thickness goes to zero the program burn region has zero physical thickness and thus represents a jump in the solution. The program burn doses, while historically prescribed purely by the definition of a discrete algorithm, actually then limit to a delta function source prescribed at the pre-determined shock location and occur as a source term in the program burn equations of motion. We consider the following question: How does one make consistent discrete approximations of detonation flows with a finite length reaction zone and spatially distributed chemistry where the reaction zone and shock is collapsed entirely to a single discontinuous front?

## Description of Program Burn as historically implemented in hydrocodes

Here we discuss the ideas behind the implementation of program burn as it traditionally exists in design hydrocodes used for explosive engineering. The algorithm has the following ingredients. i) There is a pre-determined, computational grid. The grid defines the domain of the explosive and is used to solve the Euler equations for the explosive products. ii) A graded set of "burn times" are assigned to each computational cell on the grid. The burn times are supposedly the times that the detonation shock crosses the Eulerian point, identified by the coordinates of the initial position of the computational cell. iii) A cell-based heat release algorithm is attached to the burn times. At the burn time the energy is released into the cell. Then a cell fraction is computed for each hydrodynamic time step, after the burn time for that cell. The cell fraction is typically a volume fraction $Y$ that is based on what portion of the cell has been crossed by the detonation wave, as interpolated from the field of burn times. Note that the burn times are in principle a continuos, (single-valued) spatial field whose constant value contours are the instantaneous shock locations. In general it takes several hydrodynamic steps for the shock to cross the cell, typically four or five.

The pressure starts out from some very low value and is brought up to a high value, consistent with an assumed products equation of state, ie. for $e(p, v, \lambda)$ with $\lambda = 1$. In particular, when the reaction progress variable is zero (i.e. the volume fraction of the cell that is crossed by the shock), then the pressure is necessarily assumed to be zero. The algorithm increments the pressure in such a way that the internal energy is assumed to be *finite*. One way to re-state the assumption is as follows. Let the product equation of state be given by

$$e = e(p, \rho), \tag{1}$$

then the equation of state is modified to be

$$e = e(p/Y, \rho), \tag{2}$$

such that $e$ is finite when both $p$ and $Y = 0$, i.e $p = Y = 0$ must be a fixed point. Note that this makes the strong shock approximation implicit, since $p = 0$ does not correspond to ambient condition, but rather reflects the ratio of the ambient pressure to the shock pressure. This also implies that the starting point for effective reaction zone structure corresponds to $p = 0$, and not $p = p_{shock}$, where $p_{shock}$ is the value of the pressure at the shock.

The traditional program burn algorithm starts at the unreacted state at the ambient pressure, and *not* at the shock state. If the program burn algorithm can be interpreted in terms of an effective distributed

rate law, then the corresponding detonation structure corresponds to a weak detonation, not a strong detonation. The end states that would be computed, for effective weak detonation structure, lie on the weak states that are defined by the intersection of the Rayleigh line and the products Hugoniot. Unless the detonation speed is CJ, the weak states are substantially different from the strong states, i.e. the weak endstate pressures are far below the strong state pressures, and the weak endstates specific volumes are far higher that the strong state specific volume. At the same time, the physical solutions to the Euler equations must lie on the strong branch, or limiting states of the strong branch, and generally the strong branch states are different and well-separated from the weak branch state. The *only* one-dimensional, steady exception to this is the Chapman-Jouguet detonation. Then the weak-branch and the strong-branch states are the same, and the CJ-states can in principal, be accessed either from a strong or weak detonation structure.

Thus the whole traditional PB construct is consistent only for the special case of CJ detonation. Any significant deviation from plane, CJ, detonation that employs the traditional program burn algorithm described here, will be inconsistent. And generally *any* multi-dimensional calculation, with curved detonation shock, that are under or overdriven are inconsistent, and can not produce states consistent with the full Euler equations. The original algorithm as posed is at best inconsistent, and at worst ill-conceived.

## Program burn based on Detonation Shock Dynamics

We present an alternative to the traditional program burn algorithm that will automatically achieve the end states that are consistent with those found from the theory of Detonation Shock Dynamics, which account for corrections to the sonic state due to curvature [2]. In our model, this is achieved by discarding the reactive flow variable $\lambda$ and altering the conservation equations by delta function sources in the conservation equations for the mass, normal momentum to the shock, and the streamwise total energy. Figure 1 is a comparison of a DNS of the reactive Euler equations in cylindrical geometry with our modified program burn algorithm (PB) for a detonation started as a 5 millimeter cylindrical hot spot near the origin that runs out to distances greater than 800 millimeters. Note that the physical steady CJ, ZND reaction zone is $4\,mm$. For both cases the equations are solved by a high-resolution Euler solver, namely, a third-order TVD Runge-Kutta scheme with a fifth-order WENO spatial scheme [3], [4]. Figure 2 shows a blow up of the near shock region shown in Figure 1. For the comparisons for both the DNS is $\triangle x = 0.2mm$, which puts 20 points in the reaction zone which is to be compared to the dashed PB result with $\triangle x = 4.0mm$ resolution and one point in the reaction zone, a grid 20 times coarser than the DNS simulation. We will discuss in detail the numerical analysis and algorithm that lead to this excellent comparison and discuss how the use of the PB model can lead to substantial reduction in computational costs for complex three dimensional detonation flows.

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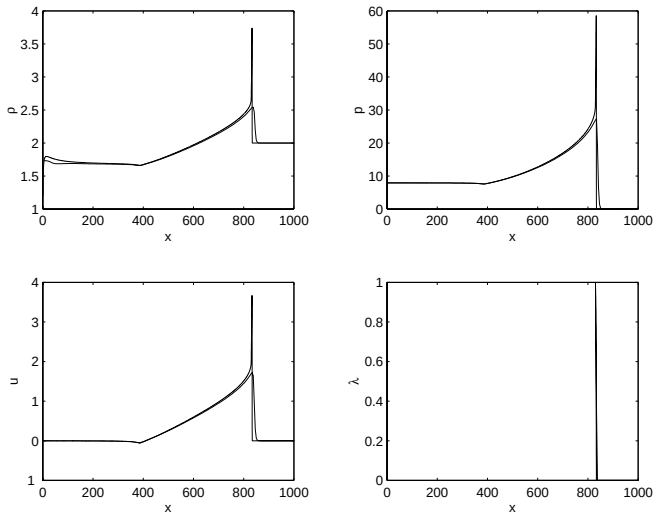


Figure 1: Plot of the DNS ($\triangle x_{DNS} = 0.2mm$) and PB ($\triangle x_{PB} = 4.0mm$) solutions for cylindrical geometry.

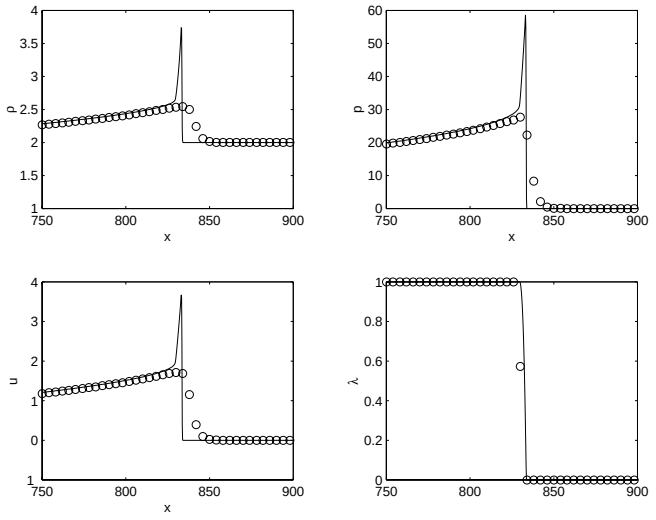


Figure 2: Blow up of the structure of Figure 1. DNS (solid) and PB (dashed).