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 on-going experimental research efforts within the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL).

The IDL staff supports the EMSL infrastructure through their ability to offer a wide variety of design and fabrication services (both hardware and software). The IDL is not only capable of providing custom engineered solutions to research problems, but also provides deep experience in the interface and control of commercial instrumentation. Since most EMSL user projects carry unique needs, the IDL staff is especially skilled in the integration of commercial and custom hardware/software packages to suit the exact specifications of the research. Some of the IDL's most recognizable services are:

- Expertise in high voltage
- RF (Radio Frequency)
- High speed analog and digital systems
- DSP (Digital Signal Processing) and FPGA (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 PDA's

In addition to providing EMSL users support within individual laboratories, the IDL also maintains a fully equipped design and fabrication facility within EMSL for the purpose of in-house electronics development and open use of its many state-of-the-art test and measurement equipment.

The IDL Business Philosophy

In an effort to reduce the cost of software development and to reduce the development time IDL has adopted the following operational philosophies:

- To develop reusable, modular, object-oriented code
- Tailoring work to suit the needs of EMSL scientific community
- Maintaining code modules (controls) within a software library, developed commercially and within the group
- Developing software specific to instrumentation, whether off-the-shelf or written in house

While the IDL is an EMSL support group, it is not limited to working only within EMSL. The IDL does offer its services to external customers, however each project must be fully funded—this includes labor, parts, and the checkout of test equipment.

Doing Business with IDL

Initiating work with the IDL team is convenient, efficient, and always customer interactive. Those wishing to do business with the IDL can make contact with IDL staff via phone, electronics shop walk-ins, the support queue, email, or by simply speaking with an IDL member in person. The specific services IDL offers are follows:

The IDL Design Laboratory offers a staffed electronics and fabrication shop for EMSL research staff and facility users, located in room 1241. 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 member. For work that is small and consumes very little time, there is usually no charge to EMSL staff for services. For larger projects staff may also access the IDL electronics laboratory and speak with an IDL 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. The IDL staff specializes 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 GPIB, Serial (RS-232), IR, TCP/IP, Analog and Digital I/O, and high-speed event counting and timing.

The IDL Maintains a Support Queue which customers can make entries into via email (idl-support@emsl.pnl.gov). The queue is monitored daily and customers are encouraged to submit their request for any type of service offered by IDL.

The IDL Website, at http://www.emsl.pnl.gov/homes/cis/idl.html, 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, fabrication, and research instrumentation support.

Collaborative Research offers many exciting aspects, and the IDL has several proven services: Design of electronics hardware, Control and monitoring software development, Data management and automated data analysis, Systems engineering, and Embedded control.

What Can You Expect From IDL

A Statement of Work (SOW) will be written for services requiring a significant amount of IDL staff time or resources. Each SOW will provide contact information, a project description, start and completion dates, and justified costing information. Statements of work are considered to be changeable documents that not only allow customers to have a clear understanding of IDL's role, but also allow internal tracking of work performed.

Full Documentation will be provided upon project completion, including; schematics, descriptions of hardware and software, flow diagrams, setup information, operating procedures, and developer contact information.

Technical Support and modifications to IDL systems will be provided.

A Commitment to Maintaining and providing state-of-the-art resources.

IDL Advisory Board

This group is composed of a representative from the IDL and one from each of the research groups the IDL serves. The committee has been instrumental in forming the current IDL project-costing model and guiding the purchases of generic test and measurement equipment the IDL maintains. Committee meetings serve as a very useful forum for the exchange of ideas, provide a regular opportunity to voice questions or concerns, and give the IDL valuable information about the strategic direction for the directorates as it pertains to their future development needs.

- Gordon Anderson, IDL (Chair)
- Mike Bowman
- Mark Engelhard
- Wayne Hess
- Nancy Foster-Mills
- Scott Studham

IDL Project Highlights

Proteomics Research Information Storage and Management (PRISM) System
GA Anderson, GR Kiebel, KJ Auberry, D Clark, ME Powers, N Tolic

The Instrument Development Laboratory oversees and manages the Proteomics Research Information Storage and Management (PRISM) System, an essential part of the laboratory facility that is being used for proteomics research (the study of proteins expressed by cells, tissues, or organisms under a specific set of conditions) on a number of different organisms. PRISM manages the very large amounts of information that the facility generates and the data processing that it requires by collecting mass spectra data files directly from multiple mass spectrometers, managing the storage and tracking of these data files, and automating their processing into both intermediate results and final products. It also collects and maintains information about the biological samples used in research experiments and the laboratory protocols and procedures used to prepare them. Finally, PRISM allows users to readily locate and examine the information that it contains, and allows other information systems to access appropriate portions of it.

Computerized Automobile Random Selection (CARS)
GA Anderson, I Allison, G Guillen, T Harper, TA Seim

The Computerized Automobile Random Selection (CARS) System will assist the security officers in random selection of vehicles for inspection. This is a system designed to assist in the selection of vehicles at entry checkpoints into secure facilities. The CARS system will log all activities and provide report files documenting the vehicle history each day.

The system will be implemented in two phases. The first phase is the deployment of the prototype system. The system consists of a laptop computer running Windows operating system. The laptop interfaces to a control unit using the USB port. The control unit allows the security offices to signal the CARS system to make a selection and to signal the results. The second phase system will position a digital camera to photograph the front of every vehicle, thus providing the ability to log useful data in any abnormal event.

Aerosol Sampler Controller
TA Seim, ME Conley

The aerosol sampler is a self-contained portable instrument that acquires samples of airborne particles. The heart of the sampler is a disk with 561 collection grids that capture the aerosol particles. Sample acquisition is fully programmable, including start time, sample time, sample mode and the number of samples.

The aerosol sampler controller is an embedded microprocessor from Rabbit Semiconductor. This microprocessor, together with a custom-designed interface printed circuit board, provides motion and pump control of the rotational sampler assembly. An analog-to-digital converter monitors air mass flow. Motion control uses a 12-volt DC motor with an effective gear ratio of 17340:1. Rotational position is monitored with an incremental optical encoder. A Compaq Personal Digital Assistant (PDA, iPAQ) implements the operator interface. The controller initializes and receives data from a particle size counter through a serial RS-232 interface.

Sensor System for Monitoring Tc-99 in Groundwater
TA Seim, GA Anderson, DC Prior, ME Conley, T Harper, MA Buschbach

With the new underground storage site for spent reactor fuel in Nevada, there is a great deal of concern for radio active leakage into the groundwater. In order to monitor the amount of Technetium 99 in the groundwater around the base of the mountain, a probe needed to be developed that would be able to sample the groundwater and return the results to the surface. Size requirements stated that the probe would be able to fit down a four inch diameter well, which greatly limited the size of the hardware components that could be used.

There are multiple pieces of hardware associated with this project. Each has a specific function within the process of sampling the groundwater. Most of the hardware that specifically deals with the sampling is concealed within a 3.5 foot by 4 inch Delron capsule. Within the capsule there are the following pieces of hardware: 3 photo-multipliers, a flow cell, a Rabbit 3000 embedded processor with Ethernet on a custom fabricated board, which contains a DAC for high voltage control as well as a CPLD for counting light pulses from the PMT's, 2 amplifier/discriminator boards, a high voltage controller board, and all the interconnect wiring. Outside of the probe capsule are the 15 and 24 volt power supplies that are mounted in a box along with a Sapphire stepper pump and its controller board. There is also a wireless modem that will be used for hardware control from a dumb terminal as well as transmitting data. Because we are using a Rabbit 3000 as the processor for this project, all the code was written in C using National Semiconductor's Dynamic C editor and compiler. The software controls all hardware associated with the sampling of the ground water. The application is broken down into separate tasks. Using the Dynamic C's Micro OS-II, we are able to assign priorities to each of the tasks by utilizing the OS's pre-emptive multitasking features.

Automation of a Bruker 9.4-Tesla ICR Mass Spectrometer and a High Resolution Capillary LC System
KR Swanson, GA Anderson, DC Prior, MA Buschbach

High-resolution mass spectrometry is an inherently intensive technique, typically requiring two or three hours of data collection per sample run, and an entire campaign devoted to the study of a single organism may include hundreds or thousands of such sample runs in order to produce conclusive results. Ideally, data collection should be as reproducible as possible, eliminating to all reasonable extent the introduction of unwanted variances which may affect the integrity of the results. Due to the length of actual data collection and the small but precisely measured volumes of sample required for each run, the process can quickly become rather tedious for the operator, possibly resulting in erroneous system operation. Therefore, it is distinctly advantageous to place as much of the data acquisition process under mechanized control—particularly those critical elements in which slight procedural variations can lead to widely disparate results.

We have developed a prototype LC/MS system which replicates a human operator with a combination of hardware devices, controls, electronics, and software. In particular, our system couples the EMSL's Bruker 9.4-Tesla ICR Mass Spectrometer with a sample delivery subsystem composed of a PAL autosampler, a set of ISCO pumps and associated controller, along with several Valco two-position and multi-position valves and actuators. The sample delivery system is under the direct control of a software program developed especially for the automation of the LC/MS system. This program (which executes on a Microsoft Windows 2000 platform) includes the timing and logic for the proper activation of the various hardware components and communicates to those devices through serial interfaces. This automation software also controls the acquisition process through communication with the XMass software running on the Bruker control computer.

The overall goal of the 9.4-Tesla LC/MS automation project is to produce a system which will maximize throughput by enabling continuous (24 hours a day, seven days a week) unattended execution of multiple sample runs, while minimizing the possibility of irreproducible and detrimental procedural variations by removing the need for a human operator. Over the past several months our prototype automation system has successfully processed hundreds of sample sequences, has run continuously with minimal human attendance for up to 60 hours at a time, and has acquired over a terabyte of useful data.

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