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COMPUTATIONAL UPGRADING

J. H. Van Velkinburgh

DEVELOPMENT DIVISION

JULY - SEPTEMBER 1971

For
System Division, Department 112

MASTER

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This project concerns the upgrading of computer technology to a level commensurate with other technologies at hand, to provide a meaningful link between Development Division and the Data Center, and to assist personnel in their computational needs.

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Section X

COMPUTATIONAL UPGRADING

ABSTRACT

Additions to our data acquisition and reduction facilities and other non-programming endeavors are discussed.

Computer codes designed to aid in the analysis and interpretation of quantitative data which were written or modified this period are also discussed.

DISCUSSION

The DEC PDP 12/30 advanced LINC System was received late this period. The system is now in the process of having final checkout and acceptance procedures done. The PDP 12/30 will provide data acquisition and computational support for the development and research activities pertaining to the thermal properties of high explosives and related materials.

A preliminary study for the acquisition of a semi-automatic optical film comparator system was begun. The optical comparator is to be used for obtaining two-dimensional spatial coordinates of points on streak camera records, oscilloscope records and raster records, and for obtaining optical density versus distance data generated by a high resolution mass spectrometer. The optical comparators being considered will afford a substantial increase in reading accuracy, repeatability and resolution over the present reading system. By upgrading the film reading capability to a level proportionate with the test firing and the data analysis and reduction technology, parameters such as detonation pressure, detonation velocity, output pressures and equation of state data can be obtained to a greater precision than was previously possible. Several possible equipment configurations have been considered, but definite decisions have not been made.

Utilization by Development Division of the CDC 3600 is outlined in Table I. A Utilization Accounting Program was written by Norma Nickerson (Systems Division Programmer) with the first formal report issued by Systems Division in July. Division usage has averaged about 25% of the total available running time. Means for increasing and maintaining an increased usage, especially with respect to number of users, have been explored. Robert Ashcraft will have initial responsibility for providing technical assistance in the operation of the large computer codes such as TRUMP and RUBY. The individual scientists and engineers will, however, still have the responsibility of recognizing potential computerized applications to their own work.

A multi-dimensional thermodynamics code, TRUMP, was made operational for the CDC 3600 late this period. The TRUMP code solves a general nonlinear parabolic partial differential equation describing flow in various kinds of potential fields, such as fields of temperature, pressure, and electricity and magnetism; simultaneously, it will solve two additional equations representing, in thermal problems, heat production by decomposition of two reactants having rate constants with a general

Table I. Development Division Usage of CDC 3600

	<u>June</u>	<u>July</u>	<u>August</u>	<u>September</u>
Total Up Time (hrs)	102.64	106.62	109.74	83.59
Total Time (hrs) Used by Dev.	18.900	25.428	23.039	29.274
Percent Usage by Dev.	18.45	23.85	20.99	34.91
No. of Users in Dev.	4	6	8	17
No. of Runs	224	144	188	228
No. of Programs	22	27	27	21

Arrhenius temperature dependence. Steady state and transient flow in one, two or three dimensions are considered. Problem parameters may vary with spatial positions, time, temperature or pressure. Initial conditions may vary with spatial position. Solutions may be obtained by use of explicit or implicit difference equations or by a combination of both. Computer time can vary from several seconds for very simple problems to several hours for the most complex problems. The code is presently being studied so that several problems of immediate interest may be solved.

A photographic emulsion and developer analysis code, NIXON2 was started. When completed, the code will utilize experimentally derived optical density and exposure data to calculate film speeds and film latitudes at various densities for different emulsions and developing procedures. The code is to employ curve fitting techniques to obtain an analytical expression for the density-exposure relationship which will in turn be used to calculate emulsion developer parameters.

An extensive test series was started on code WONDY. The testing includes comparison of experimental and WONDY calculated results from explosive-inert systems. The inerts used were water and Plexiglas. Equation of state constants used are listed in Table III. The explosives used along with their equation of state constants were listed in Table II. All computer runs assumed a constant gamma law relationship for the detonation and its products. This is, of course, not entirely physically real; however, data for performing calculations with a variable gamma (JWL polynomial coefficients) were not available for all the explosives investigated.

The gamma law predicts the pressure at the Chapman-Janquet point should be

$$P_{CJ} = \rho_0 D^2 / \gamma + 1$$

where ρ_0 is the initial density of the explosive, D is its detonation velocity and γ is its ratio of specific heats. The WONDY code, however, does not produce the pressures in explosives predicted by the gamma law. This was a very disturbing result until the ratio between the WONDY predicted pressure and the gamma law predicted pressure was calculated. It was found that the WONDY pressure in a rectangular coordinate system was about 90% of the gamma law pressure and in a spherical coordinate system was about 74% of the gamma law pressure. The ratios for the explosives tested are given in Tables IV through VII. The same type of phenomenon was found in the peak pressures transmitted to the inerts used although the ratios are different. An interesting fact about the peak transmitted pressures calculated by WONDY is that they are very close to being correct when performing graphical Hugoniot "flipping" if it is assumed that the peak pressure calculated by WONDY is the true detonation pressure. The main result or conclusion of this exercise was that in order to obtain WONDY calculations that have any significant physical reality associated with them presupposes that the user has some idea as to the closeness of agreement between calculated and experimental results. This is especially true of pressure calculations done by WONDY. The calculation of pressure histories was not the main objective which motivated the initial writing of the code; rather it was the calculation of energy histories. However even the calculation of energy histories needs a scaling or proportioning procedure applied when dealing with common explosives. WONDY calculations of all parameters usually are quite deficient when dealing with composite explosives such as aluminized perchlorate systems.

Table II. WONDY Test Parameters

<u>Material</u>	<u>Density (g/cm³)</u>	<u>Sound Velocity (cm/μsec)</u>	<u>Ratio of Specific Heats</u>	<u>Detonation Velocity (cm/μsec)</u>	<u>Initial Energy (Mbar/g)</u>	<u>Wave Width Constant</u>
PBX-9404	1.84	0.880	2.658	0.880	0.06384	2.5
LX-10-0	1.86	0.882	2.859	0.882	0.05422	2.5
LX-04-1	1.87	0.846	2.690	0.846	0.05738	2.5
Comp. B-3	1.72	0.799	2.950	0.799	0.04144	2.5
TNT	1.63	0.693	2.727	0.693	0.03731	2.5
PETN	1.77	0.830	2.576	0.830	0.06112	2.5
HMX	1.89	0.911	2.741	0.911	0.06371	2.5
LX-07-2	1.87	0.864	2.736	0.864	0.05626	2.5
PBX-9011	1.77	0.850	2.761	0.850	0.05454	2.5
Cyclotol	1.75	0.825	2.731	0.825	0.05269	2.5
LX-09-0	1.84	0.884	2.851	0.884	0.05481	2.5
Baratol	2.55	0.487	3.321	0.487	0.01183	2.5
RDX	1.77	0.864	2.909	0.864	0.05002	2.5
Tetryl	1.71	0.785	3.210	0.785	0.03312	2.5

Table III. WONDY Test Parameters

Equation of State Constant	Water	PMMA
1	1.00	1.181
2	0.1483	0.268
3	0.0244	0.033
4	0.000	0.0
5	0.000	0.0
6	0.000	0.4
7	0.124	0.0
8	6.0	0.0
9	0.0	0.0
10	5.47636	1.61
11	17.20215	0.0
12	37.19226	0.0
13	66.60373	0.0
14	106.75552	0.0
15	1.0	1.0
16	0.28	0.97
17	0.0	0.0
18	0.0	0.0
19	0.0	0.0
20	0.0	0.0
21	0.0	0.0
22	0.0	0.0
23	0.0	0.0
24	0.0	0.0
25	0.0	0.0
26	0.0	0.0
27	0.0	0.0
28	0.0	0.0
29	0.0	2.0
30	0.0	0.0
31	0.0	0.0
32	0.0	0.0
33	0.0	0.0
34	0.0	0.0
35	0.0	0.0

Table IV. HE into Water

Rectangular coordinates

	Cal Peak P_{HE}	Cal Peak P_{H_2O}	Exp* Peak P_{HE}	Exp Peak P_{H_2O}	HE/HE Exp/cal	H ₂ O/H ₂ O Exp/cal
PBX-9404	350	210	390	235 ^A	1.114	1.119
LX-10-0	340	190	378	210 ^A	1.111	1.105
LX-04-1	325	190	363	210 ^A	1.117	1.105
Comp B-3	250	170	278	188 ^H	1.112	1.106
TNT	189	130	210	144 ^H	1.111	1.108
PETN	305	190	341		1.118	
HMX	380	220	419	210 ^A	1.103	0.965
LX-07-2	335	190	371	225 ^A	1.107	1.108
PBX-9011	305	185	340		1.118	
Cyclotol	285	185	319	192 ^H	1.119	1.035
LX-09-0	335	190	373		1.113	
Baratol	125	75	140	62 ^H	1.120	0.827
RDX	305	180	338		1.108	
Tetryl	225	140	250	136 ^H	1.111	0.972

Ave=1.113

*Gamma Law Calculation

H = Hugoniot Crossing - See Table VIII

A = Aquarium Data

Table V. HE into Water

Spherical Coordinates

	Cal Peak P_{HE}	Cal Peak P_{H_2O}	Exp* Peak P_{HE}	Exp Peak P_{H_2O}	HE/HE Exp/cal	H ₂ O/H ₂ O Exp/cal
PBX-9404	290	160	390	235 ^A	1.345	1.469
LX-10-0	280	140	378	210 ^A	1.350	1.500
LX-04-1	270	140	363	210 ^A	1.344	1.500
Comp B-3	205	120	278	188 ^H	1.356	1.566
TNT	155	90	210	144 ^H	1.355	1.600
PETN	250	140	341		1.364	
HMX	310	150	419	210 ^A	1.352	1.400
LX-07-2	275	155	371	225 ^A	1.349	1.452
PBX-9011	250	140	340		1.360	
Cyclotol	235	135	319	192 ^H	1.357	1.415
LX-09-0	275	145	373		1.356	
Baratol	105	60	140	62 ^H	1.333	1.032
RDX	250	135	338		1.352	
Tetryl	185	100	250	136 ^H	1.351	1.360

Ave=1.352

*Gamma Law Calculation

H = Hugoniot Crossing - See Table VIII

A = Aquarium Data

Table VI. HE into PMMA

Rectangular Coordinates

	Cal Peak P_{HE}	Cal Peak P_{PMMA}	Exp* Peak P_{HE}	Exp Peak P_{PMMA}	HE/HE Exp/cal	PMMA/PMMA Exp/cal
PBX-9404	350	250	390	260 ^H	1.114	1.040
LX-10-0	340	240	378		1.111	
LX-04-1	325	225	363		1.117	
Comp B-3	250	195	278	216 ^H	1.112	1.108
TNT	189	150	210	167 ^H	1.111	1.113
PETN	305	240	341		1.118	
HMX	380	270	419		1.103	
LX-07-2	335	245	371		1.107	
PBX-9011	305	240	340		1.113	
Cyclotol	285	205	319	218 ^H	1.119	1.063
LX-09-0	335	245	373		1.113	
Baratol	125	85	140	78 ^H	1.120	0.920
RDX	305	240	338		1.108	
Tetryl	225	155	250	158 ^H	1.111	1.055

Ave=1.113

*Gamma Law Calculation

H = Hugoniot Crossing - See Table VIII*A* = Aquarium Data

Table VII. HE into PMMA

Spherical Coordinates

	<u>Cal</u> <u>Peak P_{HE}</u>	<u>Cal</u> <u>Peak P_{PMMA}</u>	<u>Exp*</u> <u>Peak P_{HE}</u>	<u>Exp</u> <u>Peak P_{PMMA}</u>	<u>HE/HE</u> <u>Exp/cal</u>	<u>PMMA/PMMA</u> <u>Exp/cal</u>
PBX-9404	290	190	390	260 ^H	1.345	1.368
LX-10-0	280	180	378		1.350	
LX-04-1	270	170	363		1.344	
Comp B-3	205	155	278	216 ^H	1.356	1.394
TNT	155	115	210	167 ^H	1.355	1.452
PETN	250	190	341		1.364	
HMX	310	205	419		1.352	
LX-07-2	275	185	371		1.349	
PBX-9011	250	185	340		1.360	
Cyclotol	235	160	319	218 ^H	1.357	1.36i
LX-09-0	275	190	373		1.356	
Baratol	105	85	140	78 ^H	1.333	0.920
RDX	250	180	338		1.352	
Tetryl	185	130	250	158 ^H	1.351	1.450

Ave=1.352

Gamma Law CalculationH = Hugoniot Crossing - See Table VIII**A = Aquarium Data*

Table VIII. Hugoniot Relationships

PBX-9404	$U_S = 2.5 + 2.55 U_P$	$\rho_0 = 1.84$
TNT	$U_S = 2.39 + 2.05 U_P$	$\rho_0 = 1.63$
Comp B-3	$U_S = 2.71 + 1.86 U_P$	$\rho_0 = 1.715$
Baratol	$U_S = 3.35 + 2.14 U_P$	$\rho_0 = 2.55$
Cyclotol	$U_S = 8.25 + 0.305 U_P$	$\rho_0 = 1.75$
Tetryl	$U_S = 6.90 + 1.19 U_P$	$\rho_0 = 1.71$
PMMA	$U_S = 2.68 + 1.61 U_P$	$\rho_0 = 1.181$
Water	$U_S = 1.51 + 1.85 U_P$	$\rho_0 = 1.00$

In spite of the fact that pressure calculation done in WONDY must be viewed as relative and not absolute, a plotting routine to generate pressure profiles at various times and a complete pressure distance history was incorporated into the code. Only slight modifications within the code would have to be done in order to plot other calculated parameters. The plotting routine utilizes the high speed printer for output. Fig. 1 and 2 gives a few representative frames of the plots attained. Plotting routine for WONDY and TOODY using the Computer Industries plotter are being generated by Data Center personnel.

FIG. 1. Printer Plots Obtained from WONDY
Pressure (M bar) versus distance (CM)

FIG. 2. Printer Plot Obtained from WONDY
Pressure (M bar) versus distance (cm)