Modeling shock and detonation waves with *FLAC*

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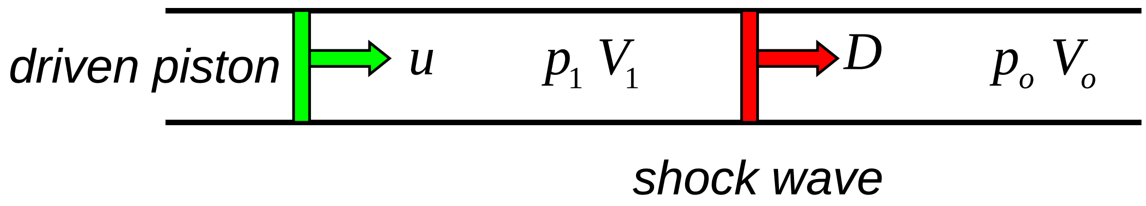
Shock waves can occur in materials that become stiffer with increasing stress – thus, high-amplitude parts of a pulse tend to overtake low-amplitude parts, resulting in a very sharp wave front (because wave speed increases with stiffness).

Detonation waves are shock waves, but internal energy is released at a rate that depends on the local pressure (mean stress) level.

FLAC is a general-purpose code that is often used to model seismic waves, but rarely (if ever) used to model shock or detonation waves. Such modeling presents a severe challenge to the code, because it involves very strong gradients (in space and time) and large local strains.

We show here the steps that are necessary for *FLAC* to model such waves accurately.

Consider the example of a piston moving a constant velocity, u, in a gas-filled tube. This causes a shock wave to develop and propagate at a greater speed, D. A shock forms because the material's stiffness increases with pressure.



Assuming the ideal equation of state (EoS) is: $e = \dfrac{pV}{\gamma - 1}$

the "bulk modulus" is $K = \gamma p$ and speed of sound is $\sqrt{\gamma p V}$

where

e	internal energy
p	pressure
$V = 1/\rho$	specific volume (1/density)
γ	ratio of specific heats

In order to solve for D, and the conditions behind the shock, we need only consider the conservation laws, applied across the jump:

$$V_0(D-u)=V_1 D \qquad \textit{mass}$$

$$Du=V_0(p_1-p_o) \qquad \textit{momentum}$$

$$D\left(\frac{p_1V_1}{\gamma-1}-\frac{p_oV_o}{\gamma-1}+\frac{u^2}{2}\right)=V_o p_1 u \qquad \textit{energy}$$

The solution is:

$$p_1 = p_o\left(1+\frac{\delta}{\Gamma}\right)$$

$$V_1 = V_o(1-\Gamma) \text{ or } \rho_1 = \frac{\rho_o}{1-\Gamma}$$

$$D=\frac{u}{\Gamma}$$

where

$$\Gamma = -\frac{(\gamma+1)\delta}{4\gamma}+\left\{\left[\frac{(\gamma+1)\delta}{4\gamma}\right]^2+\frac{\delta}{\gamma}\right\}^{1/2}$$

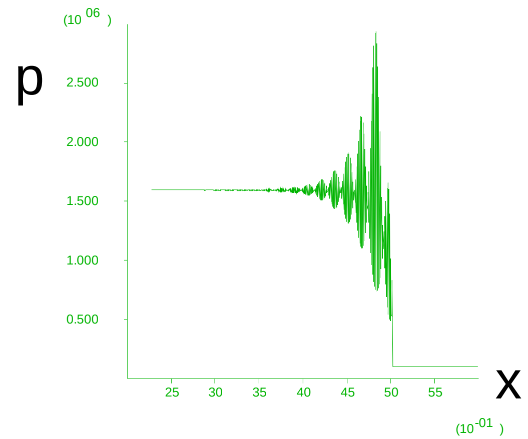
$$\delta=\frac{u^2}{p_oV_o}$$

Note that as $u \to 0$ the "shock speed" become constant: $D \to \sqrt{\gamma p_o V_o}$

Thus, at low piston speeds, an acoustic wave is propagated.

We simulate the inert shock problem with *FLAC*, using a 1D grid and the EoS implemented as a C++ user-defined function.

With no damping, there are oscillations in the pressure response, so we implement "energy leaking" between adjacent zones in proportion to pressure-difference. This is equivalent to supplying an entropy-jump across the shock, noting that



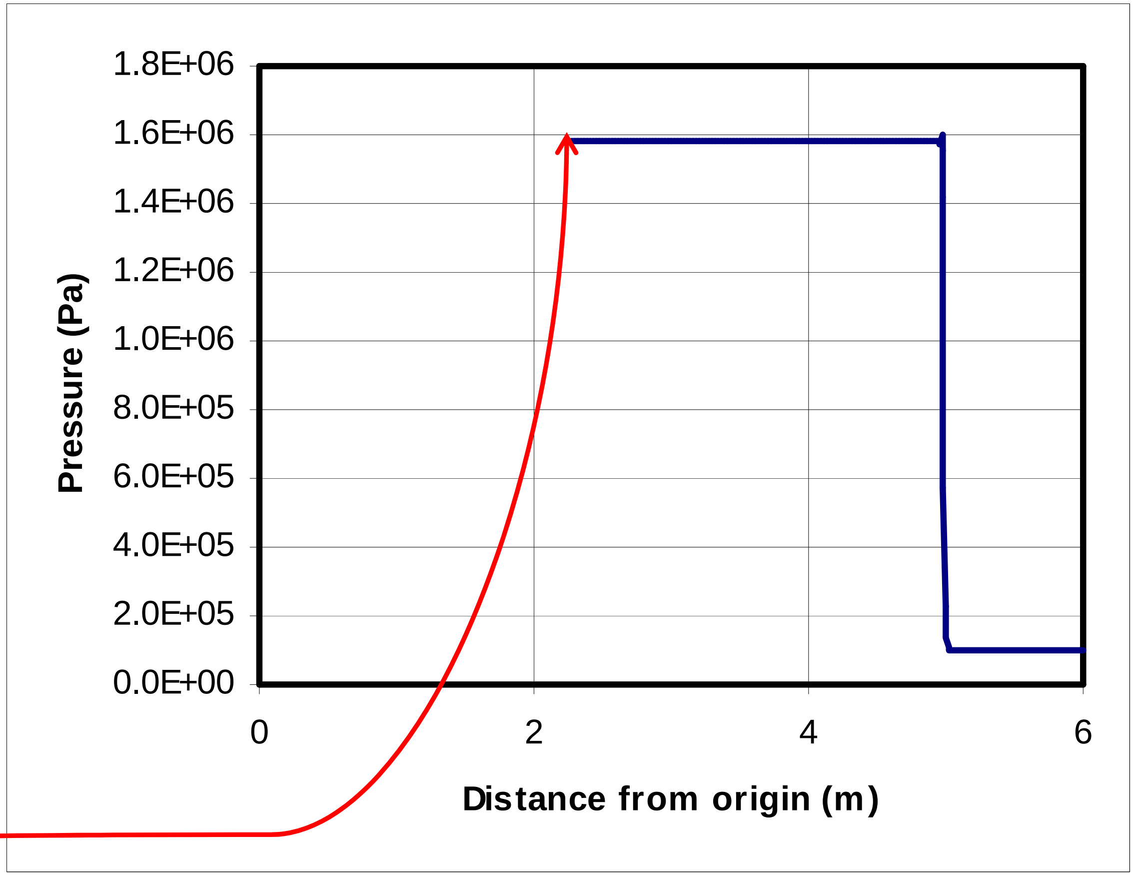
"… the entropy increase across a compression shock is entirely independent of the dissipative mechanism, and is defined exclusively by the conservation laws of mass, momentum and energy." Zel'dovich and Raizer (2002).

Thus, we implement (in *FISH*) an energy flux that is proportional to the pressure gradient:

$$\frac{\partial e}{\partial t} = \alpha \frac{\partial p}{\partial x} \frac{\overline{e}}{\overline{p}}$$

With this shock-damping scheme, and a factor (α) of 1000 m/s, we obtain a clean shock front:

Note that the simulation is done in large-strain mode. The driven piston has moved 2.27 m from its starting position.



Profile of pressure at t=3.027 ms, for u=750 m/s

Performing tests for various driving velocities, we compare results with the exact solutions for pressure, density and shock-wave velocity, for γ = 3.

u m/s	p_1 / p_0 exact	p_1 / p_0 num.	Error %	ρ_1 / ρ_0 exact	ρ_1 / ρ_0 num	Error %	D(exact) m/s	D(num.) m/s	Error %
250	3.427	3.427	0	1.447	1.447	0	809	809	0
500	8.243	8.233	-0.1	1.708	1.709	0.06	1207	1208	0.08
750	15.86	15.81	-0.3	1.832	1.838	0.33	1651	1648	-0.18
1000	26.42	26.28	-0.53	1.894	1.904	0.53	2118	2109	-0.42
1250	39.94	39.75	-0.48	1.928	1.937	0.47	2596	2583	-0.5

↑

Note that the maximum errors are 0.5%

Driving velocity

Detonation waves are treated in a similar way, but there is an additional term in the equation of state:

$$e = \frac{p}{(\gamma - 1)\rho} - Q\lambda \quad \text{where} \quad \frac{d\lambda}{dt} = \frac{1}{\tau}\left(\frac{p}{p_{\text{ref}}}\right)^{1.5}(1-\lambda)$$

Q is the total specific energy released by the explosive;

λ is the fraction released (0 to 1) – the rate equation (above) specifies how fast energy is released, as a function of pressure (τ controls the rate – low value gives rapid rate).

The solution of the conservation equations is the same, but with a different expression for Γ :

$$\Gamma = -\frac{\delta}{2\gamma}\left[\frac{\gamma+1}{2} + \frac{Q(\gamma-1)}{u^2}\right] + \left\{\left\{\frac{\delta}{2\gamma}\left[\frac{\gamma+1}{2} + \frac{Q(\gamma-1)}{u^2}\right]\right\}^2 + \frac{\delta}{\gamma}\right\}^{1/2}$$

Now, u is a free parameter, because the shock is self-propagating. We can determine u by invoking “Prigogine’s principle of minimum entropy-production” for a steady state dissipative process. By minimizing the entropy-increase across the shock,

$$\Delta S = c_v \ln\left(1 + \frac{Du}{p_0 V_0}\right)\cdot\left(1 - \frac{u}{D}\right)^{\gamma}$$

we obtain specific values for u and detonation velocity:

$$u = \sqrt{2Q\frac{\gamma-1}{\gamma+1}} \qquad D_d = \sqrt{Q\frac{\gamma^2-1}{2}} + \sqrt{Q\frac{\gamma^2-1}{2} + \frac{\gamma p_0}{\rho_0}}$$

As an example, we use the following parameters:

$$Q = 1.44\times10^6\ J/kg$$

$$\gamma = 3$$

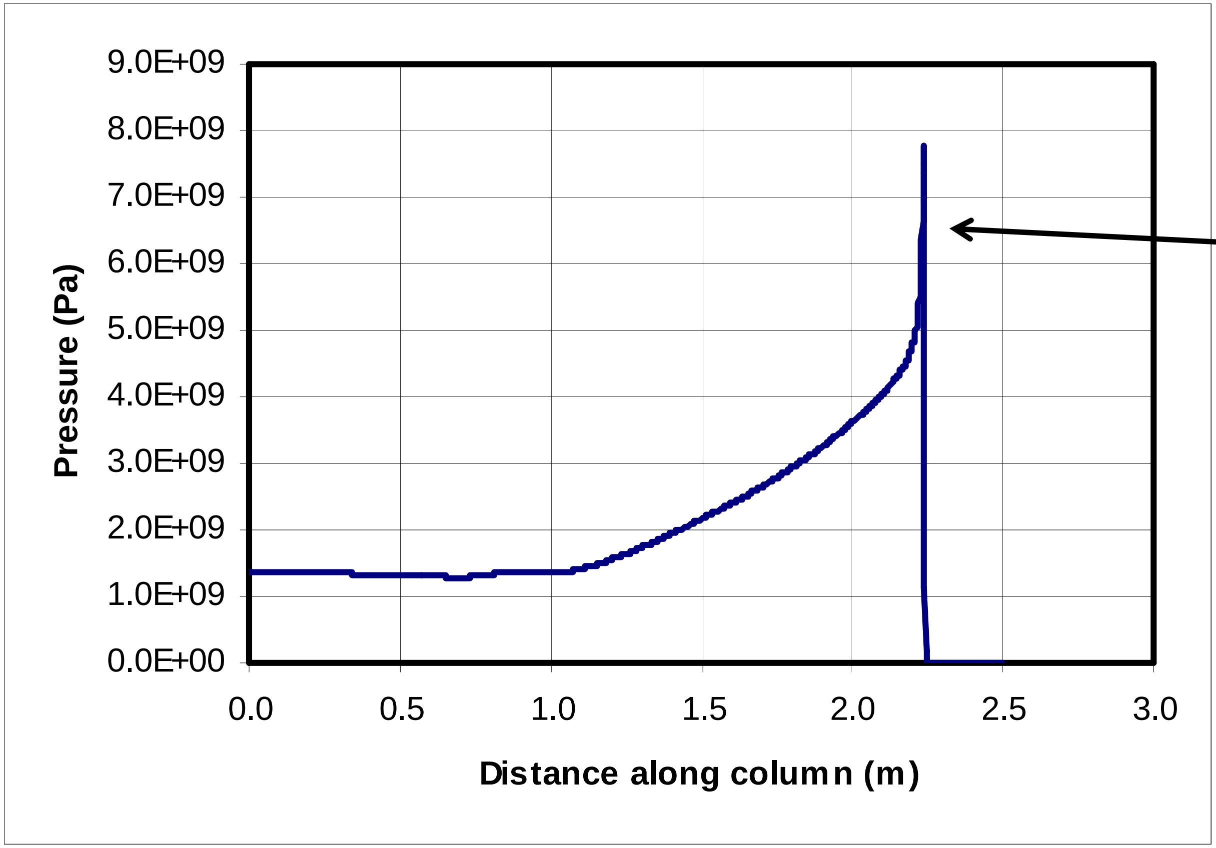
$$p_o = 10^5\ Pa$$

$$\rho_o = 800\,kg/m^3$$

$$P_{\text{ref}} = 1GPa$$

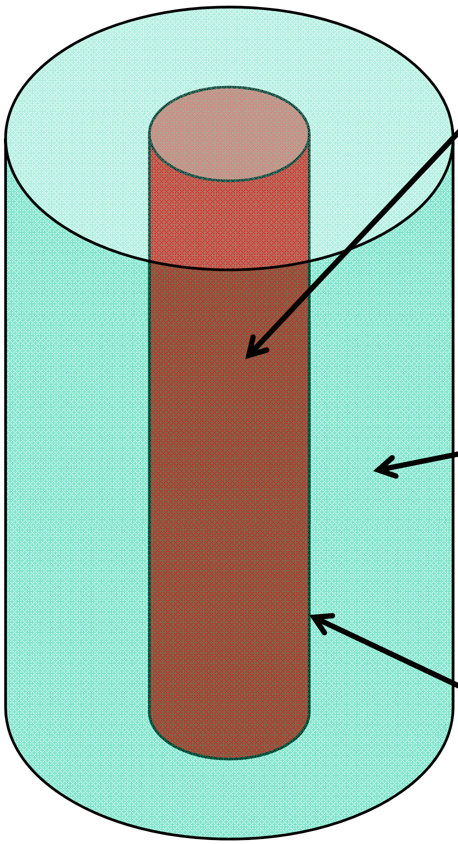
For these example parameters, the detonation velocity is **4796 m/s**

A 1D *FLAC* simulation using a zone size of 2.5 mm gives a measured detonation velocity of **4785 m/s** (an error of 0.23%), and the following profile of pressure at a time of 0.475 ms:



Note the "von Neumann spike" caused by energy being released into a pre-compressed zone at the shock front.

We perform simulations in 2D, using an axisymmetric *FLAC* grid in large-strain mode, with an interface between explosive and confining material (rock).



Explosive (ideal equation of state)

$$V_{\mathrm{IDEAL}} = 4796\, m/s$$

Rock (elastic/plastic)

$$K = 3.125\, GPa$$
$$G = 1.875\, GPa$$
$$\rho = 2500\, kg/m^3$$
$$\phi = 35^o$$
$$c = 40\, MPa$$
$$V_p = 1500\, m/s$$

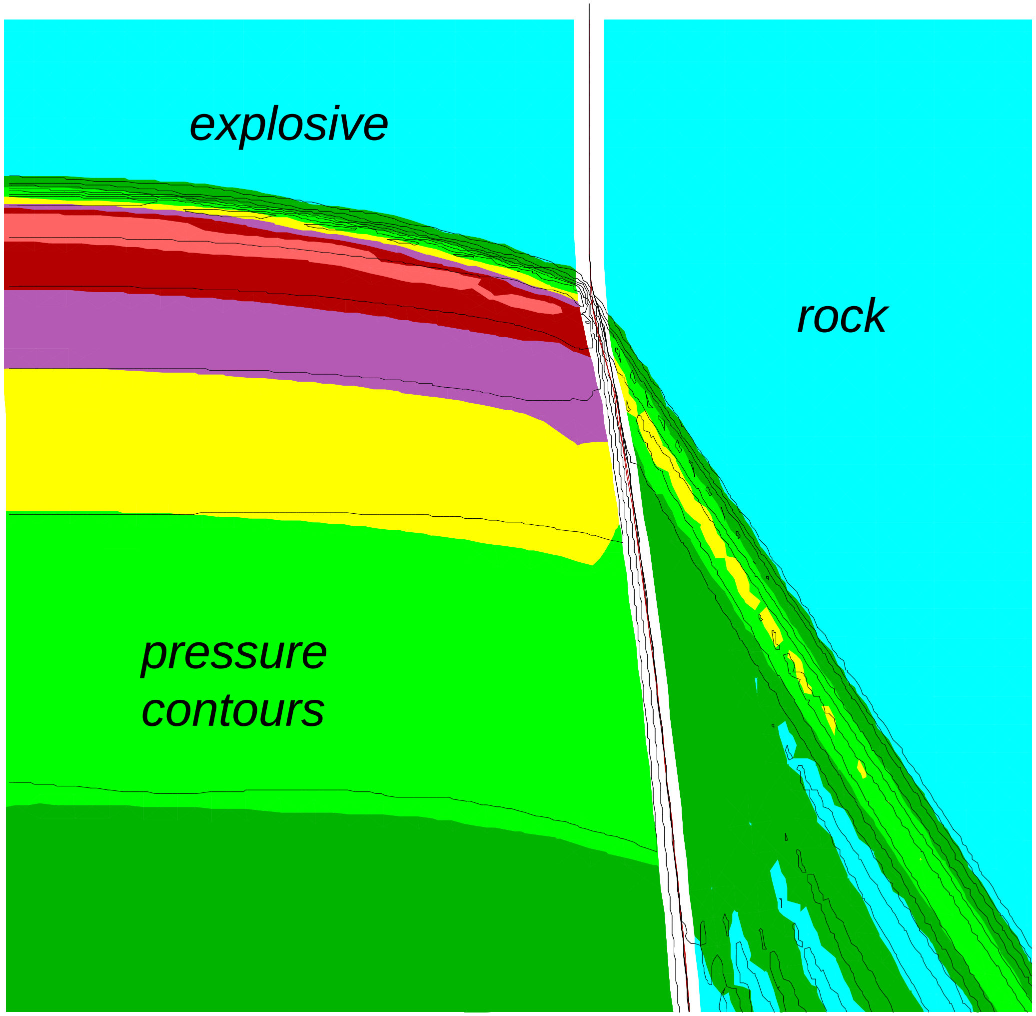
Frictionless interface

The detonation is initiated at the bottom of the explosive column.

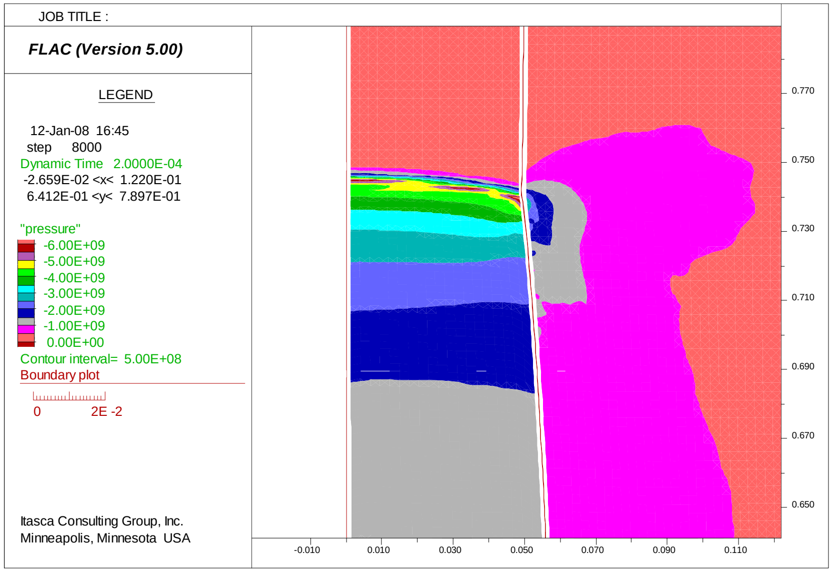
The 2D case is "non-ideal" in two aspects: (a) the confinement is not rigid, so the shock front becomes curved, and (b) the energy release is spread out over a finite region.

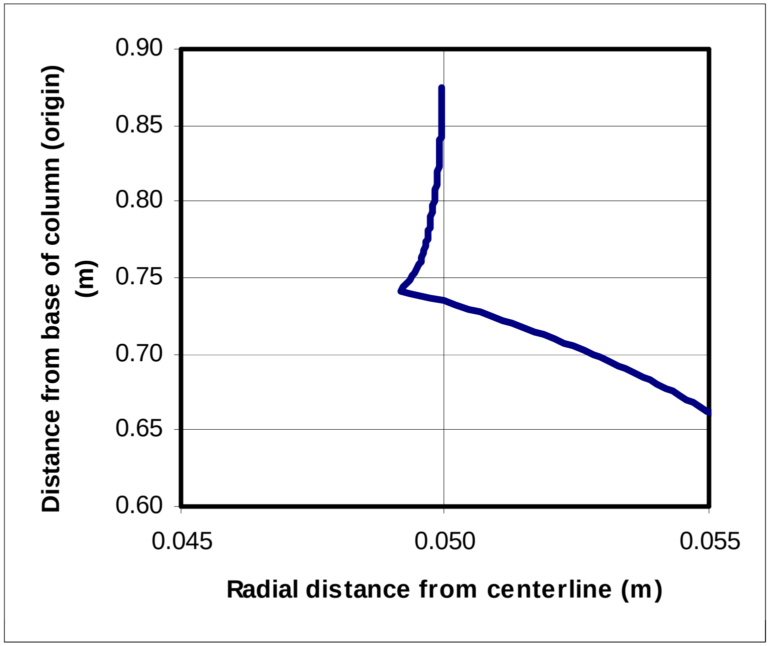
Here is a snapshot at a time of 0.2 ms, showing contours of pressure and the deformed shape of the interface (not magnified).

The color contours are for a zone size of 2.5 mm, while the black contour lines are for a zone size of 1.25 mm. (The initial explosive radius is 50 mm)



There is no analytical solution for this 2D case, but it is found that the detonation velocity (VOD) is lower than that of the perfectly confined case, conforming to field experience. Of particular interest is the case in which the VOD is lower than the p-wave speed in the rock:





Here, the advance wave in the rock compresses the explosive ahead of the shock front – note the indentation in the right-hand plot of interface profile.

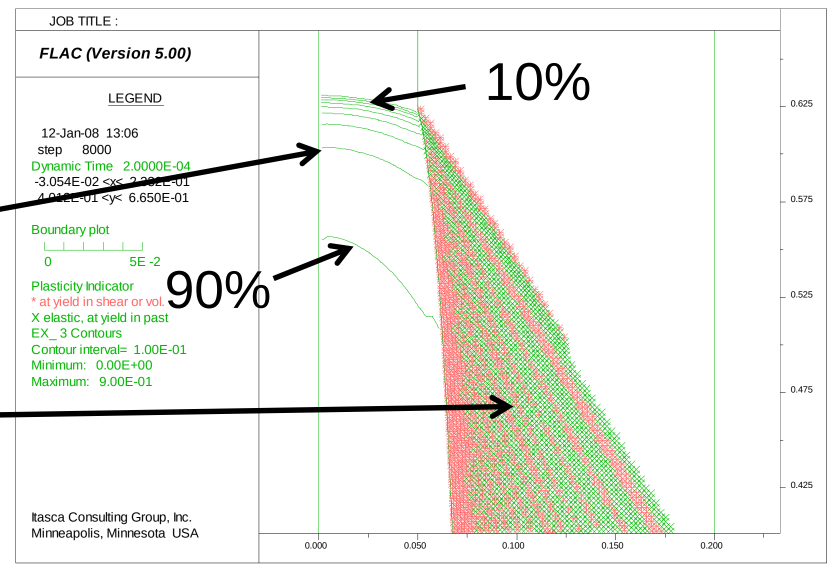
Several cases, including the two previously illustrated, were simulated – indicating how the VOD changes with rock properties.

Case	Density kg/m^3	Bulk modulus GPa	Shear modulus GPa	P-wave speed m/s	Measured D_d m/s
A	2500	3.125	1.875	1500	3016
B	2500	12.5	7.5	3000	3489
C	2500	28.125	16.875	4500	3721
D	2500	50.0	30.0	6000	3794
E	4000	50.0	30.0	4743	4029
F	-	rigid	rigid	-	4785

The simulations also show:

(a) the degree of reaction

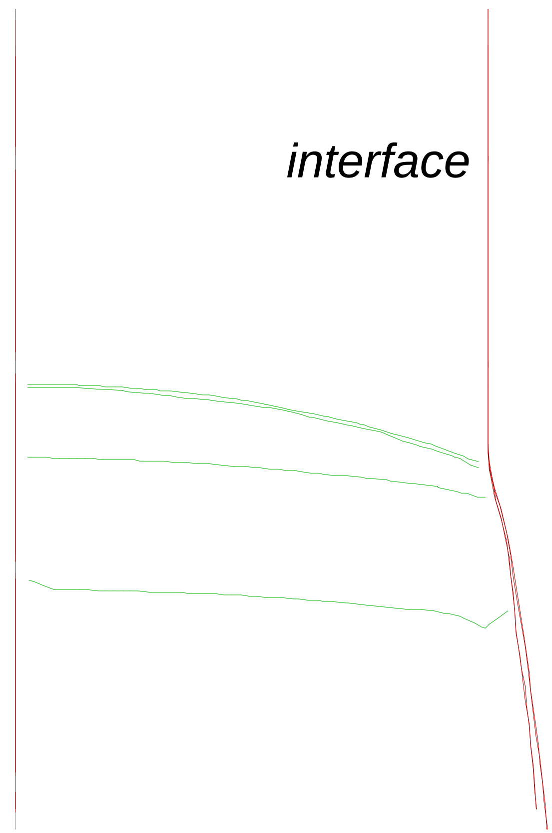
(b) the extent of plastic yield



Finally, we may identify the ***sonic locus***, which is the contour below which ***information cannot reach the detonation front*** ($u + c = D$), where u = particle velocity; c = local p-wave speed.

The plot shows sonic locus for two values of τ in the rate equation,

$$\frac{d\lambda}{dt} = \frac{1}{\tau}\left(\frac{p}{p_{\text{ref}}}\right)^{1.5}(1-\lambda)$$



The VoD is different in each case (4148 and 3016 m/s, respectively)

Conclusions

The general-purpose code *FLAC* (with user-written *FISH* functions added to the data file) gives accurate results for inert shock waves and detonation waves in 1D. Further, non-ideal 2D-axisymmetric cases of compliant and nonlinear confinement have been simulated, although no analytical solutions exist.

The 2D detonation examples (with elastic/plastic confinement) presented here took about 2 hours to simulate on a notebook machine. After replacing the *FISH* functions with compiled code, and implementing a moving-grid scheme, similar runs to determine VOD now take 4 minutes.