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DAMARIS – A flexible and open software platform for NMR spectrometer control

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Abstract

Home-built NMR spectrometers with self-written control software have a long tradition in porous media research. Advantages of such spectrometers are not just lower costs but also more flexibility in developing new experiments (while commercial NMR systems are typically optimized for standard applications such as spectroscopy, imaging or quality control applications). Increasing complexity of computer operating systems, higher expectations with respect to user-friendliness and graphical user interfaces as well as increasing complexity of the NMR experiments themselves have made spectrometer control software development a more complex task than it used to be some years ago. Like that, it becomes more and more complicated for an individual lab to maintain and develop an infrastructure of purely home-built NMR systems and software. Possible ways out are:

- commercial NMR hardware with full-blown proprietary software or
- semistandardized home-built equipment and common open-source software environment for spectrometer control.

Our present activities in Darmstadt aim at providing a nucleus for the second option: DArmstadt MAgnetic Resonance Instrument Software (DAMARIS) [1]. Based on an ordinary PC, pulse control cards and ADC cards, we have developed an NMR spectrometer control platform that comes at a price tag of about 8000 Euro.

The present functionalities of DAMARIS are mainly focused on TD-NMR: the software was successfully used in single-sided NMR [2], pulsed and static field gradient NMR diffusometry [3]. Further work with respect to multipulse/multitriggering experiments in the time domain [4] and solid state NMR spectroscopy multipulse experiments are under development.

Keywords

NMR instrumentation, spectrometer control software, open source

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1. Introduction

Reviewing a long tradition of home-built spectrometers [5,6,7,8,9] at universities and research institutes, one can see that these developments were driven by

- the need for special features, mobility or flexibility,
- the detailed understanding of the measurement procedure,
- complex pulse sequences and precise definition of data processing,
- adaption to already existing devices,
- the lack of money.

Nevertheless, such equipment is often used with great success at the very forefront of research in NMR. However, often home-built software lacks proper documentation and has no long term support. Frequently, it is designed and built up just for a single spectrometer.

In the Darmstadt case, a lab with nine rather different spectrometers had evolved with time. They were run with three different software platforms, each of them bound to specific hardware.

In attempts to keep up with novel developments, each of these spectrometer concepts revealed design limits or was found not to work properly even within its original specifications. Based on these experiences, a more general solution was sought, enabling experimentalists to use the same experimental control environment at different spectrometers and sharing the effort to improve the common parts of software.

The outcome of these endeavors is the DAMARIS concept – consisting of hardware and software components – which are described and presented on exemplary measurements in this contribution.

2. Project Outline

DAMARIS spectrometers are based on usual personal computers which are equipped with a pulse pattern generator and an analog digital converter (ADC). The computer runs a common operating system (Windows XP or Linux) which provides access to the NMR specific hardware via the vendors' drivers. The drivers are controlled by a so called “back end” program which organizes the components' interactions to a running MR spectrometer.

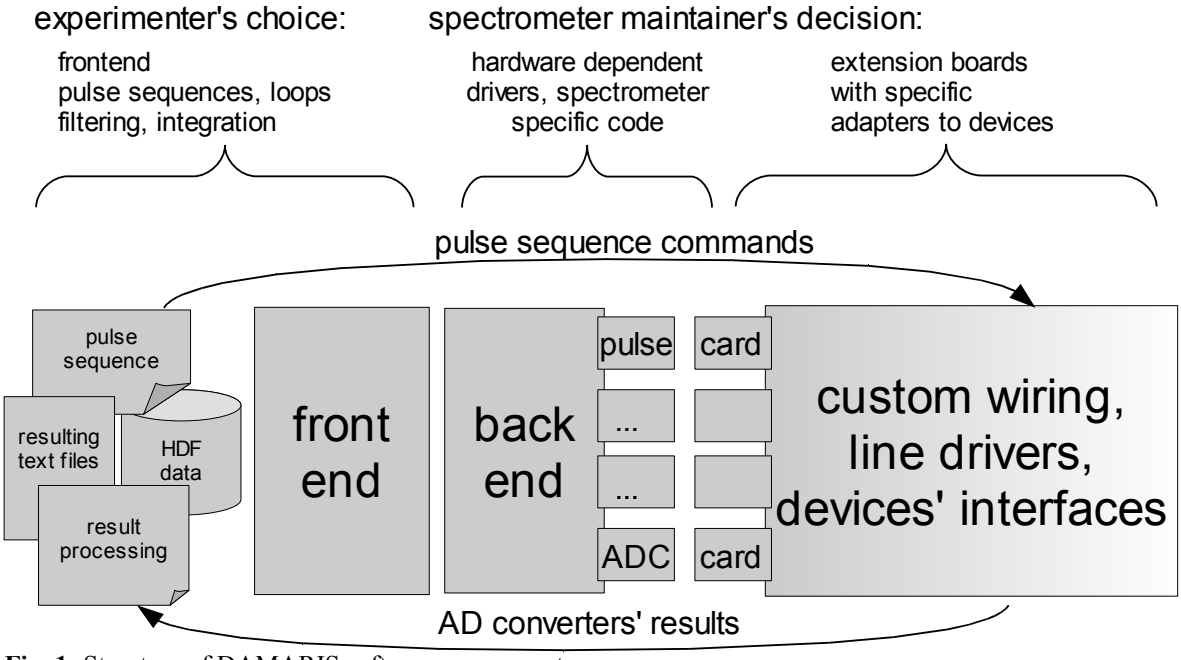

Fig. 1: Structure of DAMARIS software components

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To address the spectrometer's power components (e.g. RF amplifiers, gradient shape controls, pulse formers) a customized digital controller unit (often called the “line driver”, see figure 2) is used. It connects the pulse pattern generator with all other devices, and achieves a timing control with a precision of several nanoseconds during a single MR signal scan.

This “back end” is fed with the actual MR experiment sequences by the “front end”, which is independent of the specific hardware components, therefore the same “front end” can be used on all DAMARIS machines. Information is exchanged via file system, files written subsequently by the “front end” represent “jobs” (e.g. single shots) for the “back end”. Correspondingly data measured by the “back end” is stored in “result” files. So it is easily possible to replay experiments or analyze results on single shot level. Furthermore, this interface only requires basic programming skills to write one's own “frontend”. Modern operating systems handle file access via cache, so the performance is satisfying.

This modularized approach enables the lab staff to fit in old and new devices into the DAMARIS environment. The instrumental modularization rules the software design of the “back end”. Dedicated driver components (classes in terms of object oriented software written in C++) are provided, which are lumped together in the “back end” program. Furthermore the “back end” translates the pulse sequence into specific control signals for the individual hardware components.

Dividing the spectrometer control software into a “back end” and a “front end” part one can realize both dedicated NMR programs for well-defined use cases (“single button applications”) and more advanced options based on general scripting facilities for ongoing methods development. Presently two types of “front ends” are available: a LabView [10] based “front end” and a “front end” solely dependent on free software, which will be described in this article.

This “front end” based on Python [11] and GTK [12] is used for method development in our lab. It provides two scripts which control the experimental procedure and the data processing separately. To monitor the spectrometer while the measurement is conducted, plots of the recorded datasets can be displayed and saved online. These scripts are based on the Python scripting language, so they offer all features of a full programming language. Especially the data processing script benefits from numerical extensions like scipy and numpy [13,14,15].

This “front end” provides an unified access to research lab's MR spectrometer capabilities:

- Pulse sequences can be modified in all parameters,
- Instrumental constants (e.g. preamplifiers' dead time and gating) are accessible,
- Raw data treatment can be controlled in detail by the “front end”,
- Storage of all relevant parameters and processing results is possible in the portable data format HDF5 [16].

Furthermore the expertise on the control software and specific hardware components is collected online [1]. The source code of DAMARIS is freely available, so other labs can join this project. By founding a widespread community sharing code and documentation, mutual benefits will be achieved.

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3. Representative Spectrometer Setup

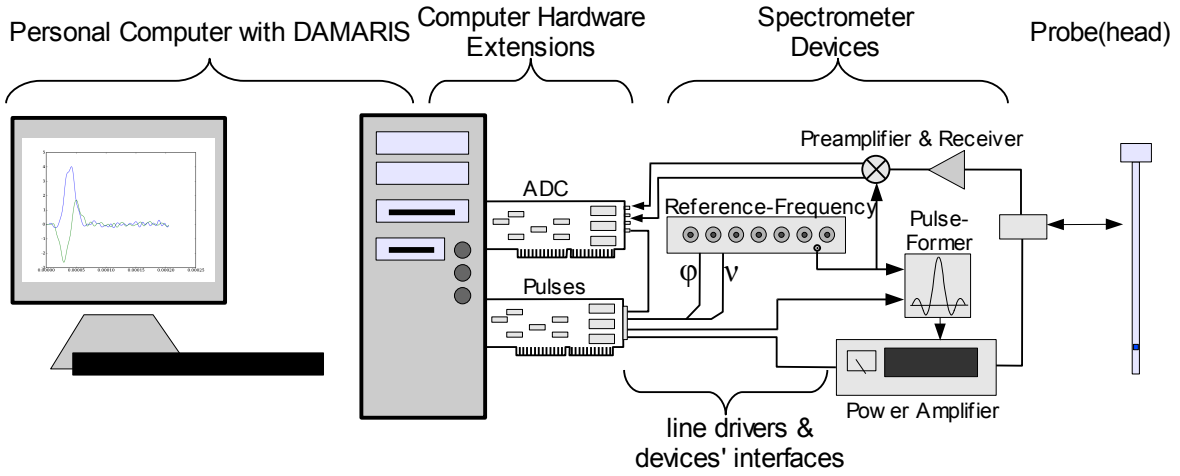

Fig. 2: Exemplary DAMARIS hardware structure

The present standard setup for DAMARIS works with a PulseBlaster 24Bit (SpinCore, Gainsville, FL) pulse programming board and a MI4021 (Spectrum GmbH, Grosshansdorf, Germany) ADC card. To address all remote controlled frequency and phase registers of PTS (Littleton, MA) frequency synthesizers, we have developed a demultiplexing device with 12 TTL lines – in contrast to 48 PTS input lines. All other devices are driven by direct connections to the pulse card. For example such a spectrometer is in operation at a static field gradient spectrometer and provides a home-built positioning stage to control the sample position relative to the magnetic field gradient.

Besides those standard components several other boards and extensions are supported:

- ADC cards from Datel (now C&D Technolgies, Blue Bell, PA), TiePie (Sneek, Netherlands) and Spectrum (Grosshansdorf, Germany)
- Pulse pattern generators and DDS frequency generator boards from SpinCore, (Gainsville, FL)
- Reference frequency generator from PTS (Littleton, MA) with phase and frequency control
- TecMag (Houston, TX) 20Bit DAC for pulsed field gradient control
- Eurotherm (Leesburg, VA) 2000 Series temperature control

All required software components are free and open source (except from some low level drivers bundled together with hardware). For Debian Linux a ready-made package is provided, which makes installation very easy, for most other recent Linux systems the base packages are contained in the standard distribution. In this case, the actual DAMARIS software has to be installed from source files. All packages are also available for Microsoft Windows, but unfortunately each must be installed manually. Detailed installation instructions are given on the homepage.

4. Example use case: Recording of primary and stimulated echo in a stimulated echo sequence

Recording both a Hahn echo and a stimulated echo attenuation curve in static field gradient NMR allows separation of T_2 and diffusion effects [3].

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