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LAWRENCE LIVERMORE LABORATORY

University of California/Livermore, California

**H-DIVISION
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October through December 1974

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FOREWORD

This quarterly report has a dual purpose: to acquaint the reader with the overall goals of each of the six groups comprising H-Division of the Physics Department; and to supply a concise statement of the status of the projects under way in each group. References and experimental details are kept to a minimum. Readers who desire additional information are encouraged to contact the individual(s) associated with each project.

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2 I. THEORETICAL EOS GROUP (R. Grover, Group Leader)

The H-Division Theoretical EOS Group has two primary tasks: the development of theoretical techniques for the description of material properties under extreme conditions; and the construction of EOS tables for specific LLL material applications.

Hugoniot Calculations for Weapon Code EOS Tables (R. J. Olness)

The shock properties of important weapon materials (D₂, ⁶LiD, U, and stainless steel) have been investigated from their tabulated equations of state. This study required the development of a computer code, MHUGO, that has several options permitting the use of various calculational procedures.

There are two principal reasons for this investigation.

- (1) It represents a natural extension of the isentrope work^{1,2} described in the preceding progress report.³ The capability now exists for determining directly from the EOS tables, without the use of a hydrocode, the two limiting extremes for purely hydrodynamic processes: isentropic and shock. In isentropic processes, the entropy change is zero; in shock processes, the maximum possible entropy increase occurs. The isentrope work showed that the most significant EOS problems occur in the low-density, low-temperature region (typically $\rho = \rho_0$, $T < 10$ eV).
- (2) Here, the problems that occur in shock processes are likely to be at least as important as those in isentropic processes, if not more so.

A Hugoniot curve, by definition, is the locus of points (ρ , P , E) that can be reached from a given initial point (ρ_0 , P_0 , E_0) in a single shock. There are a number of differential Hugoniot relations,* all equivalent for a thermodynamically consistent (TDC) EOS, which can be derived from the Rankine-Hugoniot internal energy equation,

$$E - E_0 = \frac{1}{2} (P + P_0) \left(\frac{1}{\rho_0} - \frac{1}{\rho} \right). \quad (1)$$

In the presence of thermodynamic inconsistency (TDI), certain derivatives are not single-valued, and integration of the differential relations leads to multiple-valued Hugoniots. In contrast to the isentropes, for which TDI leads to double-valued trajectories, the potential Hugoniot multiplicity is large. It is possible, however, to define two limiting cases, referred to as type T1 and type T2 by analogy with the procedure in Ref. 1, according to the derivatives employed in the differential equation. [Thermodynamic identities are used to eliminate $(\partial E / \partial \rho)_T$ from T1 and $(\partial P / \partial T)_\rho$ from T2.] The

* A differential Hugoniot treatment corresponds more closely with weapon code methods.

resulting Hugoniot for D2, ${}^6\text{LiD}$, U, and stainless steel have been examined to determine their shock response properties and to evaluate the influence of TDI.

The results exhibit effects similar to those obtained for the isentropes. The T1 Hugoniot are generally quite regular although the solutions at low temperatures often fail to satisfy Eq. (1) [rather badly below 100 GPa (1 Mbar) in ${}^6\text{LiD}$]. The T2 Hugoniot exhibit considerable irregularity with some temperatures even going negative (e.g., ${}^6\text{LiD}$ for $\rho_0 \approx \rho$ solid, $T_0 < 0.3$ eV). To examine the possible consequences in weapon applications, a number of MEG calculations were performed to determine the correspondence between the hydrocode artificial-viscosity treatment of shocks and the analytic approach employed in MHUGO.⁴ The artificial viscosity method seems to reproduce the more regular T1-type Hugoniot, for numerical (as opposed to fundamental) reasons; i.e., $(\partial E/\partial \rho)_T$ tends to be small over a major portion of the (nonphysical) artificial-viscosity track, while this term is absent by construction from the T1 calculation in MHUGO. This circumstance leads to nonpathological weapon code calculations but tends to obscure the presence of potentially serious EOS problems.

A further check has been made employing yet another method; namely a search along isotherms or isochors (fixed ρ) for solutions to Eq. (1). Some significant differences are observed in ${}^6\text{LiD}$, for example. While correspondence with the preceding methods is good above 1.0 GPa (10 Mbar) (for $\rho_0 = \rho$ solid, $T_0 = 300$ K), the agreement deteriorates with decreasing pressure and, between about 150 GPa (1.5 Mbar) and 2.0 GPa (20 kbar), there are no solutions to Eq. (1). The behavior in this region suggests that the solutions, if they existed, would lie below the zero kelvin isotherm.

Whether the problems described here are the result of tabulation distortions or errors in the underlying EOS data remains to be determined. While the artificial viscosity method produces Hugoniot which are regular and quite reasonable in appearance through regions of TDI EOS, further work (now in progress) will be required to establish whether or not the EOS problems described here are producing significant errors in current weapon code calculations, particularly in the weak shock region.

Fitting Functions for the EOS of Dense Hydrogen and Mixtures of Low Z-Elements (H. DeWitt)

The Monte Carlo data for the internal energy of the one-component plasma in the fluid regime has been fitted with a very simple and convenient function of one parameter. This functional form has been used also to fit all the Monte Carlo data generated with our Monte Carlo code that includes a realistic treatment of electron screening. With this form, the Helmholtz free energy, EOS, internal energy, and specific heat are given accurately for dense hydrogen and mixtures of light elements.

A number of algebraic fitting functions have been proposed to fit the Monte Carlo data for the classical one-component plasma as obtained in Ref. 5 and more recently by

Hansen.⁶ Recently, in an attempt to find a convenient form of the EOS for dense hydrogen along the laser-fusion track, the question of what form of fitting function is best has been examined again. A careful least-squares study of the very accurate data of Hansen for the internal energy $\bar{U}$ of the dense Coulomb fluid in the region $1 < \Gamma < 140$ [$\Gamma = e^2/kT\ell$ and $\ell = (4\pi n/3)^{-1/3}$] indicates that the function

$$\bar{U}/NkT = -a\Gamma + b\Gamma^{1/4} - c,$$

where n is partical density, is far better than any form previously proposed. In fact, the thermal energy and specific heat are so well fitted by the $\Gamma^{1/4}$ form that it seems likely that this form has some fundamental significance and should be derivable from a good theoretical model.

In collaboration with W. B. Hubbard, we have used the above form for the internal energy to fit the large amount of Monte Carlo data generated at LLL with Hubbard's Monte Carlo (MC) code that includes degenerate electron screening by means of linear response theory. We have made MC runs for hydrogen for nearly 100 temperature and density points, and thus, for the strongly coupled fluid, we have results for $1 < \Gamma < 100$ and $0 < r_s < 1$ ($r_s = \ell/b_0$ radius, a measure of electron screening for degenerate zero temperature electrons). Because of the linear response theory used in the MC code, the coefficients a , b , and c in the above fitting-form depend linearly on r_s . We have a similar number of MC runs on mixtures of fully ionized hydrogen and helium. Each coefficient in the function above has the form

$$a(r_s, Y) = a_1 + a_2 (1 + a_3 Y)r_s + a_4 Y,$$

where Y is the He/H ratio. A least-squares fit to all the MC data was used to obtain numerical values of all of the 12 coefficients needed for the fitting functions for hydrogen and for mixtures.

Since the electrons in the present MC code are at zero temperature, it is easy to integrate the internal energy and obtain the Helmholtz free energy in the form

$$F_I/NkT = -a\Gamma + 4b\Gamma^{1/4} - c\ln\Gamma + d.$$

Differentiating this form with respect to volume gives the pressure, which agrees with the MC results for the EOS. Thus thermodynamic consistency is assured.

The functions given above refer only to the Coulombic interaction of ions carrying a screening cloud of electrons. These quantities are to be added to the corresponding ideal gas quantities for the ions, plus those for electrons.

Work in progress includes a similar attempt to obtain useful fitting functions for the pair distribution function $g(r)$ as a function of Γ and r_s , and an evaluation of the constant d in the free energy so that the entropy of pure hydrogen and of mixtures can be established. The fluid structure factor, $S(k)$, is also being obtained from $g(r)$ for possible use in improved computations of thermal conductivity.⁷

The Thomas-Fermi EOS in the High-Temperature Approximation (K. W. Johnson and R. Grover)

Much equation-of-state data is based on Thomas-Fermi (TF) theory and its various modifications. We have sought to determine the validity of this data in the high-temperature limit where materials behave like nearly perfect gases. Specifically, we have found analytic corrections to the perfect electron gas EOS in the TF atomic cell. These enable us to inspect the numerical results of our TF computer calculations for correctness and accuracy at extreme conditions and will permit a simple extension of the code calculations as desired.

In the TF cell theory at high temperatures,⁸ the usual Thomas-Fermi electron distribution simplifies to a constant in such a way that one can write the EOS of a nearly ideal gas of electrons in terms of two expansion parameters, κ and Γ . κ , an ideal gas parameter, is given by $\kappa = Z\Lambda^3/2V$, where Z is the atomic number, V the atomic volume and $\Lambda = h/(2\pi mkT)^{1/2}$ is a thermal De Broglie wavelength characteristic of particles having a kinetic energy of kT . The expansion parameter $\Gamma = Ze^2/r_b kT$ is the classical plasma parameter with e the electronic charge, and r_b the atomic radius.

The expansion for the electronic pressure is then given by

$$P = \frac{kTZ}{V} \left(1 - \frac{3}{10} \Gamma + \frac{\sqrt{2}}{8} \kappa + \dots \right).$$

Similar expressions that are consistent with the virial theorem exist for the energy, electron density, and entropy.

Initially, it seemed strange that the pressures given by this expansion agreed well with our TF code calculations, while the energy expressions did not. In searching for the cause of this, we discovered another term, "near" correction, which must be added to the total electron energy to agree with code calculations. This contribution comes from a small region of the atom, near the nucleus, where the nuclear attraction far exceeds the chemical potential of the electrons. The total energy of the electrons is thus given by

$$E_T = E_{\text{near}} + E_{\text{far}} = \frac{3}{2} kTz \left[\left(-\frac{\pi}{2} \frac{\Gamma^3}{\kappa (-\ln \kappa)^{1/2}} \right) + \left(1 - \frac{3}{5} \Gamma \frac{\sqrt{2}}{8} \kappa \right) \right].$$

Figure 1 shows the regions of $\rho - T$ space (density-temperature) for hydrogen where the various corrections are obtained, the region where the numerical calculations are inaccurate, and the region where the numerical calculations are required (analytic terms are invalid).

Hugoniot of Dense LiH (F. J. Rogers)

The principal Hugoniot and some reflected Hugoniots for dense LiH have been calculated with the ACTEX code.

Fig. 1. Regions of ρ - T space that contribute to the total energy, $E_T = E_{\text{near}} + E_{\text{far}}$.

A theoretical estimate of the principal Hugoniot and some reflected Hugoniots for dense LiH are required in the design of the nuclear Hugoniot experiment. Rough estimates of these Hugoniots were previously obtained by scaling the ACTEX calculations for He. The code has since been rewritten so that it can handle multiple nuclear components.

The ACTEX code is based on an expansion in powers of the square root of the activity, and the error in the calculations can be estimated from the relative size of terms of different powers. The present code includes all terms through five-halves power in the activity. Analysis of the terms in the LiH calculation indicate that pressure errors along the Hugoniot are less than 5% for pressures greater than 1500 GPa (15 Mbar) ($T > 14$ eV). The present calculations should be considered preliminary since the importance of additional quantum diffraction corrections is still being investigated.

Ross-Lindemann Melting Criterion (R. Grover)

From the theoretical arguments and experimental data, it is concluded that the Ross-Lindemann melting criterion should apply at any pressure to the melting of all simple solids, i.e., those for which the molecular interactions do not differ in the solid and liquid phases.

The main EOS uncertainties at relatively low temperature are in the thermal properties arising from molecular interactions. Many applications in recent years have required EOS data of liquids at temperatures far above the freezing temperatures over wide density ranges including the region of the gas-liquid critical points. Previous experience has demonstrated that EOS properties of simple materials may be approximately scaled on the melting temperature of the solid.⁹ Thus, the behavior of the melting temperature as a function of density is a prime ingredient in the low-temperature EOS.

In this work, the generalized Lindemann criterion suggested by Hoover and Ross¹⁰ in terms of the excess thermal Helmholtz free energy (EFE) at melting is shown to agree with thermodynamic and high-pressure data on simple metals. A general explanation of this rule is presented making use of its validity for many-body systems with simple inverse-power law interactions as derived from computer simulations.¹¹ The rule is then applied to the melting data for metals having more complex atomic bonding and electron excitations in order to deduce information about these less well-understood properties.

These results are being considered for incorporation in the new GRAY EOS model being developed with D. Young (H-Division).

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H. CODE DEVELOPMENT GROUP ✓

(L. L. Edwards, Group Leader)

The mission of H-Division's Code Development Group is the development of time-dependent, compressible fluid mechanics programs. We are concerned with coupled-Eulerian-Lagrangian methods (CEL and CHAMP) as well as with a generalized Eulerian-mesh method (GEMINI). The motivation in each case is related to developing codes (based on either known or new methods) that are aimed at solving several general classes of fluid-flow problems.

Impulsively Started Flat-Plate Calculations (L. Edwards, A. Buckingham, and G. Wilcox)

The GEMINI code is used to calculate the boundary layer growth of flow over an impulsively started flat plate. Comparisons are made with the Stokes-Blasius solution. (GEMINI is a generalized mesh, viscous, heat-conducting, compressible, two-dimensional, time-dependent Eulerian finite-difference code.)

The interest and need for certain high-speed gas flows past rigid bodies in which viscosity and heat conduction play significant roles in the development of the flow has been the motivation for the GEMINI hydrocode package. To subject the code to a rigorous test of viscous calculations, we selected the impulsively started flat-plate problem previously calculated at Physics International Company.¹²

We present here only pictorial results. The interested reader is invited to study more details in Ref. 12. Figures 2, 3, and 4 compare the code velocity solutions with the Stokes-Blasius solution at particular times. Figures 5 through 11 give a visual aid to the development of the boundary layer by plotting velocity vectors.

In the case of the semi-infinite plate, a vortex sheet is generated at the leading edge as may be seen in Figs. 12 and 13.

The use of continuative inflow-outflow boundary conditions allows GEMINI to calculate the infinite flat-plate problem. The smoothness of this case is demonstrated in Figs. 14 through 16.

In the near future, we will document a detailed comparison of GEMINI and second-order difference-method solutions of this problem.

CEL-HEMP and Multifluid Program (CHAMP) (R. Hickman, J. Hobson, and T. Michels)

The problem generator for the CHAMP multifluid code has been completed, the first-pass modularization of the Eulerian routines for the main calculational code are being debugged, and work has begun on an EOS package.

Fig. 2. Unsteady laminar boundary layer profiles at early time.

Fig. 3. Unsteady laminar boundary layer profiles at intermediate time.

Fig. 4. Unsteady laminar boundary layer profiles at late time.

Fig. 5. Velocity vectors at $t = 0$.

Fig. 6. Velocity vectors at $t = 0.04195 \mu\text{s}$.

Fig. 7. Velocity vectors at $t = 0.1271 \mu\text{s}$.

Fig. 8. Velocity vectors at $t = 0.4272 \mu\text{s}$.

Fig. 9. Velocity vectors at $t = 0.7350 \mu\text{s}$.

Fig. 10. Velocity vectors at $t = 0.8518 \mu\text{s}$.

Fig. 11. Velocity vectors at $t = 1.033 \mu\text{s}$.

Fig. 12. Density contours at $t = 0.4272 \mu s$.

Fig. 13. Density contours at $t = 1.033 \mu s$.

Fig. 14. Velocity vectors at $t = 0.4274 \mu s$.

Fig. 15. Velocity vectors at $t = 0.7327 \mu\text{s}$.

Fig. 16. Density contours at $t = 0.7327 \mu s$.

The CHAMP (CEL-HEMP and Multifluid Program) multifluid code was formulated to provide multifluid Eulerian capabilities that are not available in the present CEL (Coupled Eulerian Lagrange) code. The utility and need for such a code has long been known.

Within the last quarter, preliminary coding and debugging were completed on the pre-generator input routines, and the programming of the CHAMP generator was completed. At that point, it was realized that the pre-generator input routines needed to be further modularized, and preliminary design plans are now being made to construct a separate Eulerian-Lagrangian grid generation module and EOS module. Work on the EOS module is almost complete, with the ability to process 12 different EOS forms.

Completion of the main CHAMP code should occur early next year. Currently, debugging is about to begin on the first-pass modularization of the present Eulerian calculational routines.

The Eulerian hydro routines, having grown by accretion over a number of years, were ill-suited to adapting to new concepts in differencing. Hence, it was necessary to rewrite them from the beginning, an undertaking which also provided an opportunity to modify coding that has led in the past to distortions of symmetry and unnecessary logic stops. The Lagrange hydro subroutines were also reordered for inclusion in CHAMP in such a way that problem dumps and mesh-altering routines could be abbreviated.

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~~III~~ EXPERIMENTAL EOS GROUP
(D. Young, Group Representative)

The H-Division Experimental EOS Group conducts investigations of the properties of materials at high pressures and temperatures. The group develops new techniques for measurements on unusual materials or for work at the extreme ranges of pressure and temperature.

Properties of Materials at High Pressure (W. H. Gust)

A study of the properties of materials at high pressure is continuing. EOS parameters for a number of materials have been determined experimentally through use of the light-gas gun and high-explosive techniques.

Experiments on a boron-loaded silastic (of interest to B-Division) are now complete. It was found that up to 60 GPa (600 kbar), the plot of U_s vs U_p was not linear. An expression for the relation has been formulated, and the data are now being used in code calculations.

Additional experiments to search for multiple shock-wave structures in tellurium, pyrolytic graphite, boron nitride and hafnium carbide have been done. These results are of fundamental interest because of pressure-induced phase transitions and Hugoniot elastic limits.

Future work will include additional light-gas gun experiments on UH_3 at pressures between 150 and 300 GPa (1.5 and 3.0 Mbar) in order to confirm the anomaly found in limited results obtained recently.¹³

Isobaric Expansion Experiment (J. W. Shaner, G. R. Gathers, and D. A. Young)

Previous thermophysical properties measurements on tantalum have been restricted to the melting region and below. This is because of tantalum's high melting temperature of 3270 K. We have applied the isobaric expansion technique to measure the equation of state, resistivity, and heat capacity of tantalum to 0.4 GPa (4 kbar) and 8000 K. In addition, we have measured the heat of fusion, as well as the volume and resistivity changes on melting.

Previous measurements of the thermophysical properties of tantalum have been restricted to the solid phase, with one exception. The exception is a Soviet measurement of the heat of fusion,¹⁴ The reason for the lack of data on liquid tantalum is its high melting temperature of 3270 K.

We have applied the isobaric expansion technique to measure the properties of tantalum in the liquid region. This technique consists of resistively heating a wire of tantalum in an inert-gas pressure vessel. The gas volume is much larger than the

sample volume, assuring an isobaric process. The sample is allowed to expand only in the radial direction, so that a streak camera record of the diameter gives the volume vs time. The energy vs time is calculated from the current and voltage vs time records. The uniformity of the expansion is monitored by a Q-switched ruby laser snapshot taken roughly 10 μ s after the end of the energy deposition. The sample temperature vs time is measured by an optical pyrometer consisting of a bandpass filter, a photodiode, and a low-noise log-preamplifier. The log-preamplifier allows the whole temperature range from 2500 to 10,000 K to be measured on a single scope.

The pyrometric record for several 0.1-GPa (1-kbar) shots is shown in Fig. 17. For these data, the light intensity was normalized to the intensity at the plateau that signaled the solid-liquid two-phase region at the known melting point of 3270 K. The temperature was then calculated assuming a constant emissivity and ignoring the small correction (<0.5%) due to the finite filter width. This diagnostic was the only one to show clear entry and exit from the two-phase region. The fact that each temperature-enthalpy trace passes through the end points of the lower energy traces indicates that the sample was near thermodynamic equilibrium at all times during each shot. Similar behavior is observed in volume enthalpy curves.

In addition to the EOS points for tantalum up to 8000 K, we have measured the parameters listed in Table 1. The slope of the melting line was calculated from the Clausius-Clapeyron relation.

Our plans for the next quarter are to apply the same techniques to measurements on stainless steel (304) and to uranium (D-38). Data on uranium to 0.2 GPa without pyrometry were reported in an earlier progress report.¹⁵ Stainless steel is a commonly used structural material for which essentially no liquid phase data is available. Presumably the lack of liquid data is because of the difficulty of maintaining a stable melt composition. Since our experiments are complete in 50 μ s, we should have no problem observing the melt region and the liquid phase.

We are also presently constructing a new three-phase EOS model that will be fitted to experimental tantalum data and will be used in hydrodynamic calculations. Our approach is to use the Hoover soft-sphere theory as the basis for both solid and liquid equations of state. The solid EOS is a Gruneisen model using the soft-sphere zero-Kelvin isotherm. This isotherm is determined by fitting it to the experimental Hugoniot. An infinite number of such fittings are possible, and the most appropriate one is chosen

Table 1. Thermophysical Properties of Liquid Tantalum.

Heat of fusion	$\Delta H_f = 0.20 \pm 0.02$ MJ/kg
Volume change on melting	$V_L/V_S = 1.05 \pm 0.01$
Resistivity change on melting	$\rho_L/\rho_S = 1.13 \pm 0.02$
Resistivity of liquid	$\rho = 130 - 150$ $\mu\Omega \cdot \text{cm}$ from 3270 to 6000 K
Heat capacity of liquid	$C_p = 3.9 \times 10^{-4}$ MJ/kg $\cdot$ K from 3300 to 7000 K
Slope of melting line	$dT_m/dP = 49 \pm 10$ K/GPa

Fig. 17. Enthalpy vs temperature for tantalum at 0.1 GPa.

on the basis of the predicted volume dependence of the Gruneisen γ and the compatibility of the solid with the liquid in the form of the melting curve. A liquid-vapor two-phase construction will be included and electronic specific heat terms added as necessary. Hopefully the model will accurately represent both the compressed and expanded thermodynamic states.

Measuring the Melting Point of Shocked Iron (L. Hord)

The melting point of iron at very high pressures is an important parameter in the understanding of the Earth's interior. Shock experiments have been designed to measure lateral rarefaction wave velocities that could give indication of melting at high shock pressures.

Samples of iron have been shocked to pressures greater than 300 GPa (3.0 Mbar) by impacting tantalum plates that were accelerated by the two-stage light-gas gun. Lateral rarefaction wave velocities were measured at these pressures in the samples and compared with plastic-wave sound velocities calculated from the iron Hugoniot. The measured rarefaction velocity should be equal to the plastic sound velocity when melting has occurred and the shear strength reduces to zero.

Results of these experiments show that the rarefaction velocity measured at 310 GPa (3.1 Mbar) is very near the plastic sound velocity calculated by the Russian Al'tshuler, et al. This would suggest that melting has occurred in the shocked iron. Further calculations of the plastic sound velocity are being made by D. Young.

Some experiments at lower pressures have been done, and they also compare closely to the earlier measurements of the Russians. However, the technique being used here does not appear to be sensitive enough to determine the discontinuity of the rarefaction velocity due to melting.

The difficulties being encountered are with the argon flash gap technique used to record shock wave arrivals. Variations in shock pressure applied to the argon also varies the light output of the flash gap. Recording such variations of light on Polaroid film becomes very difficult.

Some of the problems of light intensity variation can be solved by using a totally reflecting prism and an auxiliary light source for the shock wave arrival indicator. With this system, the light source intensity can be set in a dry run situation. Some experiments using the totally reflecting prisms are being assembled for testing.

High-Pressure Hugoniot Measurement (A. C. Mitchell, T. J. Ahrens, and N. L. Rector)

A proposed add-on experiment for the Edam event has been designed. Its purpose is to test instrumentation for future underground EOS experiments. The experiment consist of several circuits that are attached to sapphire shock-wave detectors (pins) and designed to survive in a high radiation environment.

After considering various possible objectives for an initial add-on experiment, we decided to investigate the behavior of one type of shock wave detector (sapphire) subjected to a large γ -radiation and neutron flux. The time of interest in these measurements occurs 1-50 μ sec after nuclear time. There are very little data on the properties of materials in this environment.

We are designing a diagnostic system to probe this hostile environment. One of the most promising diagnostics is a pulsed power source (No. 3 in Fig. 18). There are three advantages of this system:

- (1) It is possible to apply excitation to the pin after nuclear time, and hence, to avoid the large initial photoconductivity signals.
- (2) The circuit is relatively insensitive to radiation-induced signals.
- (3) It is possible to have more than one pin signal per cable.

The operation of this circuit is simple. If the pulse traveling down the cable senses an open circuit, it is reflected with a return pulse twice the voltage of the original. When the pin shorts, the pulse will drop to zero. One of the main problems here is identifying the location of the short, i.e., whether it occurs at the pin or in the signal cable connected to the pin. For clarification of the location of the short, we have added circuit No. 5, which consists of a signal cable ending at a junction box located above the pins.

Another circuit (No. 2) is a 100-MHz interrupted oscillator. This is a tuned oscillator circuit. In this case the pin length is $\lambda/2$, where λ is the wavelength of the oscillator signal. When the end of the pin is shorted, the circuit is detuned, and a change in signal amplitude is recorded. The advantage of this is a distinctive sine-wave signal shape which may be easier to identify in the presence of noise.

An alternative scheme (No. 1) has common mode rejection, which may reduce the background noise significantly. This circuit requires a transformer that must survive in a high radiation environment. Both circuits, No. 1 and No. 2, require one high-quality signal cable each as well as rf components not common to the Nevada Test Site. To check shorting above the pin or common mode transformer failure, circuit No. 4 is added.

Assisting this program are W. J. Nellis of B-Division who is designing a shock-wave generator, and J. H. Mallett of L-Division who is advising on the field operations. D. Faraudo of the EE Department is assisting in the electronics design.

Fig. 18. Pin-diagnostic test for Edam event.

Compilation of Shock-Wave Data (M. van Thiel)

A number of high-pressure EOS compendia exist. Only two, however, list the actual Hugoniot data from which our EOS models are derived:

- A Los Alamos Scientific Laboratory (LASL) compendium consisting of an up-to-date microfilm file of all data taken by the M-6 group.
- An LLL compendium of selected evaluated data from all laboratories producing significant results reportable in published and internal reports.

While the LASL compendium is restricted to AEC use because it contains much unevaluated data, the LLL compendium has an unrestricted distribution.¹⁶

The LLL compilation is being updated with the additional information now in the literature. The existing compilation consists of 393 entries. In addition to that number, there are 70 entries in preprint form that can be distributed without indexes to interested parties. An estimated 100-150 entries are to be extracted from the available literature for inclusion in this file. These papers cut across all disciplines interested in high pressure, as may be inferred from the types of materials studied. These vary from elements through intermetallics, carbides, oxides, silicates, and other minerals and mineral mixtures to organic compounds and their mixtures.

The major countries involved in high-pressure shock-wave research are the US and the USSR. Some work has been done in France, Sweden and England, but the current effort is low. A potential source of information is Japan, where a number of shock-wave sites (explosive and gun) are being built or are in operation. Some of the Soviet literature is not readily available. A special effort will be made to recover this work.

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IV. DYNAMIC MATERIALS RESPONSE GROUP
(W. M. Isbell, Group Leader)

The studies of the Dynamic Materials Response Group are concerned with the response of materials to a wide range of pressure, time, and temperature. Our approach in these studies is characteristic of H-Division methods, i.e., combining theory, computations, and experiments to provide computer simulation of complex phenomena major efforts include: (1) constitutive modeling and experimental characterization of porous metals, (2) advanced experimental diagnostics for shock-wave and electron-beam studies, and (3) development of gages for measurement of impulses created in underground test environments.

Recent developments include:

- Completion and experimental verification of a new constitutive model for wave propagation in porous materials.* The model, when applied to two types of porous beryllium, has provided excellent correlation with experimental measurements. Application of the new model to other porous materials, including geologic materials, is relatively straightforward.
- Completion of experimental studies of stress generation in porous metals arising from rapid radiant energy deposition.* New laser and calorimetric diagnostics were developed to measure the response of porous beryllium to pulsed electron-beams. The results of these tests will be used to evaluate the accuracy of the energy-dependent portions of the model described above.
- Beginning of a computational study to predict the damage to reentry vehicle structures caused by the internal impulse arising from warhead/RV interaction.* Calculations will be performed to assess RV damage as functions of dimensions of the internal gap, use of foam as gap fillers, etc., using a hydrocode that incorporates the model described above.
- Completion of an interferometric system capable of measuring shock-wave parameters at megabar pressures. The system is presently being tested using the H-Division two-stage light-gas gun to determine the maximum pressures at which this instrument will be useful.
- Beginning of a study of melting in copper and iron under shock-wave loading. The validity of several competing models for melting of metals at high pressures can be determined by measurements of the pressures at which metals melt under shock compression. The new interferometer, if it proves capable of making measurements at sufficiently high pressures, will be used to determine the melting pressures of copper and iron along the Hugoniot.
- Completion of an experimental evaluation of the electromechanical risetime of a recently developed impulse gage for use in underground testing.* The response of the TRIM (Time-Resolved Impulse Measurement) gage to short duration

* Indicates projects wholly or partially funded by the Defense Nuclear Agency (DNA).

impulses was measured using a gas gun to deliver 2- μ s stress pulses and a dual-beam laser interferometer to measure the motion of the specimen and of its carrier.

- Beginning of a computational/experimental study to examine possible sources of discrepancies in previous impulse measurements and to determine the characteristics of gage construction most likely to enhance the risetime of impulse gages.*

Details of some of these studies are described below.

Development of a Diffuse Surface-Velocity Interferometer (W. M. Isbell)

The H-Division version of the VISAR system has been completed and is undergoing its first series of performance tests. The initial tests will determine the maximum pressures in copper and iron at which the interferometer can be used to measure the free-surface velocity of a shocked specimen.

Laser interferometry has been used for several years now as a basic tool for measuring velocity-time histories of surfaces of shocked specimens. The systems have become capable of high resolution of both time (~ 1 ns) and velocity (better than 1%). Interferometric systems used previous to the present VISAR (Velocity Interferometry System for Any Reflector)[†] have had severe limitations on their use in any but the most rigidly controlled systems because of the following:

- The necessity of maintaining a mirror finish on the specimen surface. This rules out pressures much greater than ~ 10 GPa (~ 100 kbar), where the surface becomes diffuse upon the arrival of the shock wave.
- The decrease in measuring ability with even small amounts of specimen surface tilt. This prevents measurements involving motion in more than one dimension.
- The small depth-of-field. This restricts measurements to only a few millimeters of specimen motion.

The new VISAR system circumvents these problems and may be used to provide highly accurate measurements at high pressure [>100 GPa (>1 Mbar)], high tilt (multi-dimensional motion), and large depth-of-field (e.g., providing velocity-time measurements of projectiles accelerating down long launch tubes).

A compact version of the VISAR is shown in Fig. 19. A 4-W single-frequency laser is mounted on a table beneath the interferometer. Associated electronic instrumentation is located in adjacent racks. The interferometer design stresses portability, mechanical stability, and ease of operation.

In operation, the VISAR is placed near the specimen (distances from 1 to 30 m are common), and the laser beam is focused on the diffuse specimen surface through

* Indicates projects wholly or partially funded by the Defense Nuclear Agency (DNA).

[†] VISAR was originally developed by L. M. Barker, formerly of Sandia Laboratories, Albuquerque.

Fig. 19. Compact version of VISAR.

expendable mirrors. The light, doppler-shifted by the motion of the surface, is recollimated and returned to the interferometer where interference fringes are formed and are recorded by a photomultiplier tube and oscilloscope system. Analysis of the quasi-sinusoid traces on the resulting oscillogram is performed using a digitizer and a user-interactive computer routine. References 17 and 18 describe in detail the operation of the VISAR.

Numerical Studies of Wave Propagation in Porous Beryllium (F. H. Ree)

We report our final constitutive model of wave propagation in porous metals. It is based on similar models of Herrmann and Holt, but the new model features (1) inclusion of deviatoric stresses, (2) an option for porosity-dependent relaxation time for pore closure, (3) elastic reopening of the pores, and (4) an improved plastic compaction function.

A thin layer of porous material, coated over a solid substructure, can be used to protect the substructure against high-intensity, short-duration shock waves arising from either mechanical or other types of rapid energy deposition (e.g., sudden heating of a warhead or a reentry vehicle under x-ray attack). For such applications, it is essential to carry out computer simulations using a mathematical formulation that can accurately predict the dynamic behavior of porous materials. The DNA requested such investigations to be carried out by H-Division. Some preliminary investigation on sintered porous beryllium was reported in the preceding Quarterly Report.³

The model has been applied to plasma-sprayed porous beryllium in the as-sprayed condition (~14% porosity) and after sintering (~10% porosity). Wave profiles generated from plate impact experiments by Isbell and Horning were used to test the model under different experimental conditions. Profiles were obtained by impacting a polymethyl methacrylate (PMMA) plate onto either sintered or as-sprayed porous beryllium having carbon-Kapton in-material gages embedded at as many as six different depths within the materials. The gages were located as deep as 19 mm from the impact surface and some measurement times extended up to 4 μ s. The resulting 21 wave profiles – both attenuated and unattenuated – represent large variations in the physical parameters and enabled us to extensively test the model.

Figures 20 and 21 show comparisons between measured and computed wave profiles at high (1.7 GPa) and low (0.6 GPa) peak stress levels for as-sprayed porous beryllium. As in the case for sintered porous beryllium, (see the preceding Quarterly Report), agreement between the experimental wave profiles and those predicted from the present model is good both quantitatively and qualitatively. Slight deviations between the experimental and computed wave profiles lie mostly within the combined errors of the model and the experimental data. The largest deviations occur in the cases where the measurements were taken at impact surfaces (shot BT-A in Fig. 20 and shot BT-B in Fig. 21). We attribute the observed differences to anomalies in the experimental measurements, since the peak stress recorded in the gages lie below the peak stresses

Fig. 20. Attenuated wave profiles of the high-stress shot (shot BT) for as-sprayed porous Be: (a) experimental gage records, (b) impactor-target geometry, (c)-(h) comparison of measured and computed wave profiles at different target thickness.

Fig. 20. Continued.

Fig. 21. Attenuated wave profiles of the low-stress shot (shot BR) for as-sprayed porous Be: (a) experimental gage records, (b) impactor-target geometry, (c)-(g) comparison of measured and computed wave profiles.

Fig. 21. Continued.

recorded deeper within the material. (Compare the peak stress levels between shots BT-A and BT-B in Fig. 20 or shots BR-A and BR-B in Fig. 21.) Microstretching of the gages or macrostretching of the gage leads may account for an apparent lower stress at this surface. From Figs. 20 and 21, we note that both the compressive characteristics (wave arrival time, risetime of shock, and peak stress) and the release characteristics (arrival time of release wave and general attenuated wave shape) of shocks have been reproduced satisfactorily under different experimental conditions.

We have also investigated the influence of the in-material gage on wave profiles. Although the gage itself is very thin (≤ 0.1 mm), the discontinuity at the plane of the gage alters the wave profiles in several important ways. This is illustrated very clearly in Fig. 22, where two computed wave profiles corresponding to shot BR-D (Fig. 21) are superimposed along with the experimental wave profile. One of the computed profiles included the gage in the calculation, while the other was taken at the same position but without the gage. The importance of including the gage in a numerical wave-propagation calculation shows up rather clearly in this example. First, because the gage requires a finite ring-up time to bring the stress to that of the surrounding material, the presence of the gage reduces the measured peak stress of the attenuated wave by 0.03 GPa. The result will be substantially increased predicted attenuation. Second, the gage tends to smooth out the rather pronounced release characteristics that are calculated for the case without the gage. This release behavior gives a false impression that the material seems to be "suddenly" slowing down the release wave. As is clear from Fig. 22, this is, of course, not true; rather, the behavior is due to a time delay for the gage to "ring down," a process opposite to the ring-up process.

To obtain the correlations shown in the preceding figures, an accurate knowledge of the EOS of the impactor, gage, buffer, and backing materials was required. No satisfactory EOS expressions of these materials were available in literature. We obtained analytical EOS expressions of these materials (given in Table 2) by using a least-square fitting procedure from the original experimental Hugoniot data. These equations, their ranges of applicability, and references on the experimental sources are filed in the H-Division reference files.¹⁹⁻²²

In summary, the model constructed describes wave propagation in both sintered and as-sprayed porous beryllium layers within necessary accuracy. A computer program describing the model was included as a constitutive model in the hydrocode KO. Theoretical and computational details of the model have been documented in two LLL reports.^{23,24}

Fig. 22. Comparison of measured (dash line) with two computed wave profiles for shot BR-D (sintered porous Be): solid line is computed profile with the carbon-Kapton gage, and dotted line is computed profile without the gage.

Table 2. Expressions for equations of state of carbon-Kapton in-material gage, fused quartz, X-cut quartz, and PMMA. [P = pressure (GPa) E = internal energy per original volume (GPa).]

Material	EOS ^a	ρ_0 (g/cm ³)
Carbon-Kapton	$P = 4.310\mu + 1.904\mu^2 + 294.3\mu^3$	1.33
Fused quartz	$P = 77.56\mu - 480.7\mu^2 + 3074\mu^3 + 7.52E$	2.201
X-cut quartz	$P = 86.66\mu + 45.87\mu^2$	2.65
PMMA	$P = 10.09\mu + 6.272\mu^2 + 85E$	1.184

^aP = pressure (GPa), E = internal energy per original volume (GPa), and $\mu \equiv (\rho/\rho_0) - 1$.

Electron-Beam Techniques on Porous Beryllium (O. Walton)

Two series of exposures of plasma-sprayed beryllium to pulsed electron beams have been carried out using material in both the sintered and as-sprayed condition. The displacement-vs-time history of the free surface of each rapidly heated sample was monitored using an interferometer system of "diffuse" surfaces instead of mirrors. As expected, pronounced differences were observed in the responses of the two types of porous beryllium to the rapid (~70 ns) deposition of energy.

The semi-empirical model used to describe the properties of porous materials in present hydrocodes are based on data obtained primarily from experiments done at room temperature. The changes in these properties on heating has been hypothesized by simple mathematical expressions, but little data exist to test the validity of these expressions. Pulsed electron-beam exposures, with all of their complexity and uncertainty, are one of the few techniques available for laboratory study of the properties of rapidly heated porous materials.

The DNA-sponsored program on porous beryllium has included the development of experimental measurement techniques particularly suited for obtaining porous material property data in a hostile electron-beam environment.²⁵ We have developed and demonstrated three configurations of a DISAR (Displacement Interferometer System of Any Reflector).^{25,26} These interferometers use the "micro mirrors" of an apparently diffuse metallic surface, and obtain interference fringes in the speckle pattern reflected when an intense laser beam is focused on such a surface. We have also been developing and testing several alternative designs for thermocouple-monitored depth-dose foils that can be fielded simultaneously with a sample to give a measure of the energy density obtained in the sample independent of the notorious shot-to-shot lack of repeatability of pulsed electron beams.

Porous beryllium samples in both the as-sprayed and sintered conditions have been exposed in two test series on the pulsed electron-beam facility in building 169 at LLL. The high electron energies (~ 2 MeV) produced the desired almost flat energy deposition profile through the entire 3.6-mm-thick samples. Higher free surface velocities coupled with faster relief velocities for the sintered material imply that significantly greater pressures were generated in that material. The interpretation of this data in terms of internal pressure and elastic and plastic wave velocities will be done by modeling the experiment with the KO hydrocode using the new models for both as-sprayed and sintered beryllium developed by Ree.²³

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COMPUTER SIMULATIONS GROUP
(D. M. Norris, Group Leader)

This newly created group is responsible for calculations in the area of solid mechanics. The objective is to build in-house expertise both in the Lagrangian finite-difference HEMP-type codes and in the finite-element codes traditionally used in structural statistics and dynamics. Emphasis at this time, in addition to particular interesting applications of the software, will be to disseminate the division's software and to educate potential users.

HEMP Ground Motion Simulation of the Portmanteau Nuclear Test (D. M. Norris, M. Wilkins, and P. Weidhaas)

HEMP calculations are underway to simulate ground response from the Portmanteau nuclear test. Preliminary calculated surface velocity and spall correlate well with experimental data.

The HEMP Portmanteau calculation is designed to verify the codes's ability to predict complex ground motion surface effects from underground nuclear explosions. The calculation is the first of two calculations directed to the feasibility of full-scale missile silo testing. The work is supported by D-Division.

The HEMP Portmanteau calculation has been run to 1.6 s of actual event time. As may be seen from experimental vertical acceleration data of Fig. 23 obtained at surface ground zero (SGZ), this time carries the calculation beyond the surface wave arrival at about 300 ms and beyond the initial acceleration spike ending about 600 ms. The calculation is well into the spall time zone corresponding to the constant -1-g acceleration between about 1.5 ms to 2.5 ms (see Fig. 23).

The HEMP zoning is described in Fig. 24 which is a picture of the deformed mesh at 600 ms. We use 5498 zones in the calculation with the left boundary the axis of symmetry, the upper boundary the free surface, the lower boundary the paleozoic rock, and the right boundary a roller boundary at 1733 m. The instrumentation location (simulated silos) may be seen at the surface. The dark horizontal lines represent different material interfaces taken from the geologic containment report. The calculation was started with an overlay onto the HEMP grid from a one-dimensional SOC code calculation edited at 50 μ s.

A comparison of some preliminary results with experimental data are shown in Fig. 25. Here vertical velocity response at Station 1 at SGZ is shown vs time. Comparison plots are made of the HEMP calculation, a SOC calculation by R. Simon of K-Division and the experimental velocity data provided by G. Jackson of Nuclear Test Engineering Division. The upper diagonal line is the slope associated with the velocity due to a 1-g fall-back from spall.

The arrival of the surface velocity wave and the return to zero appear to correlate well with the experimental data. The calculation is correctly capturing the spall phenomenon. The predicted surface velocity is high by about a factor of three which

Fig. 23. Vertical acceleration at Portmanteau SGZ.

Fig. 24. HEMP mesh at 600 ms.

Fig. 25. Vertical velocity response at Station 1 at SGZ.

indicates more energy is arriving at the surface than we actually experienced on Portmanteau. Cavity growth appears normal.

Figure 26 is a contour plot of relative volume. The zones in the shaded area have increased in volume over their original volume which is a measure of the spall effect. The picture is at a time of 1 s. Figure 27 is a velocity plot at the same time.

We are in the process of plotting and interpreting the output before proceeding with the calculation. Since the calculation is relatively inexpensive at 100 min computation for 1 s real time, and is running well, we would like to carry it on beyond the "slap down" acceleration spike occurring at 2.5 s. Consideration is also being given to a second iteration on the calculation with some variation in the constitutive equations. We think it is premature to do this until we have examined all the output in more detail.

We feel we have proceeded sufficiently far with this calculation to assess the HEMP code's ability to do the silo simulation problem. This decision will be made in January 1975.

Three-Dimensional Heat Transfer Code Development (P. Grantham and D. Norris)

Improvements have been made in the HEAT3D finite-element computer program for transient heat conduction analysis.

The HEAT3D code was developed to do thermal stress analysis of three-dimensional structures. The work is supported by Advance Research Projects Agency (ARPA).

The HEAT3D code has been revised with the addition of an improved temperature diffusion model and with a convective temperature boundary condition. This boundary condition gives the surface temperature flux as proportional to the difference between the structure surface temperature and the temperature of the adjacent gas. The improved code has been checked against an available analytical transient solution with excellent correlation.

Progress with HEMP3D (G. Cronshagen)

The vectorized version is operational on the CDC 7600. The generator is partially coded. Additions have been made for MHD calculations.

To take full advantage of the CDC STAR-100 computer with its "vector" instructions, the three-dimensional hydrodynamics program HEMP3D has been reprogrammed in a "vectorized" form. Using STACKLIB subroutines to emulate STAR instructions, HEMP3D is running the LLL 7600 network. Since the coding has been written to work on both the 7600 and STAR computers, minimal effort should be required to move the program to the STAR. However, since the STAR system is still undergoing tests, initial testing of HEMP3D has been done on the 7600. The program has successfully run the vibrating plate problem detailed in a report.²⁷ Since the problem generator is not finished, and since problem (i.e., vector) sizes may affect the efficiency of the program, no definitive timings have been made to compare the vector and serial versions.

Fig. 26. Relative volume contours at $5 = 1$ s. Shaded zone is $V/V_0 > 1$.

Fig. 27. Velocity vector plot at $t = 1$ s.

To do a problem using HEMP3D, the program must have a file containing the geometry of the object under analysis, and initial and boundary conditions for the problem. Taking the grid from the mesh generator, VMESH3D, and input from the user with boundary and initial conditions, the program GEN3D will produce the problem file HEMP3D needs. The programming for GEN3D is approximately 50% complete. It will allow the user to generate problems with multiblock geometries, as well as a side range of initial (material, vector, tensor) and boundary (pressure and velocity profiles) conditions. This program should be completed by January 1975.

Magnetic-field equations have been added to the vectorized HEMP3D, in order to calculate the MHD instability of a cylindrical plasma. The analysis is under the direction of C. Hartman. Additional terms, due to magnetic field, are calculated using first-order differencing, and these terms are added into the calculation of total stress. Thus the changes in the magnetic field are due to hydrodynamic effects only.

Graphics Improvements in VPIX3D (G. Cronshagen)

A hidden-surface algorithm has been added that reduces storage and time requirements by one-half.

The graphics program, VPIX3D, used to display the results of problems run on HEMP3D, has been greatly improved. A new algorithm has been added that computes the direction of surfaces prior to passing them through the hidden-surface subroutines. Since approximately 5% of each picture is usually facing away from the viewer, this portion need not be processed. The result is production of pictures in half the time using half the space. Since less space is required and if this space is held fixed, much larger objects can be displayed. This addition, as well as the others, places VPIX3D in the forefront of programs of its kind.

Three-Dimensional Analysis of a Turbine Stator (P. Grantham, W. Feng, and D. Norris)

The thermal heat-transfer analysis of a turbine blade has been completed.

The thermal-stress analysis of three prototype turbine stator blades is underway for the Ford Motor Company under contract to ARPA. The problem taxes the capability of LLL computers and represents one of the largest three-dimensional calculations being run in the country. The three problems examine the effect of support boundary conditions on the turbine blade's thermally induced stress field.

The heat transfer analysis of one design blade has been completed (see Fig. 28) and simple checks are underway to examine the accuracy of the results. These checks include two-dimensional plane strain analyses (see Fig. 29) of the blade cross section and blade-shroud intersection using the DTVIS2 finite-element code.

(a) Stator surface, $t = 0.5$ s

°F
 A = 14.07
 B = 173.5
 C = 332.8
 D = 492.2
 E = 651.6
 F = 811.0
 G = 970.4

(b) Stator cross section, $t = 0.5$ s

(c) Stator surface $t = 1.5$ s

°F
 A = 125.5
 B = 357.9
 C = 590.3
 D = 822.7
 E = 1055
 F = 1288
 G = 1520

(d) Stator cross section, $t = 1.5$ s

Fig. 28. Temperature contours for the turbine stator with convection boundary conditions.

Fig. 29. Thermal stress analysis of the cross section of a turbine stator blade (time = 0.16 s).

Future work will complete the stress analysis with the SAP3D finite-element stress code at a specific time-edit from HEAT3D. The other two blades will also be calculated. We are also planning to study the effects of temperature-dependent material properties and radiation boundary conditions. We are considering the modification of HEMP to do a continuous stress analysis following the temperature loading.

HEMP and Finite-Element Code Comparison Studies (D. Norris)

Comparison structural-response calculations are underway to define the limitations of these two classes of software for engineering accident studies.

The finite-element codes have traditionally been used mostly in static or vibration types of structural analysis. Only recently has attention been directed to large deformation, large strain, and nonlinear type of constitutive behavior for applications in nuclear reactor type accident environments. The implicit time-solution scheme of most of this class of software has precluded wave-propagation-type analyses because of computer costs inherent in the inversion of large banded matrices at each time step.

Recent improvements in these codes makes them competitive with the HEMP-like finite-difference codes. This is done by using the finite-element procedure to discretize the spatial variables but makes use of the explicit type of time domain solution.

Studies are underway with Nuclear Test Engineering Division to determine the limits of applicability of the two types of codes. Comparisons have been made with HEMP, TOODY, NONSAP, and HONDO for an elastic/plastic deformation of a pipe with internal pressure and with one end fixed (see Fig. 30). Considerable differences have been noted in the response between the two classes of codes.

Fig. 30. Deformed elastic/plastic pipe under internal pressure loading.

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VI. SPECIAL PROJECTS GROUP
(M. L. Wilkins and C. R. Henry)

In the Special Projects Group, individuals or small groups work on new projects or special problems. The work is relatively short-term and does not logically fit into the other four H-Division groups. Projects underway include calculations on stress intensity factors in crack propagation, an improved materials properties model, a liquid metal EOS, and significant effort on various three-dimensional programs for the STAR-100.

Numerical Analysis of Underground Explosions (M. Kamegai)

The development of a computational scheme for underground explosions is in progress using a two-dimensional Lagrangian code, HEMP. This report describes the present status and the future plan for this program.

The basic format of the problem is shown in Fig. 31. A grid technique has been developed that permits polar zones to be linked with quadrilateral zones using an automatic zoner. Figure 32 shows an example of such grids. The initial phase of the explosion has spherical symmetry. Thus the polar grid allows the hydrodynamic motion to be calculated with high accuracy. The rectangular grid is provided to give better representation of motion during the two-dimensional aspects of the problem in a later phase. The transition from the polar grid to the rectangular grid is accomplished by a two-way slide plane.

We tested the grids by placing a 4184-TJ a (1-Mt) energy source in region I. A gamma-law gas EOS with the normal rock density was assumed to hold in this region. An elastic Hugoniot EOS for granite was given to regions II and III. Figures 33 and 34 show that the source expanded very smoothly, crushing the material around it. (This computation was done merely for the purpose of testing the grid. A. Leiber of B-Division coded the grid scheme, and N. Wilt ran the HEMP calculation.)

To properly account for the thermodynamic processes that the earth materials undergo in the vicinity of the explosion, a multiphase EOS was introduced which permits the materials to evaporate when the Hugoniot energy exceeds the heat of vaporization. Figure 35 shows such an equation and its unloading paths. Region 1 of the Hugoniot is an elastic region. Region 2 represents the pore-closure which is a process common to most earth materials. The equation is constructed in such a way that the unloading path smoothly approaches a gamma-law gas equation if the Hugoniot energy exceeds the heat of vaporization.

As future work, we plan to do the following:

- Develop links from one-dimensional explosion calculations on MEG to the HEMP polar grid. The MEG calculation includes thermal and radiative diffusion, and the thermal effects of neutrons and hydrodynamics.

Fig. 31. Problem configuration: region I is source; region II is ground in polar grid; region III is ground in rectangular grid.

Fig. 32. Polar-rectangular grid for underground explosion calculation.

Fig. 33. A 4184-TJ (1-Mt) source explosion at 0.3 ms.

Fig. 34. A 4184-TJ (1-Mt) source explosion at 0.7 ms.

Fig. 35. Rock equation of state: region I is elastic; region II is pore closure; region III is compacted state; region IV is gas.

- Develop constitutive models to describe mechanical and thermal behavior of the earth materials. Rock fracture and pore formation may be modeled by failure envelopes and cap model. A three-phase EOS, such as the Gray equation, must be introduced to properly account for the thermodynamic processes.
- Introduce thermal diffusion calculation for long-term steady state process as well as prompt thermal and radiative diffusion process.

CEL-HEMP Calculation of Subsurface Explosion (M. Kamegai and J. Hobson)

The objective of this problem is to study the air blast and ground motion for subsurface explosions. Since the depth of burial is shallow, a violent mixing of dirt and air is expected to take place.

The two-dimensional coupled Eulerian-Lagrangian code, CEL-HEMP, has a unique capability in that a single problem can be divided into Eulerian and Lagrangian regions, thus utilizing the advantages of both schemes. The material mixing near the explosion may be calculated with an Eulerian grid, while the ground motion is calculated with Lagrangian mesh. Figure 36 illustrates the problem. The shaded areas are the Lagrangian regions and the unshaded areas are the Eulerian regions. A tracer line marks the separation between air and ground in the Eulerian region.

The initial configuration is shown in Fig. 37. The effect of a 4.184-TJ (1-kt) energy source was examined in this problem. A gamma-law gas EOS with $\gamma = 1.33$ was assumed to hold in the source while an elastic EOS with a modulus of 54.9 GPa (549 kbar) was used for the ground. The air was assumed to be an ideal gas ($\gamma = 1.4$).

A large upward ground motion is clearly observed in the two successive snapshots of the calculation (Figs. 38 and 39). An air blast is propagating into the atmosphere.

An important omission in this calculation is thermal effect by radiation diffusion. The radiation heating is expected to have significant effects on the air blast for shallow subsurface explosions.

Future work that we plan is as follows:

- Calculation of the thermal effect by radiation diffusion.
- Application of the MEG output calculation of device to the source.
- Improvement of the EOS of the earth material.

Studies in Fracture Mechanics (W. G. Hoover and W. T. Ashurst)

Brittle fracture is being simulated using molecular dynamics to follow the motion of 1000 particles linked by Hookean springs. Fracture propagation and structure are being studied with computer-generated plots and movies.

To improve our ability to understand and describe fracture, we have studied fracture simulation based on simple force laws. We use statistical mechanics to study static cracks, and molecular dynamics to study moving cracks. The static work is described in a recent report.²⁸ We found that our cracks are consistent with

Fig. 36. Subsurface explosion for 4.184-TJ (1-kt) source.

Fig. 37. Initial configuration for subsurface explosion.

Fig. 38. Subsurface explosion at 0.6 ms.

Fig. 39. Subsurface explosion at 1.06 ms.

the predictions of linear elastic theory for crack energy and shape and with the predictions of statistical mechanics for crack entropy. The dynamic results are more complicated because a variety of boundary conditions and loadings can be used. So far we have confirmed the simple notion that increasing the breaking strength of the springs causes one to move from (1) the region of unstable catastrophic propagation through (2) the region in which cracks propagate at speeds not far from the Rayleigh speed to (3) the region in which cracks will not advance. Most of the calculations indicate forking (see Fig. 40), in which a crack propagates for some distance in a direction normal to the applied tensile stress, and then divides to form two or more cracks diverging from this direction. Movies of the propagation are being made, and we are embarking on a sensitivity study of the effects of:

- Nonlinearity in the interparticle springs.
- Nonzero initial temperature in the crystallite.
- Viscous dissipation in the interparticle springs.
- Plasticity, though we are not certain how this is to be introduced.

In addition to studying the relative importance of these effects in influencing crystal damage, we expect to use other boundary conditions (all calculations so far have used uniaxial tension) and to generate fracture failure envelopes for these simple models.

HEMPMHD (P. V. Grantham and M. L. Wilkins)

The difference equation for the thermal diffusion in HEMPMHD can be shown to have second-order accuracy.

Three test problems have been completed to verify the general accuracy of the method when a non-regular grid is used.

- Figure 41(a) shows the initial grid and calculated temperature contour from a spherical source.
- Figure 41(b) shows results of the same problem with an initially distorted grid.
- Figure 41(c) gives results for a calculation with a slide line present in the grid.

It is seen from the contour plots that the calculated results are the same in these three problems.

A review of the method used to calculate diffusion across slide lines has shown that the technique can be readily extended to include the two-way sliding in the HEMP program. Work is in progress to include two-way sliding in the thermal-diffusion calculations.

A Scheme for Developing the Nonlinear Heat-Eulerian Code for the STAR-100 (L. Truong)

This project is to develop a nonlinear heat-vector code for use on the CDC STAR-100 computer because the existing heat codes are not in vector modes. This report presents the completed scheme for the code, and to my knowledge, the ideas in this scheme are new.

Fig. 40. Typical crack pattern in a two-dimensional crystallite under horizontal uniaxial tension (vertical boundaries under constant load; horizontal boundaries periodic). The particles are joined by Hookean springs that break at preassigned stretch. The displacements of the particles are greatly exaggerated in order to make the cracks easy to see.

Fig. 41. Contour plots for three test problems to verify the general accuracy of the finite-difference method of HEMPMHD code when a non-regular grid is used.

Thus far only the two-dimensional case is being considered. The three-dimensional case can be extended from the two-dimensional one in a more or less straight-forward manner, with some work.

Specifically, the equation being considered is

$$a(u) u_t = \text{div} (f(u) \text{grad}(u)) ,$$

where $u(x, y, t)$ is the heat distribution on some rectangular region defined in the usual sense, and all necessary conditions are satisfied so that the solution of u exists. My proposed scheme is based on the alternating direction implicit (ADI) method. Split the above equation by the usual ADI method, resulting in two collections, S_x and S_y , of nonlinear tridiagonal systems, where the subscripts denote the direction of the sweep. Because of the nature of ADI, S_x and S_y are coupled collections. Therefore, the structure of all the members of S_x (and the structure of all the members of S_y) are the same. Thus the solutions for all systems in S_x can be obtained as a vector, and the solutions for all systems in S_y can be similarly obtained. A vector analog of the modified Newton iteration then is used to solve the systems in S_x and S_y . The linear systems arising from the modified Newton iteration are tridiagonal. The proposed method for solving the tridiagonal linear systems arising from S_x is a vector analog of some special Gaussian elimination or cyclic reduction, and the solution of the tridiagonal linear systems resulting from S_y can be similarly obtained.

This scheme is now in the process of being coded for testing.

H-Division Data Reduction Center (J. C. Fuellenbach)

The H-Division Data Reduction Center is now in operation and is being used for data collection and reduction. Several programs have been written for these purposes.

The center has been in development for more than a year. It was initiated for use by H-Division personnel to collect and reduce data and to develop hydrocodes. Most of the equipment has been installed for 9 or 10 months, and most of the time since then has been spent on hardware and software interfacing.

Some of the equipment installed are:

- Remote job-entry terminal (RJET).
- PDD-8/E computer.
- Cal Comp plotter.
- Grant film reader.

We are using this equipment to reduce the isobaric expansion experimental data. Programs are being written for data reduction of the two-stage light-gas gun experiment and other H-Division experimental programs.

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