Purpose of the Document:
This document describes the project outcomes of the partnership between the Ohio Supercomputer Center and Miami University to cyber-enable Ohio’s 850 MHz Nuclear Magnetic Resonance (MU-NMR) spectrometer, the first of its kind in North America.
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Glossary

**Nuclear Magnetic Resonance Spectrometer (NMR):** A computer-controlled scientific instrument used to determine supra molecular structures and functional materials in the biomedical sciences.

**Remote Instrumentation (RI):** An umbrella term that encompasses Remote Observation, Remote Operation, and Remote Monitoring of computer controlled scientific instruments such as electron microscopes, spectrometers, and telescopes.

**Remote Observation:** Term for visualization of instrument control screens and data acquisition from a remote location over the Internet.

**Remote Operation:** Term for visualization and control of instrument control screens and data acquisition from a remote location over the Internet.

**Remote Monitoring:** Term for the ability to remotely monitor progress of an experiment running on an instrument.

**Project:** Term for referring to several related sessions involving analysis of one or more samples using experiments. Also, refers to a research study using an instrument.

**Session:** Time allotted for running experiments using the instrument control PC at an instrument lab (e.g. Topspin that controls the 850 MHz NMR at Miami University).

**User:** Local or Remote person in a RI session who either is a Moderator, Observer or Operator.

**Moderator:** User who can grant/revoke session control to any of the other users; always has observer/operator privileges.

**Observer:** User who can only view the session.

**Operator:** User who can view and control the session

**KVMoIP Device:** Short for Keyboard, Video, and Mouse over IP - Appliance solutions by vendors such as Adder (http://www.adder.com) that require setting up a hardware appliance at the instrument that can be accessed via VNC (e.g. Real VNC) software on PCs.

**Web-portal:** Service hosted by OSC for multi-user RI session setup, multi-user RI session collaboration, experiment progress monitoring and data management.

**RICE:** Short for Remote Instrumentation Collaboration Environment - used for instrument desktop sharing via VNC and session status management via RI web-portal communications (i.e., Connect, Observe, Operate, Disconnect).

**Data Cache:** A server that is installed at the instrument lab to securely move the experiment data from the instrument PC to OSC storage
Executive Summary

Miami University’s 850 MHz Nuclear Magnetic Resonance (MU-NMR) shown in Figure 1 is an expensive ($2.5 Million) and rare scientific instrument, and is the first of its kind in North America. Cyber-enabling the MU-NMR instrument resources and related data sets using a remote instrumentation cyberinfrastructure can improve user convenience, avoid duplication of instrument investments and significantly reduce costs.

Ohio has long had a collaborative group of institutions which have worked together, using Ohio Board of Regents funds, to make sure that Ohio leads other states in the quality of its NMR facilities. In this project, the Ohio Supercomputer Center (OSC) partnered with MU to cyber-enable the MU-NMR by developing a cyberinfrastructure and software that leverage OSC’s software development, image processing, networking and storage resources for research and training. Specifically, OSC developed two solutions that have been deployed for the MU-NMR: (i) Remote Instrumentation Collaboration Environment (RICE), and (ii) Remote Instrumentation (RI) web-portal. RICE is a software application that provides remote observation and remote operation capabilities to multiple simultaneous users of the MU-NMR. The RI web-portal integrates RICE and has web-services that centralize handling of user accounts, user privileges, user authentication, experiments setup for projects, remote user communications, remote monitoring of experiment progress, and data management. Both these solutions have been developed with careful considerations to: instrument safety, network and data security, open-standards without licensing restrictions, extensibility to other instruments, and ease of on-going maintenance. With the help of MU NMR lab and IT infrastructure personnel at MU, the solutions have been successfully deployed in a RI cyberinfrastructure hosted by OSC.

The capabilities of the cyber-enabled MU-NMR have been demonstrated at the NSF Cyber-enabled Instrumentation Workshop, Internet2 Fall Member Meeting, ACM/IEEE Supercomputing Conference, Internet2 K-20 Advisory Committee Meeting, and NJEdge.Net Technology in Education Conference. MU is extending the remote instrumentation solutions with the help of OSC to three different instrument technologies: High Field Nuclear Magnetic Resonance Spectroscopy, X-ray crystallography, and High Performance Liquid Chromatography/Mass Spectrometry. Further, MU will use the OSC-developed solutions along with instructional materials developed at the Eminent Scholar Laboratory to demonstrate remote instrumentation at four Ohio Institutions: Bowling Green State University, Ohio University, Muskingum College, and Talawanda High School. Such demonstrations are intended to make available the MU-NMR resources and instructional materials to remote user communities who do not have access to high field NMR technologies and related instructional materials to engage students. Further, they are intended to encourage wider-adoption of the OSC-developed solutions amongst the Ohio's NMR consortium or other Ohio NMR owners/users and their national and international partners.
1 Introduction

Nuclear Magnetic Resonance (NMR) spectroscopy is a fundamental analytical technique used to study supra molecular structures and functional materials in the biomedical sciences. The data acquisition and processing of the output from these NMR systems is time consuming and limited by the computational resources available for analysis of the spectral data they produce. This project makes significant progress towards accomplishing the Chancellor’s vision to ensure that Ohio is a leader in biomedical research. The goal of this project is to establish a remote data acquisition and remote instrumentation control capability in the Eminent Scholar Laboratory in the Chemistry and Biochemistry Department at Miami University. The project leverages upon the state’s expertise in cyber-infrastructure, high performance computing and signal and image processing to the challenge of ready access and processing of NMR data. The project’s salient outcomes are a remote instrumentation cyberinfrastructure and software that enable remote access to Ohio’s 850 MHz NMR, storage and retrieval of NMR data and instructional materials for NMR spectroscopy. The outcomes are extendable to other NMR systems, by supporting storage, retrieval and higher-speed analysis of NMR data using the computational and networking resources of the Ohio Supercomputer Center.

2 User Scenarios

The user scenarios supported by the OSC developed solutions for research and training of the Cyber-enabled MU-NMR are as follows:

Web-portal Administrator

- Configures the web-portal for instruments, and registers Instrument Technicians and Remote Users in the OSC web-portal.
- Monitors active remote instrumentation sessions and can control remote access to the instruments.

Instrument Technician

- Remote Users, who are registered members in the OSC web-portal, schedule time on the instrument and submit the details of the experiment run. They ship their sample-under-study to the Instrument Technician.
- At the scheduled experiment time, the Instrument Technician can “turn-on” instrument access for the Remote Users. During an experiment that takes 2-3 days to complete, the Instrument Technician can update the experiment status for Remote Users’ progress-tracking.
- After the experiment completes, Instrument Technician can “turn-off” instrument access and initiate archiving of the experiment data using a web browser for the Remote-users to view/download.

Remote Users

- Multiple Remote Users observe and collaborate with an Operator controlling the 850 MHz NMR in a VNC session during an experiment run.
- Once the experiment is completed, the Remote Users can view the experiment data files using a web browser and use them for analytics involving computation and visualization.
3 Solutions Development

OSC has developed a peer-to-peer remote observation and remote operation software application called Remote Instrumentation Collaboration Environment (RICE). RICE can support multi-user desktop-sharing by using a keyboard-video-mouse over IP (KVMoIP) device at the NMR site and virtual network connection (VNC) software at the remote site. The KVMoIP device does not require any software installation on the NMR control computer and also does not utilize the NMR control computer resources to handle sessions with multiple remote users.

OSC has integrated RICE with an RI web portal which has web-services to centralize handling of user accounts, user privileges, user authentication, client software distribution, administration of KVMoIP device, experiments setup for projects, communications between remote users and instrument technicians, and remote monitoring of experiment progress. In addition, OSC has automated the process of archiving the instrument results in a central data repository at OSC for later retrieval by remote users for analytics involving computing and visualization.

![RICE and RI Web-portal Screenshots](image)

Figure 2: RICE and RI Web-portal Screenshots

The developed solutions shown in Figure 2 have been developed with careful considerations to: instrument safety, network and data security, open-standards without licensing restrictions, extensibility to other instruments, and ease of on-going maintenance. They function on computers using the Linux operating system. They can be used by businesses, educators and academics, and to the extent possible, does not include any sub-components with licensing terms that would bar such use.
3.1 Architecture

Our RI web-portal components shown in Figure 3 have been developed using the Pylons Python web framework. The RI web-portal interface comprises of: (a) web-pages that allow managing user accounts of the technician(s) as well as the remote users, and (b) web-pages that enable the operator(s) and remote users to request various application service processing. The application service processing corresponds to: turn ON/OFF remote observation/operation, RICE client/server download, new experiment configuration setup, experiment progress tracking, instrument technician and remote user communications, and viewing accounting/monitoring logs for tracking usage. The application service interacts with the data service for data storage at OSC’s mass storage system, and data retrieval through the web-portal. Similarly, third-party analysis clients such as Matlab or TopSpin can be made to interact with the data service for analytics-driven data retrieval and processed data storage. In addition, we developed a web-portal component to handle the collaboration tools functionality for text-chat, multi-user presence and control-lock passing through the web-portal interface. The RICE clients provide the multi-user collaboration tools functionality by interacting with this web-portal component.

3.2 Work-flows

Figure 4 shows the RI web-portal work-flows to create and view instruments, projects and sessions. Some of the work-flow states are common to both the instrument technician and the remote user(s). The other work-flow states that are applicable only to the instrument technician are shown in dotted lines. Upon user login, all the instruments supported by the web-portal are listed. Once a particular instrument is selected, both the past as well as the current projects and related RI sessions are listed. If a particular session of a project is selected, data sets corresponding to the session experiments are shown. Only the instrument technician has the privileges to create new instruments, projects and sessions in the web-portal.

Before creating a new session, the instrument technician is assumed to have taken the following steps: (i) instrument technician has obtained the experiment configuration from one or more remote users, (ii) an RI session has been scheduled on the instrument calendar and RICE client download instructions have been sent.
to the remote user(s), and (iii) the remote user sample has been loaded into the instrument at the scheduled time for the session. At this point, the instrument technician enters the project/session details into relevant forms in the web-portal. Thereafter, the instrument technician is prompted to turn ON the RICE server at the instrument side from the web-portal. Once the RICE server has started, the remote users can connect to the instrument using their RICE clients and observe/operate the instrument control-software screens using the control-lock passing. The instrument technician is also allowed to update the progress of the experiment in the web-portal for the remote users to monitor the experiment progress. Such remote monitoring is particularly useful when experiments could last for several hours or even days. After the session is completed, the instrument technician is prompted to turn OFF the RICE server. Now, the RICE client sessions expire and the remote users will no longer be able to reconnect to the RICE server with the previous session credentials. Subsequently, a data transfer is automatically initiated to copy the experiment data from the instrument computer to the mass data storage system at OSC. The instrument technician and remote users can view and download the transferred experiment data via the web-portal.

![Web-portal work-flow states](image)

**Figure 4: Web-portal work-flow states**

### 3.3 Feature Sets

#### 3.3.1 User Accounts and Privileges

The web-portal administrator can create user accounts to access the web-portal features. The web-portal administrator can also configure user groups with relevant privileges (technician, operator, observer, moderator). Example of privileges of a moderator are: can create projects/samples/sessions/experiments, grant/revoke remote operation to users, post experiment progress notes, and initiate data transfer after experiment from instrument PC to OSC storage.

#### 3.3.2 Management of Instruments, Projects, Samples, Sessions, Experiments

The web-portal administrator can create/edit new instruments in the web-portal. For a chosen instrument, the web-portal administrator can create/edit projects and sessions to manage remote access of users to an instrument and organize related experiment data. All users will be able to view a list of available instruments, corresponding projects, samples and all active or past sessions. Clicking on an instrument, project or session
will display additional information, and suggest work flows. For example, clicking on an active session will allow a user to look at the sample in the experiment and also join the session (if user has necessary privileges).

Many experiments can be performed within a session on multiple samples. For each experiment, the instrument operator (or designated remote researcher/operator) creates a new experiment and enters its name, type, and description. The source data directory on the instrument PC is located (using hints from the current project and sample) and the files may be flagged for automatic archival. The experiment may optionally be queued if it will not complete immediately. When the experiment is done, the operator/researcher must update the status in the web-portal.

3.3.3 KVMoIP and RICE Access Control
The web-portal manages ON/OFF of the KVMoIP device and user accounts to access the Topspin PC via the KVMoIP device. From the web-portal, a user with moderator privileges can turn ON the RICE server or the KVMoIP device at the instrument side. The moderator also can assign users to the session. One KVMoIP account and random password will be generated for each user only for the duration of a session. A RICE client is available via the web-portal for download. To connect to the instrument for an active session (i.e., RICE server is ON), a configuration URL needs to be used in the RICE client. A web-page in the web-portal will display list of currently online RICE client users, and their roles (e.g. moderator/observer/operator). The web-portal permits privileged users to perform control-lock passing i.e., request, yield, and/or grant remote operation status to themselves or others. After the session is completed, the moderator can turn OFF the RICE server; this will prevent any RICE clients to connect using expired configuration URLs. A KVMAdmin web-page is provided to create/edit KVMoIP device information in the web-portal.

3.3.4 Asynchronous Chat for Remote Monitoring
The web-portal allows users to maintain a list of messages for remote monitoring of session events and for generating usage reports. Some messages are auto-generated by the web-portal to indicate for example, whether a session is active. Users can create/edit messages to track various session activities in an asynchronous manner (e.g., update the status of a long-running experiment by posting the percent complete or estimated time remaining).

3.3.5 Experiment Data Archival at OSC Storage
During session setup, the user is prompted to indicate the experiments data directories on the instrument PC. After completion of experiment(s), the web-portal will scan the instrument PC data directories to find all the experiment data files. The files are automatically transferred to OSC storage from the instrument PC for archival. The archived data is available to the user(s) owning the session for viewing and download.

4 Cyberinfrastructure Deployment

With the help of MU NMR lab and IT infrastructure personnel at MU, the solutions have been successfully deployed in a RI cyberinfrastructure hosted by OSC. Using remote operation, the cyberinfrastructure has been tested for NMR instrument spectra analysis tasks such as tuning of the key parameters of the computational analysis. The cyberinfrastructure has also been tested for storage of the NMR and mass spectrometry data along with suitably de-identified data associated with the sample under test.

The RI cyberinfrastructure deployment for the MU NMR is shown in Figure 5. At the NMR lab, a hardware called IPSON contains the control electronics of all the physical NMR components. Topspin is the software that controls IPSON and runs on a Redhat Linux PC connected to the IPSON hardware. The RICE client can be used for remote observation/operation of the TopSpin computer. The web server hosted at OSC interacts with a “data cache server”. This server is used to enable the instrument technician at MU to transfer the experiment data from the NMR to OSC’s mass data storage upon experiment completion. It allows configuring data-access control for remote collaborator sites without changes to Topspin PC. Network
security issues have been addressed to allow only restricted access from OSC and remote user computers to the MU NMR lab. However, the OSC hosted web-portal is open to the Internet. Given such a deployment of OSC equipment at MU, OSC had to closely co-ordinate with the MU campus technology infrastructure group regarding on-going system maintenance and security considerations.

Figure 5: Cyberinfrastructure showing RI Solutions Deployment for the MU NMR system

5 Outreach Activities

Presentations/Demonstrations:


Peer-reviewed Publication:

Press Releases:


Appendix – I: Project Poster

Cyber-Enabled 850 MHz NMR

Leveraging Ohio’s investments in scientific instruments, wide area networking, high performance computing, and data storage to foster academia-industry collaborations involving cyber-enabled instrumentation

Remote Instrumentation Overview
Remote Instrumentation involves cyber-enabled scientific instruments (e.g., electron microscopes, spectrometers, and telescopes) over the Internet for academia and industry users.

Components of Remote Instrumentation
- Remote Site
  - Software Clients
  - Web Portals
- Remote User Site
  - Remote Observation
  - Remote Operation
  - Operator Communications
  - Lab Notebook

Why Remote Instrumentation?
Benefits
- Return on Investment (ROI) for instrument labs
- Avoids duplication of expensive (>$450K - $4 Million) instrument investments

Use Case for Research & Training
Remote Users
- Multiple Remote Users observe and collaborate with an Operator controlling the 850 MHz NMR NCE session during an experiment.
- Once the experiment is completed, the Remote Users can view the experiment data files using a web browser and download them for analysis involving computation and visualization.

Instrument Technician
- Remote Users, approved members in the OSC web-portal, schedule instrument time and submit the details of the experiment run. They ship their sample under study to the Instrument Technician.
- At the scheduled experiment time, the instrument technician can “turn-on” instrument access for the Remote Users. During an experiment that takes 2-3 days to complete, the Instrument Technician can update the experiment status for Remote Users progress tracking.
- After the experiment completes, instrument technicians can “turn-off” instrument access and initiate archiving of off-line experiment data using a web browser for the Remote-users to view/download.

Cyber-Enabled 850 MHz NMR at Miami University
OSC’s remote instrumentation web-portal features the Remote Instrumentation and Collaboration Environment (RICE) solution and cyber-enables NMR instrument and data resources

Cyber-enabled 850 MHz NMR research and training partners: Bowling Green State University, Ohio University, Muskingum College, Talawanda High School

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