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Applying the SMG Scheme to Reactive Flow

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The staggered mesh Godunov-SMG scheme for Lagrangian and Arbitrary Lagrangian Eulerian (ALE) hydrodynamics has several potential advantages for applications involving reactive flow simulations arising in the initiation and propagation of detonation. This includes the capabilities to capture discontinuities present in an expanding flow and its inherent hourglass damping property. In the current work, we add to the stagered mesh Godunov (SMG) scheme an appropriate reaction rate law and an equation of state for mixtures of reactants and reaction products, and we test the performance of the scheme to simulate the detonation initiation and propagation over an initially deformed mesh.

Keywords: detonation, initiation, modeling, reactive-flow, shock

Introduction

Flow fields of detonation products arise in various devices such as the shaped charge with a wave shaper shown schematically in Fig. 1. In this configuration the detonation wave is diffracted

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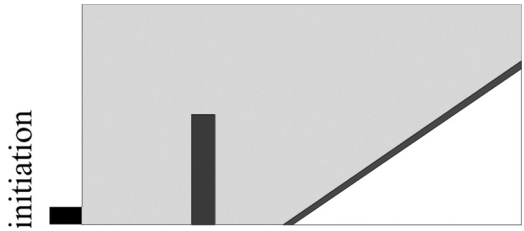

Figure 1. A shaped charge with wave shaper.

around the wave shaper, causing a coupling between the reactive fluid dynamics in the reaction zone and the detonation products flow, as well as the propagation of the detonation wave front. Our scheme is aimed at correctly simulating the flow in such situations.

Here we present the extension of the novel SMG scheme [1–3], to reactive flows and consider specifically its application to the simulation of detonation waves and the resulting products flow in a Lagrange or ALE setting. According to the classical Zeldovich-von Neumann-Doring (ZND) model, a detonation wave consists of an inert shock front followed by a narrow layer of exothermic reactive flow. In this reaction zone, the degree of reaction (or burn fraction) λ increases monotonically from 0 to 1, and the pressure and density decrease along the Rayleigh line from the von Neumann state (peak) to the sonic Chapman-Jouguet (CJ) point. The reaction rate $\dot{\lambda}$ increases with the pressure and temperature, and at fixed volume the pressure increases with λ. Such positive feedback can generate instabilities. When this tendency is well balanced by the expansion of the detonation products along the Rayleigh line, an almost steady detonation wave is obtained as a traveling wave. The criterion for stable integration of the fluid dynamical equations in the reaction zone can be obtained from linear stability analysis or, alternatively, by numerical simulations (see Sharpe [4], Erpenback [5], and Short et al. [6]). Thus, (see Short et al. [6]), for a rate law like:

$$\dot{\lambda} = c(1-\lambda)\left(\frac{p}{p_{cj}}\right)^{n} \exp^{\frac{-T_a}{T}}. \tag{1}$$

Here c denotes an inverse-time constant (see Eq. (8) where c is expressed in terms of problem parameters). A large value of the power n or of the activation temperature T_a may produce instability.

Typical detonation-induced flows involve several materials, and Lagrangian or ALE codes are the best suited to resolve the multimaterial interfaces. These codes typically have a spatially staggered mesh with the velocity defined at the zone vertices and use pseudo-viscosity to capture shocks. However, the classical quadratic von Neumann pseudo-viscosity vanishes in expansion flows. Using the von Neumann pseudo-viscosity for capturing the leading shock of a detonation wave will thus result in a scheme having no mechanism to damp oscillations in the reaction zone. Thus, numerical simulations resolving the flow in the reaction zone must include an additional linear pseudo-viscosity term acting in expansion. In order to be dissipative, this term must be negative. Using such a term in every expansion flow zone raises several problems. First, it would add unwanted dissipation and entropy to regions of smooth rarefactions. Also, according to von Neumann's original analysis, a linear term causes the shocks to be captured in an interval of ever increasing width. This problem can be partially alleviated by constraining such a term to be active only in the reaction zone. And, because its coefficient is arbitrary, choosing a sufficiently large coefficient will stabilize the solution, even if burn-law instabilities would otherwise be produced.

In Eulerian Godunov codes all variables are zone centered, with possible jumps at zone interfaces. The fluxes of conserved variables (mass, momentum, energy) at these faces are obtained by solving Riemann problems (RP) there. A second-order extension to the Godunov scheme [7,8] is achieved by solving generalized Riemann problems (GRP), obtained by taking flow variables as piecewise linear in zones (subject to slope limiting due to the necessity of imposing monotonicity constraints). When these face fluxes are used for the finite-difference time integration of conserved variables per zone, the necessary dissipation for shock capturing is produced. In a sense, the SMG scheme may be regarded as an adaptation of Godunov method

and its second-order extensions to the different setting of staggered mesh used by classical Lagrange/ALE schemes.

The difficulties inherent in extending this approach to the multidimensional staggered mesh setting of classical Lagrangian schemes has motivated us to develop the staggered mesh Godunov method (see Luttwak [1] and Luttwak and Falcovitz [1,2] which bridges the conceptual gap between classical Lagrangian (pseudo-viscosity based) and the zone-centered Godunov schemes. Kuropatenko [9] and later Wilkins [10] used the Rankine-Hugoniot shock jump relations to define the pseudo-viscosity. Christensen [11] was the first to apply second-order Godunov schemes to a staggered mesh aiming at an improved pseudo-viscosity, as outlined also in Benson's review [12].

Vitello and Souers [13] applied Christensen's scheme to reactive flow, showing that better results are obtained by letting the pseudo-viscosity to act also in expansion. Caramana et al. [14] used Christensen's approach to develop a uni-axial tensor, edge-centered viscosity. The SMG/Q scheme, as will be briefly outlined in the next section, has some ideas in common with the compatible schemes of Caramana et al. [14] and the analysis of Christensen [11]. But it also has some unique features that might be of advantage when simulating reactive flows. Like those other schemes, SMG captures shocks sharply, and it also introduces dissipation in expansion regions. Its gradient limiter, which effectively acts as a kind of shock detector, restricts the dissipative effects to the the neighborhood of a discontinuity. Its novel vector image polygon/polyhedron (VIP) type of vector limiter [15] helps improve preservation of problem symmetries. Moreover, SMG has an inherent hourglass damping capability, enabling the scheme to handle distorted meshes with a high aspect ratio, which may well occur in the presence of strong reactions. In this study we extend the SMG scheme to reactive flow by adding a reaction rate law together with the respective equation of state for the solid high explosive and the reactions products.

To test the performance of the scheme in the presence of distorted meshes we consider a test case of 1D initiation by a fixed velocity piston, once as a 1D problem and next over a distorted mesh in analogy with the well known Saltzman's shock wave test.

Theory

In studying shock initiation of detonation, the evolution of the reactive shock into a fully developed detonation wave requires an appropriate distance (referred to as *run to detonation* by Mader [16]). For the simulation of this process it is necessary to numerically resolve the details of the reaction zone. To that end, a suitably refined mesh is required, and we must also specify an equation of state for the solid (unburnt) high explosive, the reaction products, as well as the intermediate state of partially burned explosive. In addition, a reaction rate model is needed, so that its time integration specifies the fraction of the reaction product's mass in a zone. Then, using a closure law that prescribes how the released energy is shared between the reactants and products completes the modeling of the reactive fluid dynamics.

The SMG/Q Scheme

The staggered mesh Godunov SMG/Q scheme [1–3], uses a staggered mesh and, like classical Lagrange schemes, is formulated in terms of internal internal energy. But instead of the classical pseudo-viscosity, it relies on the RP solution to capture shocks. The node-centered velocities are assumed to have a piecewise linear distribution with possible discontinuities at the in-zone corner zone interfaces (marked as A in Fig. 2) that separate each pair of edge-neighbor zone vertices; for example, $(i, i+1)$ in cell k. Zone-centered velocity gradients $(\nabla v)_k$ are calculated using the velocities at the zone vertices. These gradients are limited to preserve a monotonic velocity distribution. The present SMG/Q version is staggered in time and space and therefore relies on internal, rather than total, energy. This scheme can readily be extended to the (even time-integration) compatible scheme, producing a total-energy-conserving scheme.

Formerly we used a component-wise limiter for the velocity vector. However, such a limiter is not invariant under rotation of the coordinate frame, so we subsequently developed a novel type of limiter for gradients of vectors: VIP, based on the convex hull of the vectors in a suitable neighborhood of the considered cell (cell k) [15]. The VIP key idea is to define

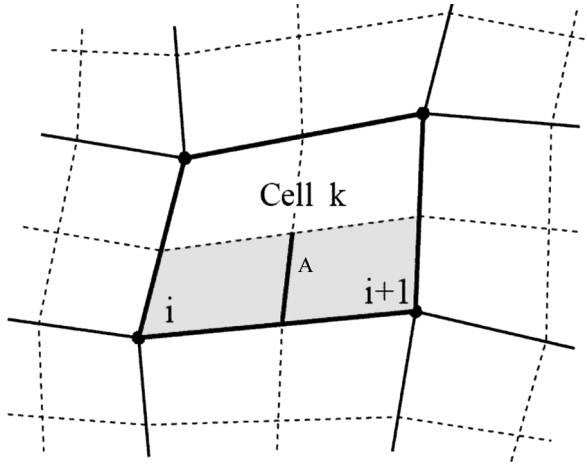

Figure 2. Corner zone interface A where an impact Riemann problem (IRP) is a set up.

monotonicity compliance by a gradient-extrapolated velocity vector as the situation where that vector is located within the edge-neighbor's VIP.

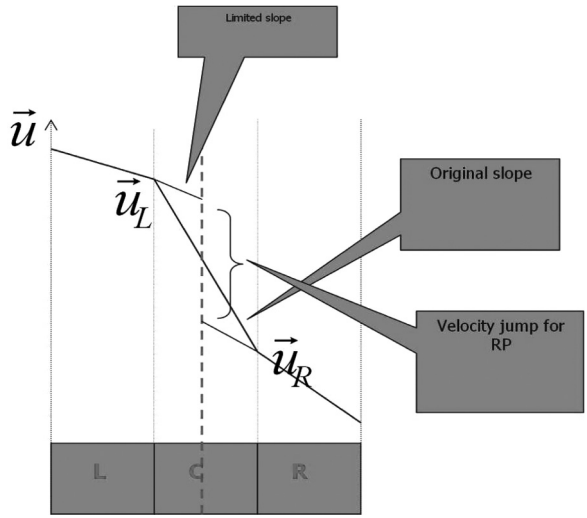

Figure 3. Scalar slope limiter.

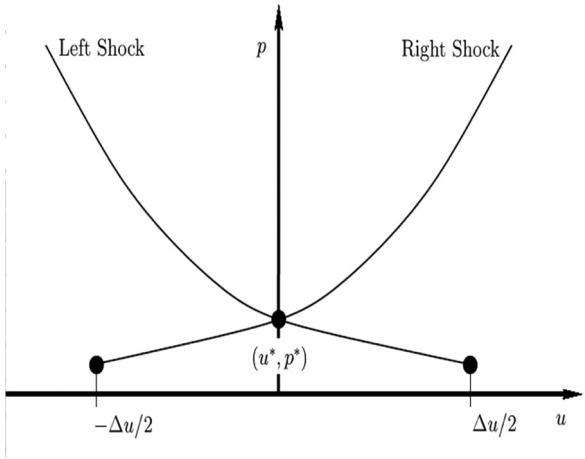

Figure 4. Solution of the impact Riemann problem.

Using the limited gradient, the velocity jumps at A are obtained. The cell-centered pressure and density are assumed to be continuous at A. Thus, we have to solve a simpler impact Riemann problem (or IRP) at A, as shown schematically in Fig. 4.

The IRP is solved in the normal to shock direction, assumed to be along the velocity difference between the pair of edge-neighbor vertices $\Delta u_{i,i+1}$. The resulting pressure p^* acts on the corner zone faces (A). Integrating the contributions from all the corner zone faces surrounding a node i, we get the lumped force on the mass associated with node i and hence its time-advanced velocity. Actually, in the SMG scheme this procedure is modified by taking the total pressure as $p^* = p_k + (p^* - p_k) = p_k + Q_{i,i+1,k}$, where $Q_{i,i+1,k} = p^* - p_k$ is regarded as a kind of pseudo-viscosity. Correspondingly, the lumped force at node i is considered as split into two terms: the first is obtained from the surrounding zone pressures p_k; the second, related to $Q_{i,i+1,k}$, is modified as a uniaxial pseudo-viscosity, exerting a force on nodes i, $i+1$ only along the direction of $\Delta u_{i,i+1}$. The reasoning supporting this genre of directional Q is that a lumped force resulting from the

pressure jump at a shock should be normal to the shock front, which is assumed along $\Delta u_{i,i+1}$. This approach is similar to the uniaxial edge viscosity proposed by Caramana et al. [14].

We emphasize that the previously outlined SMG algorithm for node acceleration is formulated in a way that inherently produces an *hourglass damping* effect. By contrast, other schemes, such as the formerly mentioned edge viscosity by Caramana et al. [14], must resort to an *additional* set of lumped node forces designed to achieve hourglass damping.

The Reaction Rate Law

Let λ be the mass fraction of the reaction products in a zone. Several reaction rate laws to describe detonation initiation, growth, and propagation have been published [16–20]. They are generally based on a semi-empirical approach. The forest fire model [16] was set up to reproduce the experimental pop-plot data. The terms in the ignition and growth model (IGG) of Lee and Tarver [17] were fitted to reproduce both thin and thick pulse initiation as seen in the pressure or velocity gauge data. These models must also reproduce the failure of detonation along cylinders with subcritical diameter. Any one of these models can be introduced into the SMG/Q scheme.

Let us briefly outline several available models, in a nondimensional form. We know that the reaction rate may depend on the degree of reaction λ, pressure p, density ρ, or temperature T:

$$\dot{\lambda} = \left(\frac{D}{\delta r}\right) y(\lambda) f(p, \rho, T). \tag{2}$$

Here D is the ideal detonation speed, and δr is a reaction zone width. Obviously the reaction rate should increase with pressure, density, or temperature. The rate dependence on λ was called the *burn topology curve* (BTC) by Partom [18]. The reaction rate should increase with λ at the ignition phase, but then it should decrease toward the burn completion due to depletion of the reactant. To get this, Partom [18] used a two-branch parabola (see Fig. 5), whereas the IGG model [17] has a $\lambda^{\alpha}(1-\lambda)^{\beta}$

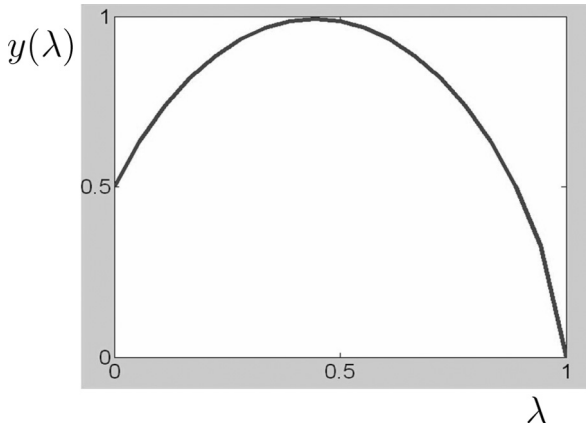

Figure 5. The burn topology curve (see Partom [18]).

dependence. In the Forest Fire model there is only a $(1-\lambda)$ depletion term:

$$y(\lambda) = \left\{ \begin{array}{ll} (1-\lambda) & \text{Forest Fire} \\ \lambda^{\alpha}(1-\lambda)^{\beta} & \text{IGG} \\ 2-\textit{branch parabola} & \text{Partom} \end{array} \right\}. \tag{3}$$

An Arrhenius type of temperature dependence can be expected from the kinetics of the reaction:

$$f(p) = \exp\left(-\frac{T_a}{T}\right). \tag{4}$$

The Partom model [18] can also provide an estimate of the activation temperature T_a. A temperature-dependent rate has the advantage that it can reproduce the lower reaction rates obtained in double shock initiation. However, most hydrocodes use an equation of state that does not compute the temperature. Moreover, temperature is not measured in typical experiments. Therefore, it is more convenient to use a pressure- or density-dependent rate. In the Forest Fire model the pressure dependence of the reaction rate is obtained by a polynomial fit

to the experimental data (pop-plot). The growth term in IGG [17] and the JWL++ rates [20] also depend on the pressure:

$$f(p) = \left\{ \begin{array}{ll} \left(\frac{p}{p_{CJ}}\right)^n & p > p_{act} \\ 0 & p < p_{act} \end{array} \right\}. \tag{5}$$

Wilkins's C-J volume burn model [21] for detonation propagation and the ignition term in the IGG model depend on density:

$$f(\mu) = \left\{ \begin{array}{ll} \left(\frac{\mu}{\mu_{CJ}}\right)^m & \mu > \mu_{act} \\ 0 & \mu < \mu_{act} \end{array} \right\}. \tag{6}$$

Here $\mu(\rho) = \rho/\rho_0 - 1$ and $\mu_{CJ} = \mu(\rho_{CJ})$, with ρ_{CJ} being the CJ density.

For the present study we assume a simple pressure-dependent rate law, similar to the one described in Luttwak et al. [22]. Let δr_c be the computational reaction zone size, which cannot be smaller than twice the cell size Δx:

$$\delta r_c = \max(\delta r, 2\Delta x). \tag{7}$$

Thus, to obtain a resolved reaction zone calculation we must have a sufficiently refined mesh with $5\Delta x < \delta r$. However, as the detonation wave develops and propagates into a region of coarser mesh, the same scheme may resolve the reaction over two or three computational cells. The rate law in the calculations that was found adequate is

$$\dot{\lambda} = \frac{D}{\delta r_c} \max\left[\phi(t - t_B),\ \max\left(\frac{p}{p_{CJ}}, \lambda^\alpha\right)(1-\lambda)^\beta \left(\frac{p}{p_{CJ}}\right)^n\right] \tag{8}$$

with ϕ being the Heaviside step function:

$$\phi(x) = \left\{ \begin{array}{ll} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{array} \right\}. \tag{9}$$

In the above, t is the time, and t_B is a time of burn (arrival of detonation front), which can be computed in advance for each

zone. Initiation is activated by a pressure $p > p_{act}$. Detonation propagation can result from initiation and growth for a resolved reaction zone calculation or be based on a programmed burn, in a coarse mesh calculation in which the time of burn can be evaluated using the known constant D or curvature-dependent detonation velocity $D(\kappa)$. The pressure-dependent term provides for an increased detonation speed in regions where the detonation wave converges, such as a Mach stem, or near a shaped charge axis.

Equation of State and Closure

For the solid reactants we assume a linear velocity relation $U_s = c_0 + su_p$ between the shock velocity U_s and the particle velocity u_p. The Gruneisen equation with a fixed Γ is used to obtain the pressure for states away from the assumed "linear $U-u$" Hugoniot. For the explosive products a Jones-Wilkins-Lee

Table 1
Detonation products JWL parameters

D	P_{CJ}	A	B	R_1	R_2	ω	e/V
8.64	35.5	871.0	13.9	4.6	1.15	0.3	10.0

Table 2
Solid reactant Gruneisen EOS parameters

ρ_0	c_0	s	Γ
1.865	2.3	2.3	1.3

Table 3
Reaction rate parameters

δr	α	β	n	p_{act}/p_{CJ}
0.08	0.0	0.95	3.5	0.01

(JWL) equation of state is assumed. Both of them can be expressed as a combination:

$$p_s(\rho, e) = F_{jwl}(\rho) + eG_s(\rho) \tag{10}$$

for the solid and

$$p_{jwl}(\rho, e) = F_{jwl}(\rho) + eG_{jwl}(\rho) \tag{11}$$

for the JWL. For closure we take a simple mix rule, assuming that the chemical (burn) energy is deposited solely in the

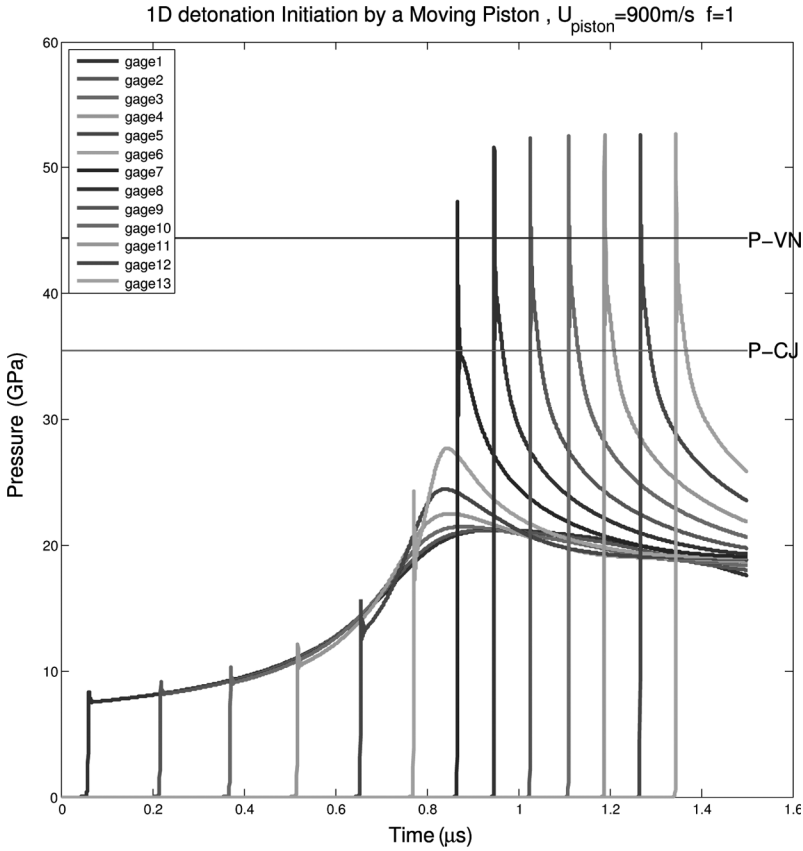

Figure 6. 1D Detonation initiation by a 900 m/s piston ($f=1$). Pressure history.

detonation products, whereas the compression work is shared by both components:

$$p(\rho, e) = \lambda p_{jwl}(\rho, e) + (1 - \lambda) p_s(\rho, e - \lambda Q) \tag{12}$$

Here the specific internal energy e includes the already released detonation energy λQ.

Test Cases: 1D Sustained Detonation Initiation

In all cases we consider an HMX-based plastic-bonded explosive with the properties given in the tables below. All units are in the

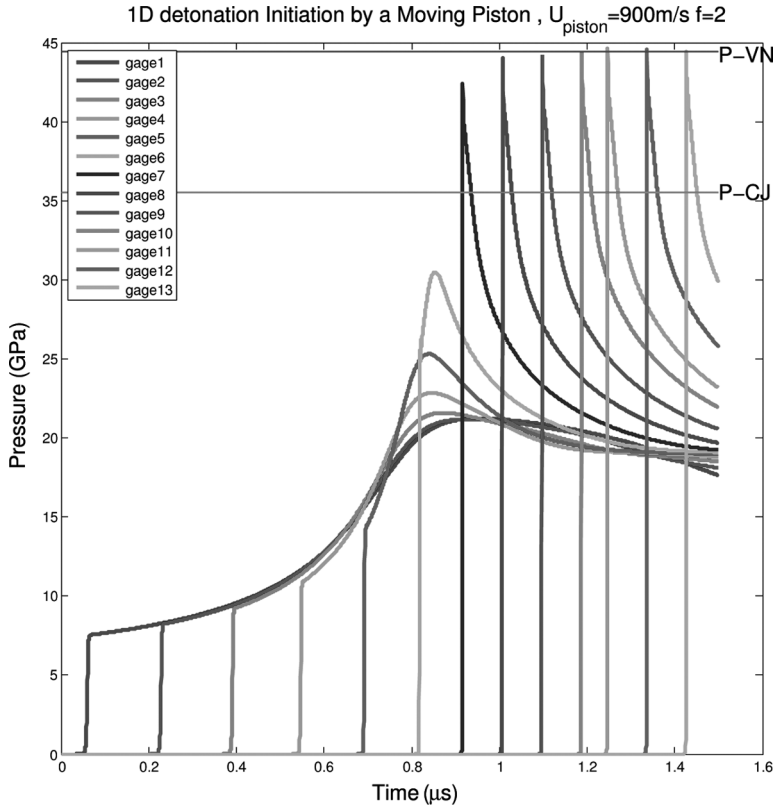

Figure 7. 1D Detonation initiation by a 900 m/s piston ($f = 2$). Pressure history.

kg-mm-μs unit system (pressure in GPa, energy in MJ). These values were chosen to check the model. The JWL parameters are taken from Dobratz and Crawford [23] for LX07. The Hugoniot parameters are close to Gustavsen et al. [24]. The reaction rate parameters similar to Lambert et al. [25] were fine-tuned to fit our model. We assume a sustained shock initiation by the impact of a 900 m/s piston. The reaction rate parameters used in Eq. (8) are given in Table 1. The solid Gruneisen parameters are given in Table 2, and the reaction rate data are given in Table 3. All the calculations were run in pure Lagrangian mode. One of the purposes of the test runs was to show how well the SMG/Q scheme can handle a distorted mesh. In the following, we consider the distorted mesh test case, preceded by the reference case of a one-dimensional detonation.

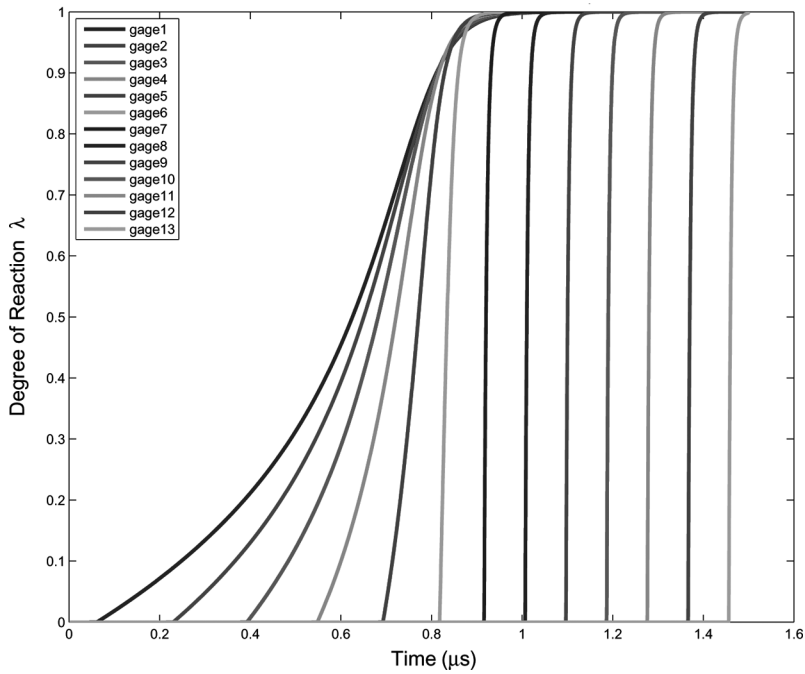

Figure 8. 1D Detonation initiation by a 900 m/s piston. Reaction degree λ history.

One-Dimensional Calculation

The 1D calculation was run in the 3D SMG code, using a single row of $1{,}000 \times 1 \times 1$ cells that mesh a slab of $10 \times 0.01 \times 0.01$ mm. In Figs. 6–8, we present the pressure and reaction rate history for 13 gauge points equally distributed along the charge. Using the SMG scheme without any modifications of the IRP solution ($f=1$) resulted in over shoot of the pressure at the leading reactive shock (von Neumann peak), exceeding the theoretical value by about 9 GPa (Fig. 6). Increasing the scheme dissipativity by taking $Q = f(p^* - p)$ with $f=2$ resulted in smooth pressure history profiles conforming to the von Neumann peak value (Fig. 7). With respect to the choice of $f=2$, we note that normally it is expected to use $f=1$, and in general shock capturing is relatively insensitive to the value of f.

For estimating the numerical convergence we conducted the 1D detonation runs with three levels of mesh refinement, using

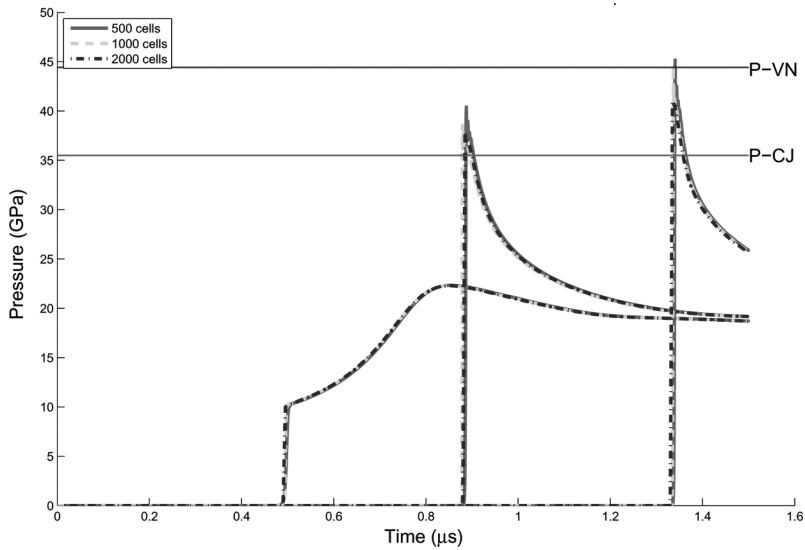

Figure 9. Mesh size dependence of 1D initiation by a 900 m/s piston ($f=2$).

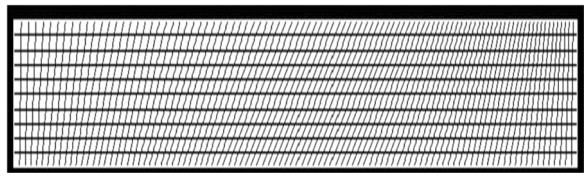

Figure 10. 2D Saltzman-like mesh block.

mesh sizes of 0.02, 0.01, and 0.005 mm, that correspond to 500, 1,000, and 2,000 cells, respectively. In Fig. 9 we present the pressure history obtained at three (nearly, but not exactly, identical) locations in each run. The resulting pressure history (Fig. 9) indicates that during the buildup to detonation the pressure profiles are almost identical. The small shift in the rise time is due only to the fact that in order to better distinguish between the profiles at the three mesh levels the gauges were located at nearly identical locations. Upon reaching a steady detonation, the reaction zone width decreases approaching

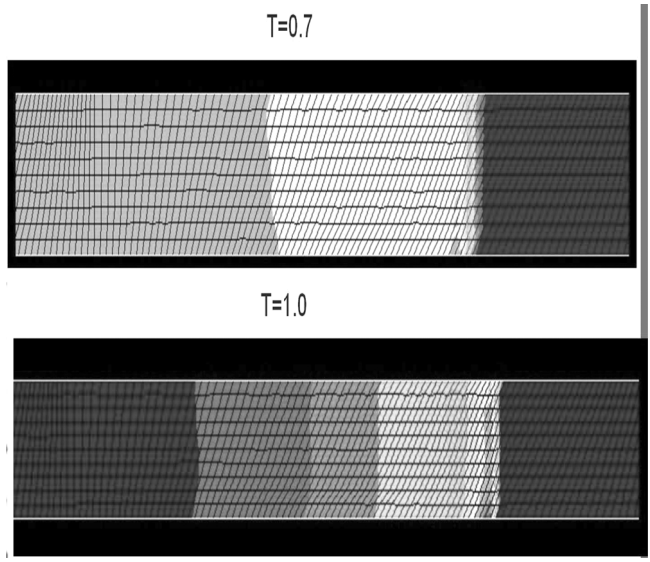

Figure 11. Detonation initiation on a skewed mesh. Isobars at $t = 0.7\,\mu s$ and at $t = 1.0\,\mu s$.

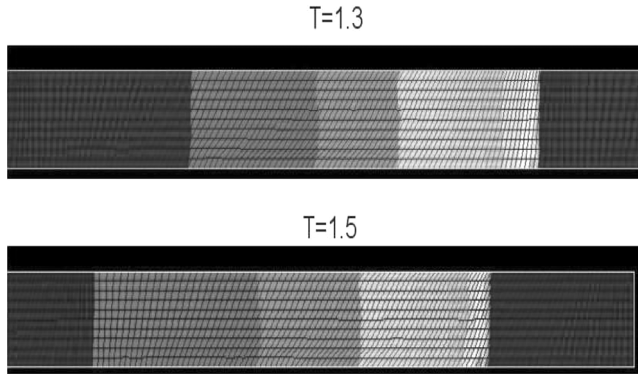

Figure 12. Detonation initiation on a skewed mesh. Isobars at $t = 1.3\,\mu s$ and at $t = 1.5\,\mu s$.

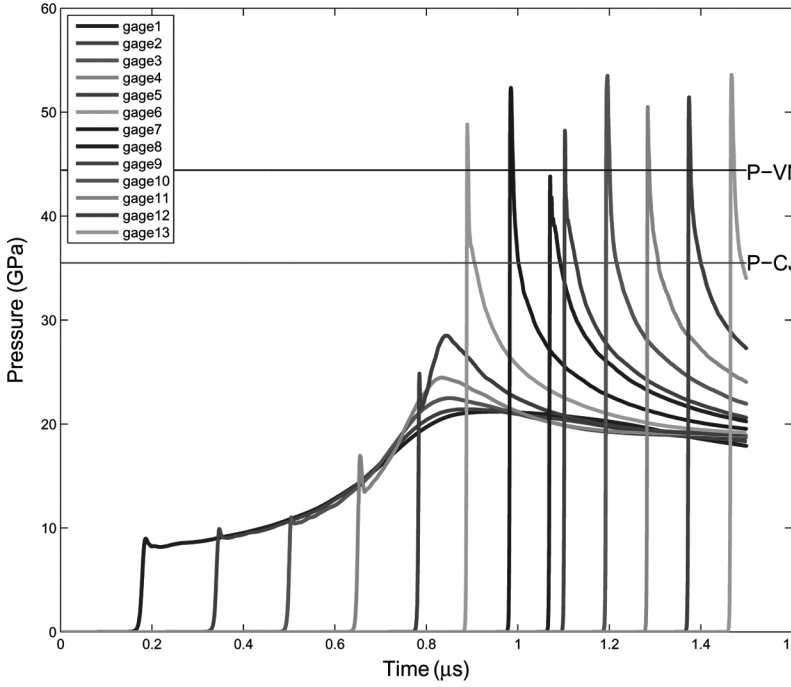

Figure 13. Detonation initiation on a skewed mesh. Pressure history along lower side.

$\delta r = 0.08$ mm (as given in Table 3), which implies that in the three mesh levels the reaction zone is resolved by about 4, 8, and 16 cell sizes, respectively. In concluding this convergence test, our main findings are that the value of the VN peak is somewhat mesh dependent, whereas the smooth reaction zone pressure profiles are nearly identical.

The Case of a 2D Skewed Mesh

To test the performance of the SMG scheme in the presence of a distorted mesh with long and thin cells, we consider a Saltzman-like mesh composed of of five blocks of $100 \times 10 \times 1$ as shown in Fig. 10. The first calculations were carried out with the original (component-wise) vector limiter and then rerun with the newly developed VIP (convex hull–based) vector limiter

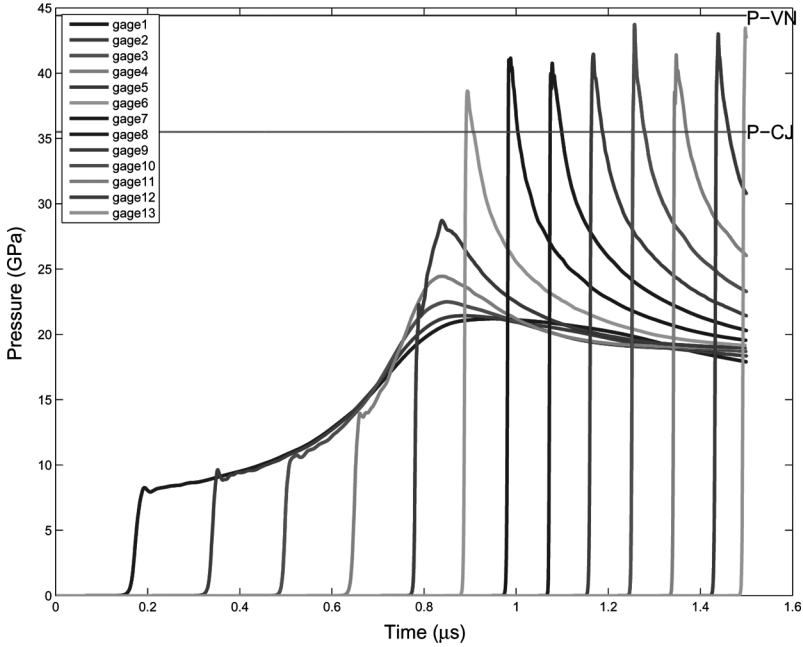

Figure 14. Detonation initiation on a skewed mesh. Pressure history along middle section.

[15], which produced an additional improvement in the problem symmetry preservation. Here we present only the results obtained with the VIP limiter. Also, as described in the previous subsection we increased the scheme dissipativity by taking $f=2$. In Figs. 11 and 12 we see the leading shock front advancing over the deformed mesh at the time sequence $t=0.7$, 1.0, 1.3, 1.5 μs. The shock front is nearly planar. Immediately behind it the pressure is higher at the lower side, but further upstream the pressure distribution becomes progressively more symmetric. In Figs. 13–15 we can see the pressure history at 13 gauge points equally distributed along the charge. In Fig. 13 the gauge points are along the lower side. In Figure 14 we follow the middle section, whereas in Fig. 15 the pressure history is given along the upper side. The differences between them display the asymmetry caused by the deformed mesh. In Figs. 16–18 we see the degree of reaction (λ) history along the charge.

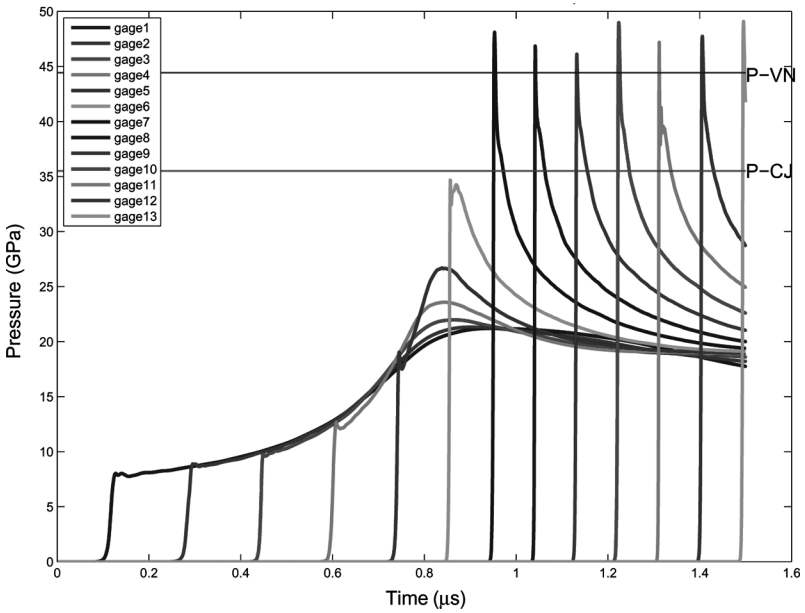

Figure 15. Detonation initiation on a skewed mesh. Pressure history along upper side.

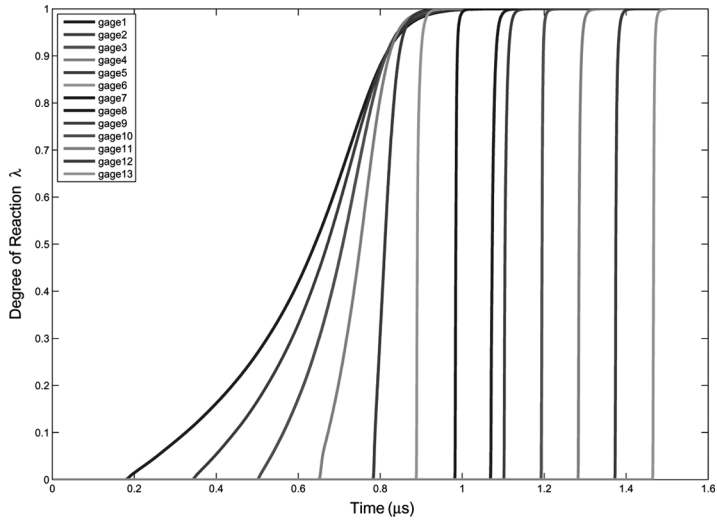

Figure 16. Detonation initiation on a skewed mesh. λ History along the lower side.

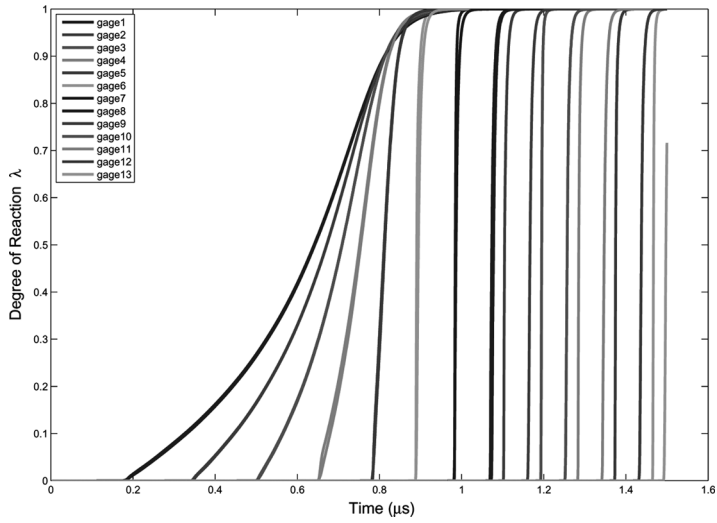

Figure 17. Detonation initiation on a skewed mesh. λ History along the middle section.

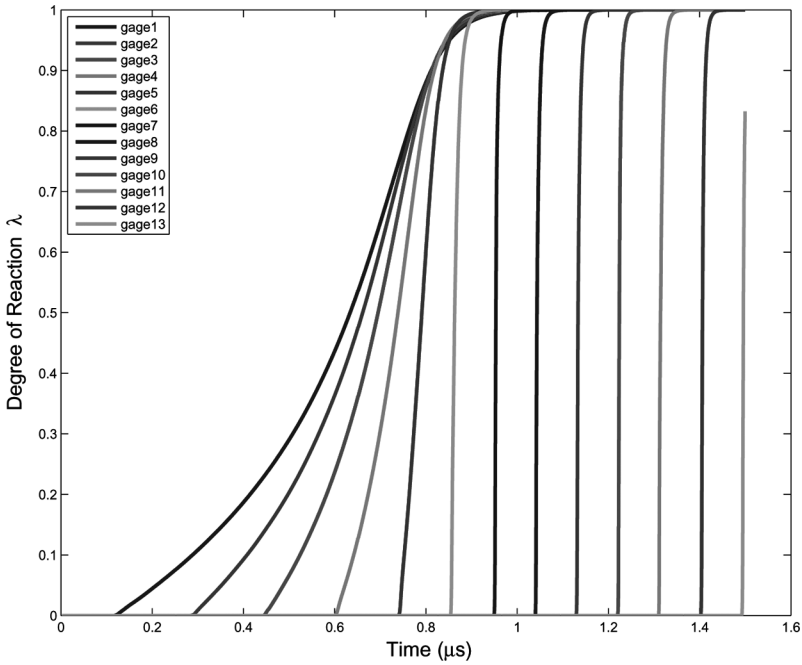

Figure 18. Detonation initiation on a skewed mesh. λ History along the upper side.

Results and Conclusions

The staggered mesh Godunov scheme has been extended to deal with problems of detonation initiation and propagation. In many real problems arising in terminal ballistics, we carry out detonation initiation and propagation calculations over already deformed meshes. In the current study, we assess this effect by considering a one-dimensional sustained detonation initiation using an initially distorted mesh, in analogy with the mesh in the (2D) Saltzman shock wave test problem. We demonstrate that the capabilities of the SMG method help minimize the disturbances arising from the deformed mesh. In particular, the SMG scheme can handle the expansion flow taking place in the reaction zone, whereas ''naturally'' damping hourglass type of instabilities that are common when using meshes with long

and thin zones. And last, here we used the VIP limiter, based on the convex hull of (neighbor nodes) vector image polyhedron for gradients of the velocity vectors. This was shown to improve the symmetry preservation for the considered test cases.

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