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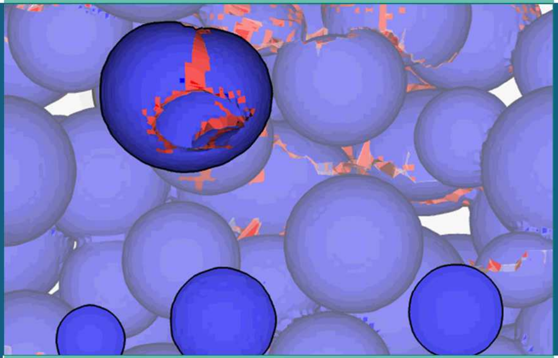
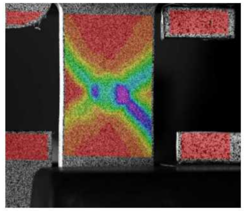
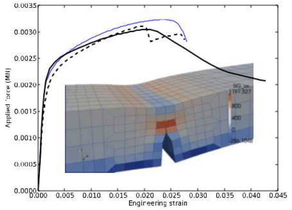
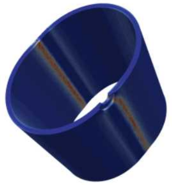


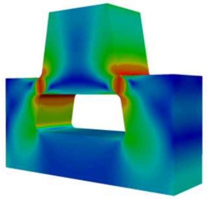
ATA/1558 Interchange

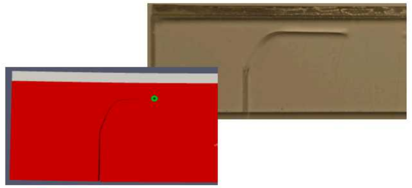
EOS for Shock











Presenter: David Kittell

[DRAFT] Anticipated UUR Content

ATA Site Visit

December 11, 2019

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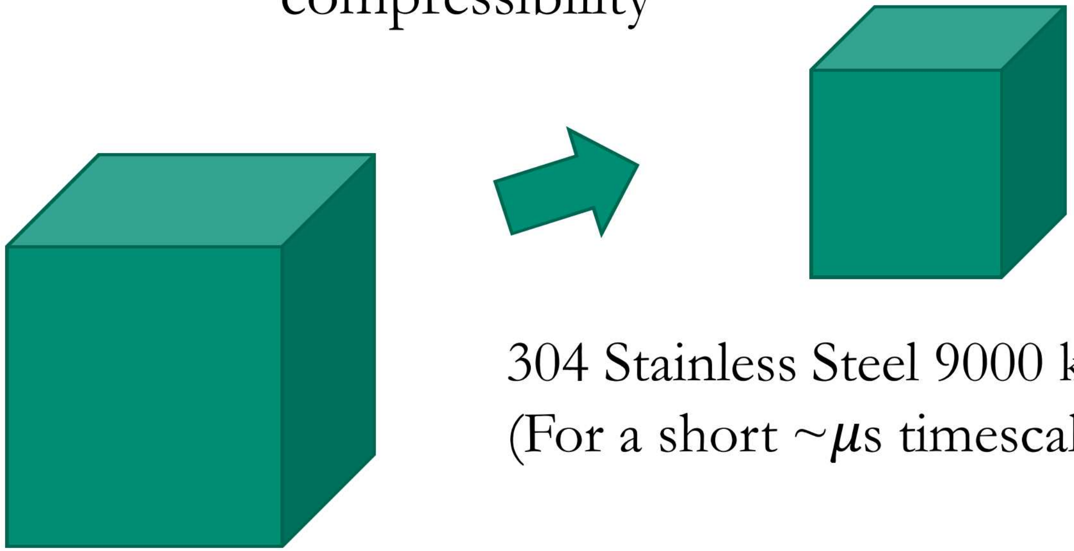
Extreme Material Behavior and Equation of State (EOS)

Problems that require the use of an EOS often coincide with and require simulation tools to handle the following

- Multidimensional domains (2D & 3D)
- Multiple materials in contact with each other
- Large deformations (not finite strains)
- **Shock waves**
- High strain rates (e.g., > 1e5-1e7 s^{-1})
- Elastic-plastic behavior
- Thermal softening
- High explosive detonation
- Fracture (spall, especially)

Think of EOS as stress due to volumetric compressibility



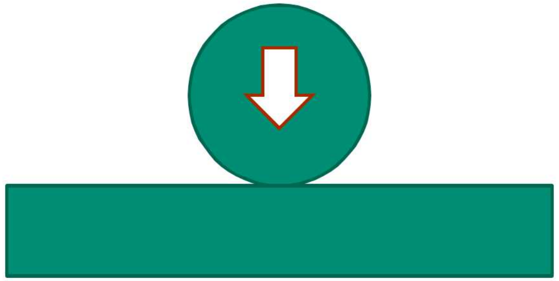
304 Stainless Steel 9000 kg/m^3
(For a short ~μs timescale)

304 Stainless Steel 7580 kg/m^3

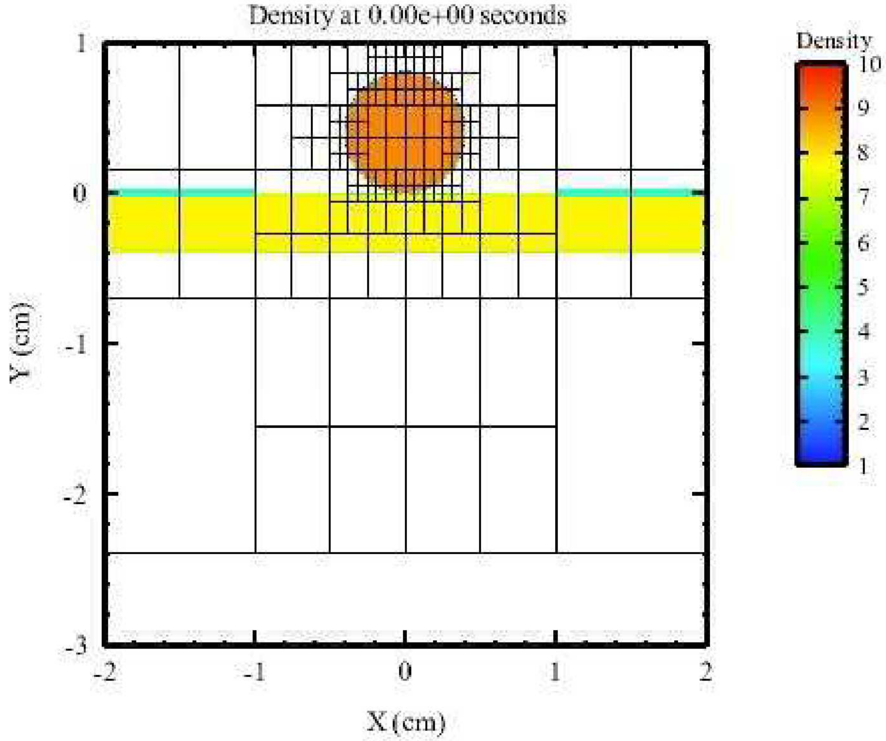
Demonstrative Example - copper penetrating a steel plate

OFHC Copper Sphere Projectile
- 4 mm radius
- Initial velocity 4.52 km/s
- Adaptive mesh refinement

That's Mach 13 !!!
(= 4520 / 344)

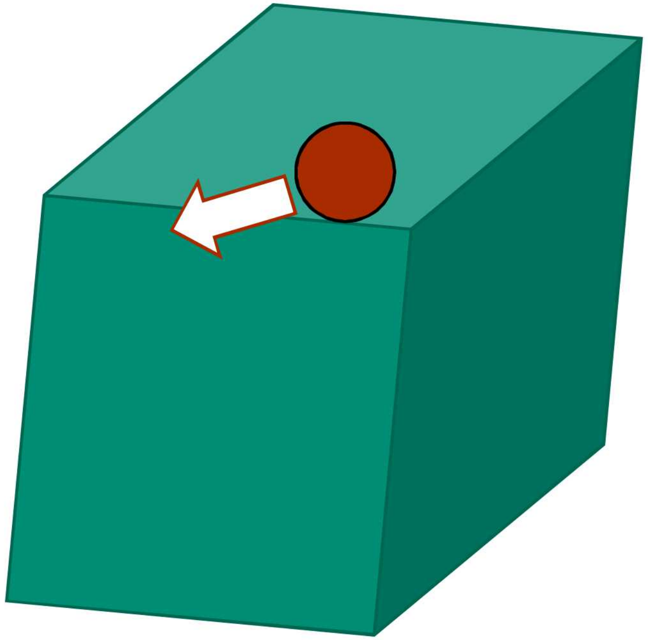


4340 Steel Target Plate
- 4 mm thick



Each Material…
- Has a user-defined **Mie-Grüneisen EOS** with 5 model parameters
- Assumes a constant isotropic yield surface (Elastic-Perfect Plasticity von Mises, EPPVM) when shocked, decreasing to zero with thermal softening
- Has 3 user-defined strength model parameters

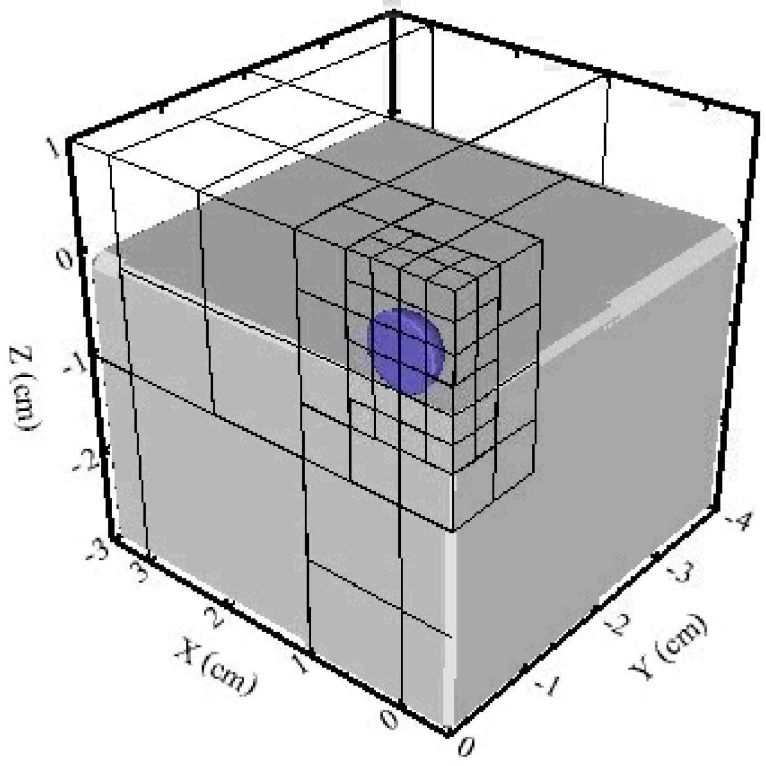
Demonstrative Example - oblique impact



14.95 degrees

-4.83 km/s in X
-1.29 km/s in Y

That's Mach 14.5 !!!

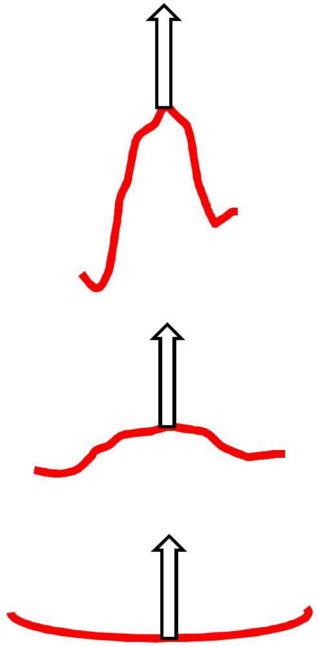


0.00e+00 secs.

Each Material…

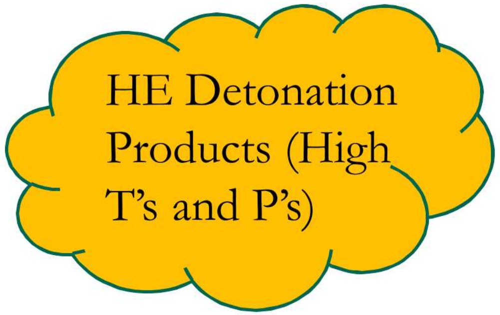
- Is 2024-T4 Aluminum
- Uses a predefined **Mie-Grüneisen EOS** from the "EOS_data" file
- Uses a predefined Steinberg-Guinan-Lund viscoplastic strength model from the "VP_data" file

Demonstrative Example - explosively formed projectile (multi-mat)



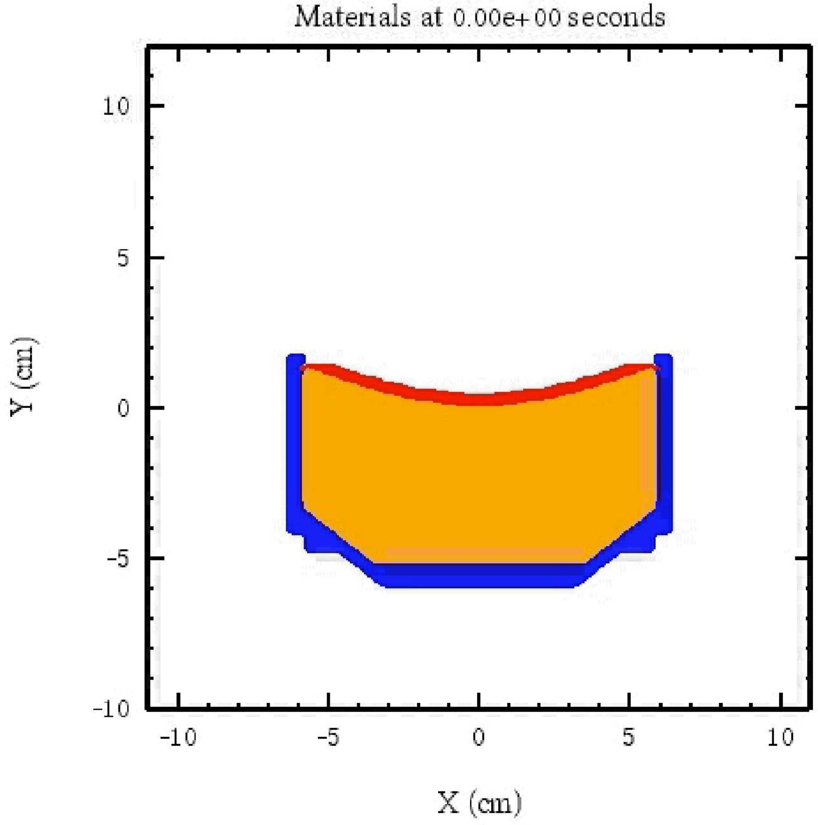
Red = OFHC Copper Lens

- Formed as the gas (i.e. detonation products) accelerates and then deforms the metal, thus launching it into flight
- Similar to how a shape charge works
- Metal stays in the solid phase
- Same **Mie-Grüneisen EOS** from Cu-impact example
- Same EPPVM strength model from Cu-impact example

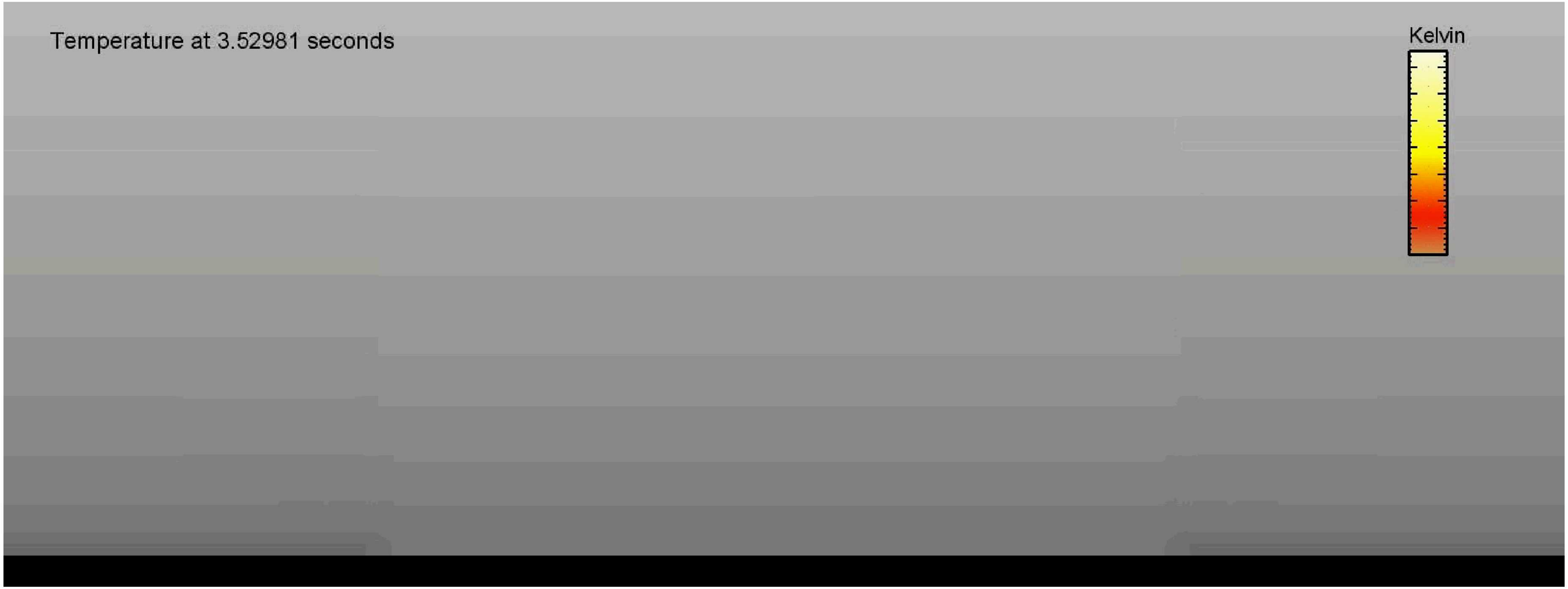


Orange = High Explosive

- Solid model assumes correct density at zero pressure
- Programmed burn converts HE to gas products
- Predefined **Jones-Wilkins-Lee EOS** from "EOS_data" file



Demonstrative Example - meteor strike on Earth (geological material)



Notes

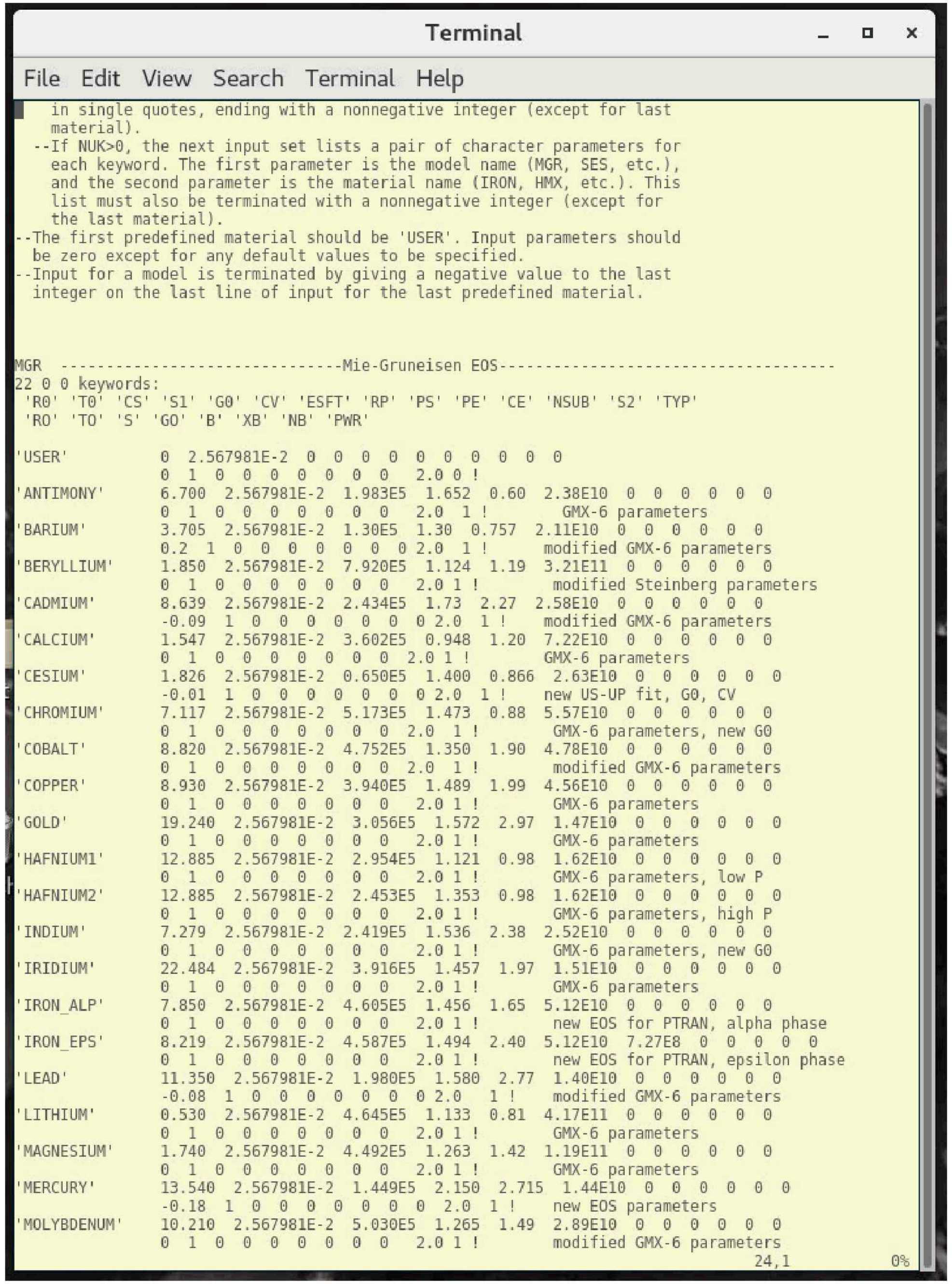
- 20 km/s Earthstrike forms a ~8 km wide crater
- Asteroid and target are predefined **ANEOS models** for quartz (Analytic Equation of State Package)
- Strength model is predefined BDL (Brittle Damage with Localized Thermal Softening, by Dave Crawford)

Some challenges exist for EOS / shock at SNL

- Where can I find an EOS to use?
  - Internal SNL ASCII data files
  - Journal papers
  - Experiments may be needed = $$$
- What is the reliability of "EOS_data" and "VP_data" files?
- Are the EOS parameters sufficient, or do I need the analytic equations as well?
- Can I write my own EOS and if so, how?
- Is the Mie-Grüneisen EOS form standardized? – NO
- Should the EOS be wide ranging (e.g., solid-liquid transition, critical point)?

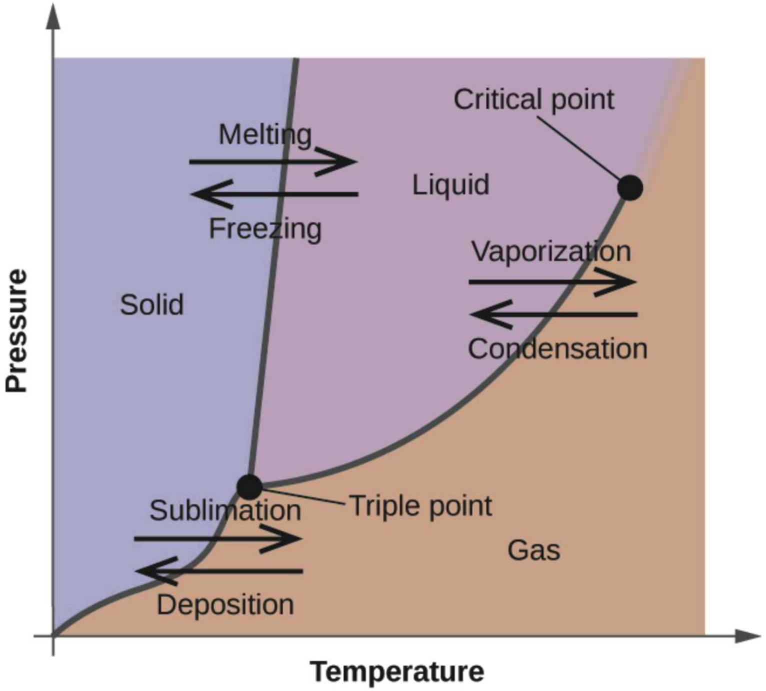
The EOS_data file (SNL-CTH)

- The "go-to" EOS library for users of CTH
- Hundreds of materials to choose from in one single ASCII file
- Little to no documentation remains of the model pedigree – it's only the parameters now
- Uses CTH's material model interface only

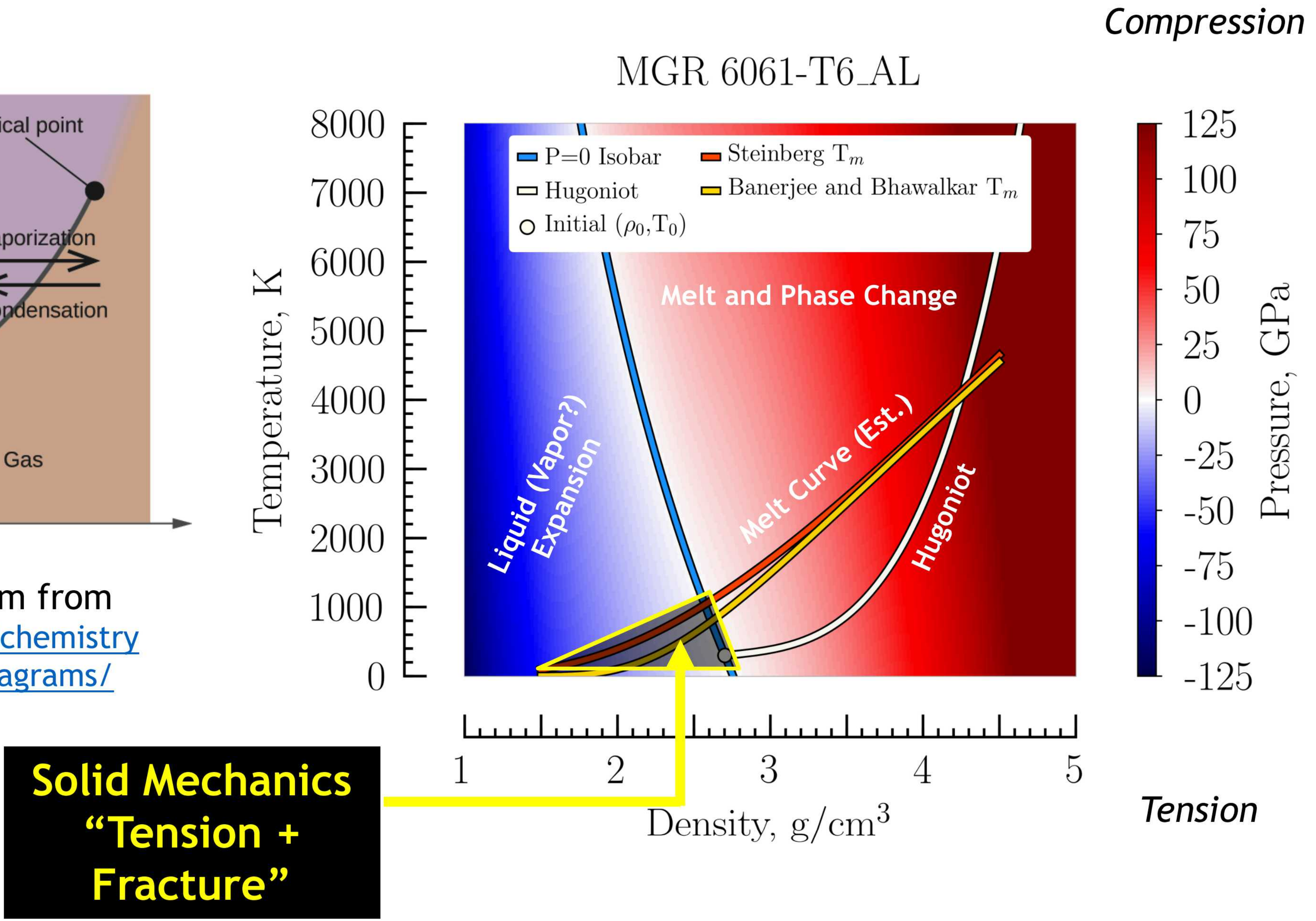



```
    in single quotes, ending with a nonnegative integer (except for last
    material).
  --If NUK>0, the next input set lists a pair of character parameters for
    each keyword. The first parameter is the model name (MGR, SES, etc.),
    and the second parameter is the material name (IRON, HMX, etc.). This
    list must also be terminated with a nonnegative integer (except for
    the last material).
--The first predefined material should be 'USER'. Input parameters should
  be zero except for any default values to be specified.
--Input for a model is terminated by giving a negative value to the last
  integer on the last line of input for the last predefined material.



MGR  ------------------------------Mie-Gruneisen EOS-----------------------------------
22 0 0 keywords:
 'R0' 'T0' 'CS' 'S1' 'G0' 'CV' 'ESFT' 'RP' 'PS' 'PE' 'CE' 'NSUB' 'S2' 'TYP'
 'RO' 'TO' 'S' 'GO' 'B' 'XB' 'NB' 'PWR'

'USER'         0  2.567981E-2  0  0  0  0  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 0 !
'ANTIMONY'     6.700  2.567981E-2  1.983E5  1.652  0.60  2.38E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0  1 !        GMX-6 parameters
'BARIUM'       3.705  2.567981E-2  1.30E5  1.30  0.757  2.11E10  0  0  0  0  0  0
               0.2  1  0  0  0  0  0  0  0 2.0  1 !      modified GMX-6 parameters
'BERYLLIUM'    1.850  2.567981E-2  7.920E5  1.124  1.19  3.21E11  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !       modified Steinberg parameters
'CADMIUM'      8.639  2.567981E-2  2.434E5  1.73  2.27  2.58E10  0  0  0  0  0  0
               -0.09  1  0  0  0  0  0  0  0 2.0  1 !    modified GMX-6 parameters
'CALCIUM'      1.547  2.567981E-2  3.602E5  0.948  1.20  7.22E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0  2.0 1 !        GMX-6 parameters
'CESIUM'       1.826  2.567981E-2  0.650E5  1.400  0.866  2.63E10  0  0  0  0  0  0
               -0.01  1  0  0  0  0  0  0  0 2.0  1 !    new US-UP fit, G0, CV
'CHROMIUM'     7.117  2.567981E-2  5.173E5  1.473  0.88  5.57E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0  2.0  1 !        GMX-6 parameters, new G0
'COBALT'       8.820  2.567981E-2  4.752E5  1.350  1.90  4.78E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0  2.0  1 !        modified GMX-6 parameters
'COPPER'       8.930  2.567981E-2  3.940E5  1.489  1.99  4.56E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters
'GOLD'         19.240  2.567981E-2  3.056E5  1.572  2.97  1.47E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters
'HAFNIUM1'     12.885  2.567981E-2  2.954E5  1.121  0.98  1.62E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters, low P
'HAFNIUM2'     12.885  2.567981E-2  2.453E5  1.353  0.98  1.62E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters, high P
'INDIUM'       7.279  2.567981E-2  2.419E5  1.536  2.38  2.52E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters, new G0
'IRIDIUM'      22.484  2.567981E-2  3.916E5  1.457  1.97  1.51E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters
'IRON_ALP'     7.850  2.567981E-2  4.605E5  1.456  1.65  5.12E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        new EOS for PTRAN, alpha phase
'IRON_EPS'     8.219  2.567981E-2  4.587E5  1.494  2.40  5.12E10  7.27E8  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        new EOS for PTRAN, epsilon phase
'LEAD'         11.350  2.567981E-2  1.980E5  1.580  2.77  1.40E10  0  0  0  0  0  0
               -0.08  1  0  0  0  0  0  0  0 2.0   1 !    modified GMX-6 parameters
'LITHIUM'      0.530  2.567981E-2  4.645E5  1.133  0.81  4.17E11  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters
'MAGNESIUM'    1.740  2.567981E-2  4.492E5  1.263  1.42  1.19E11  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        GMX-6 parameters
'MERCURY'      13.540  2.567981E-2  1.449E5  2.150  2.715  1.44E10  0  0  0  0  0  0
               -0.18  1  0  0  0  0  0  0  0  2.0  1 !   new EOS parameters
'MOLYBDENUM'   10.210  2.567981E-2  5.030E5  1.265  1.49  2.89E10  0  0  0  0  0  0
               0  1  0  0  0  0  0  0  0   2.0 1 !        modified GMX-6 parameters
                                                                    24,1          0%
```

Tabular EOS with Phase Regions



Generic phase diagram from https://opentextbc.ca/chemistry/chapter/10-4-phase-diagrams/



EOS from the Literature

This is my preferred method as an analyst…

HTML ABSTRACT + LINKS

COMPLETE EQUATION OF STATE FOR β-HMX AND IMPLICATIONS FOR INITIATION

Thomas D. Sewell* and Ralph Menikoff*

*Theoretical Division, MS-B214, Los Alamos National Laboratory, Los Alamos, NM 87545

Abstract. A thermodynamically consistent equation of state for β-HMX, the stable ambient polymorph of HMX, is developed that fits isothermal compression data and the temperature dependence of the specific heat computed from molecular dynamics. The equation of state is used to assess hot-spot conditions that would result from hydrodynamic pore collapse in a shock-to-detonation transition. The hot-spot temperature is determined as a function of shock strength by solving two Riemann problems in sequence: first for the velocity and density of the jet formed when the shock overtakes the pore, and second for the stagnation state when the jet impacts the far side of the pore. For a shock pressure below 5 GPa, the stagnation temperature from the jet is below the melt temperature at ambient pressure and hence insufficient for rapid reaction. Consequently, for weak shocks a dissipation mechanism in addition to shock heating is needed to generate hot spots. When the stagnation temperature is sufficiently high for rapid reaction, the shock emanating from the hot spot is computed, assuming a constant volume burn. For initial shocks below 20 GPa, the temperature behind the second shock is below 1000 K and would not propagate a detonation wave.

INTRODUCTION

Mesoscale simulations, which resolve the explosive grains and hot spots within a plastic-bonded explosive (PBX), are being used to better understand the initiation process. These simulations require as input the constitutive properties of the components of the PBX. A thermodynamically consistent equation of state (EOS) for the stable ambient polymorph β-HMX is developed below based on data from quasi-static compression experiments [1, 2] for the mechanical properties and molecular dynamics calculations of the crystal density of states for the thermal properties [3]. The specific heat is a function of temperature. This is particularly important for simulations that resolve hot spots since the chemical reaction rate is very sensitive to temperature.

The equation of state can be used to scope out hot-spot conditions in order to ascertain the dominant physical processes that a mesoscale simulation of initiation must incorporate. Assuming that hot spots are generated on a fast time scale behind a lead shock, their rapid heating will result in reaction that can be approximated by a constant-volume burn. The burn results in a high pressure that generates a secondary shock wave emanating from the hot spot. The pressure of the constant-volume burn and temperature of the second shock depend on the strength of the lead shock wave. These quantities are determined by the equation of state.

FREE ENERGY

A thermodynamically consistent equation of state can be defined by the Helmholtz free energy. We assume that the free energy has the form of a generalized Hayes EOS [4]

$$F(V,T) = -\int_{V_0}^{V} dV\, P_0(V) - \theta(V)\int_0^{T/\theta} \frac{d\tilde{T}}{\tilde{T}}\left(\frac{T}{\theta(V)} - \tilde{T}\right)\widehat{C}_V(\tilde{T})\,. \quad (1)$$

CP706, *Shock Compression of Condensed Matter - 2003*, edited by M. D. Furnish, Y. M. Gupta, and J. W. Forbes

157

Paper, e.g. Sewell and Menikoff, *AIP Conf. Proc.* **706** (2004)

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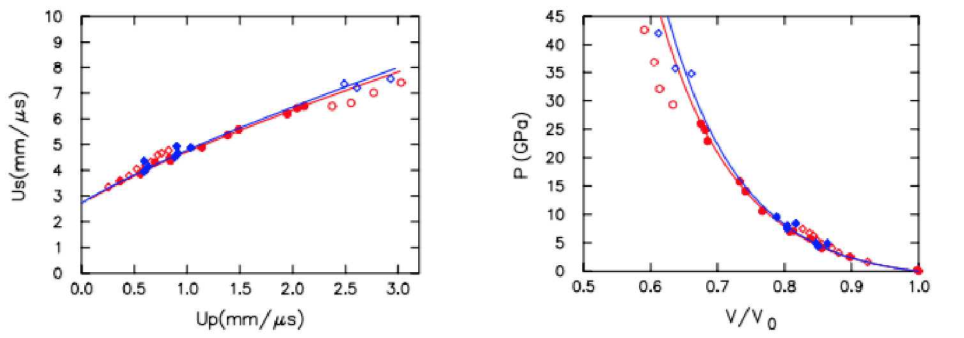

FIGURE 1. Mechanical response of HMX. Red and blue curves are isotherm and Hugoniot loci, respectively, from EOS model. Blue symbols are Hugoniot data [6, pp. 595–596] and red symbols are isothermal data [1, 2]. Open circles are above the pressure induced phase transition reported in [1] and are not used in the calibration of the EOS model.

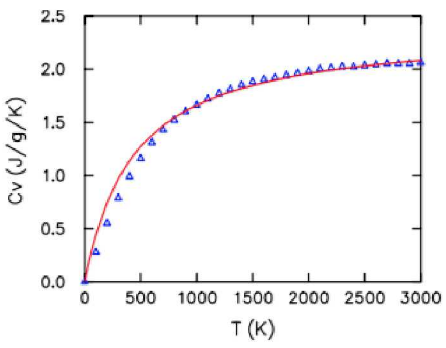

FIGURE 2. Specific heat. Symbols are from molecular dynamics calculations [3, p. 96] and red curve is fit, Eq. (3), used for the EOS model.

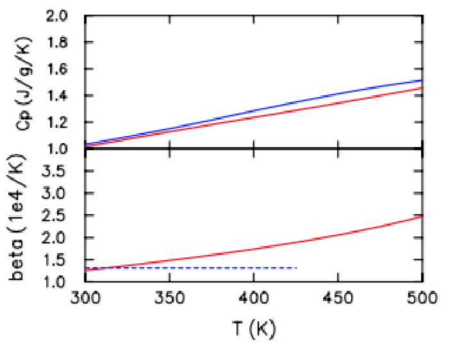

FIGURE 3. Specific heat [7] and the volumetric coefficient of thermal expansion [8] at atmospheric pressure. Blue curve is experimental data and red curve is model EOS.

A few dozen EOS data points (if lucky)

+

Implicit,
Non-linear analytic Eqns.

A Birch-Murnaghan form is used for the cold curve

$$P_0(V) = \tfrac{3}{2}K_0\left[(V/V_0)^{-7/3} - (V/V_0)^{-5/3}\right] \times \left(1 + \tfrac{3}{4}\left[K_0' - 4\right]\left[(V/V_0)^{-2/3} - 1\right]\right). \quad (2)$$

The specific heat is assumed to have the form

$$\widehat{C}_V(\tilde{T}) = \frac{\tilde{T}^3}{c_0 + c_1\tilde{T} + c_2\tilde{T}^2 + c_3\tilde{T}^3}\,, \quad (3)$$

where $\tilde{T} = T/\theta(V)$ is a scaled temperature. This form has the asymptotically correct limits: $\widehat{C}_V(T) \propto T^3$ for small T and $\widehat{C}_V(T) \to$ const for large T. The Debye temperature is assumed to have the form

$$\theta(V) = \theta_0\left(\frac{V_0}{V}\right)^a \exp\left[b(V_0 - V)/V\right]. \quad (4)$$

Consequently, the Grüneisen coefficient is given by

$$\Gamma(V) = -\frac{V}{\theta}\frac{d\theta}{dV} = a + b\frac{V}{V_0}\,. \quad (5)$$

The pressure and internal energy are determined by the standard thermodynamic relations $P = -\partial_V F$ and $e = F - T\partial_T F$.

+

Parameter Values

TABLE 1. Model EOS parameters for β-HMX.

ρ_0	1.9	g/cm^3
K_0	16.5	GPa
K_0'	8.7	—
a	1.1	—
b	-0.2	—
c_0	5.265×10^{-1}	K·kg/MJ
c_1	3.073×10^{2}	K·kg/MJ
c_2	1.831×10^{5}	K·kg/MJ
c_3	4.194×10^{2}	K·kg/MJ

Worked Example for the Mie-Grüneisen EOS

The density of 6061-T6 aluminum is increased from 2.703 g/cm^3 to 2.9 g/cm^3 and the temperature is increased from 298 K to 350 K, what is the pressure?

Hugoniot Parameters

$\rho_0 = 2.703$ g/cm^3

$C_S = 5.22$ km/s

$S_1 = 1.37$

Grüneisen Parameter

$\Gamma_0 = 1.97$

Specific Heat

$C_V = 922$ J/kg*K

Pressure EOS

$$P(\rho, T) = \overset{?}{\boxed{P_H}}(\rho) + \rho_0 \Gamma_0 C_V \left[T - \overset{?}{\boxed{T_H}}(\rho)\right]$$

Hugoniot Shock-Particle Velocity Curve

$$U_S = C_S + S_1 u_p$$

…Doesn't look too bad, right?

Worked Example for the Mie-Grüneisen EOS

The equation will change for a different Us-up and the integral requires numerical integration techniques. The answer is ~6.1 Gigapascals or 61 kilobars

$$P(\rho,T) = \frac{\rho_0 {C_S}^2 \left(1-\frac{\rho_0}{\rho}\right)\left[1-\frac{\Gamma_0}{2}\left(1-\frac{\rho_0}{\rho}\right)\right]}{\left[1-S_1\left(1-\frac{\rho_0}{\rho}\right)\right]^2} + \rho_0\Gamma_0 C_V T$$

?

$$-\rho_0\Gamma_0 C_V\, e^{\Gamma_0\mu}\left[T_0 + C_V^{-1}\boxed{\int_0^{\mu} e^{-\Gamma_0\mu}\mu^2 U_S \frac{dU_S}{d\mu} d\mu}\right]$$

where,

$$\mu = 1 - \frac{\rho_0}{\rho}$$

Few analytic EOS are explicit, partly because the EOS data that is generated is not a direct measurement of the pressure or temperature. To arrive at this kind of explicit answer, one has to use ***thermodynamic identities***. For these reasons, each EOS is usually implemented as its own model.