The Virtual Laboratory: Using Networks to Enable Widely Distributed Collaboratory Science[1]

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Abstract

Scientific research laboratories generally, and those with unique analytical instruments in particular, whose components and / or users are distributed around the Internet will provide substantially increased effectiveness for the scientific user community, and provide access to currently under-served communities like industry, K-12, Community Colleges, etc. This paper characterizes a few types of distributed laboratory environments currently being built, and the network capabilities needed to support them. While the communications requirements of the different virtual laboratories may be quite different, several labs that are now being built could make use of the vBNS as part of an experimental testbed to provide access to various university sites.

1.0 Motivation

> The fusion of computers and electronic communications has the potential to dramatically enhance the output and productivity of U. S. researchers. A major step toward realizing that potential can come from combining the interests of the scientific community at large with those of the computer science and engineering community to create integrated, tool-oriented computing and communication systems to support scientific collaboration. Such systems can be called "collaboratories."
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> "National Collaboratories - Applying Information Technology for Scientific Research," Committee on a National Collaboratory, National Research Council. National Academy Press, 1993.

A collection of emerging technologies, ranging from distributed data handling and distributed computing to the underlying multicast network infrastructure, have the potential to make it possible to create distributed scientific and industrial laboratory environments that provide complete location independent access to instruments, data handling and analysis resources, and enable remote human collaboration. These technologies will produce not so much an incremental change of today's routine use of PCs and LANs in laboratory environments, but rather the introduction of a new paradigm more akin, perhaps, to virtual reality. The vision is for a scientist thousands of miles away to get the same (or even better) sense of presence and control as if he or she were at the experiment site.

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The expected value of these geographically distributed environments includes substantially increased effectiveness in doing science by more closely integrating university and federal researchers, and an enabling capability for analytical and high-value production use of unique facilities by industry.

2.0 Introduction

The scientific community will benefit from advanced information infrastructure for several reasons. Breaking down the barriers of distance will permit routine and frequent participation by senior academic and research scientists in planning and conducting experiments that would otherwise require scheduling long in advance, flying, housing arrangements, site safety and operations training, etc. These circumstances are completely typical for today's investigators who routinely have to visit large-scale facilities to do experiments and to meet with graduate students and post docs to plan new experiments.

Establishment of remote collaboratory environments at unique or scarce facilities can also enable new capabilities for industry. This is because, in general, industry will not pack up their key personnel and go through the elaborate and time consuming procedures noted above. This is especially true of analytical and production use of remote facilities, as opposed to the few industry scientists who work at academic-like research labs. We therefore anticipate that establishing the technology for routine remote collaboration environments will add a new capability for use by U. S. industry.

The need for a distributed laboratory / scientific environment can occur by virtue of research and engineering involving the use of large and / or scarce facilities (e.g. large electron microscopes, synchrotron light sources, various types of particle accelerators, etc.); by virtue of a single experiment being unique due to its scale (e.g. a fusion reactor); or (probably most commonly) because the collaborators and / or industrial partners are at several different institutions. We anticipate that a number of technologies will be necessary to solve the problem of providing location transparency in these environments. These technologies include high speed distributed systems; use of shared networks for real-time, remote and automated control of instrumentation and sensing systems; routine and easily integrated telepresence (e.g. multimedia communication among all participants); and effective electronic publishing mechanisms to support intellectual communication during the scientific process and dissemination of results as they mature.

One model characteristic of "analytical" facilities like electron microscopes and synchrotron light sources is the following. Samples are prepared and characterized at the researcher's or industrial analyst's home laboratory. The sample is then shipped to the facility where a technician, operating while in direct video and audio contact with the sample owner, does any required final preparation, and loads the sample into the experiment chamber. The sample owner sets up the experiment / analysis, operates the parts of the experiment directly related to the sample, and collects the data in (if necessary) a confidential and secure fashion. In the future, volume analysis of manufactured items could entail robotic handling of samples in this sort of environment.

Research, development, and experimentation in testbed environments is necessary to extend, enhance, refine, and integrate the relevant technologies in ways that contribute to dramatic increases in the effectiveness of small and large scale scientific research collaborations where the scientific expertise, facilities, and instrumentation are geographically distributed. These testbeds environments need to identify, evaluate, and enhance the use of information, computing, and telecommunications technologies that will support routine "connection" among people and laboratory facilities that are scattered all over the country.

Several example scenarios illustrate the potential of an architecture that enables transparent acquisition of network resources in order to solve changing problems.

Virtual Laboratoris: The E. O. Lawrence Berkeley National Laboratory (LBNL), Advanced Light Source (ALS) is an example of a very large scientific instrument. (See: http://beanie.lbl.gov:8001/als/als_homepage.html) This national facility is used by the principle investigators (PIs) of scientific and industrial experiments, and the PIs are located all over the country. The current use-model is that users to fly to the site to conduct experiments and have graduate students and technicians live at the site.

The ALS is a unique resource that lends itself well to a remote collaborative environment or virtual laboratory. The first of the ultrabright “third generation” synchrotron radiation facilities, it can serve hundreds of users who have a broad range of applications.

One experiment that takes particular advantage of the characteristics of the ALS is the Spectro-Microscopy Facility on Beamline 7.0 (BL7 - illustrated below), which is collaborating with

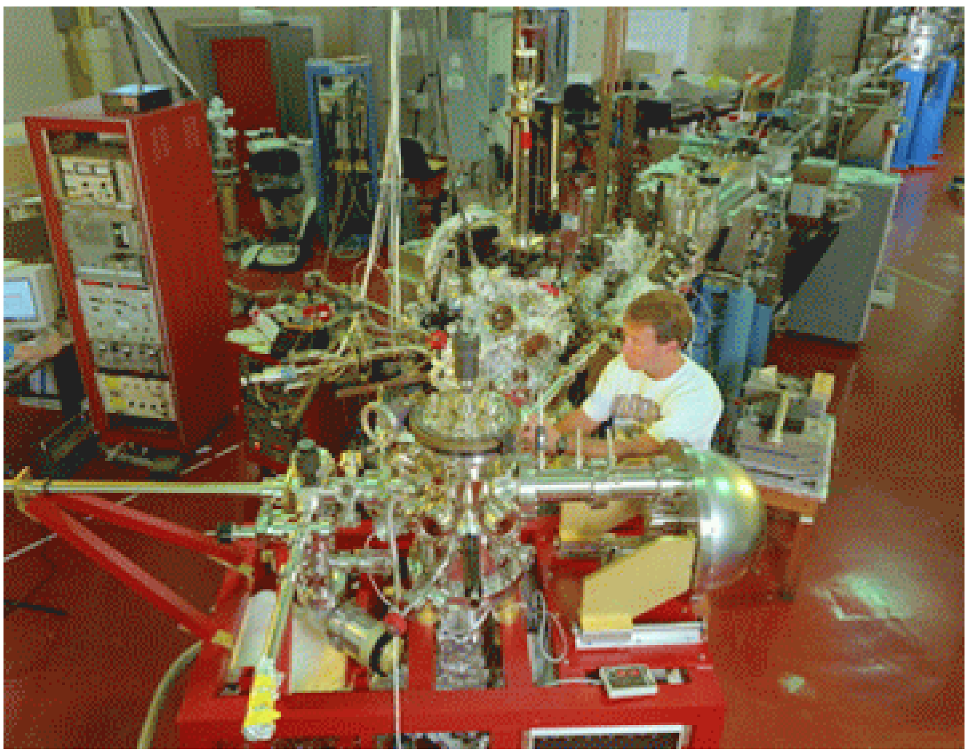

Figure 1: Spectro-Microscopy Facility at Beamline 7.0 of the Advanced Light Source

LBNL computer scientists to build a testbed virtual laboratory. This project is one of four diverse testbeds in the Distributed, Collaboratory Experimental Environments (DCEE) program described below. The overall goals are to provide easier access for users and to foster more and better opportunities for collaboration. To understand why BL7 lends itself so well to a virtual laboratory, and the basis for the design decisions, it is helpful to briefly review the functions of the beamline and its experimental end stations.

The goal of the Spectro-Microscopy Project is to take advantage of the first undulator beamline at the ALS. A 5-m-long, 5-cm-period undulator creates a small, narrow, intense cone of soft x-rays. The desired wavelength is selected with a spherical grating monochromator whose optics set new standards for surface finish and accuracy. The output of the beamline (by which we mean the undulator and monochromator) is refocused by adaptive grazing-incidence mirrors into a very small spot, less than 40 microns in diameter. This spot can be steered between two branch lines called MicroFOCUS I and MicroFOCUS II. At the end of one of these branches, the beam becomes the object point for two scanning X-ray microscopes downstream of the microfocus location. Zone-plate lenses demagnify the beam further, achieving spot sizes from 1000 angstroms down to, eventually, below 500 angstroms. These two zone-plate focal points are called the NanoFOCUS I and II stations. One application of this unique facility if nano-scale chemical analysis of crystals and chip wafers.

Many issues must be addressed in order to remotely control such a sophisticated facility, and in order to ensure success with remote collaborative environments in general. Security and access control mechanisms must prevent unauthorized access and guard proprietary data. Safety must also be addressed: not all aspects of the experiment can be safely operated remotely, and adequate safeguards are required those parts that can be remotely operated. Since the collaboratory is designed to allow multiple remote researchers to participate in an experiment, multicast data transfer mechanisms and arbitration mechanisms that determine which site is currently in control of the experiment need to be implemented. Many different kinds of multimedia communication and information sharing will have to be instantiated in order to provide effective human interaction, and to allow studies of human effectiveness and satisfaction with all aspects of this new environment.

Large-scale Science: STAR is one of two large-scale physics experiments currently under construction for use at the Relativistic Heavy Ion Collider (RHIC) at DOE's Brookhaven National Laboratory. The STAR collaboration consists of over 350 members from 35 institutions. The data processing - analysis - simulation challenge for STAR lies in the massive amount of data that will be logged by the detector (~ 25 Mbytes/second, 500 Tbytes/year). The extensive computing requirements for data analysis and detector simulations (240 GFLOPS during operation) necessitates a large-scale, cost-effective, off-line computing and storage capability; the ability to provide easy access to large numbers STAR collaborators from around the country; and flexibility and responsiveness to the experiment's needs as they evolve throughout the 10 year lifetime of the STAR physics program. These analysis systems will be built from resources located at collaborators sites, and the data and computing resources will be widely dispersed.

Further, the associated computational science community needs to be able to utilize the infrastructure for theoretical work. Nuclear matter equations of state calculations require large amounts of computing. The computational scientist will need to be able to rapidly reconfigure the computing and storage facilities used for data analysis (e.g. when experiments are not running), as well as potentially incorporating other resources, to cary out very long theoretical calculations. These many distributed resources will be configured into a single network-of-workstations (NOW) -like computational system to do the theoretical calculations.

3.0 Establishing the Requirements for Virtual Laboratories

The Distributed Collaboratory Experimental Environments of Program Lawrence Berkeley National Laboratory and DOE, Office of Energy Research, Office of Computation and Technology Research, Mathematical, Information, and Computational Sciences Division is intended to establish requirements and testbeds for Virtual Laboratories.

Five projects, beginning in early 1995 and running for about two years, will build and operate testbeds for "collaboratories." (See: http://www-itg.lbl.gov/DCEE)

The testbeds will provide remote access to the kinds of expensive, hard-to-duplicate facilities, ranging from electron microscopes to a tokamak fusion reactor. By building these testbeds and using them for real-world experiments, we will be able to study both the technical and the social aspects of controlling apparatus, taking data, and interacting with colleagues by wire. The testbeds are:

- Electron microscopy, physics, and object-oriented virtual reality: Argonne National Laboratory.

  A shared work space with persistence and history will add a virtual-reality/multi-user dimensions touch to this project. A later phase will exercise the idea of a Collaboratory internationally across a data link of varying bandwidth.

- Remote control for fusion experiments: Livermore, Princeton, Oak Ridge, and General Atomics.

  This testbed will attempt to replicate the function and feeling of real-time presence in a control room at a tokamak, a quintessentially large central facility to which today's researchers must travel.

- Remote collaboration for environmental molecular sciences: Pacific Northwest Laboratories.

  The two parts of this testbed will serve, respectively, large, highly shared NMR facilities and smaller-scale molecular-beam instruments with small user groups.

- Remote SpectroMicroscopy at the Advanced Light Source: University of Wisconsin-Milwaukee and Lawrence Berkeley Laboratory

  Distinctive features of this project include a large and geographically distributed collaboration, which is part of a much broader (and rapidly expanding) user community in the field of synchrotron radiation.

3.1 Requirements

Preliminary work at the ALS-BL7 has established a set of requirements that have been confirmed as having a lot in common with those of the other virtual laboratory DCEE projects:

- Remote experiment monitoring and control
- On-line laboratory notebook
- Tele-presence
- Security for access control, safety, and data confidentially
- Collaboration between multiple researchers at multiple sites
- Cross-platform compatibility (PC, Sun)
- Maintainability
  - minimal software duplication
- Interface coherence and usability
- Control coordination
  - automatic transfer of control
- Access from industrial sites

Many of there points relate directly or indirectly to network capability and infrastructure, so we will characterize each briefly.

3.1.1 Experiment Control

A surprisingly small number of control system strategies are in use. National Instruments' LabView is commonly used in small to medium scale systems (with up to a few hundred monitoring and control points). (See http://www.natinst.com/labview/lvindex.html and http://k-whiner.pica.army.mil/info-labview/info-labview.html) Large-scale experiments (like the DIII-D Tokamak fusion reactor) have thousands to tens of thousands of control and monitoring points. These experiments either use custom built control systems or EPICS (Experimental Physics and Industrial Control System - see http://csg.lbl.gov/OverView.html).

At the ALS BL7:

- ♦ Labview split into client and server provides
  - instrument control
  - instrument monitoring
  - user interface
  - same control software running at all sites
- ♦ Communication using TCP, UDP, multicast IP

3.1.2 Multimedia Conferencing

Although it is early in the human factors evaluation process, it seems clear that rich multimedia inter-human communication and experiment telepresence capabilities will be needed for successful remote operation and collaboration. Again, for the ALS, a specific set of capabilities has been identified, however it appears that variations of these will be common to all such environments:

- ♦ Video
  - cameras at local and remote operator/experimenter workstations
  - robotic cameras for area monitoring (remotely controlled)
  - data cameras monitoring sample chamber
  - remotely controlled video switch
- ♦ Audio
  - wireless microphone/speaker sets
  - audio mixer
- ♦ Software tools
  - vic, vat, wb, CU-SeeMe, nevot, ivs

Some of these channels are low bandwidth and some are high, but all must be multicast.

3.1.3 On-Line Experiment Notebook Requirements

An on-line notebook, especially for organizing and recording experiment parameters, data locations, etc. is a common need.

- ♦ Automated and manual data entry
- ♦ File reference capability

- Cut and paste of pictures/images
- Search functions
- Custom forms for formatted entry
- Sketching/drawing capability
- Scientific characters and symbols
- Security/access restriction
- Easy interface to other software packages (Labview, statistics, graphics)

3.1.4 Resource Arbitration

When many people at remote sites all have the possibility for controlling various aspects of an experiment, there has to be a robust mechanism for implementing whatever policy is established to permit multiple party access to the experiment.

- Resource arbitrators run locally at each site to:
  - Monitor: status of resources
  - Arbitrate: current controller
  - Negotiate: pending requests
- Arbitrators must be scalable to an environment containing many resources and collaborators, and must provide flexible access restriction and arbitration mechanisms

3.1.5 Security/Safety

- Security and safety concerns
  - network-based tampering
  - automated equipment failure modes
  - sanity checks on incoming data
- Safety architecture
  - safety mechanisms built into server control software
  - fail-safe recovery mechanisms on experiment server
- Security architecture

  With respect to remote users, one significant issue is to ensure that use-conditions of the remote resource have been met. Authentication and authorization certificates can be used in this environment to verify that some action (e.g. training) has taken place with respect to an individual. For example, Dept. of Energy operated, large experimental facilities (particle accelerators, large photon sources, X-ray microscopes, etc.) are scattered over the Internet, making security of operation an important consideration. Facility managers may, for example, require certain kinds of training prior to allowing one to participate in remote operation. This manager will also probably never physically meet many of the people who want remote access. Assuming that there are training programs at the remote institutions that qualify an operator, one model is that this operator will “present” a certificate (e.g., an X.509.v3 - like certificate) as proof of identity in order to be allowed access by the local security mechanisms, and as proof of a level of training, or other authorization criteria, to engage in operations.

In other words, a certificate mechanism that could encode various authorization criteria for individuals, and expresses the policy and identify of the grantor in an unambiguous and easily determined manner, would permit automated verification of access and usage rights for an array of circumstances.

This scenario can provide one important component of the technology needed to create distributed scientific and industrial laboratory environments which provide complete location-independent access to instruments, data handling and analysis resources, and collaborators.

3.1.6 Communication Types

From the point of view of the virtual laboratory there are several different types or uses for communication:

- Multimedia collaboration
- Experiment parameters
- Experiment results
- Collaboratory control information
- Security information
- Notebook updates and transactions

The different communication usages give rise to several different transport models:

- Status displays
  - unreliable unordered
  - reliable ordered
- Periodically updated parameters and global settings
  - unreliable ordered
- Points on a graph or notebook entries
  - reliable unordered
  - reliable ordered
- Experiment parameters (one-shot) and incremental values
  - reliable ordered

3.1.7 Throughput Requirements

The bandwidth required for communications to support virtual laboratories is fairly laboratory-specific in terms of the data that has to be transferred, but the multimedia streams for human collaboration and monitoring has a fair bit of commonality across different types of labs.

Considering specifically the spectro-microscopy experiment at BL7 of the ALS, the following parameters can be established. (Note that all numbers are in terms of application-level data. To get the corresponding numbers for, say, the SONET links for IP over ATM, multiply by about 1.4.)

- Data transmission

- 512 x 512 array of 32 bits in 30 seconds: 280 Kbits/s
- other data: 8 - 80 Kbits/s

♦ Video / image transmission

- Video images of sample positions (optical microscope):

  greyscale, 512x492, 1 - 5 Hz: 2 Mbits/s-10 Mbits/s

- Experiment chamber monitor (video):

  greyscale, 512x492, 1 Hz: 2 Mbits/s

- Video conferencing:

  compressed video transmission: 128 Kbits/s

4.0 Wide Area Network Experiments

The virtual laboratory scenario is a nice application for a high speed network testbed: The data flows are higher than current production networks could sustain (5 - 15 Mbits/s of application data, 7-21 Mbits/sec of network-level bandwidth for the ALS, BL7 example, which is an unusually low data rate device); there are real-time (though as yet uncharacterized) requirements in the control system; multiple coordinated data and multimedia streams must be multicast (using several different models) to several users and sites that are widely spread across the country; and a versatile, strong, and widely distributed security infrastructure must be in place. These are all issues that have to be addressed in research, development, prototype deployment, and experiments in the environment of a high speed network where multicast strategies, QOS, bandwidth reservation, etc. can be experimented with in the network infrastructure.