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REQUIREMENTS OF DATA ACQUISITION AND ANALYSIS FOR CONDENSED MATTER STUDIES AT THE WEAPONS NEUTRON RESEARCH/ PROTON STORAGE RING FACILITY

by

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ABSTRACT

With the completion of the proton storage ring (PSR) in 1985, the subsequent increase in neutron flux, and the continuing improvement in neutron scattering instruments, a significant improvement in data acquisition and data analysis capabilities will be required. A brief account of the neutron source is given together with the associated neutron scattering instruments. Based on current technology and operating instruments, a projection for 1985-90 of the neutron scattering instruments and their main parameters are given. From the expected data rates and the projected instruments, the size of data storage is estimated and the user requirements are developed. General requirements are outlined with specific requirements in user hardware and software stated. A project time scale to complete the data acquisition and analysis system by 1985 is given.

I. INTRODUCTION

A proton storage ring (PSR) will be added to the weapons neutron research (WNR) pulsed neutron source at the Los Alamos Meson Physics Facility in 1985. The PSR will increase the time-averaged neutron flux 25 times and the accompanying change in the repetition rate, from 120 Hz to 12 Hz, will increase the instantaneous neutron flux 250 times.

The increase in neutron production together with the improvements planned for the neutron scattering instruments requires a commensurate improvement in the fast data capture electronics and real-time data analysis provided for the neutron scattering instruments.

This report is an initial definition of the data acquisition and computing requirements for the PSR. No description of the source has been given as this is available elsewhere (Ref. 1), although the main parameters of the system have been listed to show assumptions that have been made concerning source strength.

The requirements of the system, data capture and interface presented to the user, are defined. They could be incorporated in a larger request for quotation document when possible suppliers are being sought. For this reason we have not attempted to describe specific manufacturers' hardware or software that might be used in the data acquisition system.

II. SOURCE DEFINITIONS

The overall layout of the WNR neutron source planned for early 1985 is shown in Fig. II-1. This illustrates the three main components of the facility: the PSR, the high-current target, and the experimental areas containing the neutron scattering instruments. The high-current target exists, the neutron instruments are at varying stages of development, and PSR construction has just begun.

To estimate future neutron flux levels we assumed that the proton beam delivered to the target has the characteristics listed below.

Mean proton current	100 μ A
Pulse repetition frequency (PRF)	12 Hz
Proton pulse length	270 ns
Protons per pulse (ppp)	5.2×10^{13}
Proton energy	800 MeV

When 800-MeV protons impinge on a tungsten target they produce approximately 15 neutrons per proton with a primary energy spectrum ranging from kiloelectron volts to hundreds of million electron volts. To produce short pulses of neutrons (1-100 μ s) in the thermal and epithermal region (0.01-10 eV), the target is surrounded by small hydrogenous moderators. A possible moderator configuration is shown in Fig. II-2, together with the numbered flight paths (FP).

Fig. II-1. Layout of the WNR/PSR facility. Condensed matter research uses the high-current target and several of the horizontal time-of-flight paths.

Fig. II-2. A possible target-moderator configuration. The neutron spectrum needs of the instrument can be met by viewing various moderators.

Different groups of instruments require different neutron flux-time distribution characteristics. These are realized by providing three types of moderator that have different dimensions, compositions, and temperatures. The expected coupling parameters (thermal neutrons produced per proton) and the corresponding thermal neutron fluxes for the moderators shown in Fig. II-2 are given in Table II-I.

TABLE II-I. Possible Moderators and Their Coupling Parameters

Moderator	Neutron/Proton Coupling n/eV·sr·p at E = 1 eV	Neutron Flux E = 1 eV n/eV·sr·s
1 in.	5×10^{-3}	3.1×10^{12}
1/2 in.	5×10^{-4}	3.1×10^{12}
cold	4×10^{-5}	2.5×10^{12}

The expected variation of neutron flux as a function of energy is shown in Fig. II-3. Data acquisition rates for the PSR instruments have been calculated using Table II-I and Fig. II-3.

III. THE INSTRUMENT SUITE 1985-1990

The experimental area is shown in Fig. III-1 with the neutron flight paths indicated. The present thermal neutron scattering instruments are listed with their flight path number.

A continuous program of instrument enhancement is planned for the next few years so that by the mid-through-late 1980s a suite of eight fully engineered instruments will be in operation. It is possible that in the future a new target station may be built with up to 20 beam lines.

To plan the medium-to-long term (1985-90) computing needs it would seem appropriate to assume a set of eight instruments as the target system. This number can be accommodated easily on the existing beam lines and is large enough to be representative of the computing needs of a (eventually) larger set of instruments. The suggested set of eight instruments is given in Table III-I (Ref. 2).

Figures III-2 through III-9 present characteristics of the instruments necessary to define the data acquisition rates. These parameters must be regarded as tentative because detailed plans of the instruments have not been developed.

Fig. II-3. The variation of neutron flux as a function of energy is shown for the three moderators described in Table II-I.

WNR CONDENSED MATTER INSTRUMENTS

October 81

Abbreviation	Instrument	Flight Path
GPD	General purpose diffractometer	10
SCD	Single crystal diffractometer	9
SED	Special environment diffractometer	8
FDS	Filter difference spectrometer	7
CAS	Crystal analyzer spectrometer	6
EVS	Electron volt spectrometer	3

Fig. III-1. The high-current target area and instrument layout is shown as of October 1981. Nuclear Physics (NP) will use the very long flight paths 1, 2, and 12. Flight path 4 is directed toward the low-current target area. All other flight paths are available for condensed matter research.

TABLE III-I. Planned Instruments and Flight Path Assignments for the WNR/PSR Facility

Abbreviation	Name	Flight Path
CQS	Constant-Q spectrometer	3
SCD	Single crystal diffractometer	6
FDS	Filter difference spectrometer	7
CS	Chopper spectrometer	8
BS	Backscattering spectrometer	9
SANS	Small angle neutron scattering	10
HRPD	High-resolution powder diffractometer	11
GPD	General purpose diffractometer	11

SINGLE CRYSTAL DIFFRACTOMETER

L_1 (m)	6
L_2 (m)	0.25
number of detectors	3 (64 × 64 elements = 12288)
detector area (cm ²)	1875 (3 × 25 × 25)
detector solid angle (msr)	3000
sample size (cm ³)	0.001

Fig. III-2. A schematic of the single crystal diffractometer and important instrument parameters.

FILTER DIFFERENCE SPECTROMETER

moderator	ambient (thick)
------------------	------------------------

L_1 (m)	13
L_2 (m)	0.28
number of detectors	60
detector area (cm^2)	900
detector solid angle (msr)	870
sample size (cm^3)	5

Fig. III-3. A schematic of the filter difference spectrometer and important instrument parameters.

GENERAL PURPOSE DIFFRACTOMETER

moderator	cold
------------------	-------------

L_1 (m)	10
L_2 (m)	1-2
number of detectors	120
detector area (cm^2)	1800
detector solid angle (msr)	120
sample size (cm^3)	5

Fig. III-4. A schematic of the general purpose diffractometer and important instrument parameters.

HIGH-RESOLUTION POWDER DIFFRACTOMETER

moderator	cold
L_1 (m)	30
L_2 (m)	2
number of detectors	240
detector area (cm ²)	3600
detector solid angle (msr)	90
sample size (cm ³)	5

Fig. III-5. A schematic of the high-resolution powder diffractometer and important instrument parameters.

CONSTANT-Q SPECTROMETER

moderator	cold
L_1 (m)	10
L_2 (m)	1.8-2.5
number of detectors	128
detector areas (cm ²)	1920
detector solid angle (msr)	85
sample size (cm ³)	5

Fig. III-6. A schematic of the constant-Q spectrometer and important instrument parameters.

BACKSCATTERING SPECTROMETER

moderator	cold
L_1 (m)	40
L_2 (m)	0.5
L_3 (m)	1.0
number of detectors	128
detector area (cm ²)	1920
detector solid angle (msr)	770
sample size (cm ³)	5

Fig. III-7. A schematic of the backscattering spectrometer and important instrument parameters.

SMALL ANGLE NEUTRON SCATTERING

moderator	cold
L_1 (m)	10
L_2 (m)	1-10
number of detectors	256
detector area (cm ²)	3840
detector solid angle (msr)	96
sample size (cm ³)	5

Fig. III-8. A schematic of the small angle neutron scattering spectrometer and important instrument parameters.

CHOPPER SPECTROMETER

moderator	ambient (thin)
L_1 (m)	12
L_2 (m)	1-2
number of detectors	512
detector area (cm ²)	7680
detector solid angle (msr)	192
sample size (cm ³)	5

Fig. III-9. A schematic of the chopper spectrometer and important instrument parameters.

IV. EXPECTED DATA RATES

We used source definitions in Sec. II together with the instrument descriptions of Sec. III to estimate the data rates expected when PSR becomes operational.

Whenever possible we estimated the rates for PSR instruments (GPD, HRPD, SCD, FDS) from the performance of existing instruments in operation at WNR (for example, GPD, SCD, FDS).

In other cases (CQS, SANS, BS, CS), we scaled the estimate made for similar spallation neutron source instruments at the Rutherford Appleton Laboratory.

Neutron detection rates will vary among experiments performed on the same instrument. The rates quoted are for experimental conditions producing maximal data rates.

The detection rates are given in Table IV-1 and the definition of the row headings are given below. Table IV-1 characterizes the time variability of the neutron detection problem. The detection rates quoted are for the total detector system.

All detectors record a time-of-flight spectrum by assigning a detected neutron to a particular time channel (see Fig. IV-1). The time channels may not be of constant width, but all detectors share the same time channels (that is, a single clock may be used to encode all neutrons detected). The form of a time-of-flight spectrum is shown in Fig. IV-1. Because of the value of the PRF used (12 Hz), all of the spectrum may be recorded within the frame. (The frame is the period between successive proton pulses hitting the target.)

TABLE IV-1. Detection Rates Expected During WNR/PSR Operation

	SCD	FDS	GPD (powder)	GPD (liquid)	HRPD	CQS ^a	ES ^a	SANS	CS
CR (n/s)	24000	10000	450000	96000	36000	12000	12000	48000	2000
FC (n)	2000	900	36000	8000	3000	1000	1000	4000	160
m(n/μs)	0.4	0.2	3.6	0.8	0.1	0.2	0.02	0.2	.04
r ₁ (n/μ/s)	5	1	45	2.4	3.8	2	5	2	0.5
r ₁₀ (n/μ/s)	5	1	45	2.4	3.8	2	5	2	0.5
r ₁₀₀ (n/μs)	3	1	21	2.1	1	0.8	3	1	0.2
r ₁₀₀₀ (n/μs)	2	0.4	7.2	1.7	0.2	0.4	1	0.4	0.1
r ₁₀₀₀₀ (n/μs)	---	---	3.6	0.8	0.1	---	0.1	0.3	---
t ₁ (μs)	400	900	250	250	750	1000	1000	12000	250
t ₂ (μs)	5400	4900	10250	10250	30750	6000	61000	30000	4250
DW (μs)	5000	4000	10000	10000	30000	5000	60000	18000	4000
n _t	256	1000	8000	4000	16000	2000	4000	512	4000
n _d	12288	60	120	120	240	128	128	256	512

^aThese somewhat high rates are to cope with vanadium calibration runs. In normal operation the rates would be lower.

Fig. IV-1. A schematic representation of a collected spectrum in one frame with parameters describing data collection rates.

To characterize the spectrum that may be recorded, we have used the quantities, CR, FC, m , etc., shown in Table IV-1. The definitions of these quantities given below are illustrated in Fig. IV-1.

Spectrum characteristic definitions are:

t_0 is the time a proton pulse hits the spallation target.

The frame is the time between two t_0 's.

t_1 is the time at which data collection starts.

t_2 is the time at which data collection ceases.

DW is the data collection window ($= t_2 - t_1$).

n_i is the maximum number of time channels to be employed.

The frame count (FC) is the number of neutrons arriving between t_1 and t_2 .

m is the mean count rate during the frame in neutrons per microsecond ($n/\mu s$).

Hence, $m = FC/(t_2 - t_1)$.

The overall count rate (CR) is the mean detection rate averaged over many frames. The count rate is expressed in neutrons per second.

Hence, $CR = 12 \times FC$.

The values r_1 , r_{10} , r_{100} , r_{1000} , r_{10000} refer to the highest data rates expected over periods of $1 \mu s$, $10 \mu s$, $100 \mu s$, etc., within the frame.

Figure IV-2 shows the variation of r_i with i graphically for the GPD used for powder and liquid samples. Figures IV-3, IV-4, and IV-5 show typical spectra for a powder sample (GPD), liquid sample (GPD), and an inelastic spectrum (FDS).

Fig. IV-2. The variation of r_i with i for the GPD instrument with a powder sample and a liquid sample.

Fig. IV-3. A typical spectrum for a powder sample taken on the GPD instrument.

Fig. IV-4. A liquid sample spectrum taken on the GPD instrument.

Fig. IV-5. An inelastic spectrum taken on the FDS prior to differencing.

The numbers in Table IV-I refer to the entire detector system. In some instruments where the neutrons are scattered isotropically, the detection rate per detector may be obtained by dividing the rates by the number of detectors (n_d). In other instruments, especially the SCD, the scattering is far from isotropic and the detected neutrons are concentrated in only a fraction of the detector elements. To quantify this effect, Table IV-II contains a column marked spatial anisotropy; the number the average rate per detector should be multiplied by to give the rates found in the brightest detectors. Thus an anisotropy of one implies that the scattering is isotropic.

TABLE IV-II. Spatial Anisotropy Values

Instrument	Number of Detectors	Spatial Anisotropy
SCD	12288	20
FDS	60	2
GPD (powder)	120	5
GPD (liquid)	120	2
HRPD	240	3
CQS	128	2
BS	128	2
SANS	256	5
CS	512	2

V. DETECTORS

For the purpose of the preceding calculations, all instruments (except the SCD) have been assumed to use detectors with an effective detection area of 1×15 cm. The SCD uses three area detectors providing 64×64 elements each. The average detection rate for a single detector is obtained by simply dividing the rate shown in Table IV-I by the number of detectors. (It has been assumed in most cases that the detectors are equidistant from the sample.) Because it is important that the detectors should not cause any undue dead-time correction, we have listed the average peak detection rate r_i per detector for each instrument (Table V-I). The fraction of lost counts f resulting from the detector dead time is given by

$$f = \frac{\Delta r_i}{1 + \Delta r_i} ,$$

where Δ is the dead time.

For gas detectors the value of Δ can vary considerably depending on the orientation of the charged particle track to the anode wire. For BF_3 detectors a study at the Institut Laue-Langevin (Ref. 3) has shown the dead time to be $\sim 2 \mu\text{s}$. If specially constructed* ^3He detectors may be made to run faster and in this case the dead time can be reduced to $\sim 1 \mu\text{s}$.

Scintillator detectors are inherently faster with a dead time of ~ 100 ns. If combinatorial techniques are used to encode a large number of scintillator elements with a smaller number of photomultipliers, the dead time does not refer to individual elements, but to some large fraction of the entire group.

The fraction of lost counts f is shown in Table V-I when Δ takes the values $2 \mu\text{s}$, $1 \mu\text{s}$, and $0.1 \mu\text{s}$. By using the faster ^3He detectors, the dead-time losses for both the SCD and GPD (used for powder samples) are still unacceptably high. For these two instruments the use of scintillator detectors should be seriously considered to obtain tolerable dead-time corrections.

*This information was supplied by H. Wroe, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom.

TABLE V-I. Peak Detection Rate per Detector for Each Instrument

Instrument	n_d	r_i	$r_i/\text{Detector}$	Fraction of Lost Neutrons,		
				$\Delta = 2 \mu\text{s}$	$\Delta = 1 \mu\text{s}$	$\Delta = 0.1 \mu\text{s}$
SCD	3	5	1.7	0.77	0.63	0.14
FDS	60	1	0.02	0.04	0.02	0.002
GPD (p)	120	45	0.4	0.44	0.29	0.04
GPD (I)	120	2.4	0.02	0.04	0.02	0.002
HRDP	240	3.8	0.02	0.04	0.02	0.002
CQS	128	2	0.02	0.04	0.02	0.002
BS	128	5	0.04	0.07	0.04	0.004
SANS	256	2	0.008	0.02	0.008	0.001
CS	512	0.5	0.001	0.002	0.001	0.000

In other instruments (especially SANS and CS), the use of scintillators may be considered for their advantages in fabricating annular ring detector geometries.

VI. DATA CAPTURE ELECTRONICS

The data capture electronics (DCE) must perform the function of a large multichannel analyzer. All neutrons detected are assigned a descriptor constructed from the detector and time information appropriate for that particular event. This descriptor then is used as an address for a read-increment-write operation on a large random access memory. This large memory, which is emptied at the start of a run, contains the complete record of the neutrons detected during the run. It is sometimes referred to as the run histogram.

In some cases, the descriptor will be constructed from two time subdescriptors instead of the usual one. This occurs when time-dependent phenomena are being studied. The two times are t , the time of arrival of the neutron measured from the time the protons hit the spallation target, and p , a period count measuring the time elapsed since the sample environment was changed.

The requirements of the DCE are listed below.

1. Record the neutron event by first registering the time of arrival. Because the neutron detection rates reach tens of megahertz in some cases (Table IV-I), it is important that the DCE should not introduce any excessive dead-time corrections (dtc). In any case, the highest dtc should not exceed 4% and in general should be well below 0.5%.
2. The time of arrival is recorded as an n_t -bit time descriptor so that $2^{n_t} \geq n_t$, where n_t is the maximum number of time channels required for a particular instrument. The values of n_t are given in Table VI-I.
3. The time descriptor specifies the time channel where the event occurred. The time channels may have a constant width $\Delta t = c$, but provisions should be made to allow the user to choose a regime where the width of the time channels increases at longer times. For example, $\Delta t_i = c + a \cdot t_i$, where c and a may be set by the user.

TABLE VI-I. Memory Requirements for Each Instrument

Instrument	Number of Spectra n_s	Number megawords		Word Size (bytes)	Memory Size (Megabytes)
		n_t	in Run Histogram ($n_s \times n_t$)(bytes)		
SCD	12288	256	3	3	9
FDS	12	1000	0.01	3	0.03
GPD (p)	120	8000	1	3	3
GPD (I)	120	4000	0.5	3	1.5
HRPD	64	16000	1	2	2
CQS	128	2000	0.25	2	0.5
BS	128	4000	0.5	2	1
SANS	256	512	0.13	3	0.5
CS	128	4000	0.5	2	1

- [illegible]

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7. In a similar way the period p subdescriptor may be incorporated $D = t + n_t s + n_t n_s p$.
8. Each DCE should contain its own large random access memory to contain the run histogram. The size of this memory (in words) is dictated by the length of the longest descriptor that might be reasonably used on a particular instrument. This is determined by the maximum number of spectrum and time channels that are required. These quantities are given in Table VI-I. The lengths of the words used in the memory are determined by the size of the count in each channel that will be required and by the method adopted in dealing with overflows. All counts must be accurately recorded and either the word length should be long enough to cope with the highest count required, or a mechanism must be used to store the overflow addresses. For low-count rate instruments a word length of 16 bits may be adequate. This permits a maximum count of 64K before overflow occurs. For many instruments it may be inconvenient to work with the large number of overflows that would occur with a word length of 16 bits, and in these cases a word length of 24 bits has been suggested in Table VI-I.
9. The memory size (in Mbytes) for each instrument is given in Table VI-I. Note that for two of the instruments the size exceeds 2 Mbytes. A reduction in the memory size required by the GPD instrument (in powder use) could be achieved if the detectors were arranged on an isochronous surface (time focusing). The current proposals suggest that a resolution focused locus will be used that requires the detectors to be treated separately. The large memory size required by the SCD instrument may only be reduced by decreasing the number of area detectors to one or two. Even so, each area detector will require a megaword of DCE memory to store the run histogram.

VII. THE USER INTERFACE: REQUIREMENTS

The user interface is the description of the data acquisition and control system as presented to a scientific user of the system. It includes the physical methods by which the user must interact with the system—the screens, plotters and keyboards—and of equal importance, the command language available to him to perform his tasks. Before attempting to specify the hardware/software interface, it is essential that the user's requirements be listed. These fall into two categories: requirements needed to successfully initiate, record, and file a run or series of runs (data taking); and those necessary to analyze the data. The division is important because the first is a real-time requirement that has a substantial penalty (in the form of an underused expensive resource) if it is not met.

A. Data Taking

In this section the user's requirements fall into three areas: initiating a run or sequence of runs after setting the appropriate parameters; displaying the results for the current and previously recorded runs; and filing and cataloguing the results.

Some requirements are common to all three categories. The user should be able to control an experiment using a concise set of keyboard instructions. It should be impossible for a user to issue commands to more than one instrument. The instructions should be self-checking to prevent the accidental use of an inappropriate

command that could adversely affect the user's experiment. After a hardware failure and reloading of the control programs, the user should be able to return to the prefailure state without interrupting the operation of the DCE. A HELP command should be available that provides information to new users on how to use the system.

Before explaining the user's needs in more detail it is necessary to provide two definitions.

A run is the basic unit of data collection. It is a period of data acquisition with the detectors, sample position, and sample environment in a fixed state. Thus, during a run all parameters should stay constant. An example of a run might be:

Collect data with the time channels set to be $\Delta = t/500$, $t_1 = 1000 \mu\text{s}$, $t_2 = 10000 \mu\text{s}$ from an area detector with the sample in the orientation $\omega = 20.1^\circ$, $\chi = 2^\circ$, $\phi = 10^\circ$. The sample temperature is $240 \pm 2\text{K}$. Stop data collection when the monitor counts reads 10^7 .

If the temperature, time channel width, or any other parameter is changed it is considered a separate run. Each run is identified by a run number.

The end-product of a successful run is a file containing a list of all the parameters that may be set to define a run, together with the time-of-flight spectra (the run histogram) recorded in the DCE memory. To be useful as a starting point for a data analysis sequence the file should contain all other parameters that might be needed. These parameters cannot be changed by the user (for example, the primary flight path L_1 or the detector angle) and therefore are not unique to a particular run.

1. Initiating Runs: User Requirements. The user must be able to change parameters in the DCE or the sample environment by keyboard commands. Ideally the DCE parameters (for example, time channel widths or boundaries, detector mapping table, etc.) should only be changeable by keyboard commands to prevent any inadvertent change during a run. If panel switches must be used they should be computer readable. The user then starts a run or sequence of runs for a preset monitor or time count. When a sequence of runs is specified, it will involve DCE parameter changes or sample environment changes between runs. These should be implemented by a stored list of commands. The user should be able to stop or pause/restart runs at any time, even interrupting a predefined run sequence.

2. Display: User Requirements. It is extremely important that the user is provided with a fast, versatile, and physically meaningful method of displaying spectra from the run currently being collected or runs recently completed.

The graphics screen display should enable arbitrary choices of the x,y scale sizes and their origins, linear and logarithmic plots, and the simultaneous display of two or more spectra (not necessarily from the same run). In particular, the user should be able to select physically meaningful scales such as the lattice spacing d , momentum transfer Q , energy transfer E , etc.

The display command language should permit the user to perform simple arithmetic operations on a run or group of runs. For example, it should be possible to display the spectrum c^i , where $c^i = (aR_1^i - bR_2^i)/cR_3^i$, c^i = i -th element of spectrum c , R_1 , R_2 , R_3 are separate runs, and a , b , c are constants chosen by the user.

It should be possible to produce a hard copy of anything displayed on the screen. This hard copy should have a moderate quality and be produced within a few seconds.

Because the display of current or recently completed runs is a very frequently used function, the methods of switching from one spectrum to another and changing scales should be made as simple as possible. For example, the user should be able to display the entire spectrum for a particular detector (or group of detectors) and then zoom-in on a particular region of interest by using the x-y cursor or simple keyboard commands to define the new scale limits.

When area detectors are used it will be necessary to display intensity maps of a particular plane or projection of the x,y,t space. These may be represented on a conventional screen by two-dimensional histograms or contour maps. The data would be more clearly represented by the use of a display using gray scales or color.

The requirement that current and recently recorded spectra should be displayed quickly, within five seconds, is paramount. Table VII-I lists the storage location of the system for displaying data files as a function of their ages. In this table 'current' means the run currently being collected or the last recorded run.

'Attached' is a category of files that have been marked for immediate display and must be stored locally.

3. Filing and Cataloguing. Upon completion all runs should be filed without the experimentalist's intervention. This may occur when the preset monitor or time count is reached, or when a run is ended prematurely by a user command. This copy of the run, the primary file, will be used for local display up to 48 hours after the run has been recorded.

Users should be able to make a file copy of the current run in progress by use of a single command.

TABLE VII-I. Data File Storage Locations and Sizes as a Function of Age

Age	Storage Location	Number of Files^a
'Current'	local disc 30 Mbytes	1
'Attached'	local disc 30 Mbytes	20
48 hr.	hub disc 500 Mbytes	40
7 days	hub disc 500 Mbytes	100
30 days	archive medium locally stored	500
1 yr	archive medium warehoused	5000

^aBoth the number of files and their size will vary from instrument to instrument. See Table VII-II for an estimate of the number of files per day for each instrument.

Provision should be made for users to archive the run as soon as a primary file has been created. The archive copy should be on a physically different medium from the primary file and after 48 hours the archive copy should be duplicated to provide two long term copies of the data. The archiving process should be an extremely simple command to permit the archiving of multiple runs. The user should not be required to mount tapes or in other ways involve himself with computer hardware.

The deletion of primary runs should be the responsibility of the user. A warning message and a further user response should be required for the deletion of runs not previously archived.

To ensure that the system has sufficient space for the creation of primary files, users should be warned if insufficient space is available when a new run is started. The space required to start a run should be stated. The user should be able to easily determine the amount of local storage space available and be able to list quickly the primary and attached files and their sizes so that they could be archived and/or deleted.

A catalogue of the last 5000 runs performed on the instrument should be immediately available (within 25 seconds) on a screen or hard copy terminal. The form of the catalogue should be a single line entry for each run. The line should be 60 characters long to print/display on a variety of terminals. It should contain the following information.

run no.	(6)
extension	(6)
date	(6)
time	(4)
state	(2) (attached, archived)
user	(12)
title	(20)
size	(4)
run duration	(5)
type of dump	(1) (intermediate or final)

Runs that were deleted before archival should not be included. Users should be able to invoke simple commands that would display subsets of the catalogue. For example, a user should be able to recall all runs performed by a particular user, runs between given dates, or runs containing a particular character string within the title.

To judge the amount of file storage capacity that will be required both locally and in the archival system, it is necessary to know both the size of the data files and the frequency with which they are produced. These estimated figures shown in Table VII-II furnish the required information for calculating traffic expected on the computer network.

B. Data Analysis

Data analysis consists of two problems, that of providing an immediate display of physically meaningful spectra ($S(Q)$ vs. Q , etc.) to the user while a run is in progress, and the larger computational problem of reducing the entire run histogram to a form suitable for comparison with theory or for the least-squares refinement of structural models.

TABLE VII-II. Estimates of Daily Storage Requirements

Instrument	Runs/Day	Run	Megawords/Day
		Histogram Size (Megawords)	
SCD	10	3	30 ^a
FDS	10	0.01	0.1
GPD	20	1	20
HRPD	10	1	10
CQS	2	0.25	0.5
BS	2	0.5	1
SANS	10	0.13	1.3
CS	2	0.5	1

^aThis large volume of data could be reduced at least 10 times if a local computer is used to extract integrated intensities.

1. Immediate Display. The requirement for immediate display has already been mentioned under the display function. In this section we attempt to quantify the amount of input/output (I/O) and central processing unit (CPU) power required.

The programs that provide immediate displays during data collection should be capable of transforming and displaying a single time-of-flight spectrum in a few seconds. Two dimensional data, consisting of many individual spectra, may take a few tens of seconds.

The data transformations will typically require (for single spectrum) the copying of 3 spectra to memory, about 10 floating point operations per data point, and the output of the transformed file.

A single spectrum typically contains a few thousand data points. In the case of two-dimensional data roughly 20 times as many data points may be involved.

2. Bulk Data Analysis. Although the final analysis of the data from different instruments varies considerably, there is a common problem that may be quantified. There is a need to remove the instrument dependent characteristics such as background spectrum, energy dependent incident beam intensity, and the detector response.

The computational size of this problem may be estimated from the size of the run histograms, the frequency at which runs are recorded, and the amount of processing required per histogram element.

These quantities are estimated in Table VII-III. Benchmark tests may be employed to convert the figures in Table VII-III to specific hardware requirements.

The rest of the bulk data analysis problem is difficult to quantify, but experience suggests that this activity requires a machine with a power of approximately 1.0 MIPS (1 MIP = 10^6 instructions/second) or the proportional share of a larger machine.

TABLE VII-III. Parameters Indicating Daily Computational Needs of Each Instrument

Instrument	Run Size Megawords	Run Frequency Runs/Day	I/O Megawords/Day	CPU MFLOPS/Day^a
SCD	3	10	---	---
FDS	0.01	10	0.5	1
GPD	1	20	80	200
HRPD	1	10	40	100
CQS	0.25	2	2	5
BS	0.5	2	4	10
SANS	0.13	10	6	15
CS	0.5	2	4	10

^aMFLOPS = million floating point operations.

VIII. THE USER INTERFACE: HARDWARE

To control and interpret a series of runs on a particular instrument, the user should have exclusive use of the following configuration. A medium sized (~0.25 MIPS) minicomputer with a hardware floating point unit containing 0.25 Mbytes of memory should be available for user or display programs. The peripherals should include a hard copy alphanumeric terminal, a graphics display screen (with or without a separate keyboard), disc file space, 5 Mbytes for program development, and 20-50 Mbytes for run file storage. Five Mbytes should be allowed for storage of standard control and display programs, a parallel interface to the DCE, and communications interfaces to shared resources should be available.

He should have shared use of a lineprinter (600 lpm), a hard copy graphics device, and a file archiving system for both data and programs. The user should have access to a more powerful computer (~1 MIPS) for bulk data processing and model fitting. There should be adequate hardware and software links between these two computers to enable data and program files to move easily between them.

The hard copy terminal is necessary to provide a record of the course of the run. It will log instructions issued and any fault condition messages. It can be slow (30 characters/second) and inexpensive.

The graphics screen should have a resolution of at least 1000 (x) by 500 (y), and it should provide a display area of at least 12 in. (high) by 14 in. (wide). The size of the screen is especially important for displaying three-dimensional information, and the increased use of area detectors or pulsed sources will make this a common requirement. Either a storage tube or a refresh display could be used, although the latter would provide a greater flexibility in use. The screen should be capable of drawing a single spectrum (1000-4000 points) in 2-3 seconds. On those instruments with area detectors it would be advantageous to have a screen with a gray scale capability. This enables an intensity map of the detector to be easily displayed.

The screen should be equipped with a crosshair graphics cursor controllable from a joystick (or similar device) preferably with two-speed operation. The cursor is essential for fast interaction with the graphics display. This includes finding peak positions, calculating background levels and peak heights, identifying areas to be redrawn on a larger scale, and marking areas over which a spectrum integral is displayed.

The minicomputer will be used to provide the normal graphics display facilities previously outlined in Sec. VII. It is likely that some users will develop their own display and/or analysis programs, and for this reason a certain amount of disc space (5 Mbytes) should be available for this purpose. This will be in addition to the larger volume of file space (20-50 Mbytes) reserved for run data files. The size of disc space to be provided locally may be estimated from Tables VII-I and VII-II.

The communications link from the minicomputer to the file archiving system is very important. The number and size of the runs to be archived may be estimated from Table VII-II.

The line printer, hard copy graphics output, and archiving file store are expensive items that should be shared.

The hard copy graphics device should have a similar resolution to the screens. It should be capable of reproducing any picture from a screen display, preferably by the simple operation of a 'hard copy' command. It should be fast enough to produce a 10- by 8-in. copy in a few seconds.

IX. THE USER INTERFACE: SOFTWARE

The users will control the course of the experiment by a command driven dialogue that will provide both the control and display functions. This command language must be logical and concise with consistent argument or parameter form to be quickly learned and correctly used by new users.

Outlines of the commands that might be used for both the control and display functions are given in Sec. IX-A and Sec. IX-B.

In addition to this supplied software however, the user should have at his disposal the facilities of a modern operating system and utility programs for the development of his own display or analysis programs.

It is also important that a common file structure and naming convention be adopted for filing the completed runs. This is discussed in Sec. IX-C.

A. The Control Commands

Because certain sequences of commands are either nonsense (for example, stopping a run before it has started) or likely to lead to faulty data taking (for example, changing the time channel width during a run), they must be prevented. This is achieved most easily by considering the instrument to be in one of a number of 'states,' and while in a particular state only a restricted set of commands may be used.

Examination shows that there are only three permissible states of an instrument.

SETUP—data are not being taken; DCE or sample environment parameters may be set in preparation for a run.

RUN—data are being taken (unless hardware inhibits are in effect); parameters may not be changed.

HALT—data are not being taken, and parameters may not be changed. (This is a temporary pause condition.)

These arise from the fact that there are four fundamental states (data taking on or off combined with parameters changeable or fixed) of which one, changing while taking data, is forbidden.

All possible movements between these three states may be achieved by four commands. These are illustrated in Fig. IX-1. Thus, when in a SETUP state only the BEGIN transition command may be issued. The effects of the four transition commands are given in Table IX-I.

In addition to the four transition commands, three other commands are necessary, SET, DUMP, and DISPLAY. The meaning of these commands are given in Table IX-II. The first two are input/output commands, the third is a command that removes the user from control mode to display mode where a set of display commands are available.

Thus, the seven commands

BEGIN	S
END	RH
PAUSE	R
CONTINUE	H
SET	S
DUMP	RH
DISPLAY	SRH

are the control commands. The instrument states, SETUP (S), RUN(R), and HALT(H), in which they may be used as shown by the letters following the command.

Fig. IX-1. The three states of data acquisition with the transition commands.

TABLE IX-I. Transition Commands and Their Effects

Command	Effects
BEGIN	Issues a new run number. Asks the user to type in the run title. Uses all of the information stored in the run control file (RCF) to set the necessary parameters in the DCE. Checks for possible inconsistencies between parameters and reports errors. Clears the run histogram memory in the DCE. Initializes the clock or monitor scalers that provide the intermediate dump interrupt. Removes inhibit from data collection. Sets flag in RCF to run state. Informs user of new state. When the run duration scaler limit has been reached an END command is automatically executed.
END	Inhibits data collection. Creates a run data file (RDF) from parameters stored in the RCF and the run histogram in the DCE. Copies the RDF to local disc storage. Sets flag in the RCF to SETUP state. Informs user of new state.
PAUSE	Inhibits data collection. Sets flag RCF to HALT state. Informs user.
CONTINUE	Removes inhibit from data collection. Sets RCF flag to RUN state. Informs user.

TABLE IX-II. Additional Commands Necessary for Data Acquisition

Command	Argument	Effect
SET	Parameter/ values	<p>Change the value of a parameter in the DCE, sample environment or RCF (a file containing the title, run, number, dump interval, duration, etc., of the next run to be started.).</p> <p>When a parameter is changed in the DCE, a return should be made after this has been completed.</p> <p>When a sample environment parameter is changed (for example; θ, T), a return should be made when the information has been received by the control system—not when the physical parameter has been changed. Hardware inhibits should be used to halt data collection of any sample environment parameters are beyond limits.</p> <p>A SET command without argument should display the parameters and their current value.</p> <p>It should be possible to input values from files.</p>
DUMP	---	A command that takes the current contents of the run histogram, DCE parameters, and creates a new RDF on local disc storage. A new run extension number is chosen.
DISPLAY	---	Moves the user to display mode.

The commands should be self-checking. A record of the current state of the instrument should be kept and checked against the commands as they are issued. Invalid commands should result in an error message to the user. Automatic checks should be made on the values issued by SET commands. A record should be kept of the limits between which a given parameter may be set, and the command checked against these values. These control commands may be issued from the keyboard or they may be read from a control instruction file (CIF). To initiate reading from a CIF one further instruction is required, OBEY filename. On receipt of an OBEY command, the file specified is used as the source of commands. Each command is acted upon in turn until a BEGIN command is reached. This is acted upon, but control reverts to the keyboard until the run has completed (to allow for manual END, PAUSE, DUMP, or DISPLAY commands). At the end of a run, control reverts to the CIF until the next BEGIN is encountered, and so on. When the last instruction has been read from the CIF file, control reverts to the keyboard.

B. The Display Commands

As mentioned in Table IX-II the use of the DISPLAY command should remove the user from control mode and take him into display mode. In this mode a set of commands will provide the type of display functions outlined in Sec. VI.

These cover three main areas; the graphical display of a single spectrum or multiple spectra; the alphanumeric display of parameters, either DCE, or run control file information for the current run or from the parameter block of a completed run; and the display of the catalogues of recorded runs. Because it will be necessary to archive or delete runs after consulting this catalogue, these commands (ARCH, DELETE) should be within the display level.

The types of commands that might be used for line spectrum displays, for example, are given in Table IX-III. The values of all parameters that may be set by a command, (for example, spectrum number, run number, axis units, axis minimum and maximum, summed zone) should be stored in a display information table. These values should be used as the defaults in all display operations. Changing any of the values should result in a redrawing of the display (except in the case of AS).

When it is required to display arithmetic combinations of runs, first combine the runs in a scratch file by using a series of commands like those illustrated in Table IX-IV. The scratch file would be used as input to the display commands NS or AS. Frequently required manipulations, such as $c = (s_{i1}/m_1 - s_{i2}/m_2)a$, where s_{i1}, s_{i2} = spectrum i of run 1 and 2, m_1, m_2 = monitor spectrum run (1,2), and a = constant, could have a single command.

TABLE IX-III. Examples of Spectrum Display Commands

Command	Argument	Effect
NS	spectrum/ run number	New spectrum. Draws a single spectrum with the default values of x and y stored from previous run.
AS	spectrum/ run number	Add spectrum. Adds a single spectrum to the current display.
N	---	Next. Like NS but draws the spectrum following the previously drawn spectrum.
AN	---	Add Next. Add next spectrum to current display and display sum.
CA	axis/mode	Change Axis. This command enables the user to change the units of a particular axis. The unit picture is redrawn with the new axes.
SC	x-min, x-max, y-min, y-max	Scale change. By specifying c for x-min the cursor is displayed and may be used to define the new limits.
IN	x_1, x_2	Display the integral between limits. By specifying c for x_1 display cursor and use to define x_1, x_2 .
CON	---	Leave display mode and return to the control mode.
CU	---	Display cursor and use it to print x,y position chosen.

TABLE IX-IV. Arithmetic Commands in Display Mode

Command	Argument	Effect
ADD	run 1, run 2 or run 1→run2	Adds all spectra of the runs specified. run 1→run 2 implies all runs from run 1 to run 2 inclusive. Store in a scratch file, display scratch file name used.
SUB	run 1, run 2	Subtract run 2 from run 1.
DIV	run 1, run 2	Divide run 1 by run 2.
MUL	run 1, run 2	Multiply run 1 by run 2.
SCA	p, run 1, run 2 or run 1→run 2	Multiply all of the runs listed by the value p.

*In all cases a scratch file name may be used instead of a run number.

C. The Format of the RDF

The RDF Sec. VII, should contain all information necessary for subsequent data analysis. Its structure should be the same for all instruments, to enable standard reading routines to be used in different data analysis or display programs. A possible structure for the RDF is shown in Fig. IX-2.

The abstract is used to identify the file and should contain the following information.

Instrument	4
Run no.	6
Run no. extension	3
Duration	5
Time	6
Date	6
User	8
File type	2
Title	25

Fig. IX-2. Format of the RDF.

The figures denote the number of characters that might be used for each field. The abstract will have the same format for all instruments. The parameter block is a large but fixed length block that records all of the parameters necessary for subsequent data analysis. Most importantly, this block will contain those parameters that may be varied from run to run (for example, time channel width, rotor period, detector ganging arrangements). It should also contain those parameters that change infrequently (L_1 , L_2 ,... etc.), but that are vital for display programs or subsequent data analysis. The parameter block is fixed in the sense that it is of a fixed length for a particular instrument, but may vary among instruments. For this reason its length is included as the first parameter.

The scratch block is simply a free area for the user to record any notes or parameters.

The run histogram is the copy of the spectrum stored in the DCE. It will be of variable length depending on the number of time/spectrum channels chosen. It should contain the data in spectrum order. If time-dependent effects have been studied, all of the spectra for one time domain should be grouped together.

Finally, the RDF file name should be carefully chosen to be as meaningful as possible. It should begin with a one or two letter instrument code and include the run number and run number extension.

Run data files may be produced in one of four ways: on completion of a run, either by an END command, by the run duration scaler reaching its preset limit, by a DUMP command, or by an automatic, intermediate dump. This last provision is important. If it is not possible to inhibit data collection when the sample environment changes, it is necessary to take intermediate records of the run. This could be achieved by providing a second preset scaler, the dump scaler. On reaching its preset value the DCE would produce a dump interrupt, causing a DUMP command to be issued without user intervention. The dump scaler would then be reset at its previous value and the run continued.

X. TIME SCALES

We have summarized the stages necessary to realize a complete data acquisition and analysis system by early 1985 in Fig. X-1. This illustrates that many man years of effort are involved and that decisions are required very quickly regarding the funding and implementation of the project. Many of the time scales suggested are far too short, especially with regard to the design of the high-speed electronics.

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Fig. X-1. Stages and time schedule necessary to complete data acquisition and analysis systems are diagrammed.

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