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Design, Control System and Software Organization of Multi-purpose NMR Spectrometers

I. The Basic Requirements and Overall Design

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This first paper in a series of three deals with the basic requirements and the overall design of multi-purpose NMR-spectrometers. The second paper will concentrate on the control and acquisition system and the third paper concerns all the non-time-critical software and future trends. In the first paper the requirements for spectrometers in general and their consequences for the design of an NMR-system are given. A non-detailed analysis of different control systems is presented, and the analogue part of NMR-spectrometers is shortly described. The general computer requirements for spectrometers are analysed, and the partitioning of the software NMR-system is given. A characteristic of the system is an operator communication language that has been adapted to the different types of experiments. For reasons of flexibility and ease of upgrading, the control and acquisition tasks are as much as possible performed by software.

KEY WORDS Design Software NMR Spectrometers

INTRODUCTION

After 35 years, there still remain many developments in NMR-techniques. Especially, the introduction of two-dimensional spectroscopy[1] has provided an enormous stimulus for new techniques during recent years. More than ever we need spectrometers capable of performing experiments which were unknown during the design phase of the spectrometer.

The performance of novel experiments without writing any software and the possibility of an easy extension of software and hardware, were two of the major design goals of the 7-T superconducting spectrometer, constructed in Delft.[2]

Experience with many 2D-techniques[3] proved the correctness of the design.

This paper will deal with the basic requirements and overall design of spectrometers in general, with reference to the Delft system, in particular. It is the first in a series of three concerned with the design, the control system and the software organization of multi-purpose NMR-spectrometers. The last two papers concern the control and data acquisition system and the non-time-critical software.

THE SYSTEM DESIGN

The chronological design of a spectrometer consists of:

(a) The design of the overall system. This consists of a distribution of all the spectrometer tasks over the following three main systems:

 (i) the software system
 (ii) the hardware control and acquisition system
 (iii) the rest of the spectrometer.

(b) The design of the main systems. This consists of a distribution of the main tasks over general purpose (usually external manufactured) and dedicated (home-built) software and hardware.

(c) The design and development of the subsystems.

For each spectrometer the most important points, determining the design of the overall and main systems are in general terms:

1. The type of spectrometer and the types of experiments that must be performed on the spectrometer system.
2. The way in which the spectrometer is to be operated.
3. The desired modification and/or extension capabilities.
4. The optimization of the effort required for construction, modification, extension and service/maintenance of the spectrometer system.
5. The present capabilities of hardware and software.

The subsystems design is mainly determined by: the system design that is chosen, the desired area of experimental applications and the desired accuracy of the experimental results.

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CCC-0734-3051/83/010003-08$01.00

DESIGN GOALS AND REQUIREMENTS

A translation of the general points 1–5 into specific design goals and requirements for a multi-purpose NMR-spectrometer gives:

1. The type of spectrometer and the types of experiments that must be performed on the spectrometer system.
   (a) A multi-purpose high field NMR-spectrometer.
   (b) The execution of the HR NMR-techniques of any importance must be possible for all nuclei that possess a magnetic moment.
   (c) The capability to perform an experiment that is not endemic to the software must be possible without writing new software, of course, within the limits of the hardware.
2. The way in which the spectrometer is to be operated. This point is mainly determined by the fact that a multi-purpose spectrometer must be suited for the development of new techniques, for sophisticated experiments and for routine experiments.
   (a) Both a simple to use menu-driven and a fast code-driven command language are necessary.
   For experiments which are implemented in the software, the number of commands must be minimized and the conversation must be dedicated to the particular experiment.
   For novel experiments the spectrometer control language is system-oriented and the data-processing language is mathematics-oriented.
   (b) The spectrometer must be a multi-user system without degrading the control and acquisition performance.
   (c) Parameters needing different settings in one or more experiments, and of which it is advantageous to determine their values in other experiments in a fast interactive way, should have the capability of computer *and* manual setting.
   (d) A change of nucleus must be possible with a simple change of hardware.
   (e) The surface area of the front panel and the number of knobs must be minimized. The grouping of the front panel controls must be logical.
3. The desired modification and extension capabilities.
   (a) Hardware as well as software should be modular.
   (b) A hardware reserve for spectrometer control must be created.
4. A minimization for the effort of the construction, modification, extension and service/maintenance of the spectrometer system.
   (a) A structured, decomposed and hierarchical system. This point is especially important for the software.
   (b) An overall system which makes the hardware of the subsystems as simple and as small as possible.
   (c) A balanced ratio between software and hardware. The modification and extension requirements make in general a realization on software bases more favourable than a hardware realization.
5. The present capabilities of hardware and software.

The most important development is in microprocessor technology, array processors and peripherals.

In the software system the following general principles are used:

One software package with small software parts, completely dedicated to a certain type of experiment, is the basis for the simple performance of routine experiments.

A completely general software package, that is suitable for all experiments can be used for the performance of novel techniques. Many generally written modules are common for both packages. Assembly and micro assembly language are only used when necessary or when a high level language would degrade the speed.

A multi-user operating system is used, which is completely interrupted if the spectrometer needs attention.

In this way, experiment preparation, data processing, data plotting and software development can be done simultaneously, without degrading the acquisition and control potentialities.

A decomposed and modular structure is used for software and hardware and the system is as software-oriented as possible. Therefore a modification of the system for the implementation of a new technique is, in general, only a software modification.

The top level software package is split into four parts: the experiment preparation software, the experiment executing software, the data end-processing software and the display software.

The experiment executing software and the display software are completely general. The data processing is matrix oriented. Each row of the matrix has either one (e.g. absolute value) or two (e.g. absorption and dispersion) vectors.

In the hardware system the following principles are used:

(a) Multinuclear observing, irradiation and lock capabilities.
(b) Separate channels for both frequency generation and timing for observing, homonuclear irradiation and locking purposes.
(c) Direct time averaging in double precision on the background storage (disc) at high input rates.
(d) A reserve is created to handle many computer generated control words for a spectrometer upgrade.
(e) Fast terminals are used for intensive dialogue between the operator and the computer.

In this paper the separate subsystem requirements will not be discussed. Rather the way in which one can cope with these requirements is described. The subsystem requirements for a spectrometer can be divided as follows:

1. Requirements such that, if it appears that they cannot be fulfilled or must be changed in the future, changes are necessary in the subsystem as well as in the main systems.
2. Requirements such that, if it appears that they cannot be satisfied or must be changed in the future, changes are necessary only in the subsystem.

It is clear that, before one starts realizing the spectrometer, the consequences of the requirements of group 1 must be analysed. This can be done with the aid of calculations, computer simulations[4] or measurements on another spectrometer provided it has sufficient capabilities to measure the instrumental consequences of a particular requirement.

The technical consequences of the requirements of group 2 can be analysed in the same way as those of group 1. Moreover, sometimes it can be of benefit to determine the consequences of a certain requirement of group 2 by way of a measurement on the spectrometer that is under development. This can be done via a measurment on an appropriate sample if the spectrometer is in its final stage of development. Thus, the modification or extension of the subsystem can be done in the most justified way.

THE OVERALL SYSTEM

Only spectrometers that are equipped with a general purpose computer are considered. The design of the overall system of these spectrometers is, to a large extent, determined by the way in which the spectrometer control is accomplished.

Three possible solutions for the control function can be distinguished.

1. During the entire measuring time the spectrometer is controlled by an autonomous dedicated control system.[5–12]
2. The computer directly controls the spectrometer.[13]
3. Solutions which are a combination of 1 and 2. These combinations can be of different kinds:

   (a) Time critical adjustments are controlled by the dedicated hardware. Less time critical settings are directly controlled by the computer.

   (b) During a certain time of the measuring sequence, which will be called a *stretch*, the spectrometer is autonomously controlled by the dedicated control system. The data needed by the control system for the next stretch are transferred from the computer at a non-time-critical moment during or immediately after the current stretch.[3,14–16]

The advantages and drawbacks associated with the above solutions are listed below.

The main advantage of solution 1 is the capability of generating measuring sequences with very short time intervals. Another advantage is that the computer is not burdened with the control task. The setting of the dedicated control system can either be done manually or by computer. In the case of computer setting, the software for this task is rather simple. During the control time, no advantage can be taken of the flexibility of the general purpose computer. This is the main disadvantage of solution 1. A rather complicated and extensive hardware system is necessary for complex sequences.

Solution 2 requires a minimum of dedicated hardware, but can result in timing problems for time critical intervals. The computer is completely occupied during the measuring time.

The main disadvantage of system 3(a) is that, although it still needs a dedicated timing part, some timing is inaccurate because of the direct computer control. This drawback can be devastating for generation of novel techniques.

In 3(b) the time accuracy is completely determined by the dedicated control system. For the generation of complex sequences advantage can be taken of the flexibility of the computer. The computer is occupied with the control task for a relatively short time.

Within system 3(b) a range of different solutions with two extremes is evident. These extremes are:

(i) A very simple and small hardware control system with a rather complicated control software where the minimum stretch time is just long enough for the transfer of new control words by the computer.

(ii) A hardware control system that can autonomously control almost all measuring sequences. This control hardware is quite similar to the hardware needed for solution 1, but now the contents of the hardware registers can be refreshed by the computer while retaining the time accuracy.

As is clear from the above, the two most promising solutions are 1 and 3(b). In the second paper of this series the different hardware/software ratios that can be chosen in the latter solution will be discussed. Since the extreme of a powerful hardware control part in system 3(b) comes very close to solution 1, this discussion includes also solution 1.

Figure 1 shows the overall block diagram of a spectrometer system. The communication from the operator to the computer is done through keyboards and through front panel controls. In the Delft system the front panel controls consist of potentiometer(s) and a 4 × 4 array of push buttons that assign the functions of the potentiometer(s).

1. Hardware system

A block diagram of the hardware system is shown in Fig. 2. It can be grouped into three parts:

(i) The magnet and the radio/audio frequency system

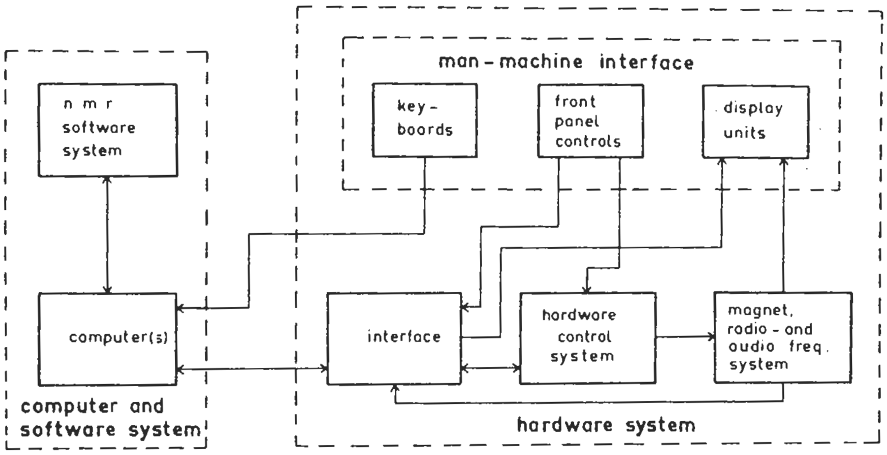

Figure 1. The overall spectrometer system.

(ii) The hardware control system
(iii) The interface

In the radio/audio frequency system the synthesizers generate the excitation frequencies for the transmitters and the reference frequencies for the receivers. The response of the probe to the transmitter signals is detected in the receivers. The outputs of the receivers are an observing signal and a lock signal. The first signal passes an ADC and is transferred to the interface. If the spectrometer operates in the slow passage mode, this signal also can be directly transferred to the plotter. The lock signal is conducted to the magnet in order to correct the H_0 field.

The hardware control system performs the control of the radio/audio frequency system. The inputs to the control system are: (a) the timing data from the interface and (b) the setting and selection data from the interface and from the knobs on the front panel.

Here only information about the radio- and audio-frequency system is presented whereas the control system and the interface are discussed in the second paper of this series.

Radio and audio frequency system. In order to apply HR NMR-techniques of any importance we need the following RF magnetic fields: one field to observe the NMR-signal, one field to stabilize the H_0 field/frequency ratio, and two fields to apply homonuclear and heteronuclear double resonance. With the last two fields only irradiation takes place without signal detection.

As stated above, 4 different frequencies: one observing, one homonuclear irradiation/lock, one heteronuclear irradiation and one heteronuclear lock frequency are needed.

In many applications the stability of the ratios of these frequencies must be better than 1 part in 10^9. Thus, the four frequencies are generated by four synthesizers and one master oscillator as a reference. (see Fig. 3). From each synthesizer one frequency is needed to generate the RF fields for the probe. Two additional frequencies must be generated by the observing and the lock synthesizer to serve as reference frequencies for their respective receivers.

There are 5 transmitters: one high power observing transmitter, one low power observing transmitter and 3 transmitters for the other 3 frequencies. In the transmitters the RF powers can be amplified, amplitude modulated and phase modulated.

The probe output contains the observing and the lock signal. The latter may be either homonuclear or heteronuclear. Fig. 3 shows how the input and reference signals to the lock receiver are switched from homonuclear to heteronuclear stabilization.

2. Computer and NMR software system

Computer. An excellent introduction of theory and application of digital measurements emphasizing the use of minicomputers is written by Soucek.[17] A similar book written by Korn[18] presents this subject in more

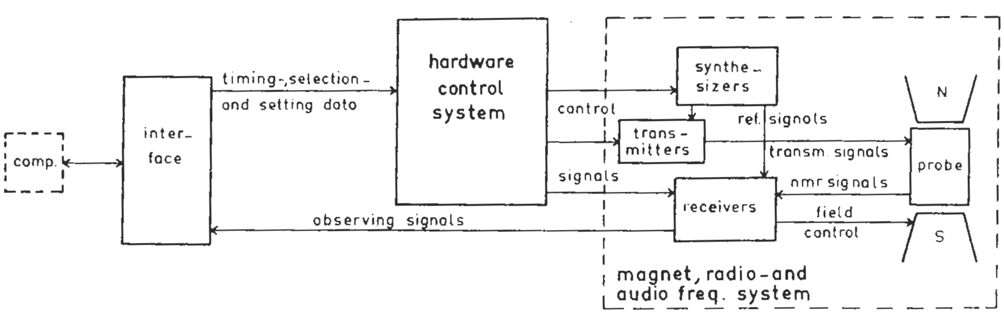

Figure 2. The hardware system.

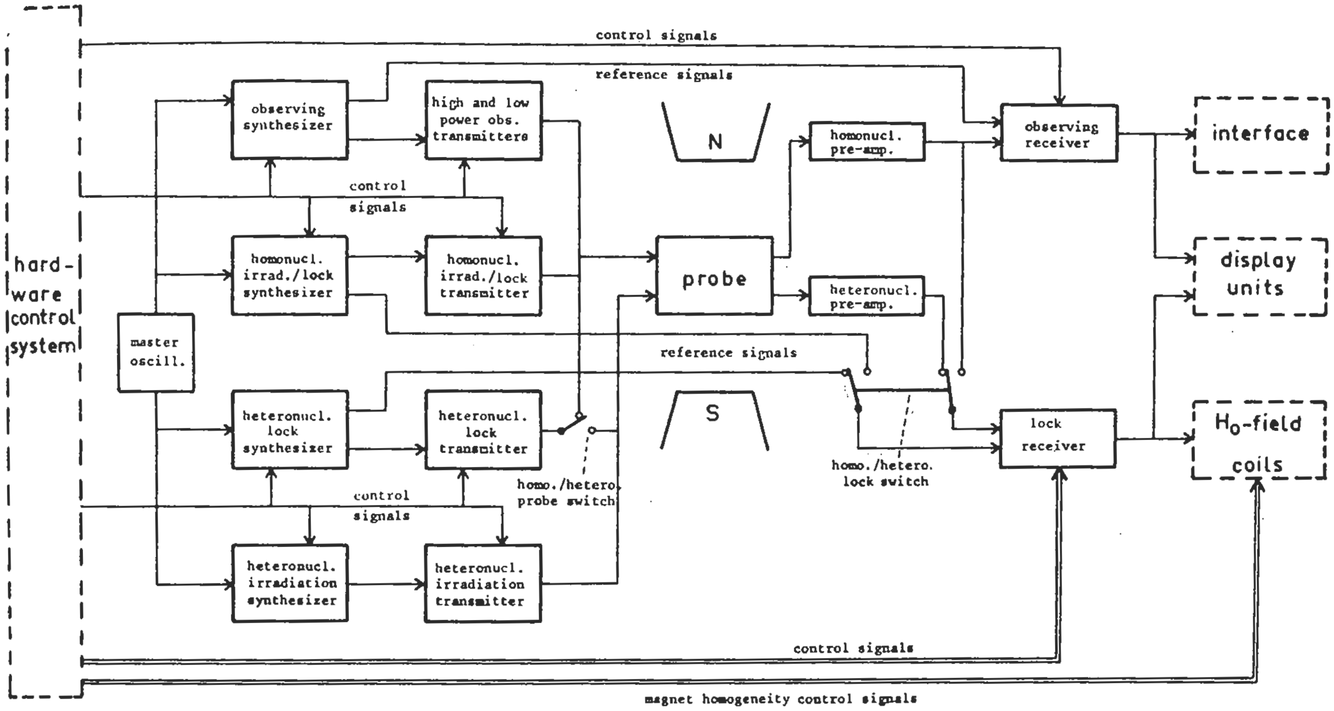

Figure 3. The radio- and audio-frequency system.

detail. Cooper's book[19] about the PDP 11 was written from the viewpoint of NMR-applications.

Of course a minicomputer, as well as a microprocessor based computer system can be used as long as the system satisfies all the requirements. For one of a kind home built spectrometers, a minicomputer based system is more attractive with respect to needed manpower. Two very important criteria are the expected long term service of the computer manufacturer and the peripherals that can be added in a facile manner.

In the following a brief discussion of some computer characteristics and their relationship to NMR-application is given.

Operating system. For the non-time-critical NMR tasks a multi-user disc-oriented operating system is the best choice. For the time-critical tasks (data acquisition, on-line data reduction and spectrometer control) such a system can be a serious limitation.

To avoid this limitation two solutions are available.

(i) The time critical applications are handled by a separate stand-alone processor.
(ii) When the spectrometer requires servicing from the computer, the former operates in the stand-alone mode and is totally devoted to the spectrometer; during the rest of the time it has a multi-user operating system.

Programming capabilities. As high level languages Fortran, Pascal, C and Ada can be considered. Fortran is the most commonly used language but does not force the programmer to employ structured programming. This disadvantage can be prevented by a Ratfor precompiler. An excellent choice is C,[20] which is a powerful structured language with a high execution speed. C will limit the use of the assembly and micro-assembly language to a minimum.

Full advantage of the virtual disc storage can be achieved if a type of segmented programming is possible. For a multi-user environment, program locking is of benefit.

Input/output capabilities. In NMR the spectrometer control, data acquisition and data reduction software has the most severe I/O requirements. At least two dynamically assignable DMA channels are needed for the acquisition and reduction of large decays (>32 K). For the spectrometer control a conditional and an unconditional non-interrupted program transfer mode is necessary (see for details paper two of this series).

In general the interrupted program mode should be avoided in time-critical programs.

Regarding processing speed in multi-dimensional spectroscopy it is very important that the main processor can act as a host for an array processor.[21]

Word length. For a straight, on line, time averaging operation where no scaling procedure is applied, the needed number of bits in the computer (η_c) is given by:

$$\eta_c = \eta_a + {}^2\log R_m \qquad (1)$$

To calculate the maximum number of time averaged scans (R_m) we assume a maximum measuring time of a weekend (64 h) and a maximum scan repetition rate of 1 Hz. As can be calculated[3] fourteen ADC bits (η_a) are always sufficient for a receiver bandwidth of 3000 Hz or more. Substituting these figures in equation (1) results in:

$$\eta_c = 14 + {}^2\log 2.3 \times 10^5 = 31.81 \text{ bits} \qquad (2)$$

Thus time averaging in integer double precision with a 16 bit computer satisfies the most stringent requirements. Upon completing the time averaging the data may be divided by the square root of the number of time averagings without the introduction of serious digitization noise. After the division the maximum needed word length is 23 bits. Thus, the common used floating point 32 bit words, which possess a 23 bit mantissa are just right. A transformation from integer double word to floating point double word will not introduce round-off errors.

There are 4 sources that limit the dynamic range: (1) linearity of the receiver, (2) spectral purity of the synthesizer reference frequencies, (3) finite ADC-wordlength and (4) finite register-wordlengths in the computer. As has been pointed out[3] the synthesizer spectral purity is the dominant one in a balanced design.

The consequences of dynamic range effects of finite register length in the signal processing, executed after the time averaging, are discussed by Oppenheim and Schafer[22] and Rabiner and Gold.[23] Cooper *et al.*[19] pay special attention to the influence of finite register lengths with respect to an FFT algorithm for NMR applications.

The AP 120 B array processor of the Floating Point System has a word length of 38 bits with a mantissa of 28 bits. Extrapolation of the 23 bits needed for the time domain signal with a bandwidth of 3000 Hz shows that this mantissa satisfies the very high dynamic range requirements after a Fourier transformation of such a time domain signal of a few seconds.

Memory size. Data processing on large data blocks and data output to fast display units will take less time if a large main memory is available. For direct data reduction with interactive use of the disc, a data buffer of 3 times the disc track is necessary if the highest input rate must be achieved (see paper two of this series). On the basis of the above, some of the partitions in a multi-user system must be of the order of 30 K. In order to avoid multiple swapping, about 4 partitions are needed if all tasks are done in one computer. This gives a total memory size of about 128 K 16 bit words, including the general purpose operating system.

NMR software systems. Only the internally generated software packages are described in the remainder of this section. The four main tasks which can be distinguished for the spectrometer software are:

(a) The initiation of the measurement.
(b) The control of the spectrometer and the on line data acquisition and data reduction of the spectrometer responses.
(c) The end-processing of the collected data.
(d) The display of the data.

It is possible to service these four tasks with either of two different software designs.

1. A design in which, for each type of experiment, a complete software package must be available if the experiment is to be performed by an operator with only minimal knowledge of the spectrometer system, the measuring sequence, the data operation modules and the processing chain.
2. A design, in which for each task (a), (b), (c) and (d), a separate software package is available. These software packages are written as generally as possible.

Thus for the second design the extra software necessary to perform a new type of experiment in a simple way can be kept very much smaller than in the first design. If many different measuring methods are implemented the total amount of software is less with the second design. Thus, the maintenance of the software is easier. If different workers develop software for different measuring methods on the spectrometer, they are forced to design much more standard types of software under the constraints of design 2 than design 1.

Another advantage of design 2 is that it automatically leads to a modular software system with a structured design. In general, for design 2 a fast mass storage device must be available. When starting, one might automatically choose design 1, to perform the first experiment as soon as possible. However, when the amount of software drastically increases design 2 is the proper choice.

The system flow chart of the NMR-software, showing the connections between the operator, the four software packages, and the mutual links between the four packages is presented in Fig. 4.

The questions, instructions and information of the pre-experiment dialogue software are displayed on a CRT-screen. The answers are given via a keyboard. It is always possible to perform a measurement with exactly the same parameters as the preceding experiment of the same type without entering new parameters. Hence it is necessary to store the information regarding the measuring sequence of each type of experiment on a disc file.

The processing and display information available during the experiment preparation is also stored in this file. After the control words for computer and spectrometer are generated the experiment executing software is started. The NMR signals are displayed after the preset number of scans are executed or after a manual stop command is given. After a study of the displayed signal one can decide either to continue the measurement or to store the collected data in a disc file. The processing and display information to be used for the data management, that was gathered in the pre-experiment software is also stored in that file. Then the file name is reported to the operator. After the file name has been reported, the spectroscopist can, for instance, decide to proceed to another type of experiment with the same sample, to repeat the same measurement on another sample, or to process the collected data.

The NMR data, questions, instructions and file name of the processed data are displayed on a CRT-screen or a storage scope. The operator input for

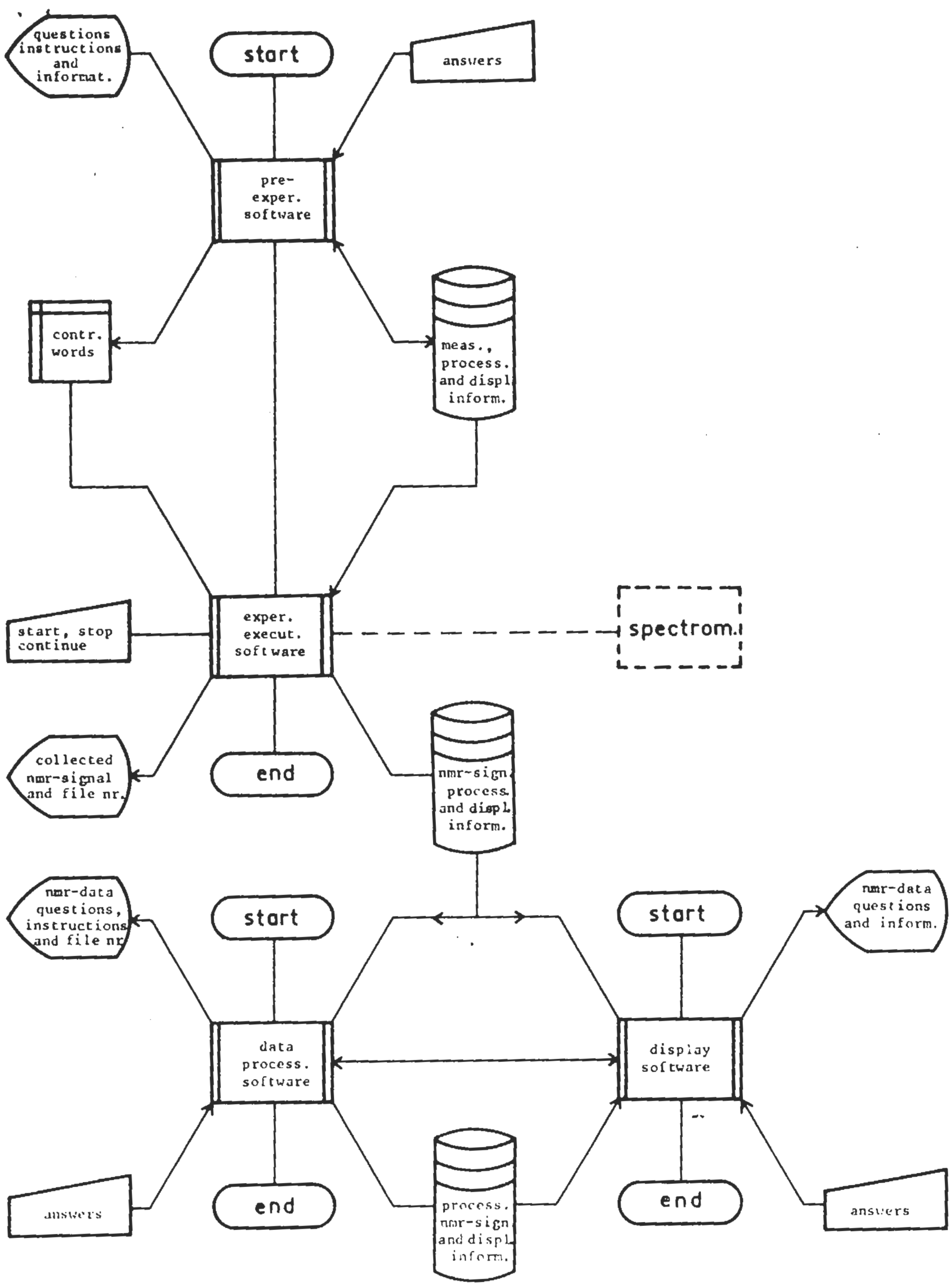

Figure 4. System flow chart of the NMR-software.

the data processing is given either by the way of a keyboard or via a 4×4 array of push buttons in combination with one or two potentiometers.

If the display software is used separately it can make use of all the input and output devices of the processing software plus the plotter.

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Received 7 May 1982
Accepted 12 July 1982