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How to Plan and Analyze an Isentropic Compression Experiment (ICE)

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Abstract

This report is a how-to manual for planning and analyzing an Isentropic Compression Experiment (ICE). Here the specific task is to find the unreacted Hugoniot of high explosive (HE) using Sandia National Laboratories Z-machine facility. However, many of the principles are broadly applicable to general ICE problems.

Contents

1. Introduction

This report will discuss only the method employed at Sandia National Laboratory's Z-machine for executing ICE experiments. There, the compression ramp wave needed for ICE is generated by the Lorentz force or magnetic pressure from an enormous electric current interacting with itself (Fig. 1). The ramp wave compresses a sample along a path which generally lies somewhere between the isentrope and the single shock Hugoniot in terms of how much specific entropy is generated in the sample. For a fluid in which the energy dissipation is caused by viscosity and heat conduction it can be shown [1] that the loading path is much closer to the isentrope than to the shock Hugoniot whenever the pressure gradients are small compared to those that would be found in a steady shock in the same material to the same final pressure (i.e. when the ramp duration is long compared to the shock rise time, final pressure being the same). When the sample strength can be neglected it may be that nearly isentropic compression is achieved.

However, this conclusion is very case-by-case dependent and for a strong material taken just beyond its elastic limit there may well be almost no difference between the specific entropy generated by a ramp wave and a shock wave. That being said, we recognize that the ramp wave at least holds the possibility in some cases of nearly isentropic compression and call these Isentropic Compression Experiments according to established convention. Excellent general references describing the ICE technique at Z-pinch are found in the literature [2,3].

ICE is particularly useful for measuring the unreacted Hugoniot of an explosive. In the ZND theory of detonation, the unreacted Hugoniot establishes the location of the von Neumann point, i.e. the pressure spike at the head of the shock wave that propagates the detonation [4]. Shock compression techniques can only probe the unreacted Hugoniot of HE to very low pressures, because of the tendency of all HEs to undergo a shock-to-detonation transition, some at quite low shock strengths.

The ICE technique can take HE to significantly higher pressures without reaction than conventional shock compression techniques as can be seen experimentally in Fig. 3 for LX-04 [5]. In many explosives this is probably due to a heat-conduction effect resulting in the suppression of hot-spot temperature by the relatively long void collapse times of the ramp wave rather than to a genuine isentrope versus shock adiabat temperature effect. The summary of all LLNL HE ICE experiments at Z-machine up through June 26, 2004 is given in Appendix C.

2. Sample and strategy

Ideally what you would like to do is get the unreacted isentrope of the explosive sample up to as high a pressure as possible without any shock wave formation within the ramp wave. You would also like to be able to verify that reaction did not occur. In theory it takes only one good sample velocity history and one good reference velocity history to infer the unreacted Hugoniot. My own preference is to have redundant samples. I will discuss standard panels for our shots that will readily accommodate eight samples and four reference surfaces. A reference surface gives a velocity history in which all Hugoniot data is already known. It is used to deduce the pressure drive that is needed to find the unknown EOS of the sample.

A very common reference surface is a LiF (100) window directly on the panel. Both LiF (100) and the panel material Al 6061-T6 have well known Hugoniot data. The values for these two materials are taken out of D.J. Steinberg's "Equation of State and Strength Properties of Selected Materials" [6]. The NaCl (100) data were taken from the LASL Hugoniot reference [19] and the data below 23 GPa (below any shock-induced phase transition in NaCl) refit to a linear U_S ,u_P. Γ_0 was computed from common thermodynamic data.

Table 1

material	ρ_0(g/cc)	C_0 (cm/us)	S_1	Γ_0	b

NaCl (100)	2.163	0.356	1.28	1.51	Assumed 0.
Al 6061-T6	2.703	0.524	1.40	1.97	0.48
LiF (100)	2.638	0.515	1.35	1.69	0.34

S_1, Γ_0, and b are dimensionless. "b" is a compression-dependent correction on Γ.

$$\text{Eq. 1:} \quad \Gamma = \frac{\Gamma_0 + b\mu}{1 + \mu}$$

$$\text{Eq. 2:} \quad \mu \equiv \frac{\rho}{\rho_0} - 1$$

b = 0 is the same as the commonly made "constant gamma / volume" assumption. I recommend using a LiF (100) window directly on the (aluminum) panel as the reference no matter what windows you may wish to use on your samples. The reason is that the LiF is an excellent shock impedance match to the aluminum and this makes it possible to infer the pressure or current drive in a very simple way without having to resort to backwards integration techniques.

3. Choosing a panel

For an explosive at ambient temperature there are several good panel designs already available. For lower pressures (peak around 200 kbar) I would stick with the panel and hardware design of shot 1067 (LLNL HE ICE, LX-04, shot date 3/19/03; the "low pressure hardware"). The 1067 panels with samples and windows mounted are shown in Fig. 2. The design team at Sandia (Terry Gilliland: design coordinator: (505) 845-7365) has these experiments and the drawings and documents archived. For higher pressures I would recommend the panel design used in shot 1221 (LLNL HE ICE, LX-17, shot date 12/9/03; the "high pressure hardware").

If you choose one of these pre-existing panel designs, then respecify the floor thickness. I would recommend a 600 μm floor for all sample and reference locations unless there is a compelling specific need for doing otherwise.

For a heated shot, a basis to start with would be the panel design that Jean-Paul Davis and D.E. Hare did together in shot 1265 (LLNL HE heated LX-04 shot date 3/16/04). This arrangement took eight samples to approximately 150 ^{0}C but temperature control wasn't as good as had been hoped for. Hopefully there will be even better designs available in time for the next heated shot.

LLNL HE ICE effort has not yet (as of June 2004) attempted any sub-ambient temperature shots.

4. Samples

The samples are disks, 6.0 mm in diameter by various thicknesses typically between 200 and 800 μm thick. These samples are typically lapped to final thickness starting from thicker disks (1 or 2 mm) at the 6.0 mm diameter. The samples are then carefully glued to the correct panel floor locations as per the kickoff plan with the appropriate epoxy and after that the windows are glued to the samples in like fashion. Often, the slot in which the windows and samples lie is potted with additional epoxy. This seems to be a good idea for ambient shots but we have found that this doesn't work well for heated shots. I wouldn't do this for cooled shots either. The stress generated by differential thermal expansion of the various bonds and materials is likely to damage samples and windows in both cases. Spring-loaded mechanical contacting of window to sample to panel may be the way to go, perhaps with some appropriate grease or oil to insure intimate gapless contact between panel, sample, and window.

It is important to keep the glue bonds as thin as possible to preserve the accuracy of the measurements. You want to be measuring the EOS of sample, not glue.

The minimum necessary accurate measurements needed for the simulation are the thickness of the floor and the thickness of the sample at each sample or reference location. It is even better, if time allows, to also measure window thickness and the thickness of the glued (floor + sample + window). That way you have two independent measurements of the sample thickness: the direct measurement, and the measurement inferred from (total thickness – window – floor). If the glue bonds are thin the two measurements should agree to within a few μm. This is very reassuring.

It is important to stick fairly closely to the sample thicknesses you have called out at the kick off because the SNL VISAR probe assembly staff will offset the probes an estimated 250 μm from the window surface based on your estimated sample thicknesses given in your shot plan. So if you do have to change sample thickness for some reason, let the probe assembly people know as soon as possible. They don't like to be surprised two weeks from shot date.

5. Windows

The windows are approximately 6.00 mm diameter by 3.0 mm thick. I have used LiF (100) or NaCl (100). There are other possibilities: sapphire and PMMA are used in some applications. The windows may be supplied by SNL (in the order put in at kickoff time along with the panel and shot hardware) or purchased from an independent vendor. They are typically coated with 200 nm of silver on one side and an anti-reflection coating (AR coating) on the other side. It is possible to use windows without AR coatings but I recommend always using them: It makes your measurement more robust against possible probe positioning errors and it can help protect the fragile NaCl surface against water vapor in the air. The silvered coating always goes up against the sample (or floor in the reference case).

The velocity-per-fringe (VPF) information for NaCl and LiF is required by the fringe-to-velocity conversion program. I have taken this from Wackerle and Stacey [7].

(no window VPF)/1.29 = (NaCl VPF)

(no window VPF)/1.28 = (LiF VPF)

(NaCl VPF) = (LiF VPF)*1.28/1.29

This data applies as follows: When the VISAR operators set up the VISAR for your experiment they will report their VPF settings either as “free surface” or “LiF window”. For example, if they reported in the “LiF window” format and you in fact did use a LiF window at that location, then you will use their VPF directly without correction. On the other hand, if instead you used a NaCl window at that location then you would have to multiply their stated “LiF” VPF value by 1.28/1.29 = 0.992 to arrive at the correct VPF appropriate for a NaCl window at that particular VISAR setting.

6. Designing the current pulse

Jean-Paul Davis is the present SNL contact for current pulse design (505) 284-3892. What he will require is the current history you will want from the Z-machine to get the drive that you need. David Reisman here at LLNL has designed current pulses for many ICE experiments. Alternatively you may want to design the pulse yourself. To do that you will have to have some kind of educated guess of what the unreacted Hugoniot will be for your HE sample. Let’s design a pulse for LX-16.

LX-16 is PETN based. There is no ICE data on it so far. We decide to keep the initial shot peak pressure low, say 120 kbar peak in the LX-16. We would like to try and get data out of 600 μm thick samples without any shock-up. If you can find unreacted Hugoniot data in an HE reference [8], use it. We will use:

$$U_S = 0.23 \text{ cm/us} + 2.3*u_P$$

for the approximate Hugoniot and take the density as 1.7 g / cc

We start by working backwards from what we want. Since we don’t want any shock formation at 600 μm we imagine a fully developed shock wave to exist at 800 μm in the LX-16. We propagate the velocity history of the fully developed shock wave at 800 μm backwards in Lagrange coordinate space to 0 μm. We will make use of an important expedient design tool, namely that the Lagrange sound speed C_L is approximately related to the shock speed U_S by:

Eq. 3: $$C_L \approx C_0 + 2S_1u_P$$

whenever

Eq. 4: $$U_S = C_0 + S_1u_P$$

C_0 and S_1 are the usual Hugoniot coefficients. The basis for this approximation is given in Appendix D. Thus the Lagrange sound speed for LX-16 will be approximately:

$$C_L = 0.23 \text{ cm/us} + 4.6 * u_P$$

What value of u_P will give 120 kbar? About 1320 m/s. It happens that the usual steady shock formula;

Eq. 5: $$P = \rho_0 U_S u_P$$

will give the correct answer (within this approximation) for converting between P and u_P even though we will be using it in an unsteady ramp wave instead of a steady shock wave (Appendix D). Having established peak u_P we now use:

Eq. 6: $$\Delta t = \frac{\Delta x_0}{C_L}$$

to go from the velocity history at x = 800 μm to x = 0 μm. For example, for u_P = 1320 m/s then C_L = 8370 m/s. Δx_0 is set to –800 um. This gives Δt = –95.6 ns. So the peak of the velocity arrived at the x = 0 μm interface at –95.6 ns and at x = 800 μm at 0 ns. Now apply this formula not just to the peak u_P but to the entire u_P range from 0 – 1320 m/s. Repeated application for u_P in 100 m/s increments up to 1320 m/s gives Fig. 4.

What we have done so far is to generate the velocity history at the panel / sample interface (0 μm) that would shock up abruptly at 800 μm. This was done using just 15 velocity points and EXCEL (Microsoft). 100 points would have been better.

We still have to go backwards through the 600 μm of Al of the panel floor to get to the drive. It would take a backwards integration code, like that described by D.B. Hayes [9] to do that accurately. This is because the significant multiple reflections at the aluminum / LX-16 interface and aluminum / vacuum interface can't be easily treated by the Eq. 6 formula. We will have to do it approximately.

Convert the LX-16 velocity history to an LX-16 pressure history using Eqs. 4 and 5 and the assumed LX-16 EOS data. Convert the pressure history to a current history using the accurate semi-empirical formula:

Eq. 7: $$p = \frac{\mu_0 i^2}{32 a^2}$$

For a square anode-cathode geometry "a" is (0.92 mm + width of cathode stem) [10]. So for the low pressure hardware a = 20.92 mm (20.92E-3 m) and for the high pressure hardware a = 11.92 mm (11.92E-3 m). Eq. 7 is an MKS formula, use meters, amps, etc. The current history (caution, the current must be further transformed into a psuedocurrent before use in Trac-II. See Appendix A) should be put back in the Trac- II code and the problem simulated. The pressure can be scaled up or down to tweak in the peak pressure in the HE. The time base can be expanded if necessary to extend the run-to-shock-formation distance. How to run the Trac- II hydrocode is in Appendix A.

When you are satisfied with the current pulse, send it to Jean-Paul Davis. He will come back with current pulses that they believe they can achieve that are close to what you want. Simulate the pulses he comes back with and decide on one. This latter interaction will usually happen after the kickoff.

7. The kickoff

The kickoff occurs 14 weeks out from the scheduled shot date. It has thus far been on a Tuesday at 9:00 in the trailer there next to Z-machine at SNL. At the kickoff you will discuss 1) what you are trying to do 2) the panels you need. 3) the windows and special hardware you will need. 4) the sample layout with thicknesses 5) the diagnostics you will want (standard VISAR, line VISAR, how many VISAR probes you want on each sample).

8. At SNL during the shot

I would be at SNL a full day before the scheduled shot. At SNL, there may be some last minute pulse design modifications. You will decide how to assign the VISAR channels to the samples, witness the shot, and collect the data. Keep in close contact with your Sandia contact as the shot date approaches. Shots can slip or advance a day or two and this will impact your travel plans.

You will get together with your Sandia collaborator or the VISAR operator to assign the VISAR probes to the various sample and reference locations. In an ideal world each location would get two probes of different VPF (this provides a definitive assignment of velocity jump in the case of shock formation) However, in practice there never seem to be enough probes of the right VPF to go around. Some information to consider:

1) The thickest samples are the most likely to shock up. They are most in need of verification by two independent VPFs.
2) The reference locations are the least likely to shock up, and therefore least in need of independent VPF velocity verification. In good circumstances the references of the four panels of the assembly are likely (but not guaranteed!) to be in close agreement. However, remember that the accuracy of the data of both samples on a panel depends directly on the accuracy of the reference on the same panel (i.e. you can’t really afford to get no data at all at any reference location). Not all VISAR channels are created equal. Don’t assign a single marginal VISAR channel to a reference location. Ask the VISAR operator which channels are marginal in performance.

9. After the shot: Converting the VISAR fringe records to velocity histories.

This can be tedious and involve a lot of effort. Up to 22 VISAR signals need to be correctly syncronized in time. I have done this myself a few times and it takes me a couple or three days to do it, per experiment. Mike Furnish at SNL is an expert at this and might be able to help you on this. The other option is to do it yourself. This is covered in Appendix B.

10. Analyzing the velocity histories to obtain the unreacted Hugoniot using the Trac- II hydrocode

You will need at least one reference velocity history, and at least one sample velocity history. It is very helpful to also have the experimental current history, but in theory you can do without it. It is best if the reference history is from the same panel as the sample you wish to analyze.

In theory, you could conduct an EOS analysis of the sample without a reference velocity history if you had the experimental current history and the sample velocity history (correctly syncronized timewise). In practice this is inferior to having a good reference and is to be avoided except as an act of desperation (i.e. the reference data is lacking).

If you don't have the current history, you can backwards integrate [9] the reference history to find the drive. If you don't have a backwards integration code you can propagate the velocity history backwards in space using the Lagrange sound speed trick (Eq. 6). This works best if the reference is a LiF (100) on aluminum because of the excellent impedance match of the two. However, even in this most favorable of cases it is more accurate and therefore better if you have access to a backwards integration code.

After you propagated the reference backwards to obtain the drive it is important to then run the resulting drive forwards, simulating the reference with Trac- II. If the backwards – forwards simulation result matches the experimental reference well then you know you have obtained the correct drive. If the backward-forward velocity does not agree perfectly with the experimental record you started with then tweak the drive until good agreement is obtained. One simple tweek is to multiply the current (or the square of the current, which is pressure) by a constant.

If you do have the experimental current history then start with it to run the reference geometry with Trac- II. If the peak pressure in the window is not correct, scale the current until it is. At that point the simulation reference velocity history should be very similar to the experimental velocity history. You will probably have change the time by a constant to force the current start to turn on at t = 0 in the simulation (the code likes the current to turn on at t = 0). Then this same constant time offset should also show up between the experimental reference and the simulated reference.

When you have the current really tweaked-in well, simulating the reference geometry should accurately reproduce the experimental reference velocity history. Because of this, the drive is considered to be known and you can now run it forward in the sample geometry. The simulated sample velocity history now will not reproduce the experimental velocity history unless you have the correct sample Hugoniot.

The following is a routine for fitting a simple the experimental sample data to a simple linear Hugoniot (i.e. $S_2 = S_3 = 0$ assumed: Appendix A, p17). You start by already knowing the density of your samples. You can also readily compute a Gruneisen gamma Γ_0 from thermodynamic data [11]. I simply set b = 0 (the constant gamma / volume assumption). ρ_0, Γ_0, and b = 0 are considered known and I do not iterate them during the procedure. Only C_0 and S_1 are iterated.

Let's say you focus on three specific values of u_P in the sample velocity history. Let's say your sample velocity peaks at 0.20 cm/μs, so you pick 0.02, 0.10, and 0.18 cm/μs to focus on. (Two points is the absolute minimum. More is always better but increases the level of effort if you do the fitting procedure manually. Four or five velocity points are manageable). Based on your simulation of the reference and the experimental velocity history you know the times at which 0.02, 0.10, and 0.18 should show up in the sample simulation when C_0 and S_1 are correct.

Form a quantity which is the sum of the square of the difference between the times when 0.02, 0.10, and 0.18 were reached in the sample simulation versus when they were predicted to be reached based on the experimental sample history. This "sum of squares" is always greater than or equal to zero and is a goodness-of-fit parameter. It will go to zero for perfect agreement.

1) Choose $S_1 = 2$

2) Increment C_0 at fixed S_1 and run Trac- II. Do this for a series of C_0 values (for example 0.15, 0.20, 0.25, 0.30, 0.35 cm/μs) and plot the sum of squares versus C_0. Choose the value of C_0 that minimizes the sum of squares.

3) Now choose a series of C_0, S_1 pairs such that $C_0 + 2*S_1*(u_{MAX}/2)$ is a constant. This constant quantity is approximately the Lagrange sound speed at half the maximum particle velocity. Plot the sum of squares versus S_1 and choose the C_0, S_1 pair that minimizes the sum of squares.

4) With this new value of S_1 from step 3 held fixed, go back to step 2.

Repeat the process until satisfactory convergence on the minimum sum of squares is reached.

There may exist routines that will run and increment a code in this fashion automatically.

In theory you certainly could do a higher order U_S vs. u_P fit in which S_2 (or S_2 and S_3) were not assumed zero. You would need a cooorespondingly larger number of velocity points to fit. Unfortunately I don't know, and therefore can't give guidance on, what would be a good search algorithm for the coefficients in these higher order cases.

However, at least in the case of LX-04, a non-linear fit of the most current ICE data would definitely represent the data more accurately than a linear fit. It is worth expending some thought on how one would go about this.

11. Analyzing the velocity histories using the Lagrange analysis

For the most accurate analysis I would recommend not using this method as first choice. The hydrocode method is more general in its applicability and it gives the Hugoniot directly (at least to the extent to which the Gruneisen gamma EOS model is accurate) and has the ability to accurately handle partial shock up of the data (an undesirable but common enough occurrence in real data). The Lagrange analysis method gives the isentrope directly, which then must be converted into a Hugoniot. The Hugoniot-to-isentrope conversion is well covered in the shock compression and detonation science tutorial of J.W. Forbes [12] and isentrope-to-Hugoniot conversion is a straightforward reversal of the process. The Lagrange analysis method in the elementary form as I employed it is strictly speaking not applicable unless the flow is both isentropic (no shock formation) and simple (window is well impedance matched to sample) [13]. The hydrocode method doesn't have these limitations. I will not discuss the Lagrange Analysis method here but there are two good references both to the theory of the method [14,15] and one applying the analysis to infer the unreacted Hugoniot of LX-04 [5].

Although not first choice, this method has been used in the past and gives an interesting alternative way of looking at and thinking about the ICE data. If you would like to try the Lagrange Analysis, first look at the data analysis in [5], then read [14]. Reference [15] is advanced reading.

12. Acknowledgements

Many, many people have contributed to the LLNL HE ICE effort. Jim Asay, Marina Bastea, Jean-Paul Davis, Allen Elsholz, Jerry Forbes, Mike Furnish, Frank Garcia, Leroy Green, Dennis Hayes, David Reisman, Kevin Vandersall, Sally Weber., The technical staff of the Z-machine facility at SNL.

David Reisman is responsible for much of the recent development of the Trac- II hydrocode and I gratefully acknowledge his assistance in getting me started in its use.

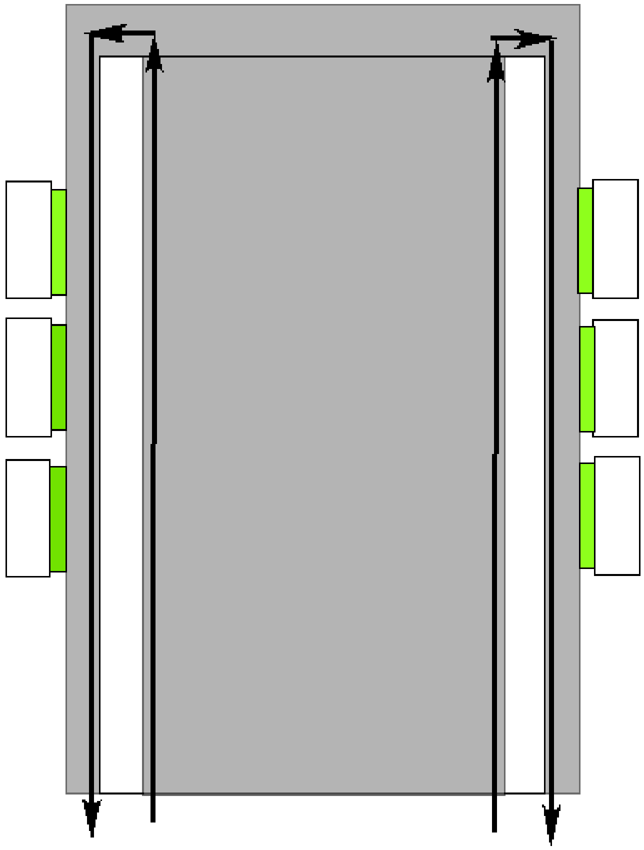

Figure 1: A side view sketch of the stem and sample assembly indicating current flow (black arrows), samples (green), and windows (on top of samples, white). The current comes up through the stem and then returns through the panels, staying near the vacuum gap between them. This generates a large Lorentz force pressure that drives the ramp wave that originates in the panel floor near the insulating vacuum gap and subsequently propagates into the samples.

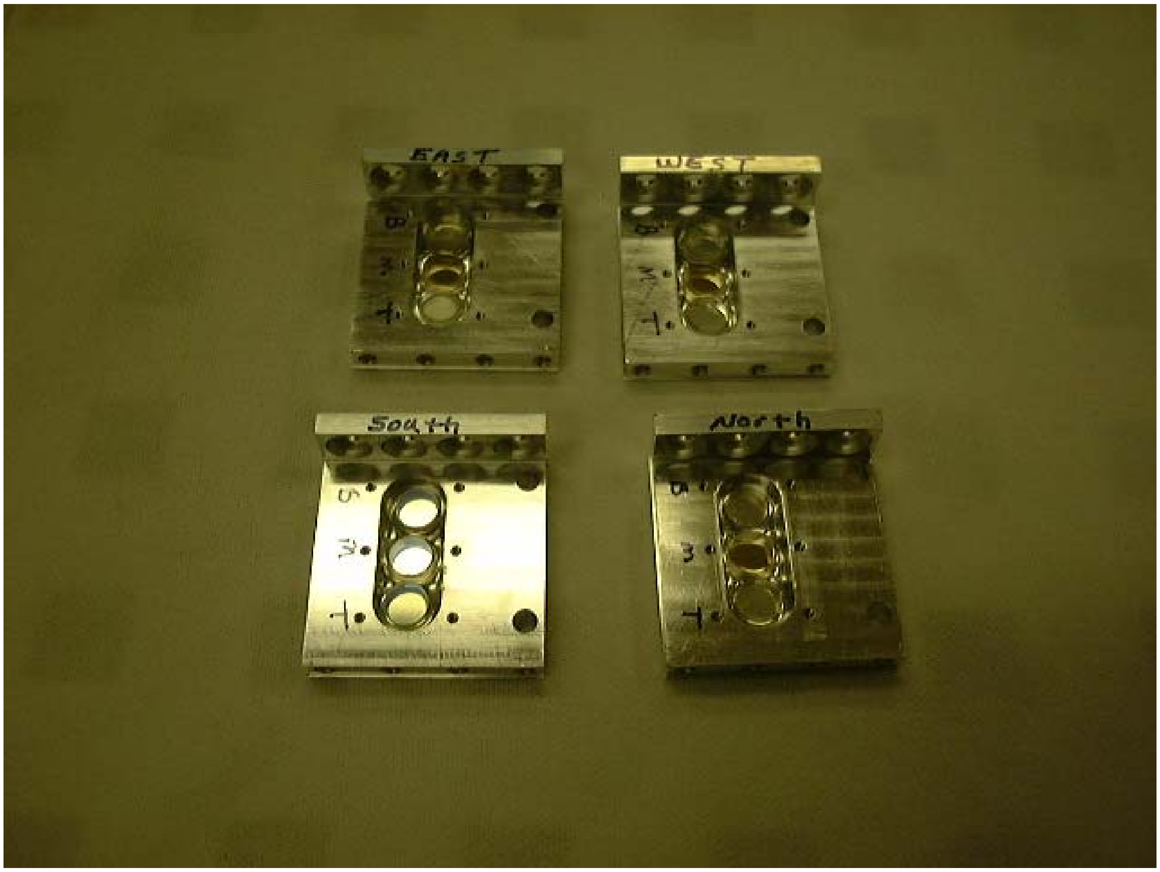

Figure 2: The finished panels, with samples and windows mounted, ready to go: shot 1067 LX-04.

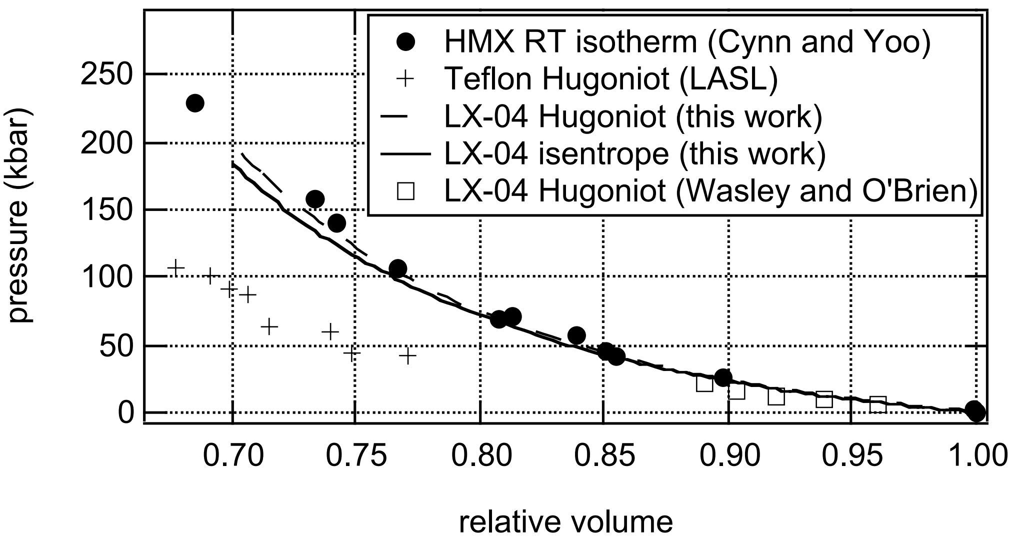

Figure 3: A comparison of the LX-04 ICE loading data of shot 1067 (3/19/03), labeled "this work"; with the Hugoniot data of Wasley and O'Brien [16] generated by conventional shock compression techniques. Notice that the final pressure reached by the ICE technique is more than six times the maximum pressure achieved by Wasley and O'Brien. Attempts in their same work to reach higher compressions resulted in severe reaction and were not plotted here. Also shown here is the room temperature DAC isotherm of HMX by Cynn and Yoo [17] as well as the LASL Teflon Hugoniot [18]. Teflon has a Hugoniot similar to the 15 % Viton-A binder component of the LX-04. The other 85 wt % is HMX. This figure was taken from reference [5]

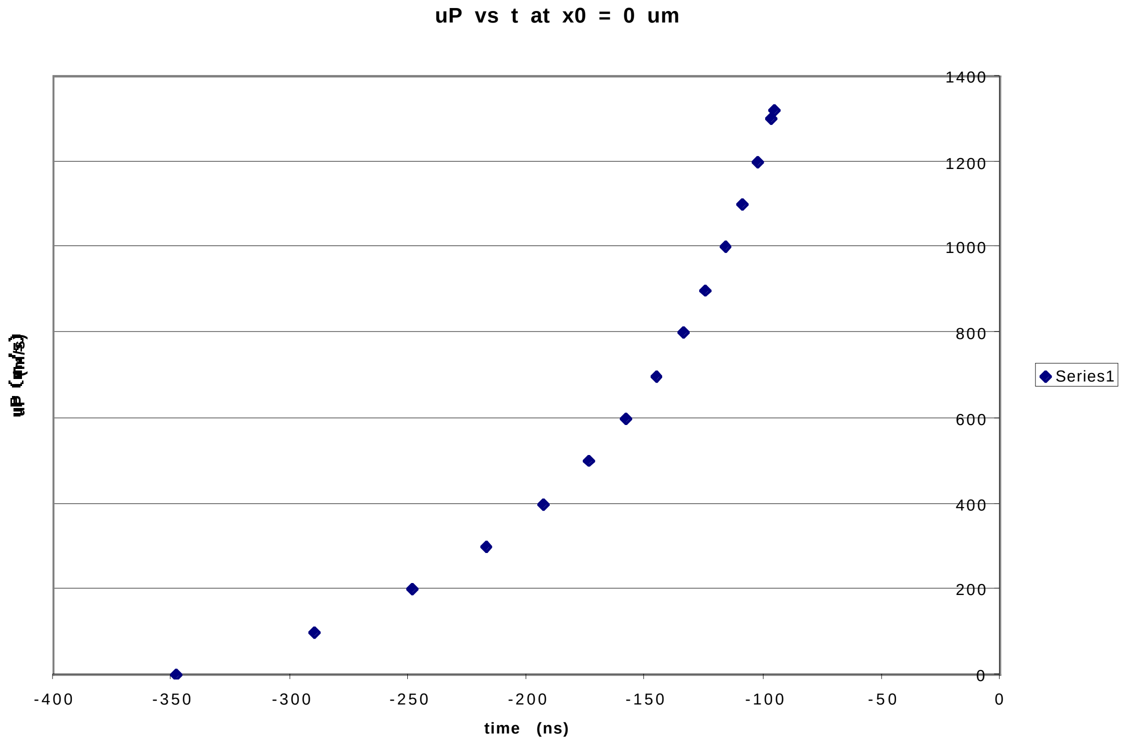

Figure 4: The velocity history in LX-16 at 0 μm that should simultaneously shock up at 800 μm at t = 0 ns, given the Lagrange sound speed approximation used.

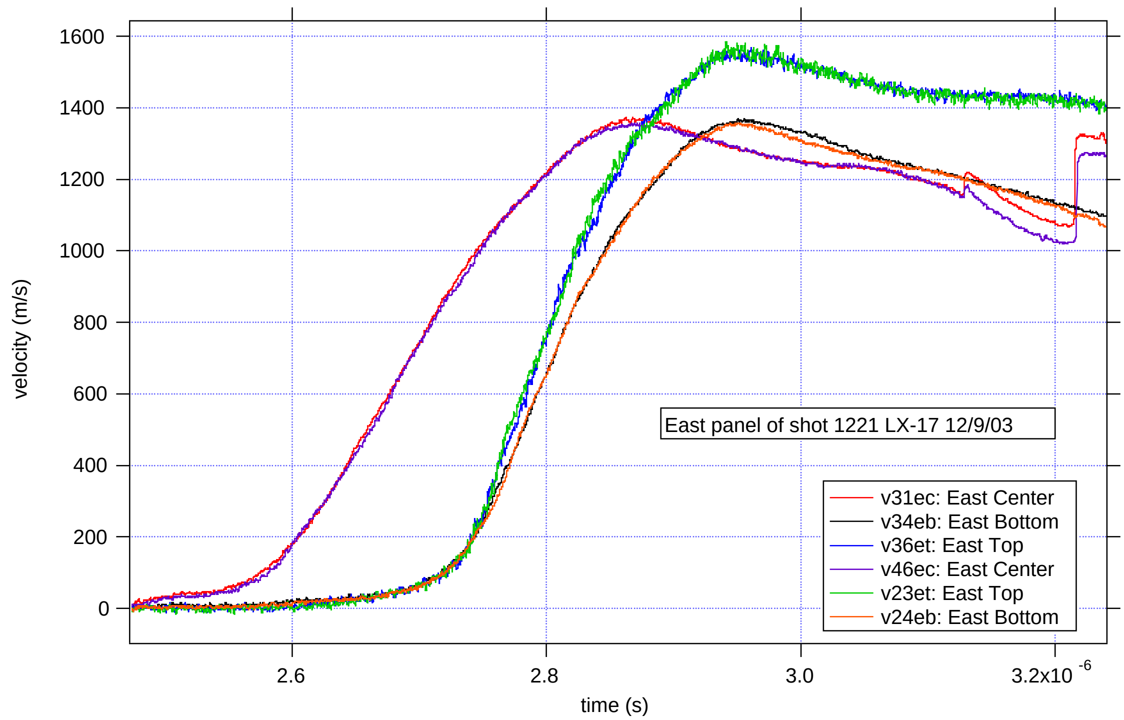

Figure 5: The velocity histories for East panel for shot 1221 12/9/03. All time corrections have already been applied. East Top thicknesses: 1012 μm Al 6061 T6 panel floor, 811 μm LiF (100) sample, NaCl (100) window. East Center thickness: LiF (100) window directly on 1014 μm Al 6061 T6 panel floor. East Bottom thicknesses: 1013 μm Al 6061 T6 panel floor, 793 μm LiF (100) sample, LiF (100) window. The East Center – East Bottom pair would also be ideal candidates to try the Lagrange Analysis on, since the waveforms are shockless and the windows are perfectly impedance matched to the samples (simple flow). In the Lagrange Analysis context East Center is essentially a LiF (100) sample of zero thickness.

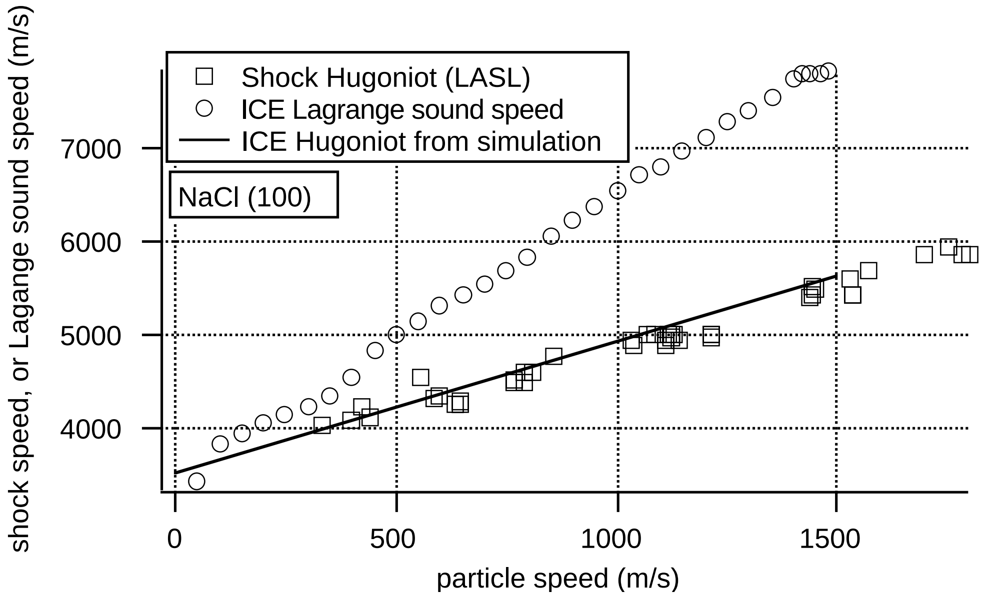

Figure D1: Although not an explosive, data on single crystal NaCl (100) orientation (a common window material in ICE experiments) makes a good set for illustration purposes. The squares are the shock Hugoniot data from Los Alamos from their classic compendium of shock data [19]. The circles are the Lagrange sound speed as measured in an ICE experiment, using the Lagrange Analysis technique. The straight line is the Hugoniot that was obtained by the iterative hydrodynamic simulation of that same ICE data, using the Trac-II code. Note that the Lagrange sound speed data has the same Up = 0 intercept and roughly twice the slope of the shock Hugoniot results.

The NaCl ICE data are from shot 1067 3/19/03. This same figure and caption are taken from a submission to the LLNL HE reference guide [8].

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13. Appendix A

How to run the Trac- II hydrocode.

Trac- II is a cylinderical 2-D geometry magnetohydrodynamic code that can be used to find the unreacted Hugoniot of HE ICE samples. The input is a current history, which is applied to the outside boundary of a cylinder. The cylinder outside radius is 100 cm. The ramp wave is propagated radially inward. Since the sample plus floor thickness taken together is under 0.2 cm the inner cylinder radius is on the order of 99.7 cm (about 0.1 cm of window material included). In theory, there is a pressure increase due purely to the cylindrical flow convergence that is not present in a true plane wave geometry. In practice the increase in velocity or pressure due to this convergence effect is less than 0.3 % with these dimensions. So at the 0.3 % accuracy level, this input deck or one of similar dimensions will mimic a plane wave geometry.

There is however an important conversion that needs to be done between the experimentally measured current and the current input to give the equivalent drive conditions in Trac- II. The simulation current (or pseudocurrent) is obtained from the experimental current by:

Eq. A1: $$\frac{i_{SIM}}{2\pi(100)} = \frac{i_{EXP}}{4(W + 0.092)}$$

W is the width of the cathode stem in the experiment, in cm. This mapping makes the linear current density nearly the same for the simulation and the experiment. For example, for a current of 20.5 MA (MegaAmps) in the experiment with the low pressure design (W = 2.00 cm) the Trac- II simulation current required for the same drive effect would be 1.539 GA. Since the fundamental unit of current in Trac- II is the 1. E+7 A the correct entry in the current input file would be 153.9

The units of Trac- II.

Mass: g
Time: μs
Space: cm
Velocity: cm/μs
Density: g/cc
Current: 10 MA
Pressure: Mbar

The input for Trac- II.

The two files the user needs to prepare for Trac- II input are the input deck and the simulation current history input (current input for short). The current input is related to the experimental current history by the transformation given above (remember Trac- II likes current in 10 MA units and time in μs). I have always run simulations with the current input and input deck in the same directory as Trac- II.

Below is an example of an input deck that runs. It was used to simulate the “West-Top” LX-04 sample in shot 1067.

```
'WTlx04fine'
1 0. 99.7552  2 1. 99.7552  3 1. 100.00  4 0. 100.00
0
fblok 1  1 2 3 4  1 900 1 2 3 4 1. 1. 1. 1.
$
vgen 1  1  1 601 1 900 2.703 2.5e-5 2.5e-5 2.5e-5 0.0
vgen 2  1  1 436 1 600 1.87 2.5e-5 2.5e-5 2.5e-5 0.0
vgen 3  1  1 1 1 435 2.163 2.5e-5 2.5e-5 2.5e-5 0.0


eos 1 4 .524  1.40 0. 0. 1.97 0.48 '6061 T6'
refd 1 2.703
eos 2 4 .3102  1.876 0. 0. 1.251 0. 'LX04'
refd 2 1.87
eos 3 4 .35596  1.2821 0. 0. 1.513 0. 'NaCl (100)'
refd 3 2.163



resbc=0 tkbc=0 vbc=3
bdy 2 0 0 0 0 0 0. 0. 0. -1. 0. 0.
bdy 4 0 0 1 0 0 0. 0. 0.  0. 0. 0.
bdy 3 0 0 0 0 3 0. 0. 0. -1. 0. 0.
bdy 1 0 0 0 0 3 0. 0. 0. -1. 0. 0.

dt 1.e-6 qvism 0. qvislm 0. qvisdm 0. qaprm 0. eicfac 0.
hdtm .1  eedif 0 eidif 0 eedifx 1. eidifx 1.
rad 0  hdifx 1. hdif 0 tkefac 1. radtab 0 rhomin 1.e-5
qeos bondcor dtmax 1.e-3
t0volt 0. ifstr 0
currinp lx04curr1.inp


hvst 1 0 9500000 10   1.e10  100. .01
hvst 2 9500000 9500000 10   0.0 1. .0002
hvst 3 0 9500000 1000  1.e10 100. .01
hvst 4 9500000 9500001 0   .60  .61 .01
hvst 5 1000000 1000000 0 0. 1.1 .1

fvst 2 ekin ethe ethi $
```

```
fvst 2 etot ebdy echk $              vstfile 2 2 energy.vst
fvst 3 eqvis $                        vstfile 2 3 eqvis.vst


fvst 10 pta 1  1 900 1 900 $
fvst 10 pta 1  1 600 1 600 $
fvst 10 pta 1  1 435 1 435 $
fvst 10 pta 1  1 1 1 1 $          vstfile 2 10 ptot.vst

fvst 11 vra 1  1 900 1 900 $
fvst 11 vra 1  1 600 1 600 $
fvst 11 vra 1  1 435 1 435 $
fvst 11 vra 1  1 1 1 1 $          vstfile 2 11 vr.vst


fvst 14 etot ehfd erdf echk $                  vstfile 2
14 erdf.vst
fvst 15 eohm $                          vstfile 2 15
eohm.vst
fvst 16 curr2 $                         vstfile 2 16
curr.vst
fssh 1 rc pi den vr q $
sshfile 5 1 tg.ssh
stoprun 4
ttyedit 1 2
lag
onedl
/
```

Establishing the length scale.

```
'WTlx04fine'
1 0. 99.7552  2 1. 99.7552  3 1. 100.00  4 0. 100.00
0
```

The length of the mesh is established in this statement. Here we see that the mesh extends from 100.0 cm (the boundary where the current is applied) to 99.7552 cm. This makes the mesh 2448 μm from one end to the other. (Note: This particular length was chosen to make the 816 μm thick Al floor exactly 300 zones)

The number of zones.

```
fblok 1  1 2 3 4  1 900 1 2 3 4 1. 1. 1. 1.
```

This simulation has 900 zones. Change the number 900 to alter this. You will also have to alter zone reference in the vgen statements and fvst statements consistent with this, as will be discussed shortly.

The vgen statements:

```
vgen 1  1  1 601 1 900 2.703 2.5e-5 2.5e-5 2.5e-5 0.0
vgen 2  1  1 436 1 600 1.87 2.5e-5 2.5e-5 2.5e-5 0.0
vgen 3  1  1 1 1 435 2.163 2.5e-5 2.5e-5 2.5e-5 0.0
```

The mesh is being filled with three different materials. Material 1 and the zones it occupies are covered in the vgen 1 statement. Material 1 occupies zones 601 to 900. 2.703, 1.87, and 2.163 are the respective densities of the three materials filling the mesh. Make sure they match the densities in the eos statements.

The eos statements:

```
eos 1 4 .524  1.40 0. 0. 1.97 0.48 '6061 T6'
refd 1 2.703
eos 2 4 .3102  1.876 0. 0. 1.251 0. 'LX04'
refd 2 1.87
eos 3 4 .35596  1.2821 0. 0. 1.513 0. 'NaCl (100)'
refd 3 2.163
```

eos 3 fills region 3, etc. This is the Hugoniot EOS format. Let's look at eos 1 which is supposed to be the panel material. There are six numbers in a sequence:

```
.524  1.40 0. 0. 1.97 0.48
```

they are, respectively, C_0, S_1, S_2, S_3, G_0, b. C_0 is in cm / μs. All the other coefficients are dimensionless. This will accommodate a non-linear Hugoniot and a Gruneisen gamma given by Eqs 1 and 2.

The form of the Hugoniot is:

Eq. A2: $$U_S = C_0 + S_1 u_P + S_2\left(\frac{u_P}{U_S}\right)u_P + S_3\left(\frac{u_P}{U_S}\right)^2 u_P$$

In practice S_2 and S_3 are often zero. Setting b = 0 is equivalent to the constant gamma/volume assumption and is expedient when better gamma information is not available. The density for each material should usually be the initial density. It should match that given in the vgen statement.

The current call:

```
currinp lx04curr1.inp
```

This statement calls the file lx04curr1.inp, which is the current input.

The file looks like this:

```
26
0 0
0.0487 5
0.0608 10
0.0709 15
0.0803 20
0.0890 25
0.0977 30
0.1068 35
0.1162 40
0.1263 45
0.1403 50
0.1613 55
0.1810 60
0.1948 65
0.2068 70
0.2180 75
0.2291 80
0.2394 85
0.2492 90
0.2591 95
0.2688 100
0.2786 105
0.2892 110
0.3016 115
0.3282 120
1.0 120
```

This is a pretty simple example. The first number says that there are 26 time, current pairs. Time in μs, simulation current in 10 MA units. Remember this is the simulation current which is related to, but different from, the experimental current as was previously discussed.

The experimental current can be manipulated in either EXCEL or IGOR PRO (WaveMetrics, Inc.) to obtain the simulation current file. My notes on this process are below. (Note: I use the term “psuedocurrent”. This is synonymous with simulation current.

Starting from SNL-supplied actual current:

- Discreetize the current, using IGOR, into a small file of about 30 – 50 points (for ease of handling. I don’t believe this step is necessary but I have taken to doing it for reasons of conceptual simplicity) The number of t,I points in the file has to be the first number, followed by a left time column, and a corresponding right current column.

- Convert actual current into Trac- 2 psuedo-current using panel dimensions (stem width and AK gap) and the procedure given in the simulation notebook. I believe this can be done in either Excel or Igor. I did it in Excel. I believe Trac- 2 will accept either tab or space delimited general text input.
- Copy to laptop. put in the same directory with Trac- 2

Starting from Al-LiF velocity history:

- Propagate the time array backwards using the panel floor thickness and the approximate Lagrange sound speed in 6061 T6 (the panel material) CL = A + 2*B*u, A and B from Steinberg blue book.
- Convert velocity to pressure using Hugoniot.
- Convert pressure to (approximate) experimental current using panel geometry and formula of p from I excel worksheet.
- Convert current to pseudo-current for Trac- 2.
- Discreetize psuedo-current (optional?)
- Run psuedocurrent as input in Trac- 2 using the Al –LiF geometry.
- Because Al and LiF are not perfectly Z matched there will be some disagreement between the simulated and actual velocity histories. Rescale the pseudo-current amplitude (in Excel?) and run simulation again. Remember current goes like sqrt(p). Consider performing this iteration at least twice to get best agreement.

Setting the location of the pressure and velocity history interfaces.

```
fvst 10 pta 1  1 900 1 900 $
fvst 10 pta 1  1 600 1 600 $
fvst 10 pta 1  1 435 1 435 $
fvst 10 pta 1  1 1 1 1 $          vstfile 2 10 ptot.vst

fvst 11 vra 1  1 900 1 900 $
fvst 11 vra 1  1 600 1 600 $
fvst 11 vra 1  1 435 1 435 $
fvst 11 vra 1  1 1 1 1 $          vstfile 2 11 vr.vst
```

fvst command writes the history of some function at a given zone location. pta gives the pressure, vra gives the velocity. Four history locations are chosen here: 900 is the drive interface (aluminum-vacuum boundary), 600 is the panel-sample interface, 435 is the sample-window interface, 1 is the window-vacuum interface. I would recommend this as the minimum set of interfaces to watch. The VISAR measurement will correspond to the 435 velocity interface, so this is the thing that gets compared to the data.

These histories are combined into two files that are output from the simulation:

ptot.vst
vr.vst

These are TECPLOT files (Tecplot, Inc). Thus TECPLOT is needed to read the output of the simulations. The velocities in vr.vst will be negative due to the geometry of the problem.

You have to play around with the TECPLOT files to get the hang of things but a few useful menu items are “define x-y mappings” (under the “xy” menu) where you choose which data gets plotted against which. There is also “edit” (under the “axis” menu) where you can rescale the axes.

There is also the ability to look at the data in spreadsheet or table form. This is to be found in the “spreadsheet” menu (under the “data” menu). This is useful for reading off the vr.vst file simulation velocity versus time points and thus closely comparing the simulation and experimental VISAR velocities.

Practice data

East panel data of shot 1221 is very good data to practice simulating. This data is shown in Fig. 5. The sample is LiF (100) which is a material with a well-known Hugoniot so that we know what answer we should get. Simulate the sample using Trac-II to find C_0 and S_1, treating the sample as though these quantities were unknowns. If things are working right you should converge on values pretty close to those given in Table 1. The figure with its caption and table 1 contain all the information needed to find C_0 and S_1 for the sample. Step-by-step:

1 Assume that the panel floor and window Hugoniot information is completely known. Use the values in the table. (Note that for the LiF (100) in the window, you assume its data is completely known. For the LiF (100) in the sample position you treat its Hugoniot as an unknown and attempt to find it.)
2 Assume ρ_0, Γ_0, and b for the sample are known. Take the values for LiF (100) from table 1.
3 Assume that C_0 and S_1 (for the sample!) are not known. They are to be determined by the simulation process.
4 Take the reference data (East Center) and propagate it backwards through the reference panel using Eq. 6.
5 Convert velocity (u_P) to pressure using Eq. 5 and the data in table 1 for 6061.
6 Convert pressure to current using Eq. 7.
7 Convert current to pseudocurrent (Appendix A)
8 Simulate the reference geometry (East Center) using the pseudocurrent above. Scale psuedocurrent if necessary to optimize agreement between simulation and East Center data.
9 When pseudocurrent is tweeked in to give best agreement in the reference geometry, use it as the drive to simulate East Bottom using the procedure described in this Appendix. You will not be tweeking the pseudocurrent from now on: it is now considered a given, having been verified by the reference simulation. When you simulate East Bottom you know the drive. You are pretending like you don’t know what C_0 and S_1 are for the sample (Although you do know what they

are for the purpose of the window entry. It just so happens that in this particular exercise the window and the sample are the exact same material). How do your sample C_0 and S_1 values determined by simulation compare with those given for LiF (100) in table 1?

16. Appendix B

The fringe-to-velocity data reduction and synchronization of the velocity histories.

The fringe to velocity conversion process is fairly routine and is covered by standard software such as VALYN VISAR data reduction software or its equivalent. The important extra step is that the time synchronization of multiple simultaneous velocity records is very important in ICE. The precision of an ICE isentrope measurement is directly impacted by the accuracy with which the reference and sample velocity histories are correct in time relative to one another. It is this time synchronization aspect that is covered here. As we speak there can be up to 22 VISAR probes on a single experiment, all potentially needing to be synchronized relative to one another.

A general comment is that since there are small time corrections between the two fringe histories corresponding to the same VISAR signal it is best if the velocity synchronization is all done while the data is still in fringe form (i.e. before the fringe-to-velocity conversion is done).

Here we assume that the VISAR fringe conversion process will be done using the VALYN VISAR routine.

The records the experimenter will receive will be of two formats: Sandia-owned VISARS (MP1 and MP2) and Bechtel Nevada-owned VISARS (03C and 04C).

The experimenter will also need the VISAR timing data spreadsheet and the VISAR scope assignment data spreadsheet, both supplied by Sandia.

The Sandia VISARs

The SNL VISARs are four beam each. The data files are labeled T1 thru T8. The correspondence is:

MP1-1 = T1 (MP1-1 is channel 1 on MP1)
MP1-2 = T2
MP1-3 = T3
MP1-4 = T4
MP2-1 = T5
MP2-2 = T6
MP2-3 = T7
MP2-4 = T8

The SNL files come stripped of their time array, which the user must reinsert (I do this in IGOR PRO (wavemetrics)). The time increment is 200 ps per point. There are four columns of numbers in this order: data 1, data 2, beam intensity monitor, and the time mark. The beam intensity monitor signal is non-zero only on T1 (representing all of MP1 VISAR) and T5 (representing MP2 VISAR).

The time array has to be shifted as follows: An EXCEL spreadsheet giving VISAR timing information will be supplied by Sandia at the same time the data is delivered. It will list four types of delays. For each data channel you will form the time quantity:

(Machine time at which nanofast fires) + (time mark delay) – (optical delay) – (VISAR timing delay)

For each SNL data fringe the time array should be offset such that 10 % full height on the time mark occurs at the above time. Note that each data fringe will have its own unique time array.

Below I have a procedure that I used for doing this using IGOR PRO. (Note!!!! The VALYN VISAR routine will not accept data file input in just any format.). I had IGOR PRO installed on my MAC and the VALYN data reduction program installed on a PC laptop. Hence the strange references such as“load on laptop”, load back on MAC, etc.

SNL VISAR data T1-8:

- load into Igor
- add time array (each T-file contains its own time fiducial)
- adjust time according to timing spreadsheet and time fiducial, both D1 and D2 get their own unique time correction. They are frequently close but not identical.
- output as a general text file. Use CRLF terminator and deselect “write wave names” option. The time array needs to be the first column and you will often have to go to the command line using “to cmd line” button to alter the order of the arrays.
- load on laptop. VALYN will ask for VPF of the window and you will have to know this before hand. Make velocity histories.
- load back on MAC
- If fringes need to be inserted, I do it by hand in the IGOR routine.

<u>The Bechtel Nevada VISARs</u>

The BN VISAR output is in a more typical scope output format: two column: time array and fringe signal. Thus the time array doesn’t need to be added although it does still need to be shifted.

The tricky thing about the BN time correction is that the time mark doesn’t show up on every file, it only shows up on channel 1 of each digitizer. Therefore for these guys you have to know the digitizer assignments. This is given in an EXCEL sheet that looks something like Z1067.xls for shot 1067, etc.

Again for the time quantity:

(Machine time at which nanofast fires) + (time mark delay) – (optical delay) – (VISAR timing delay)

each fringe data time array is now shifted such that the its time array would put the 10 % full height of the scope's channel 1 time mark at the above time quantity.

I would do this in IGOR PRO. The checklist is shown below:

BN VISAR data

- load into IGOR
- locating the fiducial is a little tricky. It is on channel 1 of what ever scope the fringe data got recorded on. You need to have the data-scope assignments to psyche this out.
- adjust time via timing spreadsheet and fiducial
- output as general text file, and continue further processing in exactly the same manner as above SNL example

17. Appendix C

Summary of all LLNL HE ICE experiments done at SNL Z-machine up to 6/26/04

The author D.E. Hare participated in the design of HE ICE 6 thru 10 and the analysis and write-up of HE ICE 5. Information about ICE 1 thru 4 has been obtained through D.B. Reisman and others.

HE ICE 1
Shot number 679
Sample: LX-04
Shot date: 12/18/00
Summary: basic preliminary isentrope data

HE ICE 2a
Shot number 754
Sample: LX-04
Shot date: 5/29/01
Summary: basic preliminary isentrope data

HE ICE 2b
Shot number 755
Sample: ultrafine TATB
Shot date: 5/30/01
Summary: Basic preliminary isentrope data. Strongly shocked-up due to porosity of samples.

HE ICE 3
Shot number 844
Sample: LX-17
Shot date 12/19/01
Summary: basic isentrope data

HE ICE 4
Shot number 896
Sample: HMX
Shot date: 4/9/02
Summary: basic isentrope data

HE ICE 5
Shot number 949
Sample: single xtal HMX
Shot date: 8/2/02

Summary: initial search for phase transformation data. The data were analyzed and will be published in Appl. Phys. Lett., Hare, Forbes, and Reisman, July 2004.

HE ICE 6
Shot number 1067
Sample: LX-04
Shot date: 3/19/03
Summary: Isentrope data for NaCl (100) and LX-04 were taken to 170 kbar.

HE ICE 7
Shot number 1146
Sample: viton-A and LX-17
Shot date 8/5/03
Summary: isentrope data for viton-A was attempted. The data is of limited use because of the difficulty of controlling the thickness of the samples. LX-17 data was good.

HE ICE 8
Shot number 1221
Sample: LX-17
Shot date: 12/9/03
Summary: data ready to simulate.

HE ICE 9
Shot number: 1265
Sample: heated LX-04
Shot date: 3/16/04
Summary: Had problems with heater run-away and sample bonding at elevated T. Two samples appeared to yield data.

HE ICE 10
Shot number: 1289
Sample: single xtal HMX phase transition
Shot date: 4/23/04
Summary: Data ready to simulate.

18. Appendix D

What is Lagrange sound speed? How it is related to the Hugoniot?

Lagrange sound speed relates the time it takes an acoustic disturbance to propagate between two points to their seperation when written in terms of the original, uncompressed distance between the two points. (Their Lagrange coordinate distance).

Eq. D1: $$C_L = \frac{\Delta x_0}{\Delta t}$$

On the other hand the common (Eulerian) sound speed definition uses the lab coordinate distance between the two points. The relationship between the two is:

Eq. D2: $$C_L = \frac{\rho}{\rho_0} C_E$$

The usefulness of the Lagrange sound speed is that it is a convenient way of computing the transit time of an acoustic disturbance between two Lagrange gauges. Lagrange gauges flow with the medium and the VISAR reflective surfaces are Lagrange gauges. Thus ramp wave transit time between two VISAR surfaces is most simply related to C_L.

It is a common approximation in shock compression physics to treat the release isentrope as following the same path as the Hugoniot in pressure – particle velocity (p-u_P) space. We show that to the extent that you have a standard linear Hugoniot and that the Hugoniot and isentrope overlay in p-u_P space, then:

$$U_S = C_0 + S_1 u_P \text{ implies } C_L = C_0 + 2Su_P$$

Suppose that C_L has a linear form. (The subscript is dropped on u_P for convenience.)

Eq. D3: $$C_L = A + Bu$$

For a simple forward facing isentropic wave the relationship between p and u is given by:

Eq. D4: $$dp = \rho C_E du = \rho_0 C_L du = \rho_0 (A + Bu) du$$

The first part of Eq. D4 is the statement that the Rieman invariant along all backwards facing characteristics is zero everywhere. This is integrated, starting from p = u = 0 to give:

Eq. D5: $$p = \rho_0 (Au + \frac{B}{2} u^2) = \rho_0 (A + \frac{B}{2} u) u$$

But, the standard steady shock relationship between p and u is:

$$\text{Eq. D6:} \qquad p = \rho_0 U_S u$$

If the isentrope and Hugoniot follow the same path in p-u space then by comparison:

$$\text{Eq. D7:} \qquad U_S = A + \frac{B}{2}u$$

implying:

$$\text{Eq. D8:} \qquad C_L = C_0 + 2S_1 u$$

Figure D1 compares experimental shock and Lagrange sound speed data on NaCl (100).

19. Appendix E

Definitions

Drive: The pressure boundary condition generated by the current flow in the floor. As the pressure is caused by the current the term drive can refer either to the pressure or the current.

Floor: the flat thin section of the panel where the current is conducted and the ramp wave is generated which then subsequently propagates into the sample.

HE: high explosives

History (like velocity, pressure, current history, etc); a time record of some variable, in this report all histories are at a fixed Lagrange point in the material. Thus a velocity history is velocity versus time at some interface, which moves with the particle flow of material, such as the VISAR interface or the vacuum-aluminum interface, etc.

ICE: Isentropic Compression Experiment: The use of a ramp compression wave instead of a shock wave to determine the dynamic high pressure properties of a material.

Lagrange Gauge: A gauge which moves with the particle flow. In contrast an Eulerian gauge is fixed in the lab reference frame. The VISAR interface is a Lagrange gauge for measuring velocity history.

Pseudocurrent / simulation current: The current required by the Trac-II 1-D geometry to give the same current density (and hence same drive pressure) as the experimental current (Equation 8).

Reference velocity history: The velocity history at the floor / window interface of a floor / window assembly. All Hugoniot information is considered known to high accuracy. The purpose of the reference is to determine with accuracy the correct drive to use for the simulation of the sample velocity history.

Sample velocity history: The velocity history at a sample / window interface of a floor / sample / window assembly. This contains the (unknown) sample Hugoniot information to be determined through agreement between simulation and experiment.

Window: A material through which light can be transmitted for the purpose of laser Doppler interferometry such as VISAR or Fabry-Perot. The window serves two purposes: it allows light access to and from the sample and it tamps the sample surface. LiF (100) is an excellent all around window but its shock impedance is somewhat higher than most explosives. NaCl (100) is a better impedance match but it should be avoided above 250 kbar because it has a pressure-induced phase transition. It is also water-soluble and slightly hygroscopic and so needs some protection against a humid environment.