

The UIUC Virtual Spectrometer: A Java-Based Implementation of a Learning Environment

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ABSTRACT

The development of the UIUC Virtual Spectrometer (UIUC-VS), an interactive, Java-based simulation and tutoring system, is discussed. The system utilizes the apprenticeship model of learning to create a learning environment for the study of a one-proton nuclear magnetic resonance (NMR) experiment. The development of a learning environment is driven by the goal of linking theoretical knowledge with practical operational experience. Active, exploratory, apprentice-style learning is supported via modes of operation within the system. Students can flexibly choose to "observe the expert" perform and explain operational steps, or to "act as an apprentice" and carry out the steps autonomously. Students can switch between these modes at their discretion, giving them control of the level of intervention by the system. In addition, students can explore and reflect on an "information space" of objects, procedures, and related concepts. The UIUC-VS project is an extension of a previous tutorial application, LEMRS, and uses Java-based, Web-capable technologies to provide a basis for a shared simulation environment for teaching NMR. In creating a computer-supported collaborative learning environment, the system includes a method of asynchronous communication, where the student can post questions and comments to a "question board", complete with the ability to capture the current state of the system and make annotations on the screen capture. Formative evaluations involving undergraduate chemistry students were crucial to inform redesign of the system.

I. INTRODUCTION

In the physical and engineering sciences, students experience both classroom and laboratory instruction. Typically, classroom instruction focuses on theoretical principles, while laboratory instruction focuses on practical tasks such as running experiments using equipment. It is important that the links between theory and practice are strong and clearly articulated. Learning, furthermore, is a social process[1],[3],[4]. Our interest is in using information technology to link theory and practice in the context of a collaborative, simulation-based learning environment. This paper describes the UIUC Virtual Spectrometer, a Web-based learning environment for nuclear magnetic resonance (NMR) spectroscopy. The UIUC Virtual Spectrometer teaches operational procedures in a safe, simulated environment that allows exploration of relevant theoretical concepts. Additionally, mechanisms for asynchronous communication are provided to allow for collaborative interaction and peer tutoring. For a more detailed description, the reader is referred to the Technical Report associated with this project[1]. The UIUC Virtual Spectrometer is based on an earlier stand-alone application, LEMRS[2].

The UIUC Virtual Spectrometer's learning methodology is based on the theories of cognitive apprenticeship[3],[4] and legitimate peripheral participation[5]. These theories emphasize learning-by-doing in the context of the activity where the novice learner interacts with an expert. The UIUC Virtual Spectrometer supports a simple form of apprenticeship learning where the student can choose

the role of an observer as an "expert" runs the experiment, or can choose to "act as an apprentice" and perform the experiment with a variety of tutorial resources.

II. MOTIVATION

NMR spectroscopy is an operational task that rests on a great deal of theoretical knowledge of physics and quantum mechanics. In our studies, we found that even after class exposure to NMR theory and application, an overwhelming majority of undergraduate students have only a rudimentary understanding of NMR. An interactive tutoring system that addresses the theory of NMR spectroscopy and the routine operating procedures associated with using a spectrometer provides individualized, stable, and consistent training[6] that explicitly attempts to activate relevant theoretical knowledge in the context of practice with a simulated instrument. Legitimate peripheral participation[5] or cognitive apprenticeship[7] is an educational paradigm that can support such an agenda.

III. SITUATED COMPUTER-SUPPORTED COLLABORATIVE LEARNING

Situated action theory emphasizes the local management of activity as mediated by relevant environmental cues[8][9]. The implications for learning are that appropriate actions are generated from a recognition of appropriate opportunities given the context. Apprenticeship learning is a means through which situated learning can occur, where apprentices are active participants in an activity, usually with an expert. Apprentices' process of learning moves from peripheral to full participation in the activities of a community of practice, as the expert "fades" from engagement of the activity. The support for active contextualized learning[10] lends itself well for the teaching of procedural knowledge and operational skills. Vygotskian theories of learning stress that individuals gain skills by engaging in tasks with an "adult or more capable peer"[11]. In general, four overlapping stages of pedagogy can be identified[3]: (1) Modeling, through the observation of expert performances, (2) Coaching, with expert guidance and help, (3) Fading, where expert assistance is gradually withdrawn, and (4) Reflecting, student self-monitoring and reflecting upon past performances.

Computer-Supported Collaborative Learning (CSCL) argues that learning is generally seen as a collaborative activity that is situated in its environment. Collaboration promotes convergence of a shared relational meaning[12]. Knowledge is constructed incrementally through a process of mutual contributions via interaction. For a more in-depth review of situated learning and the use of computer technology in education, the reader is referred to the Technical Report associated with this project[1].

IV. UIUC VIRTUAL SPECTROMETER

Nuclear Magnetic Resonance Spectroscopy.

Nuclear magnetic resonance (NMR) spectroscopy is a technique used to study molecular structures via the interaction of radio frequency electromagnetic radiation with nuclei immersed in a strong magnetic field[13]. NMR spectrometers are instruments which support this type of analysis. Spectrometers typically consist of a computer (which provides software that allows the user to input parameters, run an experiment, and examine the results of an experiment) and the following apparatus: a spinner (to spin the test tube holding the sample), a magnet with electronic "shim coils", a lock system (to stabilize the magnetic field), and a radio frequency transmitter and receiver. The usual procedures of a basic NMR experiment involve sample preparation and insertion, locking and shimming the magnet, setting of experimental parameters, and processing and analyzing of the

resulting spectrum. Locking and shimming the magnet to form a stable, homogeneous magnetic field is the critical part of the process.

Conceptual Overview.

The UIUC Virtual Spectrometer is a Web-based system written in Java. It is an interactive learning environment for the procedures and theories involved in conducting a generalized Nuclear Magnetic Resonant (NMR) spectroscopy experiment. It supports active, apprenticeship-style guidance and exploration. Support for apprenticeship learning is provided via demonstrations by an expert and tools for exploration and reflection. Students have the option of flexibly switching between two instructional levels, which are (1) *Observe Expert*, where students observe an "expert technician" perform and explain an NMR experiment and (2) *Act as an Apprentice*, and carry out the procedure themselves. Thus, rather than the system making macro-level decisions about when to "coach" and when to "fade", the student has control over this aspect of the learning process. Tools for exploration and reflection consist of options to explore related theoretical concepts and ask "what if" questions.

Once the student has selected a level of expert guidance, an NMR experiment begins. The system will supply experimental scenarios to the student. The base simulation models all of the important aspects of a real NMR experiment, including locking and shimming and acquisition. Students may vary lock and shimming parameters and observe their effects on the lock level and lineshape displays. The lock level display supports general shimming procedures (e.g., maximize the lock level) while the lineshape display allows direct visualization of the individual effects each shim value has upon the magnetic field (e.g., each shim produces specific aberrations in the line shape). Students also engage in the acquisition portion of an NMR experiment by iteratively setting values of various parameters (e.g., magnetic strength, number of scans, spectral width). Data acquisition filters, and Fast Fourier Transforms of the spectrum are also superficially supported.

Throughout the simulation, students are able to browse an "information space" of object definitions, relations, and procedures. These types of non-directive support have been shown to be extremely useful[14]. The *More Info* option allows the student to explore theoretical concepts (what is this and why is it important?) and hypothetical situations (what if...?) that are relevant at that point of the lesson. The *Let Me Try* option displays a context-sensitive checklist to provide guidance on operational procedures. The *Show Me* option allows the student to switch into *Observe Expert* mode. Finally, when the student has successfully completed the current part of the scenario, the *Done* button advances him or her to the next part of the lesson. Overall, with these relatively simple mechanisms, the system allows the student a great deal of flexibility and discretion in training.

Migration to the World-Wide-Web.

One major direction of interest is to support groups of student apprentices in learning about NMR spectroscopy by extending the original stand-alone application, LEMRS[2], to be a computer-supported collaborative learning environment. A first step towards collaborative support is a Web-based implementation. The UIUC Virtual Spectrometer (<http://tortie.me.uiuc.edu:8000/UIUC-VS>), is implemented as a series of Web pages utilizing Java applets.

The goals of the project are to re-implement LEMRS in Java as a Web-based interactive simulation environment and provide initial mechanisms for asynchronous collaborative learning, including an "organizational memory" of comments from previous users via a Question Board with organized annotations.

Architecture of UIUC-VS.

The UIUC Virtual Spectrometer has three primary conceptual area: (1) main lessons for conducting

NMR experiments, (2) a context-dependent information index (*Let Me Try* and *More Info*) and (3) expert knowledge, narrative "voice-overs" while in the *Observe Expert* mode. Each conceptual area is encapsulated by a distinct Java applet, each running in its own window (the Main Window, the Information Window, and the Expert Window, respectively). Additionally, it is important for evaluative purposes to track the student's actions, so a separate (non-visible) applet records the student's actions. Finally, an applet in the Menu Window keeps track of the student's present position within the system.

User Interface and Implementation.

The UIUC Virtual Spectrometer's user interface, like the original LEMRS interface, is a generalization of the interfaces offered by common NMR machinery. NMR laboratory equipment can come in many forms and there exists no standard interfaces. This extends not only to interface design, but functionality as well. For instance, some NMR machinery may have automatic shimming while others may require manual shimming. Additionally, simulation and visualizations are built into the UIUC Virtual Spectrometer to support student's reasoning and comprehension tasks (i.e. "what-if" reasoning) and are not found on actual NMR machinery.

The Five-Window Layout. The system splits the browser into five "windows" or frames, as demonstrated in Figure 2. The top window simply holds a title for the UIUC-VS system. The Main Window (center-right) is where the main lessons are conducted. The Menu Window (upper left) displays the current and completed lessons. The Information Window (middle left) displays the results of pressing the *Let Me Try* or *More Info* buttons (i.e., a context-dependent checklists of procedures and hierarchies of information and concepts that the student can explore, respectively). Finally, the Expert Window (bottom), displays the expert knowledge of the system in the form of answers to questions, what-if scenarios, and demonstration tutorials. This information is conveyed in text and voice form.

Figure 1. Illustration of the UIUC Virtual Spectrometer in *Observe Expert* mode, in the Magnet lesson.

Mode Selection Page. Once the full system has loaded, the student can choose which tutorial mode the system will conduct the lesson: the *Observe Expert* mode or the *Act as an Apprentice* mode.

Observe Expert. Using both audio (optional) and text, the student is taken on a step-by-step tour of the six lessons that comprise an entire NMR Experiment. Figure 1 illustrates the system in *Observe Expert* mode, demonstrating the steps necessary to insert the sample into the magnet. The student simply keeps pressing the *OK* button to continue to the next step of the tutorial after reading (or listening to) the description of the present step. The Main Window is automatically updated throughout the demonstration. The student may stop the demonstration at any time, and switch to the

Act as an Apprentice mode.

Act as an Apprentice. There are six lessons in a basic NMR experiment: (1) *Goals*, (2) *Sample*, (3) *Magnet*, (4) *Lock & Shim*, (5) *Experiment*, and (6) *Analysis*. Most of the lesson pages contain buttons labeled *Show Me*, *Let Me Try*, and *More Info*, as well as multiple levels of hint support. The student is free to work through each lesson, and upon successful completion, the appropriate box is checked. The Menu Window record progress and as the student enters a specific lesson page, the name of that page is highlighted.

Goals. Details the learning goals of the lessons to follow.

Sample. This lesson displays information about the sample and the lock solvent used in the experiment, with the possibility of choosing a different lock solvent.

Magnet. The student is presented with a menu listing the required lesson (Sample Insertion, illustrated in Figure 1) and two optional lessons: (1) View Current Parameters, displaying the present status of experimental parameters such as nucleus information, nuclear spin state energies, magnet strength, temperature, and nuclear spin quantum numbers, and (2) Look at Other Nuclei, where the student can view the experimental parameters when a different nuclei is used, as well as adjusting the magnet strength or the temperature and see the resulting changes in the experimental parameters.

Lock & Shim. Figure 2 depicts the Lock & Shim lesson, where the student attempts to shim the magnet to create a uniform magnetic field. The Lock & Shim Page provides direct visualization of the lineshape. The student can load a shim table, select a shim and adjust it, and vary the lock gain. The resulting lock level is depicted via a bar graph. Figure 2 also shows the result of pressing the *More Info* button. The student selected the topic Lineshape and pressed *What is It and Why is It Important?* and the resulting answer appears in the Expert Window.

Figure 2. The UIUC Virtual Spectrometer in *Act as an Apprentice* mode, in the Lock & Shim lesson.

Experiment. The student calculates experimental parameters based on the current acquisition parameters. The calculations are based on several formulas, which can be found in the information within the *More Info* hierarchy.

Analysis. The student sets the line broadening characteristic, performs a Fast Fourier Transform on the data, and views the resulting spectrum and free induction decay graph. The student can zoom the spectrum for greater resolution of regions of interest.

Show Me. The *Show Me* button will start the demonstration mode for the present lesson. The Expert

Window takes over control of the interface again, and the student is led through a step-by-step tutorial of the procedures necessary to successfully complete this portion of the experiment. The student can stop the demonstration at any time, and control of the Main Window passes back to the student, with the settings prior to the invocation of the *Show Me* demonstration mode restored.

Let Me Try. A step-by-step checklist of procedures appears in the Information Window, as shown in Figure 1. As each step is successfully completed, the corresponding box is checked. The student can press *Reset Lesson* to reset this portion of the lesson to its starting values.

More Info. A selection list of topics appears in the Information Window. After selecting a subject, the student presses the *What is It and Why is It Important?* button, and an answer appears in the Expert Window (see Figure 2). Additionally, the student can explore "what-if" scenarios by pressing the *What if...?* button.

Multiple Levels of Hint Support. If the student attempts to leave the present lesson by pressing *Done* without successfully completed the lesson, a window pops up to let the student know that some parameters are set incorrectly. If the student erroneously presses *Done* a second time, the popup window message is more specific about which parameters are set incorrectly. If the student again erroneously presses *Done*, the popup window message inquires if the system should set the correct parameters automatically (after explaining in detail what needs to be done to successfully derive the correct parameters). Thus the system attempts to tailor hints to the student's actions.

V. FORMATIVE EVALUATION AND REDESIGN

A pilot formative evaluation was conducted to assess the usability of the UIUC Virtual Spectrometer. Formative evaluation techniques are used early in design to provide feedback to designers in order to improve the usability and functionality of the system. For the design of tutoring systems, students can interact with the system in unexpected ways, which are difficult to predict. Formative evaluations can be a powerful method in obtaining this type of information[15]. Four Chemistry undergraduate students were recruited to come in and work through the system. All the students in the study had some familiarity with NMR spectroscopy, and averaged 15.5 hours per week on computers. The students were asked to first work through the *Observe Expert* mode, and then attempt to do the experiment themselves in *Act as an Apprentice* mode. All their computer actions were logged, and the sessions were tape recorded. The transcripts (both verbal and the logging data) were analyzed for common themes and incidents. The following problems were identified.

S No students looked to the lineshape display for feedback when adjusting the shims.

S All students asked what the lock solvent was and what was it used for.

S Students consistently used the formulas incorrectly.

S With the audio in *Observe Expert* mode turned off, students often prematurely went to the next step, not realizing that the text in the Expert Window extended beyond what was visible.

S Students did not check previously adjusted shims when finished adjusting current shims

S Students did not always know what had changed on the display in the Main Window during *Observe Expert* mode.

When analyzing the problems, it is important to consider overall causes apart from the details of the

problem itself. Some redesign ideas are simple fixes to existing, specific problems. Other redesign ideas, however, are addressed to larger issues, where the problems encountered served to as examples to identify methodological problems. The analysis of the problems (and the resulting redesign decisions) are as follows:

S The lineshape display was invariant during the *Observe Expert* mode, so the students never learned to look to it for feedback as they adjusted the shims. The demonstration was changed to include a dynamically changing lineshape display.

S A short explanation of the lock solvent and its uses was included with the lock solvent information in the Sample page.

S The formulas were re-written to include units and express themselves more clearly.

S Various problems with the *Observe Expert* mode stemmed from the fact that the navigation through the demonstration was one-way. Clicking *OK* advanced the demo, but students were unable to revisit the previous step unless they restarted the demonstration from the beginning. The interface was modified to allow students a mechanism (a *Previous Step* button) to reverse their actions if desired.

S In order to increase visibility of the salient events on the Main Window during the demonstration mode, widgets that are affected by pressing *OK* would briefly flash yellow, to draw the student's attention to them.

As more functionality is added to the UIUC Virtual Spectrometer, more formative evaluation of this type will be performed to assess usability and alert the designers to problematic aspects of the design.

VI. ASYNCHRONOUS COLLABORATION VIA THE QUESTION BOARD

One of the key goals in the development of the UIUC Virtual Spectrometer is to use its Web-based technology to create mechanisms for collaborative learning tools. In order to provide a forum for asynchronous communication between students, the Question Board was developed. The Question Board, shown in Figure 3,

Figure 3. Illustration of the Question Board.

is a messaging system that functions somewhat like an Internet newsgroup. That is, students have the ability to post messages to a central server, which then makes all messages available for inspection by others. Through this messaging system, students can communicate asynchronously as they hold discussions of a topic of interest, ask and answer questions, and generally inform and learn from each other. The Question Board supports "context capture" by allowing the students to attach to their message a snapshot of the Main Window. In this way students can relate pictorially the present state of their system. Additionally, students can highlight, with transparent colored boxes, portions of the snapshot in order to draw attention to salient features germane to their question or comment. When students respond to the message, they can overlay their own highlights (in any of nine colors) if they wish to demark another portion of the snapshot. Thus students have a common object which they can annotate and share in the course of a discussion.

The Question Board can be used by students as they engage in tutoring each other. The system may also be used as a way to involve outside expert or teachers in answering student questions. We are in the process of designing experiments to evaluate the UIUC Virtual Spectrometer with the Question Board.

VII. ON-GOING AND FUTURE WORK

The UIUC Virtual Spectrometer, in its present incarnation, offers an excellent starting point to further explorations of machine-mediated learning. Work is underway with the National Computational Science Alliance (NCSA) to integrate the UIUC Virtual Spectrometer into the NCSA Habanero environment, an experimental framework that imports single-user Java applications and recasts them a multi-user, collaborative work environments (c.f.

<http://www.ncsa.uiuc.edu/SDG/Software/Habanero>). Once the UIUC Virtual Spectrometer is recast as a Habanero tool, users will be able to simultaneously share the interface when working on different machines. Each user sharing the tool will see the real-time actions of the other participants as they manipulate the interface. Thus the tool becomes a computer-supported collaborative learning environment[16] that supports both asynchronous collaboration (via the Question Board) and synchronous collaboration (via its incarnation in Habanero).

VIII. ACKNOWLEDGMENTS

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