Minutes of the CAALS Workshop on Modularity and Communications Standards

National Institute of Standards and Technology
June 25 and 26, 1991

Members in Attendance:

ABC Laboratories, Inc. - J. Upham
Applied Analytical Industries - R. Miller, W. Struve
Department of Energy/National Laboratories - M. Griesmeyer
Digital Equipment Company - R. Lysakowski, S. Tilden, J. Currie†
E. I. DuPont de Nemours Co., Inc. - L. Falkenau, R. Weimar
Eastman Kodak Company - W. Sonnefeld, B. Seiler, C. Houck
Environmental Protection Agency - V. Laurie
Hewlett-Packard Company - D. Hawk
The Perkin-Elmer Corporation - W. Barnett
Union Carbide Corporation - R. Dillon

NIST Personnel in Attendance*:

G. Kramer (CAALS Project Manager), J. DeVoe (Chief, IARD), H. Kingston (Supervisory Research Chemist, IARD), F. Ruegg (Physical Scientist, IARD), M. Salit (Research Scientist, IARD), J. Petersen (Research Associate, IARD), P. Walter (Guest Scientist, IARD).

Summary

This Workshop was organized similarly to the previous meeting. After a presentation by Scott Tilden on Instrument Interfacing, three of the four Working Groups met individually. The Strategic Planning Committee did not meet at this Workshop, but it held a meeting in April; the minutes of that meeting are included. The Physical Link and Transport Committee has defined the requirements for the link connecting modules to their controller, examined a new ASTM standard for low-level communication, and is determining what fits into to the various layers of the ISO model. The Module Requirements Group has proposed a process control model, has defined the core functionality, and has listed the requirements for a Standard Laboratory Module. The Software Engineering Group proposed that a document detailing the CAALS Modularity Architectural Specification be prepared and presented a working outline. The future structure and charters of the committees and the decision making criteria of the Workshop itself were questioned. These items will be examined in greater detail at the next Workshop.

†via Phone Link; * IARD = Inorganic Analytical Research Division

not a conf.
Working Group
jcp 3/16/95

MASTER

Presentations

The attendees were welcomed by Gary Kramer. After a plenary session on the first morning, the Workshop broke into three of its four Working Groups. The Workshop reconvened as a whole on the following morning for summary presentations by each Working Group and general discussions.

Dr. Scott Tilden from Digital Equipment Corporation (via Kodak) presented a talk on World-Wide LIMS Implementation Strategies. Scott pointed out that it is not possible to decouple analytical methods concepts, networks and LIMS technology from instrument interfacing. The cost of interfacing analytical instruments to information management systems is very large—about half the cost for laboratory automation is for instrument interfacing. Scott described a hierarchy of method descriptions with a General Method covering procedures for analyses of a class of analytes. Below the General Method lies the Method Set which is a collection of conditions for analyzing a subset of the analytes. The lowest level is the Instrument Method (also known as a Test) that contains the conditions for handling a single analyte. Scott stated that ISO-9000, FDA, EPA, and other regulatory documentation procedure hierarchies allow for a few "methods" each specifying several "tests." Scott went on to describe an ideal instrument interfacing scheme. His vision includes a four-level architecture, very like the CAALS concept, with a Service Request Host, Service Control Hosts, Test Stations, and Test Devices; these translate in CAALS parlance to Information Management System, Method Controller, Test Station Controller, and Standard Laboratory Module. All of the Networking Elements must support a wide-area network based on the OSI standards and must provide a communications protocol that will guarantee error-free delivery of messages, which can range from simple alphanumeric strings to complicated multi-dimensional data utilizing standardized data formats. Test Devices must allow buffering of needed test request information from multiple Service Request Hosts and should be capable of stand-alone operation by buffering completed test data. Test Stations must allow multiple types of workstations to "front-end" test devices and must support the network protocol. A Service Control Host must maintain the integrity and auditability of the methods it is supervising, should support temporary archiving of raw test data, and should participate in a networked approach to controlling and archiving data centrally in accordance with ISO-9000 and GLP. The Service Control Host is responsible for maintaining service logs, calibration data, device and protocol limits and must ensure that all data sent from the test equipment has been validated by appropriate procedures. Scott concluded his presentation by discussing models for inter-level communication links in his interfacing scheme.

Discussions

This section will delineate only the items that are not covered in the following committee reports.

Our lack of formal agreement on the definition of important terms is a growing problem. It was agreed that the creating of a glossary of terms should be a priority item. Dick Weimar volunteered to manage the glossary, and everyone was asked to submit definitions for consideration.

There was a substantial discussion on the roles and charters of the committees. There was general agreement that the Module Requirements Committee had completed most of its tasks (with the notable exception of writing up its decisions). It was suggested that this committee, having defined the Standard Laboratory Module, might continue by taking on the Test Station Controller, much as the Physical Link Group has expanded its charter to examine the whole issue of message transport. There seems to be some overlap between the Software Engineering Group's interests in defining an overall architecture and this suggested expansion of the Module Requirements Committee's assignment. There also appears to be an overlap between some activities of the Software Engineering Group and the Strategic Planning Committee. Several new items needing committee attention were listed: Workcell Functionality, Threading Architecture and its Justification (Client-Server Definitions, Multi-tasking, etc.), Session and Presentation Layer Problems, and Scripting Language. It is unclear whether new committees are needed or whether our existing groups can assume these tasks. Committee charters will be an agenda item for the next Workshop.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

It was pointed out that the Modularity Workshop lacks formal precepts for its group decision making. This has not been a liability in the past when we were still in an information/learning phase; however, now that decisions are to be made, it is imperative that we explicitly define how our process will work. It was suggested that we examine the processes used by other standards organizations, such as IEEE, ISO, and ASTM, and that we also look into the guidelines used by our member organizations for product development. This will also be an agenda item for the next Workshop.

Committee Reports

Strategic Planning Committee

The Strategic Planning Group met in Great Valley, PA on April 25, 1991. Bill Sonnefeld (Chair), Larry Falkenau, Charlie Houck, Mike Griesmeyer[†], and Rich Lysakowski[†] attended. The following minutes of that committee meeting were provided by its chairman, Bill Sonnefeld.

The Strategy Planning Group meeting consisted of three major elements:

1. Identification of "Driving Forces" for automation requirements.
2. Identification of major programs aimed at developing standards which impact automation efforts.
3. Discussions around the control level software lying above the actual modules.

1. The Strategy Committee has the task of compiling information concerning the various "Driving Forces" acting on the laboratory environment which ultimately become requirements for automated systems. Many of these requirements may be passed down into modules and need to be identified so that module specifications are correct. Some of these "Driving Forces" are coming from government regulatory agencies, international agreements, internal quality programs, and accreditation agencies. Other requirements are being developed for specialized businesses, but may cross over into the domain of the analytical laboratory sometime in the future. We identified several major efforts which are having an impact on how laboratories operate, and we are starting to compile information on these. These efforts and those in charge of gathering information about them are:

ISO 9000 Requirements - Bill Sonnefeld

GLP (Good Laboratory Practices) Requirements - Rich Lysakowski

Clinical Chemistry [E31.(11,12,13,14)] - Rich Lysakowski

LIMS (Laboratory Information Management Systems) Requirements - Rich Lysakowski, Bill Sonnefeld

Process Control Requirements - Larry Falkenau

EPA Requirements - Bill Sonnefeld

The group will attempt to collect this information by the end of June and then decide on how to reduce the information down to a manageable level.

2. There are a variety of major programs developing standards which have an impact on automation in manufacturing operations or laboratories. These include:

AIA - Analytical Instruments Association

ADISS - Analytical Data Interchange and Storage Standards

ASTM - E31 Subcommittees on LIMS, Clinical Labs

EIA - Electronic Industries Association

MAP - Manufacturing Assurance Plan

SEMI - Semiconductor Equipment and Materials International

SCPI - Standard Commands for Programmable Instruments Consortium

The CAALS members have heard presentations from representatives of several of these groups, and CAALS members are active in some of these organizations.

There are several issues here:

- A: Which of these efforts should be monitored by CAALS?
- B: Which efforts should be adopted by CAALS for us to build on?
- C: How should we monitor the status/results of these other efforts?
- D: Where is the overlap of these efforts and what are the differences?
- E: What is the proper terminology for all of the issues being addressed?
- F: What emerging technologies will be available in the near future?

The Strategy Committee agreed that one of the highest CAALS priorities should be to develop a common glossary of terms so that we can avoid the general confusion which results when items are not defined. This is the first recommendation. The other issues will be discussed in our next session.

3. The Module Requirements Committee is dealing with definitions of a module, but not with the specific control-level software that will be needed to run the modules in an integrated environment. This is called cell or workcell control software in the process control arena. Issues involved with this area are: Calibration, Maintenance, Method Scripts, QA Control, Equipment Performance Criteria, Sample Tracking, Error Recovery, Resource Allocation, Report Generation, Data Storage, and Materials Management. This is a fundamental area in which CAALS members should develop a common system hierarchy.

The Strategy Committee recommends that a new committee be formed to address this area and that this be opened up to anyone interested in joining this effort. The mission of this new committee will be to develop the functional design of the workcell control level software, to develop a script language standard, to develop the database structure required, and to develop the scheduling algorithms. It would be expected that this committee would work closely with the Strategy, Module Requirements, and Software Engineering Committees. Specific elements of this might be considered as modules which could be developed by other groups.

Physical Link and Transport Committee

The Physical Link Committee met via a telephone conference on May 29, 1991. Jim Currie, Dave Hawk, Brian Seiler, and Gary Kramer were present. The group sees its mission to:

1. Develop the framework within CAALS into which the communications link will fit.
2. Derive the requirements that communication links must satisfy.
3. Survey the industry for well-supported communications links. "Recommend" the most appropriate links and "list" the others. It is expected that the link which is "recommended" will change over time.
4. Develop recommended practices for the "recommended" links and encourage similar developments by others for "listed" links.

The primary result of this meeting was the following list of requirements for a CAALS Physical Link:

1. The link should support up to 15 devices.
2. Interface link must be supportable on mainstream computers using common operating systems.
3. Controller resource requirements must be minimized.
[I/O Slots, DMA Channels, Interrupt Lines]
4. The link implementation must be low cost.
5. The link must be easy to incorporate into instrumentation.
6. The link must provide for controller capability.
7. The application program interface must be consistent with out regard to the actual physical link.
8. The physical link must assure an error-free message transmission; if a message cannot be delivered, an exception must be raised.
9. Communications protocol failure must not allow the physical link to lock-up the system.
10. The physical link should operate in a "real-time" rather than a "store-and-forward" mode.

The Physical Link and Transport Committee met at the June 25 Workshop. Dave Hawk (Co-chair), Jim Currie† (Co-chair), Brian Seiler, Fillmer Ruegg, Ray Miller, and Gary Kramer were present. The Group decided accept the recommendation of the Workshop to expand its charter from solely the physical link to include message transport issues, hence the change in the name of this committee to the Physical Link and Transport Committee. The following minutes were provided by the co-chairman, Dave Hawk.

We are basing our work on the OSI model. The intention is to use OSI to provide a link-independent framework on which several different communications links can be utilized. We are currently recommending IEEE-488 as a primary communications link and are also looking at recommendations for RS-232 links for small systems. The intention of the link independence is to allow relatively easy conversion to LAN technologies when they make sense (maybe 5-10 years?).

We have made a first pass at defining the functionality required for each OSI layer. We have decided to assume direct connections between the computer and the devices, so for our purposes, there will be no need for a network layer. Application layer models will come from the Module Requirements Committee. We are working on presentation, session, transport, physical and data link requirements.

We spent some time discussing good practices for IEEE-488 systems. Despite the fact that -488 is already very well standardized and supported, there are some areas where agreeing upon common practices can make things easier—such as a standard mechanism for signaling message-available (service request and parallel poll), standard message terminators (LF and EOI), and so forth. There also need to be some rough guidelines to ensure that devices are implemented using appropriate technology to ensure that many -488 devices can operate simultaneously on the same bus (e.g. using DMA for high data-rate devices).

We also favorably reviewed a recently passed ASTM standard for RS-232 interfaces for clinical instruments (ASTM E1381). Jim Currie served on the ASTM committee which approved it.

ASTM E1381 addresses the physical link and data link layers of OSI. It specifies a 25 pin connector (DTE at the instrument, DCE at the computer) with 3 wires plus shield. All messages are broken up into 240 byte (max) packets. Each packet is checked with an eight-bit checksum, and there is a retransmission scheme for bad packets. Line direction is simplex, and there is a simple contention mechanism for grabbing the line to send a message. There is also a means by which a message in progress may be aborted by the receiver to grab the line for sending a priority message. The overall scheme looks fairly straight forward and should be fairly easy to implement.

Our committee did have several concerns about this standard. The eight-bit checksum is weak, the connector is oversized for three wires, binary data cannot be directly accommodated because certain characters are reserved as protocol characters, and the simplex nature of the link and slow data rates would extend response times for alarm messages. We felt that these concerns could be mostly overcome and were probably outweighed by the fact that this standard had been approved and adopted by the ASTM for a similar application area.

Within CAALS, we intend to layer a complete CRC around each message to ensure accurate message delivery (this gets around the weakness of the eight-bit packet checksums). We also intend to provide some "escape" mechanism to allow forbidden binary characters to be mapped into the allowed character stream.

Module Requirements Committee

The Module Requirements Committee held a meeting on May 23 and 24 at Sandia National Laboratories in Albuquerque, NM that was attended by John Upham, Mike Griesmeyer, Marc Salit, Jim Petersen, and Bill Sonnefeld†. The committee agreed that the terms *common command* and *generic command* were too confusing and recommended that these should be replaced by *core functionality* and *process control commands* respectively, with class-specific commands, and

proprietary commands ruling out the possible CAALS command types. A process control model was proposed for a Standard Laboratory Module (SLM). The requirements for such a model are a standard state model, standard process commands, asynchronous event reporting of state transitions and other events, monitoring of alarm and other conditions of interest, controller-settable parameters and enabling of monitoring and reporting, controller querying for status, and debugging facilities such as logging, tracing, and spooling. Process commands are required for operation control, data collection, parameter and variable set and query, and alarm management. The operational control commands for an SLM are: status query, set-up operation, start operation, pause operation, resume operation, and abort operation. Data collection occurs through predefined reports, event reports, custom reports, trace reports, and requested reports. Ancillary data collection functionality must include the capability to enable or disable reports, to trace and log occurrences, as well as to key reports to specific events. It must be possible to set SLM parameters, status, and data variables by ID. Furthermore, existing parameters, status, and data variable values and attributes must be available for external query by ID. Reporting is tied to the occurrence of events such as state transitions, selected processing activities, completion of extended commands, material-supply notifications, and user-defined variable limits. Figure 1 shows an applicable process operation state diagram for an SLM, along with a listing of state transition events, based on the General Equipment Model (GEM) defined by the SEMI Implementation Task Force (SEMI SITF).

Figure 1. SLM Operation State Diagram.

The Module Requirements Committee met at the June 25 Workshop. John Upham (Chair), Bill Sonnefeld, Marc Salit, Jim Petersen, Skip Kingston, Charlie Houck, Mike Griesmeyer, Bill Struve, and Scott Tilden were present. There was a general discussion of where the intelligence should be placed in the system. For the purposes of this discussion, the system is composed of SLM's and a Test Station Controller (TSC). It was decided that SLM's handle all of the defined functionality for a module, but SLM's are owned by only one TSC. The TSC has a world model data store which is kept up to date by the SLM's as events occur. SLM's must have the ability to

implement monitoring functions. This does not mean that the SLM must handle monitors or have values that are monitorable.

The discussion turned to the TSC and its controller, the Method Controller (MC). The MC produces method script sequences that determine the overall method, e.g. the number of samples, which samples, which standards, which controls, etc. The MC also handles scheduling and sequencing and quality assurance issues. The TSC takes method scripts from the MC and converts them into SLM control scripts and coordinates and synchronizes tasks among the SLM's that it owns. A *task* is an operation that can be performed by an individual SLM. A *supertask* is an operation that requires operations by more than one SLM for completion.

The need for standardizing terms became evident repeatedly throughout the discussion. The following is a partial list of such terms: test station controller, test, standard laboratory module, method controller, method, alarm, event, monitor, command, device, report, task, supertask, world model, task token, parameter, process, process flow, data dictionary, symbol table, work list, script, resource, consumable, scripting language.

Software Engineering Committee

Rich Lysakowski (Chair), Larry Falkenau, Mike Griesmeyer, Ron Dillon, Peter Walter, Dick Weimar, and Bill Barnett participated in the meeting of the Software Engineering Group at the June 25 Workshop. This group devoted a substantial portion of its effort to understanding the four-level modularity architecture depicted in the Object-Oriented Analysis schematics shown in Figures 2, 3, and 4. There was general agreement that explaining the architecture was going to be a major, but essential, undertaking. To expedite this process, the group proposed the development of a CAALS Modularity Architectural Specification Document. A working outline is shown in Figure 5. This document will be a major CAALS deliverable. Initial elements of the document are to be complete by the next Modularity Workshop in September. It is hoped that the version 1.0 of final document can be completed and released by the first quarter of 1993. Rich Lysakowski agreed to be the editor of the document and solicited contributions for the sections in the outline.

Future Workshops - The next two CAALS Modularity and Communications Standards Workshops will be a day and a half session to be held on Thursday, September 12 and Friday, September 13 and a two and a half day affair scheduled for Wednesday, December 4 through Friday, December 6. The Workshops will be held at NIST.

Respectfully submitted,

Gary W. Kramer.

Figure 2. OOA Schematic of CAALS Analytic System

CAALS ANALYTIC SYSTEM
00A MODEL
REVISION 6/18/91

Figure 3. 00A Schematic of CAALS Analytic System

CAALS Modularity Architectural Specification Document

Executive Summary

Introduction

- Document Audience
- CAALS Mission
- Scope of CAALS Architecture
- Motivation for and Needs Satisfied by CAALS Architecture
- General Terminology
- CAALS Project Description
 - What is Modularity?
- Intended Usage and Endpoints for Usage
 - Context - Lab, Quality, and Manufacturing Systems
 - What is not Covered in CAALS
- Scalability
 - What is Scalability
 - Commercial and Technical Aspects of Scalability
 - Entry Points for Manufacturers and Implementors
- Low End
- High End

Module Requirements

Architectural Models

- General Terminology for Architectural Modeling
- Device Complexity Classes/Categories
 - Dumb Instruments
 - Intelligent Instruments
 - Standard Laboratory Modules
- Work Flow Model Examples
- Process Model Examples
- CAALS System Hierarchy Logical Model
 - Introduction to System Hierarchy Modeling
 - CAALS System Logical diagram
- Class/Object Hierarchy Diagrams
 - Introduction to Object-Oriented Modeling
 - CAALS Class Hierarchy Diagram

Architectural Components

- Standard Laboratory Model
 - Definition
 - Example of Commercial Implementation(s)
- Test Station Controller
 - Definition
 - Example of Commercial Implementation(s)
- Method Controller
 - Definition
 - Example of Commercial Implementation(s)
- Information Management System
 - Definition
 - Example of Commercial Implementation(s)

Physical Link

Example Implementations

Appendix

- Glossary of Terms
- Bibliography

Figure 5. Proposed Outline for the CAALS Modularity Architectural Specification Document.