Appendices

A. Effect of a Second Shock on the Principal Hugoniot

Given an equation of state

$$P = a\mu + b\mu^2 + c(1+\mu)E,$$

where

$$\mu = \frac{1}{V} - 1, \qquad V = \text{relative volume.}$$

We wish to find how much a second compression from a point on the principal Hugoniot differs from the principal Hugoniot.

The principal Hugoniot is obtained by substituting in the equation of state the relation $E = E_0 + 1/2(P + P_0)(V^0 - V)$ where $E_0 = 0$, $P_0 = 0$, and $V^0 = 1$. For the given equation of state this yields

$$P = \frac{a\mu + b\mu^2}{1 - c\mu/2} \qquad \text{(principal Hugoniot).} \tag{A.1}$$

For $\mu < 0.25$ we may write

$$P \sim a\mu + \left(b + \frac{ac}{2}\right)\mu^2 + \frac{1}{2}c\left(b + \frac{ac}{2}\right)\mu^3. \tag{A.2}$$

To calculate the Hugoniot starting from the point (P_1, V_1, E_1) on the principal Hugoniot (Fig. A.1), we substitute in the equation of state the relation $E = E_1 + 1/2(P + P_1)(V_1 - V)$. Let $V_1 = 1 - \delta$, then $E_1 = 1/2P_1\delta$.

We have

$$\begin{aligned}
P &= a\mu + b\mu^2 + c(1+\mu)\left[E + \frac{P + P_1}{2}(V_1 - V)\right] \\
&= a\mu + b\mu^2 + \frac{c}{2}\left[P_1\frac{\delta}{V} + P\left(\mu - \frac{\delta}{V}\right) + P_1\left(\mu - \frac{\delta}{V}\right)\right] \\
&= a\mu + b\mu^2 + \frac{c}{2}\left[P\left(\mu - \frac{\delta}{V}\right) + P_1\mu\right].
\end{aligned}$$

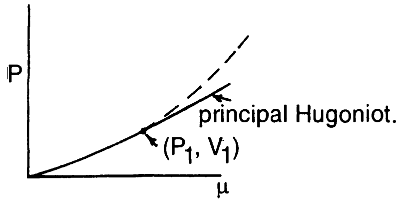

Fig. A.1. Hugoniot from point (P_1, V_1) on principal Hugoniot

The Hugoniot for points above the initial point $\left(P_1, V_1 = 1 - \delta,\ E_1 = \frac{P_1 \delta}{2}\right)$ is

$$P = \frac{a\mu + b\mu^2 + \frac{c}{2} P_1 \mu}{1 - \frac{c}{2}\left(\mu - \frac{\delta}{V}\right)}. \tag{A.3}$$

Expanding, we get

$$\begin{aligned} P &= a\mu + b\mu^2 + \frac{c}{2} P_1 \mu + \frac{ac}{2}\mu\left(\mu - \frac{\delta}{V}\right) \\ &\quad + \frac{bc}{2}\mu^2\left(\mu - \frac{\delta}{V}\right) + \frac{c^2}{4} P_1 \mu\left(\mu - \frac{\delta}{V}\right) + \frac{c^2}{4} a\mu\left(\mu - \frac{\delta}{V}\right)^2 \\ &= a\mu + \left(b + \frac{ac}{2}\right)\mu^2 + \frac{c}{2}\left(b + \frac{ac}{2}\right)\mu^3 - \frac{ac}{2}\mu\frac{\delta}{V} \\ &\quad - \frac{bc}{2}\mu^2\frac{\delta}{V} - \frac{c^2}{2} a\mu^2\frac{\delta}{V} + \frac{c^2}{4} a\mu\frac{\delta^2}{V^2} \\ &\quad + \frac{c}{2}\mu P_1\left[1 + \frac{c}{2}\left(\mu - \frac{\delta}{V}\right)\right]. \end{aligned}$$

Rearranging the terms and replacing P_1 by (A.2) we obtain

$$\begin{aligned} P = {} & \underline{a\mu + \left(b + \frac{ac}{2}\right)\mu^2 + \frac{c}{2}\left(b + \frac{ac}{2}\right)\mu^3} \\ & - \frac{c}{2\mu}\left[a\frac{\delta}{V} + \left(b + \frac{ac}{2}\right)\mu\frac{\delta}{V} - \frac{c}{2} a\frac{\delta^2}{V^2}\right] \\ & + \frac{c}{2}\mu\left[a\mu_1 + \left(b + \frac{ac}{2}\right)\mu_1^2 + \frac{1}{2} c\left(b + \frac{ac}{2}\right)\mu_1^3 + \ldots\right]. \end{aligned} \tag{A.4}$$

The underlined terms in (A.4) are the same as the principal Hugoniot. Since $\frac{\delta}{V} \sim \mu_1$ and c is usually between 1 and 2, equation (A.4) is very nearly equal to the principal Hugoniot except for high order terms.

B. Finite Difference Program for One Space Dimension and Time

The partial differential equations and the corresponding finite difference equations are those used by the KO computer program. Time-dependent flows in one space variable, r, are described for plane ($d = 1$), cylindrical ($d = 2$), and spherical ($d = 3$) geometries.

B.1 Fundamental Equations

1. Equation of motion

$$\frac{\rho_0 \dot{U}}{V} = \frac{\partial \Sigma_r}{\partial r} + (d-1)\frac{\Sigma_r - \Sigma_\theta}{r},$$

   where U is the particle velocity.

2. Conservation of mass

$$\frac{\mathrm{d}M}{\mathrm{d}t} = 0$$

   with M a mass element.

3. First law of thermodynamics

$$\dot{E} - V[s_1\dot{\varepsilon}_1 + (d-1)s_2\dot{\varepsilon}_2] + (P+q)\dot{V} = 0.$$

4. Velocity strains

$$\dot{\varepsilon}_1 = \frac{\partial U}{\partial r},$$

$$\dot{\varepsilon}_2 = \frac{U}{r}.$$

5. Stress deviators

$$\dot{s}_1 = 2\mu\left(\dot{\varepsilon}_1 - \frac{1}{3}\frac{\dot{V}}{V}\right),$$

$$\dot{s}_2 = 2\mu\left(\dot{\varepsilon}_2 - \frac{1}{3}\frac{\dot{V}}{V}\right),$$

$$\dot{s}_3 = 2\mu\left(\dot{\varepsilon}_3 - \frac{1}{3}\frac{\dot{V}}{V}\right).$$

   Note: Three stresses are identified here, even though they are not all required in order to maintain an analogy with the two and three dimensional programs.

6. Pressure equation of state

$$P = a(\eta - 1) + b(\eta - 1)^2 + c(\eta - 1)^3 + d\eta E$$

   with $\eta = 1/V = \rho/\rho_0$ and where a, b, c, and d are equation-of-state constants.

7. Total stresses

$$\Sigma_r = -(P+q) + s_1$$
$$\Sigma_\theta = -(P+q) + s_2.$$

8. Artificial viscosity

$$q = C_0^2 \frac{\rho_0}{V} \left(\frac{\partial U}{\partial r}\right)^2 (\Delta r)^2 + C_{\mathrm{L}} \frac{\rho_0 a}{V} \left(\frac{\partial U}{\partial r}\right) \Delta r,$$

where C_{L} and C_0 are constants, $a = \sqrt{P/\rho}$, and Δr is the grid spacing.

9. Von Mises yield condition

$$(s_1^2 + s_2^2 + s_3^2) - \frac{2}{3}(Y^0)^2 \leq 0$$

with Y^0 the plastic flow stress.

B.2 Finite Difference Equations

1. Mass zoning

$$m_{j+\frac{1}{2}} = \frac{\rho_0}{V_0} \left[\frac{(r_{j+1}^0)^d - (r_j^0)^d}{d} \right] \qquad \begin{cases} \text{plane:} & d = 1 \\ \text{cylindrical:} & d = 2 \\ \text{spherical:} & d = 3 \end{cases}$$

where ρ_0 is the equation-of-state reference density and V_0 the initial relative volume.

2. Equation of motion

$$U_j^{n+\frac{1}{2}} = U_j^{n-\frac{1}{2}} + \frac{\Delta t^n}{\phi_j^n} \left[(\Sigma_r)_{j+\frac{1}{2}}^n - (\Sigma_r)_{j-\frac{1}{2}}^n \right] + \Delta t^n (\beta_j^n)(d-1),$$

where

$$(\Sigma_r^n)_{j+\frac{1}{2}} = \left[-(P^n + q^{n-\frac{1}{2}}) + s_1^n \right]_{j+\frac{1}{2}},$$

$$(\Sigma_\theta^n)_{j+\frac{1}{2}} = \left[-(P^n + q^{n-\frac{1}{2}}) + s_2^n \right]_{j+\frac{1}{2}},$$

$$\phi_j^n = \frac{1}{2} \left[\rho_{0_{j+\frac{1}{2}}} \left(\frac{r_{j+1}^n - r_j^n}{V_{j+\frac{1}{2}}^n} \right) + \rho_{0_{j-\frac{1}{2}}} \left(\frac{r_j^n - r_{j-1}^n}{V_{j-\frac{1}{2}}^n} \right) \right],$$

$$\beta_j^n = \frac{1}{2} \left\{ \left[\frac{(\Sigma_r)_{j+\frac{1}{2}}^n - (\Sigma_\theta)_{j+\frac{1}{2}}^n}{\frac{1}{2}(r_{j+1}^n + r_j^n)} \right] \left(\frac{V^n}{\rho_0} \right)_{j+\frac{1}{2}} + \left[\frac{(\Sigma_r)_{j-\frac{1}{2}}^n - (\Sigma_\theta)_{j-\frac{1}{2}}^n}{\frac{1}{2}(r_j^n + r_{j-1}^n)} \right] \left(\frac{V^n}{\rho_0} \right)_{j-\frac{1}{2}} \right\}.$$

3. Conservation of mass

$$V_{j+\frac{1}{2}}^{n+1} = \frac{\rho_0}{m_{j+\frac{1}{2}}}\left[\frac{(r_{j+1})^d - (r_j)^d}{d}\right]^{n+1},$$

$$r_j^{n+1} = r_j^n + U_j^{n+\frac{1}{2}}\Delta t^{n+\frac{1}{2}}.$$

4. Calculation of velocity strains

$$(\dot{\varepsilon}_1)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{U_{j+1}^{n+\frac{1}{2}} - U_j^{n+\frac{1}{2}}}{r_{j+1}^{n+\frac{1}{2}} - r_j^{n+\frac{1}{2}}},$$

$$(\dot{\varepsilon}_2)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{U_{j+1}^{n+\frac{1}{2}} + U_j^{n+\frac{1}{2}}}{r_{j+1}^{n+\frac{1}{2}} + r_j^{n+\frac{1}{2}}},$$

$\dot{\varepsilon}_2 = 0$ for $d = 1$.

5. Calculation of stresses
   (a) Stress deviators

$$(s_1)_{j+\frac{1}{2}}^{n+1} = (s_1)_{j+\frac{1}{2}}^{n} + 2\mu\left[(\dot{\varepsilon}_1)_{j+\frac{1}{2}}^{n+\frac{1}{2}}\Delta t^{n+\frac{1}{2}} - \frac{1}{3}\left(\frac{V^{n+1} - V^n}{V^{n+\frac{1}{2}}}\right)_{j+\frac{1}{2}}\right]$$

$$(s_2)_{j+\frac{1}{2}}^{n+1} = (s_2)_{j+\frac{1}{2}}^{n} + 2\mu\left[(\dot{\varepsilon}_2)_{j+\frac{1}{2}}^{n+\frac{1}{2}}\Delta t^{n+\frac{1}{2}} - \frac{1}{3}\left(\frac{V^{n+1} - V^n}{V^{n+\frac{1}{2}}}\right)_{j+\frac{1}{2}}\right]$$

$$(s_3)_{j+\frac{1}{2}}^{n+1} = -\left[(s_1)_{j+\frac{1}{2}}^{n+1} + (s_2)_{j+\frac{1}{2}}^{n+1}\right].$$

   (b) Pressure equation of state

$$P_{j+\frac{1}{2}}^{n+1} = A(\eta_{j+\frac{1}{2}}^{n+1}) + B(\eta_{j+\frac{1}{2}}^{n+1})E_{j+\frac{1}{2}}^{n+1}.$$

6. Von Mises yield condition

$$(s_1^2 + s_2^2 + s_3^2)^{n+1} - \frac{2}{3}(Y^0)^2 = K^{n+1}.$$

If $K^{n+1} \leq 0$ the material is within the elastic limit. If $K^{n+1} > 0$ multiply the stress deviators by $\sqrt{2/3}Y^0/\sqrt{s_1^2 + s_2^2 + s_3^2}$.

7. Artificial viscosity

$$q_{j+\frac{1}{2}}^{n+\frac{1}{2}} = C_0^2\rho_{j+\frac{1}{2}}^{n+\frac{1}{2}}(U_{j+1}^{n+\frac{1}{2}} - U_j^{n+\frac{1}{2}})^2 + C_{\mathrm{L}}a\rho_{j+\frac{1}{2}}^{n+\frac{1}{2}}|U_{j+1}^{n+\frac{1}{2}} - U_j^{n+\frac{1}{2}}|.$$

Calculate only if $U_{j+1}^{n+\frac{1}{2}} < U_j^{n+\frac{1}{2}}$ and $(V_{j+\frac{1}{2}}^{n+1} - V_{j+\frac{1}{2}}^{n}) < 0$. Here $a = \sqrt{P/\rho}$, where P is the local pressure and $C_0 = 2$; $C_{\mathrm{L}} = 1$.

8. Energy equations
   The change in the internal energy, ΔE, is composed of a hydrodynamic component and a distortion component:

$$\Delta E = -(P + q)\Delta V + \Delta Z.$$

The change in distortion energy, ΔZ, is

$$(\Delta Z)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = V_{j+\frac{1}{2}}^{n+\frac{1}{2}} \left[s_1 \dot{\varepsilon}_1 + (d-1) s_2 \dot{\varepsilon}_2\right]_{j+\frac{1}{2}}^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}},$$

where

$$s_1^{n+\frac{1}{2}} = \frac{1}{2}(s_1^{n+1} + s_1^n) \quad \text{etc.}$$

The total internal energy, E, is

$$(E)_{j+\frac{1}{2}}^{n+1} = \left(\frac{E^n - \left\{\frac{1}{2}[A(\eta^{n+1}) + P^n] + \bar{q}\right\} [V^{n+1} - V^n] + \Delta}{1 + \frac{1}{2}[B(\eta^{n+1})][V^{n+1} - V^n]} \right.$$

where

$$\bar{q} = \frac{1}{2}(q^{n+\frac{1}{2}} + q^{n-\frac{1}{2}}).$$

This equation assumes that the equation of state has the form

$$P = A(\eta) + B(\eta)E.$$

9. Time steps

$$\Delta t^{n+\frac{3}{2}} = \frac{2}{3} \left. \frac{\Delta r^{n+1}}{\sqrt{a^2 + b^2}} \right|_{\text{min over } j},$$

$$\Delta r^{n+1} = r_{j+1}^{n+1} - r_j^{n+1}$$

where a is the local sound speed and

$$b = 8(C_0^2 + C_{\mathrm{L}}) \Delta r^{n+1} \left(\frac{\dot{V}}{V}\right)^{n+\frac{1}{2}};$$

$$b = 0 \text{ if } \frac{\dot{V}}{V} \geq 0.$$

If $\Delta t^{n+\frac{3}{2}} > (1.1)\Delta t^{n+\frac{1}{2}}$, use $\Delta t^{n+\frac{3}{2}} = (1.1)\Delta t^{n+\frac{1}{2}}$

$$\Delta t^{n+1} = \frac{1}{2}(\Delta t^{n+\frac{3}{2}} + \Delta t^{n+\frac{1}{2}}).$$

B.3 Boundary Conditions

At an outside regional boundary J (Fig. B.1)

$$\phi_J^n = \frac{1}{2} \rho_{0_{J-\frac{1}{2}}} \left(\frac{r_J^n - r_{J-1}^n}{V_{J-\frac{1}{2}}^n}\right)$$

$$\beta_J^n = \left[\frac{(\Sigma_r)_{J-\frac{1}{2}}^n - (\Sigma_\theta)_{J-\frac{1}{2}}^n}{\frac{1}{2}(r_J^n + r_{J-1}^n)}\right] \left(\frac{V_n}{\rho_0}\right)_{J-\frac{1}{2}}.$$

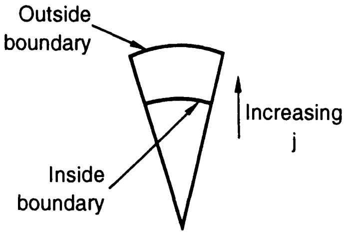

Fig. B.1. Grid boundary scheme

At an inside regional boundary J

$$\phi_J^n = \frac{1}{2}\rho_{0_{J+\frac{1}{2}}}\left(\frac{r_{J+1}^n - r_J^n}{V_{J+\frac{1}{2}}^n}\right)$$

$$\beta_J^n = \left[\frac{(\Sigma_r)_{J+\frac{1}{2}}^n - (\Sigma_\theta)_{J+\frac{1}{2}}^n}{\frac{1}{2}(r_J^n + r_{J+1}^n)}\right]\left(\frac{V^n}{\rho_0}\right)_{J+\frac{1}{2}} .$$

For a free surface at $j = J$, the stresses are set to zero at $J + \frac{1}{2}$ for an outside free surface or at $J - \frac{1}{2}$ for an inside free surface.

B.4 Opening and Closing Voids

Many calculations require a routine that will permit a material to break or spall. An additional requirement is a routine that will allow two materials originally separated to join during the course of a calculation. Details of these routines are given below.

(a) Opening of a void

Let

$$P_j^n = \frac{1}{2}(P_{j+\frac{1}{2}}^n + P_{j-\frac{1}{2}}^n)$$

$$V_j^n = \frac{1}{2}(V_{j+\frac{1}{2}}^n + V_{j-\frac{1}{2}}^n).$$

If $P_j^{n+1} < P_S$ and $V_j^{n+1} > V_S$ where P_S, V_S are material constants, then introduce a new interface at j with the label V (Fig. B.2), with

$$r_V^{n+1} = r_j^{n+1}$$

$$U_V^{n+\frac{1}{2}} = U_j^{n+\frac{1}{2}}.$$

In subsequent time steps, both j and V are treated as free surfaces where V is an outside boundary and j an inside boundary (refer to Sect. B.3). The criteria for the opening of a void given above are meant to serve as an example. In general, the criteria for the calculation of spall involve other parameters, stress gradients for example.

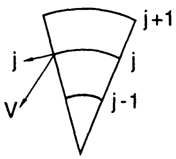

Fig. B.2. Scheme for void opening

(b) Closing of a void

At the beginning of each time step, the new positions of r_V and r_j are calculated first, using a Δt that is 20% larger than the normal Δt for this time step. If $r_V^{n+1} < r_j^{n+1}$, calculate all grid points with the normal Δt. If $r_V^{n+1} \geq r_j^{n+1}$, solve for a new Δt as follows:

$$W = U_j^{n-\frac{1}{2}} - U_V^{n-\frac{1}{2}},$$
$$R = r_j^n - r_V^n,$$
$$A = \left[\frac{(\Sigma_r^n)_{j+\frac{1}{2}}}{\phi_j^n} + \frac{(\Sigma_r)_{j-\frac{1}{2}}^n}{\phi_V^n} + (\beta_V^n + \beta_j^n)(d-1)\right],$$
$$B = 2W + A\Delta t^{n-\frac{1}{2}}.$$

Note: In the calculation of ϕ and β, the subscript V refers to an outside regional boundary and the subscript j to an inside regional boundary, see Sect. B.3. Then

$$A(\Delta t^{n+\frac{1}{2}})^2 + B\Delta t^{n+\frac{1}{2}} + 2R = 0.$$

To solve for $\Delta t^{n+\frac{1}{2}}$:

$$\Delta t_i - \Delta t_{i+1} = \frac{A(\Delta t_i)^2 + B\Delta t_i + 2R}{2A\Delta t_i + B}.$$

Start with $\Delta t_i = 0$ and iterate until $(\Delta t_i - \Delta t_{i+1}) = 0$. Solve equations of motion for one time step with:

$$\Delta t^{n+\frac{1}{2}} = \Delta t_{i+1}$$
$$\Delta t^n = \frac{1}{2}(\Delta t_{i+1} + \Delta t^{n-\frac{1}{2}}).$$

Remove the free surface boundary condition on j and set

$$r_V^{n+1} = r_j^{n+1}$$
$$U_j^{n+\frac{1}{2}} = \frac{m_{j+\frac{1}{2}}\,{}^*U_j^{n+\frac{1}{2}} + m_{j-\frac{1}{2}}U_V^{n+\frac{1}{2}}}{m_{j+\frac{1}{2}} + m_{j-\frac{1}{2}}},$$

where ${}^*U_j^{n+\frac{1}{2}}$ is the velocity of interface j when the void closed.

Note: no attempt has been made to conserve energy after setting the velocity U_j to the value required to conserve momentum.