Instrument Development Laboratory

The Instrument Development Laboratory (IDL) designs, builds, and deploys advanced state-of-the-art instrument systems and custom application software in support of the ongoing experimental research efforts in the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL). As depicted in Figure 1, the IDL staff support EMSL researchers and users by providing a wide variety of design and fabrication services for hardware and software, custom engineered solutions to research problems, and in-depth experience in the interface and control of commercial instrumentation. Because most EMSL user projects have unique needs, the IDL staff are especially skilled in the integration of commercial and custom hardware/software packages to suit the exact specifications of specific research projects.

Capabilities

Some of the IDL's most recognizable expertise and capabilities fall into the following areas:

- high-voltage expertise
- radio frequency (RF) expertise
- high-speed analog and digital systems
- digital signal-processing and field-programmable gate array technologies
- databases
- laboratory automation
- data acquisition
- instrument control
- common communications methodologies
- software design and implementation (C, C++, Visual Basic, JAVA)
- embedded systems and personal digital assistants.

Figure 1. The IDL and its staff members provide a wide variety of technical support to EMSL users.

The IDL Design Laboratory offers a staffed electronics and fabrication shop for EMSL research staff and facility users. IDL customers will find a fully stocked parts supply, electronic components and small hardware, test, and measurement equipment available for checkout, and ready assistance during business hours. For immediate hardware assistance, customers may access the IDL electronics laboratory and receive assistance from any IDL staff member. For work that is limited in scope and not time-consuming, there usually is no charge to EMSL staff for services. For larger projects, staff may also access the IDL electronics laboratory and speak with an IDL staff member, who will happily assist the customer in defining the work to be done and begin the process of designing solutions.

Custom Software Design, Development, and Support are critical services offered to IDL customers. IDL staff members specialize in several key services related to research: data acquisition, instrument control, laboratory automation, systems integration, data analysis and visualization, data management and archiving, and handheld and embedded systems. Using a modular code design model as their basis, IDL software developers can efficiently develop software in a number of languages, tools, and scripts (e.g., Visual Basic, Java, C, C++, Labview, Assembly, Access, and SQL Server). In addition, software developers are skilled in a number of instrument control strategies, including General Purpose Interface Bus (GPIB), Serial (RS-232), infrared (IR), Transmission Control Protocol/Internet Protocol (TCP/IP), Analog and Digital I/O, and high-speed event counting and timing.

The IDL Support Queue is accessible by customers via email (idl-support@emsl.pnl.gov). The queue is monitored daily, and customers are encouraged to submit their requests for any type of service offered by IDL.

The IDL Website at http://idl.emsl.pnl.gov provides a full description of IDL capabilities, access to the support queue, team highlights, recent projects, statement-of-work access, and a downloadable business plan.

IDL Technical Support is readily available to assist research by providing software modifications, troubleshooting, equipment fabrication, and research instrumentation support.

Future Directions

Field-programmable gate array (FPGA) technology is being exploited in a new field known as reconfigurable computing. Programmable logic implements algorithms instead of sequential stored instructions. Performance gains of several orders of magnitude are possible with select algorithms. Future efforts will include FPGA architecture investigation, inter-FPGA communication, algorithm design and implementation, and testing and validation.

Emerging high-throughput nuclear magnetic resonance (NMR) technology has the potential to transform the rate at which NMR experiments can be performed, and thus expand the applicability of NMR to processes with much shorter time scales. Hardware interfaces and software implementation and automation of new experimental protocols will require new and ongoing development and support within IDL

Confocal Microscope with Field-Programmable Gate Array Processing

MS Sowa,[a,b] JC Solinski,[a] HS Wiley,[a] KA Perrine,[a] DF Hopkins,[c] and T Seim[c]
(a) Pacific Northwest National Laboratory, Richland, Washington
(b) University of Maryland, Baltimore, Maryland
(c) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

Cellular communication is a dynamic process involving various proteins and small molecules. Understanding how cells sense their environment and communicate with one another is essential to developing a mechanistic understanding of human disease and possible intervention strategies. The study of cellular communication using fluorescence microscopy requires high-speed processing of digital image data. This aim, currently being pursued in the Instrument Development Laboratory through the use of field-programmable gate arrays, has significantly advanced the state of-the-art in multi-spectral confocal microscopy by providing near-real-time imagery of processed data.

The high-speed confocal microscope (formerly in the W.R. Wiley Environmental Molecular Sciences Laboratory [EMSL] and now at the University of Maryland) can simultaneously acquire two-color images at speeds up to 30 frames/sec, providing the capability to perform near-real-time fluorescent resonance energy transfer (FRET) and ratiometric analysis of confocal images. Confocal capabilities are necessary for three-dimensional reconstruction and correlation of image slices with identified signaling and propagation chemistry, using observation of the fluorescence originating from spatially localized portions of cells. Such information is important for two reasons: it adds to the existing knowledge base related to cellular signaling in general, and it also provides primary data that can be used to critically test developing spatial models of intercellular signaling.

The high-speed confocal microscope is designed to simultaneously capture output from two intensified charge-coupled diode cameras. Software provided by the EMSL Instrument Development Laboratory (IDL) controls laser output from the microscope via an eight-channel acoustic-optic tunable filter. This custom software also controls both the XY axis of the microscope, using a high-resolution Ludl stage, and the Z-axis, using a PT piezo focus drive. Images from the two cameras are acquired synchronously and merged using a software package developed at Pacific Northwest National Laboratory. To maximize the flexibility of the control software, this software package uses a text-based script engine that exposes the functionality of all hardware components of the system, allowing the operating scientist to build or customize *ad hoc* experiments.

The fundamental software/hardware infrastructure needed to conduct "real-time FRET" includes 1) two cameras matched and aligned to the pixel level so alternate frames are acquired using alternate excitation wavelengths and 2) the ability to capture images from both cameras simultaneously. The capability to match and fuse two images in real time is being developed by IDL staff using a field-programmable gate array as a reconfigurable processor. Additional manipulations include averaging of multiple images, co-adding images to create 16-bit pseudo-color images, and achieving a ratio of different images with a correct registration of pixels.

Control System for an Inexpensive and Configurable Ion Trap Mass Spectrometer

ML Alexander,[a] DF Hopkins,[b] K Swanson,[b] and MA Buschbach[b]
(a) Pacific Northwest National Laboratory, Richland, Washington
(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

Development of a low-cost, easily configurable ion-trap mass spectrometer will make a new, inexpensive, and flexible research capability available to small laboratories and universities.

This project involved development of an ion trap mass spectrometer that is both inexpensive and flexible. The development of this instrument will integrate ion-trap mass spectrometry (ITMS) with hardware and software platforms that will allow the construction and deployment of systems with capabilities tailored to the specific needs of a variety of scientific applications. These systems will focus on the use of chemical ionization techniques to address the need for highly sensitive and specific measurements, as well as analytical needs dictated by focused research areas such as atmospheric chemistry, catalysis, materials science, biology, and inhalation toxicology.

This ITMS platform can be used to develop and deploy systems for critical applications such as chemical weapons detection and nuclear proliferation monitoring. Although commercial ITMS systems are available, their hardware and software are tailored to specific, focused needs and are not easily modified. Additionally, the cost of commercial systems (i.e., $60,000 to $200,000 for commercial systems versus $20,000 for the new ITMS platform described in this paper) places them beyond the financial means of many academic researchers, particularly those at smaller institutions. Thus, we have created a platform using inexpensive, commercially available computers, data acquisition systems, and control equipment combined with open source software for instrument control, data acquisition, and analysis. As such, the software can be readily tailored to different applications, in contrast to commercial ITMS systems, which as mentioned above tend to be tailored to specific, focused needs.

The hardware and software developed as part of this project enhance and extend the capabilities of two instruments used in the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL): the proton transfer ion-trap mass spectrometer and the laser-desorption, ion-trap mass spectrometer (LD-ITMS). As an illustration of one application the newly developed system, the control system includes components specific to the LD-ITMS system for the analysis of single biological and non-biological particles. The remainder of the system can be used by a wide range of ITMS applications.

The control and acquisition hardware consists of four National Instruments peripheral component interconnect boards that provide the signal generation, timing, and data acquisition for the system. An optional component of the system is a field-programmable gate array-based particle discriminator. Developed in the EMSL Instrument Development Laboratory, this particle discriminator is used to trigger an ablation laser as a particle passes through its beam. To take advantage of the Visual Basic's rapid application development and its straightforward integration with the control hardware, the control software was written in Visual Basic 6.0.

Novel Cooling Technology

RS Studham,[a] ND Tenney,[a] and T Seim[a]
(a) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

We are investigating technology that addresses the major barrier to future supercomputers – heat removal. The patented spray cooling technology discussed below has the potential of removing 500 times as much heat as conventional air cooling.

Researchers from the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL), Pacific Northwest National Laboratory, and Isothermal Systems Research are collaborating to install and evaluate SprayCool™, a novel cooling technology patented by Isothermal Systems, on a portion of the EMSL supercomputer. This evaluation will be conducted to measure and document any improvements in computational speed and system reliability resulting from the use of SprayCool.

Heat generation is one of the most critical limitations in high-performance computing and electronics in general. Electronic circuits consume power, and the heat generated is directly proportional to the clock speed of the circuit. With clock speeds now well into the gigahertz range, performance is often limited not by semiconductor technology but by how much heat can be removed. If heat is not adequately removed, it will destroy the circuit. This process is analogous to an automobile engine that overheats under load and, thus, must be slowed to avoid permanent damage. Next-generation microprocessors have potential power dissipation of more than 100 watts, which is well beyond the capacity of current air-cooling technologies. This limitation currently is resolved by slowing the microprocessor, which in effect reduces its computing capacity and, thus, negatively impacts the effective computational rate of the supercomputer.

SprayCool technology addresses this problem by replacing the typical cooling medium (moving air) with Fluorinert™ a liquid that is sprayed in a finely atomized stream directly on the component being cooled. The liquid vaporizes on contact, and the heat of vaporization is supplied by the component, effectively cooling it. The vapor is removed from the cooling apparatus and sent to a heat exchanger outside the equipment cabinet. The heat exchanger cools the vapor and converts it to liquid form, which can be reused in the cooling process. The system is completely closed, with none of the cooling liquid vented to the atmosphere. The SprayCool technology can potentially remove 500 times more heat than conventional forced-air cooling methods.

Staff

Daniel J. Gaspar, Scientist, Acting Technical Lead (See also Interfacial and Nanoscience Facility)
(509) 376-2413, daniel.gaspar@pnl.gov

Gordon A. Anderson, Chief Engineer, Acting Deputy Director
Technical Lead (January – October)
(509) 376-9558, gordon@pnl.gov

April L. Green, Administrator
(509) 376-0591, april.green@pnl.gov

Kenneth J. Auberry, Senior Research Scientist
(509) 376-1453, kenneth.auberry@pnl.gov

Michael A. Buschbach, Scientist
(509) 376-7207, michael.buschbach@pnl.gov

Eric Y. Choi, Scientist
(509) 376-4509, eric.choi@pnl.gov

James L. Eick, Technician
(509) 376-4540, james.eick@pnl.gov

James C. Follansbee, Research Scientist
(509) 376-4689, james.follansbe@pnl.gov

Gabriel F. Guillen, Student
(509) 376-1727, gabriel.guillen@pnl.gov

Navdeep Jaitly, Senior Research Scientist
(509) 376-6160, Navdeep.jaitly@pnl.gov

David C. Prior, Technologist
(509) 376-3923, david.prior@pnl.gov

Samuel O. Purvine, Senior Research Scientist
(509) 376-3013, Samuel.purvine@pnl.gov

Thomas A. Seim, Senior Research Scientist
(509) 376-2533, thomas.seim@pnl.gov

Kerry D. Steele, Chief Engineer
(509) 375-2880, kerry@pnl.gov

Kenneth R. Swanson, Senior Research Scientist
(509) 376-0826, kenneth.swanson@pnl.gov

Beverley K. Taylor, Technician
(509) 376-5095, beverley.taylor@pnl.gov

Nikola Tolic, Senior Research Scientist
(509) 376-3090, nikola.tolich@pnl.gov

We would also like to acknowledge the contributions of David A. Clark, Marie C. Gibbons, Gary R. Kiebel, Brian L. LaMarche, Nathan D. Perry, and Elena S. Peterson.