**The Environmental and Molecular
Sciences Laboratory**

**Computing and Information
Sciences Preliminary
Engineering Design Study**

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The Environmental and Molecular Sciences
Laboratory

**COMPUTING & INFORMATION SCIENCES
PRELIMINARY ENGINEERING DESIGN STUDY**

Prepared by the EMSL C&IS Engineering Team

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Abstract

This document presents the preliminary design concept for the integrated computing and information system to be included in the Environmental & Molecular Sciences Laboratory (EMSL) at the Pacific Northwest Laboratory, Richland, Washington, for the U. S. Department of Energy (DOE). The EMSL is scheduled for completion and occupancy in 1994 or 1995 and will support the DOE environmental mission, in particular hazardous waste remediation. The focus of the report is on the Computing & Information Sciences engineering task of providing a fully integrated state-of-the-art computing environment for simulation, experimentation and analysis in support of molecular research. The EMSL will house two major research organizations, the Molecular Sciences Research Center (MSRC) and part of the Environmental Sciences Research Center (ESRC). Included in the report is a preliminary description of the computing and information system to be included. The proposed system architecture is based on a preliminary understanding of the EMSL users' needs for computational resources. As users understand more about the scientific challenges they face, the definition of the functional requirements will change. At the same time, the engineering team will be gaining experience with new computing technologies. Accordingly, the design architecture must evolve to reflect this new understanding of functional requirements and enabling technologies.

Summary

Pacific Northwest Laboratory^(a) (PNL) is creating a collaborative research facility for molecular sciences research, the Environmental and Molecular Sciences Laboratory (EMSL). The EMSL will support the DOE environmental mission, in particular hazardous waste remediation, and is scheduled for completion and occupancy in 1994 or 1995. The period between 1990 and facility operation is devoted to facility design and construction, development of the Molecular Sciences Research Center (MSRC) and part of the Environmental Sciences Research Center (ESRC), and design and implementation of a fully integrated state-of-the-art computing and information system.

The focus of this report is on the Computing & Information Sciences (C&IS) engineering task which is responsible for the design and implementation of the integrated computing and information system. Included are the C&IS scope, objectives, design goals, system architecture, and technical approach.

Plans for the EMSL call for an integrated computer and information system providing a complete suite of computing, electronic communications, and information management services to facility staff and visitors. This integrated system will support simulation, experimentation, and analysis. It is intended to significantly enhance technical productivity through application of modern information and computing technology in the research enterprise. The major C&IS deliverable is a fully functional advanced computing environment for the EMSL, the first version of which will be operational in an interim facility prior to EMSL occupancy. It is intended that this information system represent a major advance in the use of information technology to support scientific research.

Goals for C&IS Engineering Task

The following are the goals of the C&IS engineering task:

- Build a computing environment that meets the technical requirements of EMSL staff, visiting scientists, and off-site collaborators and users.
- Provide efficient and seamless management of data and information from simulations, experiments, technical databases and publications.
- Provide an integrated computing environment where a single multi-functional workstation can be used as the standard user-interactive device to access computing services available in the facility.
- Accommodate new requirements and new computer technology through modular expansion without total systems redesign/replacement.
- Achieve a reasonable cost of development and operation by using commercially acquired equipment and technologies whenever possible.

To reach these goals, the state of the art in the application of information technology to support scientific research will need to be extended. Prototypes will be developed for many of the systems that will make up the planned computing environment in interim facilities before those systems and components are installed in the EMSL. Prototype development will promote a better understanding of enabling computer technologies, help prepare for EMSL operation, and provide the equipment needed to support ongoing research in the interim facility.

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Architecture

An integrated network will be the foundation of the EMSL computing environment. The network will consist of a computer-to-computer network which will be used to couple high speed systems, many end-user subscriber networks that will provide network attachment points for equipment located in science laboratories and offices, and a backbone information network interconnecting all high speed computing systems and end-user subscriber networks. Video communication services will also be provided by the integrated network.

The computer-to-computer network will service the high performance computers, experimental computer system, data management systems, and the Graphics & Visualization Laboratory. Together, these computing resources will be known as the Molecular Sciences Computer Facility (MSCF).

High performance computing will be supplied by one or more advanced architecture (parallel) computers. A network of scientific workstations will also be available as a loosely coupled parallel high performance "computer." The experimental computer system will be a leading-edge high-performance system. It will provide an opportunity for scientists to evaluate new computer architectures in advance of selecting the next generation of high performance computers. The data management system will store simulation and experimental results, technical databases, and scientific publications (stored in electronic format). This system will have both on-line media and extensive archival storage capability. Advanced graphics workstations and software will be available in the Graphics & Visualization Laboratory. This equipment will be used for animation, display, and manipulation of molecular models, for analysis and display of experimental or computer generated data, and for viewing in real-time the progress of simulation and analysis codes running on the high performance computer.

Additional elements of the computing infrastructure will be the Interface Development Laboratory (IDL), the Facility Training Center, and a considerable amount of distributed computing equipment. The IDL will support the EMSL laboratory automation activity by providing the tools and environment necessary to develop instrumentation interfaces. The Facility Training Center will be used for demonstrations, presentations, workshops, seminars, and training sessions involving large groups of people. It will be tied to the Northwest Educational System. A client-server computing model will be adopted for user workstations and network servers. User workstations will be mid- to upper-range scientific workstations that have a good balance of graphics and general computational performance.

The EMSL computing environment will be built using existing commercially available products whenever possible. Appropriate standards will be specified in all procurements and adopted for all development projects.

Challenges

The greatest challenges in implementing the EMSL computing architecture lie in delivering an integrated MSCF. The performance that scientists will demand of the MSCF is essentially everything that can be delivered by leading-edge high-performance computers, data management systems, and graphics and visualization systems. To make these systems usable by theoretical and experimental scientists, and to couple them together in a seamless manner, will be a challenging task. The engineering staff will involve outside collaborative partners in industry, academia, and government research organizations. We expect that the computer industry will supply many of the required technologies. The challenge will lie in integrating them into a cohesive computing environment.

Where proven computing technology will meet our needs, we will use it. Where our requirements exceed current capabilities--for example, in the area of high performance computing and scientific information management--we will push as far to the edge of technology as we can while, at the same time, providing a usable and manageable system.

The proposed technical approach, that of coupling a traditional engineering approach with prototype development, is the best way to control the risk associated with the project. It is important that the systems and components of the architecture be delivered to users in increments that do not exceed our understanding of the problems that the systems are supposed to solve. In this manner, those who will implement the architecture will have the benefit of seeing their creation as a functioning entity, rather than as a paper model, and will be able to alter course as needed to engineer a better solution to the EMSL users' computing needs.

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1.0 Introduction

The Pacific Northwest Laboratory (PNL)^(a) is creating a collaborative research facility for molecular sciences research, the Environmental and Molecular Research Laboratory (EMSL), with emphasis on the support of the DOE environmental mission, in particular hazardous waste remediation. The EMSL is scheduled for completion and occupancy in 1994 or 1995. It will house two major research organizations, the Molecular Sciences Research Center (MSRC) and part of the Environmental Sciences Research Center (ESRC). The facility will incorporate significant computational capability for experimental and theoretical analysis. The period between 1990 and facility operation is devoted to facility design and construction, design and prototype of an integrated computing and information system, and development of the MSRC and ESRC research programs.

Plans for the EMSL call for an integrated computer and information system providing a complete suite of computing, electronic communications, and information management services to facility staff and visitors. This integrated system is intended to significantly enhance technical productivity through application of modern information and computing technology in the research enterprise.

Computing and Information Sciences (C&IS) engineering tasks cover the design and implementation of the integrated system. The major C&IS deliverable is a fully functional advanced computing environment for the EMSL, the first version of which will be operational in an interim facility by the time the EMSL is completed and ready for occupancy. This integrated system will represent a major advance in the use of information technology to support scientific research.

This section of the report introduces the EMSL project for PNL by presenting the C&IS scope, objectives, and design goals.

1.1 Scope

The purpose of the C&IS engineering task is to design and implement an integrated computing and information system. The following will comprise the integrated system:

- Integrated Network
- High Performance Computer System (*)
- Data Management System (*)
- Graphics & Visualization Laboratory (*)
- Experimental Computer System (*)
- Interface Development Laboratory
- Distributed Systems
- Facility Training Center

System components marked above with an asterisk (*) will be located within the EMSL in a facility to be known as the Molecular Sciences Computing Facility (MSCF). The MSCF will be central to the EMSL Theory, Modeling, & Simulation program.

While the EMSL is being designed and constructed, development of an integrated system will be carried out in PNL's Physical Sciences Laboratory and Mathematical Sciences Laboratory. The majority of the C&IS Engineering tasks will be carried out while the research staff and laboratories are located in this interim facility.

1.2 Objectives

The following are the C&IS engineering objectives:

- Implement a fully integrated computing environment for simulation, experimentation and analysis in support of molecular research
- Demonstrate and transfer modern information system technologies to other DOE facilities and cooperative organizations.

1.3 Design Goals and Critical Success Factors

The C&IS design goals specify the manner in which the engineering objectives will be accomplished. Critical success factors are the metrics

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by which the success in achieving the design goals will be measured.

Goal: Build a computing environment that meets the performance requirements of EMSL staff, visiting scientists, and off-site collaborators and users.

- The system will become the user's first choice as a simulation and analysis tool and source of scientific information.
- The system will provide high performance computing resources to ensure on-time response to user requests for information and services.

Goal: Provide efficient and seamless management of data and information from simulations, experiments, technical databases, and publications.

- Data will be available to authorized users at any location and will be accessible to application programs operating on any EMSL computing resource.
- Information access will be granted to authorized users and denied to unauthorized users.
- The system will support timely and efficient information exchange with external organizations.

Goal: Provide an integrated environment where a single multi-functional workstation can be used as the standard user-interactive device to access computing services available in the facility.

- The user interface will be consistent across applications.
- Minimum training time will be required to effectively use the system.
- Training will be facilitated by using the inherent capabilities of the system to assist and guide users.
- Visitors will make effective use of the system during a temporary assignment to EMSL.

Goal: Maintain an open architecture that can embrace new developments in computer technology. Accommodate new requirements and new computer technology through modular expansion without total systems redesign/ replacement.

- The design will be based on applicable industry and government standards.
- The system will be incrementally expandable to accommodate future growth.

Goal: Achieve a reasonable cost of development and operation by using commercially acquired equipment and technologies whenever possible.

- Maintenance of applications and systems will not be so time consuming as to preclude development of new capability by EMSL staff.
- Distributed computing resources will be effectively managed from a central location.

To reach these goals, it will be necessary to extend the state of the art in the application of information technology to support scientific research.

2.0 System Architecture

Shown in Figure 1 is a block diagram of the integrated system. Major system components are described in this section.

2.1 Integrated Network

A network that provides facility-wide communication services will be the foundation of the system architecture. It will be built using several technologies selected to provide the necessary range of data and video communication services. These services are as follows:

- coupling high speed systems that must inter-operate in a seamless manner
- interconnecting distributed and centralized resources
- distributing video to all offices, laboratories, and conference rooms
- reconfiguring the network for performance tuning and fault isolation.

A computer-to-computer network (C2N) will be used to couple the high performance computer system, data management system, experimental computer system, and high performance graphics and visualization workstations. Distributed systems located in scientific laboratories and offices will be attached to one of many end-user subscriber networks (ESNs). A backbone information network (BIN) will interconnect high speed systems with the ESNs that service the laboratories, computing centers, and distributed systems.

The BIN will be a high speed network that is typified by 100 Mbps or greater data transfer rates, high reliability, and a relatively small number of connections. The connections will consist of network routing devices that transfer network traffic between the ESNs and the BIN if a destination address is outside the local service area. The fiber data distribution interface (FDDI) would be the technology of choice if the BIN were to be implemented today. Giga-bit network technology may, however, emerge as an alternative for the BIN.

The ESNs will service the science laboratories, C&IS laboratories and computing centers, and the EMSL office complex. The ESNs will provide a low cost connection point for a variety of computer resources, including workstations and personal computers, network printer and file servers, and computers servicing the science laboratories.

Emerging network technologies that operate in the 100 Mbps range may in the near future be sufficiently mature for production use as ESNs. Ethernet technology, operating at 10 Mbps, is the predominate technology in use today and is the fall back technology for EMSL. Ethernet is compliant with the open system interconnection (OSI) compliant communication standards, which promises interconnectivity of heterogeneous resources. Ethernet will be used within the interim facility at the ESN level. ESNs will be interconnected via the BIN.

Network technologies that operate above 1 Gbps are needed for the C2N but are still in an early stage of development. Many different approaches for high speed networking are being proposed by vendors. There is not yet a clear leader. Candidate technologies will be selected for further study and testing before a decision is made on the C2N technology to employ within the EMSL. Evaluation of emerging BIN and ESN technologies, and how these will integrate with the C2N candidate technologies, will also be a part of this activity.

Access to existing site PNL networks will be through a network bridge/router that partitions the EMSL BIN from the PNL networks, transferring data only as appropriate. Access to networks external to PNL will be through a gateway system that attaches directly to the BIN or to one of the ESNs.

The video system envisioned for the EMSL would provide full color multi-channel video to each office, laboratory, and conference room. The video system could be used to support the graphics laboratories as well as provide informational services (for instance the NW WERTS video seminar system).

Figure 1. EMSL Network

2.2 High Performance Computer System

The high performance computer system (HPCS) will provide the computational power needed to run complex molecular modeling codes. These codes range from semi-empirical and *ab initio* electronic structure and molecular geometry prediction to molecular scale models of physical processes. Sophisticated studies of environmental molecular systems typically require state-of-the-art computing resources, and beyond. The HPCS will also be used for the analysis of experimental datasets and the correlation of that analysis with model predictions. Modeling, analysis and correlation are key activities of the EMSL, and HPCS is the primary resource for these services.

There is a direct correlation between the execution speed of the simulation codes and the productivity of the EMSL scientists. Consequently, there is considerable emphasis on re-engineering existing computational chemistry codes and developing new codes to take best advantage of high performance computers. The nature of these codes is such that both shared memory vector processors and distributed memory parallel processor can be effectively applied. Therefore, we are considering the possibility of providing both architectures in one integrated system.

Highly parallel machines are now the subject of research in the industry, government, and university sectors, but they cannot yet be applied to scientific computing. Evaluation and development of this technology will be undertaken through strategic alliances with other research groups, and through prototype development within the interim facility.

Working prototypes are now in use that consist of a supercomputer and parallel computer that are coupled over a high speed link to form a metacomputer system. This metacomputer strategy will be used in the interim facility. It will provide a limited scale resource for execution of production codes and the development of new algorithms that take advantage of the dual architecture system. The system will be built using commercially available distributed memory and shared memory computers that are coupled over a network link. To augment this system, strategic linkages have been established with the Caltech Concurrent Supercomputing Facility. Parallel codes developed in the

interim EMSL can be ported to the more powerful Caltech facility for production execution. However, the dual architecture aspects cannot be used at Caltech.

The interim HPCS will support ongoing research activities and provide valuable experience with competing parallel architectures. This experience will lead to developing a set of performance specifications used to procure the production quality HPCS for the EMSL.

2.3 Data Management System

Another key element of the MSCF is the data management system (DMS). High performance computers will support a modest amount of on-line data storage for codes running on the system. However, there will be a large volume of data that must be accessible, not only to the HPCS but to other systems distributed throughout the EMSL and to offsite collaborators and users. This data will include simulation and experimental data, technical databases, and research literature. The DMS will be the home for this data.

A major challenge in the design and implementation of the DMS is the organization, maintenance and application of large amounts of heterogeneous scientific data. Improvements in instrument and computer technology are yielding dramatic growth in the size of experimental data sets and computer generated simulation datasets. The scientific literature is undergoing explosive growth, and the announcement of major new technical databases is a common occurrence. Hardware and software tools for efficient management of scientific information are just now becoming available. However, they are not fully developed and we expect that the implementation of the DMS will be a significant challenge. The architecture of the DMS will be a two-level hierarchy, each level distinguished by its storage capacity and access time. One level will provide fast access with limited capacity and the other will provide slower access with extensive capacity.

The limited capacity/fast access tier will be implemented using on-line read/write media. Using today's technology, this media would be magnetic disk storage. The storage capacity of this system is anticipated to be 80 to 100 GB at a minimum. (For the interim DMS, the capacity will be less

using conventional disk drive arrays that store 1+ GB per spindle.) The on-line storage system will connect to the HPCS over a high speed C2N channel.

The high capacity/slower access tier will use off-line media stored in a juke-box type assembly. A mechanical selector will load the media on to a playback device where the data will be transferred to on-line storage devices over a C2N channel. The capacity requirements of this system are expected to be on the order of 100 times that of the on-line system. High capacity optical media that provide direct file access (after they are loaded on the playback device) are expected to be available for use in the interim facility and the EMSL.

Software to operate the hierarchical storage devices will be implemented as a common file system (CFS). The CFS will appear to users as an "infinite" extension of their local storage devices. Software to support this concept is commercially available but must be extended to provide scientific information management features not currently supported. For example, procedures must be developed for extracting key items of information out of flat files, collecting other "metadata" as required, and integrating this information into a scientific database accessible through the DMS. The CFS must be extended to become a data management system with tools that support the design, creation and maintenance of scientific databases and provide convenient and efficient user access to data and information.

2.4 Graphics & Visualization Laboratory

The Graphics & Visualization Laboratory (GVL) will support advanced graphics workstations and software that will provide a full range of capability, from simple two-dimensional graphics to complex multi-dimensional renderings.

The laboratory will contain several high performance graphics workstations. Other scientific workstations will be distributed throughout the facility. Workstations located in the GVL will be distinguished by their performance and high speed C2N connection to the HPCS and DMS. These workstations will be selected from commercially available products that operate at the top end of the performance envelope.

GVL equipment will be used for production and development tasks. In production mode, animating, manipulating, and displaying molecular models will be fundamental tasks performed in the laboratory. In addition, the workstations will be used to present a real-time window into the progress of simulation and experimental analysis processes. In development mode, visualization techniques and user interfaces will be implemented and tested using software engineering tools available on the workstations.

A physical environment will be established within the GVL that is optimized for user viewing. Video equipment will be integrated with the workstations to facilitate the recording, playback and projection of scientific information displayed as images. In addition, video editing capability will be available to allow for the proper presentation of scientific material. This video system will be available for use by scientific teams and to present information to visitors. This laboratory will be a primary demonstration and discussion center for small groups.

2.5 Experimental Computer System

The experimental computer system (ECS) will be a test bed for new generation high performance computers. It will provide access to new computer technologies that show potential for extending the range and reducing the cost of molecular computations.

The service life of the HPCS is expected to be approximately three years. The ECS will be the prototype for the next generation HPCS. It will also provide an opportunity for scientists to evaluate new supercomputer architectures specific to the needs of the EMSL in advance of selecting a production machine. Experience gained here will provide a technical basis for writing procurement specifications for the next generation HPCS.

The typical machine purchased for evaluation will be a small scale resource suitable for testing and evaluation. It will not be a fully configured production machine. The machine will be attached to the C2N for access to the DMS and GVL.

The ECS will not be an element of the interim EMSL, although the interim HPCS discussed

above will be a test bed for investigating competing parallel architectures.

2.6 Interface Development Laboratory

The Interface Development Laboratory (IDL) will support the EMSL laboratory automation activity by providing the tools and facilities necessary to develop instrumentation interfaces. In addition to electronic test equipment and board level fabrication equipment, the lab will provide computer hardware and software for the development of real-time data acquisition and instrument control applications. An important part of this activity will be to encourage the development of guidelines and standards for EMSL instrumentation interfaces.

Because of the great variety of instrumentation to be used within the EMSL, the IDL must be able to accommodate a mix of interface architectures. For example, interface technologies that are now commonly used for instrumentation include CAMAC, IEEE 488, VMEbus/VXIbus, ISA, various serial protocols such as RS232 and RS422, and special parallel protocols for high data rate instruments. At least four development platforms are needed to support these architectures, currently represented by a Macintosh, personal computers (with MCA and EISA bus architectures), VMEbus system, and a UNIX workstation.

An IDL capability will be established in the interim facility to support the development of interfaces and data acquisition systems for instruments currently undergoing prototype development. This activity will provide the experience necessary to evaluate evolving technologies and standards, thus providing a good basis for developing guidelines and recommendations. Prototype development will involve addressing several issues, such as high performance data acquisition and control requirements, low cost personal computer applications, and integration of vendor data acquisitions and control systems into the EMSL computing architecture.

2.7 Distributed Systems

The primary user access to EMSL computing resources will be through workstations located in

the offices of the research and support staff. These workstations will be medium- to high-performance scientific machines equipped with large display screens and performance specifications at or above the current median performance for scientific workstations. These will be mainstream products available from established vendors and will likely use reduced instructions set computer (RISC) technology. This technology is predominant in today's market and is improving rapidly in performance.

The client-server computing model that is becoming the standard computing architecture for the 1990s will be adopted. This model relies on the presence of network server resources to support the workstations. Servers provide file storage for client workstations and are the load and control point for the client operating system and application software. Management and administration of the user workstations centers around the maintenance of software stored on the server, which is an enabling factor for efficient system administration. It is intended that distributed file servers will be integrated with the DMS to provide a common file system.

Other user services will be provided by network accessible resources. These include access to computer servers, shared printers, and other peripheral devices and support for electronic mail.

There is currently considerable activity in distributed computing technologies within standards setting bodies, research organizations, and the computer industry. Examples are the Athena project (a joint industry/university research project), the recent call for distributed computing technology by the Open Software Foundation (OSF), and products that are being developed and marketed by computer companies such as Sun Microsystems, Digital Equipment, and Hewlett-Packard. This activity will result in robust commercial grade products that will operate well in heterogeneous computing environments. Therefore, it is likely that establishing a production quality client-server workstation environment within the EMSL will not require us to develop fundamental software.

The UNIX operating system is the focus of the standards setting activity. POSIX (Portable Operating System Interface for Computer Environments) compliant UNIX will be the operating

system of choice for EMSL. This policy is consistent with government guidelines and is in the best interest of the EMSL, in that it will provide the most economical solution to distributed computing needs and the most flexibility to select and use products from a large vendor base. The POSIX suite of standards now includes software portability specifications (POSIX.1) and, in the future, will address system security, administration, networking, and other services provided by the operating software.

A key element of the EMSL computing environment will be the user interface presented on the scientific workstation. In selecting this technology, the C&IS strategy, as in the choice of operating systems, will be to adopt and use accepted industry and government standards. The X Window System will be the underlying client/server display model. The user interface will perform interactively and provide advanced graphics features, including three-dimensional and rendering capability. The selection of a high level

window manager (Open Look and Motif are examples) will be based on the suitability of the various models for scientific use, quality of supporting development tools, and portability to different platforms.

2.8 Facility Training Center

The Facility Training Center (FTC) will be used for demonstrations, presentations, workshops, seminars, and training sessions involving large groups of people. Computer equipment located in the FTC will include scientific workstations similar to those distributed throughout the EMSL offices and laboratories and high resolution projection devices. All workstations will be connected to an ESN serving the FTC. The unique aspect of the FTC will be the effective educational environment created by its physical architecture. Computer equipment located here will be similar to that distributed throughout the EMSL. There will not be an FTC in the interim facility.

3.0 Technical Approach

The strategy for implementing the EMSL computing architecture relies on the use of commercial products, approved and emerging standards, and a combination of traditional engineering practice and prototype development.

3.1 Design Rules

Two design rules apply universally to systems to be included in the EMSL computing environment.

The first is to use existing commercially available products whenever possible. There are many challenges ahead in implementing the EMSL computing architecture, so effort spent developing code, tools, and systems that can be purchased would be at the expense of progress in more important areas. Vendors will often tailor their products to fit specific requirements and do so at less expense and with better results than developing custom solutions in-house. Use of commercial products generally means fewer operating problems and lower maintenance costs.

The second rule is to specify appropriate standards in all procurements, and to use appropriate standards in all development projects. National, international, and industry standards are now in place for many of the EMSL's traditional computing requirements. The EMSL computing architecture will adopt and use these standards, which will include the following:

- Open System Interconnection (OSI) compliant communications standards
- Portable Operating System Interface for Computer Environments (POSIX) standards for operating systems
- POSIX compliant UNIX operating systems
- X Window System standard for client-server graphical user interfaces
- GKS, PHIGS+, and PEX graphics standards.

As other standards are developed and put into practice, they will be studied for possible use in the EMSL computing architecture.

It is clear that the range of computing products needed for EMSL must be supplied by many vendors, and a standards-based strategy will promote the interoperability of heterogeneous computing resources. The strategy will promote the selection of the best performing and most cost effective equipment during phased procurement cycles.

3.2 Implementation Strategy

Implementation of many elements of the computing architecture will be accomplished through a prototype development that leads to specification and procurement of the required resources. Prototypes for the HPCS, DMS, and GVL will be developed in the interim facility. Prototypes for the integrated network, distributed systems, and the IDL will also be developed.

Prototype development for these systems will provide computing resources for the operation of the interim facility and feed information to the engineering process. In many cases, prototype systems will be incorporated into the EMSL computing environment.

The engineering process includes the following activities:

- Preliminary Design
- Functional Design
 - Enterprise Modeling
 - Functional Requirements Definition
 - Conceptual Design
 - Functional Specification
- Detailed Design
 - System Specification
 - Connectivity Specification
 - Operation Specification
 - Acquisition Package Preparation
- Implementation
 - Procurement
 - Installation
 - Acceptance Testing
 - System Integration
- Operations

These activities will occur for each of the major systems of the computing architecture. However, execution of the process will not occur at the same time for all elements.

This formal methodology will satisfy the DOE requirements for project engineering.

3.3 Prototype Development

Prototype development is a valuable activity because it minimizes the risk associated with aggressive technology development. Many of the technologies needed to realize the EMSL vision are in their infancy today. One of the motivating factors for prototype development is the need for more information about these technologies before they can be factored into the engineering process. This development will provide an avenue to explore how leading edge technologies can be effectively used to perform scientific research.

Prototype systems will be used in the interim facility to conduct research. This experience will lead to a much better understanding of user needs and the capabilities of new technologies. This information will feed into the engineering process with the result that equipment and systems installed in the EMSL will be much better suited to their task. Table 1 summarizes the objectives and technical issues associated with the development of each prototype. The relationship

between prototype development and the engineering design process is illustrated in Figure 2. For those technologies where further development is needed, the prototype program will provide the necessary equipment and tools. The maturation of prototype systems into production systems will support research in the interim facility and provide experience that will help prepare for EMSL operation.

3.4 Engineering Plan

In Figure 3 is a summary of the overall C&IS project schedule as it stands in late 1990. The schedule is based on an EMSL occupancy date of early 1995. The engineering process follows a traditional schedule profile. However, as explained above, there is considerable coupling between the prototype development and the functional and detailed design activities of the engineering process. Lessons learned during prototype development will be captured in the engineering process and result in a more appropriate solution to computing needs in the EMSL. Shown in Table 2 are the labor and non-labor resources needed to perform the engineering and prototype development from FY 1991 through FY 1995. Labor resources are listed for each year in terms of full time equivalent (FTE) charges. A mix of junior and senior level professionals will be needed to staff the project. Non-labor charges listed in the table are for equipment, and are costed in FY 1990 dollars.

Table 1. System Prototypes

Prototype System	Objectives	Technical Issues
Integrated Network (Sec. 3.1)	<ul style="list-style-type: none"> • Test & evaluate emerging high performance technologies • Develop and verify network model for design process • Evaluate proposed EMSL network architecture 	<ul style="list-style-type: none"> • Relative merits of high performance technologies • Multi-protocol routing • Importance of redundant connections • Traffic loads imposed by distributed file system and hierarchical network architecture
High Performance Computer System (Sec. 3.2)	<ul style="list-style-type: none"> • Evaluate alternative supercomputing architectures • Demonstrate and evaluate dual architecture system • Provide platforms for parallel computational and experimental chemistry code development • Provide platform for developing, testing and evaluating tools for parallel code development 	<ul style="list-style-type: none"> • Feasibility and benefits of dual architecture design via a possible alternatives • Software tools for partitioning of problems across multiple architectures • Connection of high performance multiprocessors to graphics engine • Scalability of parallel algorithms
Data Management System (Sec. 3.3)	<ul style="list-style-type: none"> • Test and evaluate technology for large scale data management in distributed, heterogeneous environment • Support data management requirements for MSRC research 	<ul style="list-style-type: none"> • Feasibility of unified distributed file system and archive • Performance of distributed file system and archive
Graphics and Visualization Laboratory (Sec. 3.4)	<ul style="list-style-type: none"> • Evaluate competing visualization technologies • Demonstration multiprocessor graphics engine construction • Provide platform for visualization and user interface software development • Support research in interim MSRC facilities 	<ul style="list-style-type: none"> • Software portability • Techniques for connection of parallel computers and graphics engines
Interface Development Laboratory (Sec. 3.6)	<ul style="list-style-type: none"> • Evaluate alternative data acquisition and instrument control technologies • Support selection of data acquisition technologies and electronic interface standards for EMSL • Support development and control of data acquisition systems for MSRC instruments • Support design and specification of EMSL IDL • Build a group of instrumentation specialists to staff EMSL 	<ul style="list-style-type: none"> • Viability of CAMAC/LabView technology • Suitability and availability of electronics for VME and VXI bus technology • Integration of instrumentation into UNIX environment • Data, communication, and user interface standards for instrumentation • Availability of mature technology for icon-driven experiment configuration and control
Distributed Systems (Sec. 3.7)	<ul style="list-style-type: none"> • Evaluate alternative workstation models • Provide effective, distributed workstation and server environment that can be operated at reasonable cost • Support visitors in interim MSRC facilities 	<ul style="list-style-type: none"> • Efficient operation of distributed, heterogeneous computing system • Merits of alternative workstation architectures • Interoperability

Figure 2. Relationship Between Design and Prototype Development

Figure 3. Engineering Schedule

Table 2. Project Resource Requirements

<u>Labor (FTE/Year)</u>	<u>FY 1991</u>	<u>FY 1992</u>	<u>FY 1993</u>	<u>FY 1994</u>	<u>FY 1995</u>
High Performance Computer System	0.6	1.0	1.1	0.8	1.3
Experimental Computer System	0.0	0.0	0.0	0.0	0.9
Data Management System	0.2	1.0	1.9	3.2	4.5
Graphics & Visualization Laboratory	0.6	1.0	1.0	1.0	1.0
Network	1.0	1.5	3.0	4.4	7.0
Laboratory Automation	1.5	3.0	4.5	5.0	6.7
Facility Training Center	0.0	0.0	1.0	1.0	2.7
Distributed Systems	0.0	1.0	3.0	3.0	7.0
Integrated System Design	1.5	3.0	3.5	2.0	2.5
Total FTE Per Year	5.4	11.5	19.0	20.4	33.6

<u>Non-Labor</u>	<u>FY 1991</u>	<u>FY 1992</u>	<u>FY 1993</u>	<u>FY 1994</u>	<u>FY 1995</u>
High Performance Computer System	* \$500,000	* \$500,000	\$2,000,000	\$0	\$15,200,000
Experimental Computer System	0	0	0	0	1,000,000
Data Management System	615,000	* 345,000	* 100,000	*5,420,000	0
Graphics & Visualization Laboratory	* 320,000	75,000	*370,000	*500,000	600,000
Network	135,000	720,000	400,000	1,020,000	230,000
Laboratory Automation	150,000	355,000	320,000	385,000	170,000
Facility Training Center	0	0	0	605,000	358,000
Distributed Systems	<u>* 255,000</u>	<u>* 535,000</u>	<u>* 470,000</u>	<u>*1,812,000</u>	<u>* 730,000</u>
Total Non-Labor Per Year	\$1,975,000	\$2,530,000	\$3,660,00	\$9,742,000	\$18,288,000

Note: Estimates in Table 2 are based on a five-year implementation schedule
Asterick (*) denotes programmatic funding.

Appendix A

Acronyms and Initialisms

Appendix A

Acronyms and Initialisms

BIN	backbone information network
CFS	common file system
C&IS	Computers and Information Sciences [project]
C2N	computer-to-computer network
DMS	data management system
ECS	experimental computer system
EISA	extended industry standard architecture
EMSL	Environmental and Molecular Sciences Laboratory
ESN	end-user subscriber network
ESRC	Environmental Sciences Research Center
FDDI	fiber data distribution interface
FTE	full time equivalent
GB	giga-bytes
Gbps	giga-bits per second
GKS	graphics kernel standard
OSI	open systems interconnection (compliant communication standards)
HPCS	high performance computer system(s)
IDL	Interface Development Laboratory
ISA	industry standard architecture
Mbps	mega-bits per second
MCA	micro channel architecture
MSCF	Molecular Sciences Computer Facility
MSRC	Molecular Sciences Research Center
OSF	Open Software Foundation
PEX	PHIGS extensions to X
PHIGS	Programmer's Hierarchical Interactive Graphics Standard
PNL	Pacific Northwest laboratory
POSIX	Portable Operating System Interface for Computer Environments
RISC	reduced instruction set computer

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