CONF-9010211--3

WSRC-MS-90-246

# AN EXPERT SAMPLE ANALYSIS PLANNER (U)

WSRC-MS--90-246

DE91 005124

by

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A paper proposed for presentation at
***Department of Energy Complex Conference***
***"AI in the DOE Complex"***
Idaho National Engineering Laboratory
Idaho Falls, ID
October 9-11, 1990

and for publication in the proceedings of the meeting



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This article was prepared in connection with work done under Contract No. DE-AC09-89SR18035 with the U. S. Department of Energy. 

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## ABSTRACT

Analytical chemists are faced with the problem of choosing an appropriate analytical technique for a particular sample and weighing the options as they affect precision, time, and cost. This paper describes a computer technique to assist managers in reviewing the alternatives and to match needs with the resources available.

This paper proposes an expert system, knowledgeable of analytical chemistry techniques, to create sample plans. Sample planning is an appropriate topic for expert systems because scarce human expertise is required to complete sample plans. A sample plan is the description of how samples received at the Savannah River Laboratory are handled, controlled, measured, and dispositioned. Sample planning is difficult because multiple experts are needed, planning is not a static function, and planning is time consuming.

An **E**xpert **S**ample **A**nalyses **P**lanner (XSAP) is proposed to create sample plans for laboratory managers. XSAP supplements the scarce knowledge of analytical techniques creating sample plans based on analysis constraints, methods available, and time requirements. XSAP interacts with the chemist to suggest sample plans. XSAP considers equipment available locally, at other Savannah River laboratories, at other Department of Energy facilities, and at other commercial laboratories. XSAP allows options on scheduling: best solution, cheapest solution, best local solution, and fastest solution.

## INTRODUCTION

The task of The Analytical Services Group (ASG) personnel is to develop consistent plans to assure quality-analyses/cost-savings to the customer. Assurance of quality analyses requires attention to analysis scheduling and methods. Assurance of cost-savings depends on the development of unambiguous sample plans for the technicians of ASG.

A sample plan must be established before any analysis can be conducted by ASG. The sample plan is the description of how samples received at the ASG laboratory are handled, controlled, measured, and dispositioned. The development of sample plans is not a static function; periodic reviews are conducted for established customers because analytical methods change.

ASG assigns a chemist or "planner" to create sample plans. The planner is familiar with the routine analytical methods and instruments offered by ASG. And the planner is familiar with offsite laboratories to supplement ASG services.

The planner programs the ASG Laboratory Information Management System (LIMS) to support the customer. The planner sets default instructions for ASG to safely handle samples and notes instructions for assigned methods. Samples logged into the LIMS data base become permanent records to identify the sample, determine the hazards, perform the analyses, and dispose of the sample. The planner must know the Customer, the Study, the Material, the Profile, and the Parameters to create the LIMS record. The information required for LIMS:

**CUSTOMER**
(e.g., Actinide Tech, DWPT TNX, REACTORS, M AREA, etc.)
**STUDY**
(e.g., Pu Scrap, IDMS, J. Bibler)
**MATERIAL**
(Glass, Sludge, Pu Scrap, etc.)
**PROFILE**
(lists of analytical methods, e.g., SEM/XRD)
**PARAMETERS**

ASG (Receiver Initials) ..... used to activate ASG
Description ..... brief description
Radioactivity ..... how much and what
Fissionable ..... no or yes, what and how much
Chemical Hazards ..... warn ASG personnel
Submitter ..... who gets the results
Disposal ..... return or dispose of sample
Sample Size ..... helps identify sample
Heterogeneous ..... if multiphase give instruction
Requester ..... technician or other contact
Analyses ..... specific instructions (e.g., IC: chloride, nitrate)
Comments ..... special message to ASG

Planners are expert in one or two areas of analysis but cannot be expert in all analyses. The planner relies on existing plans and other analytical experts to create customer sample plans. Relying on existing plans requires that the plans

be accurate. Relying on other experts requires the customer to wait until experts are available. Overlap of analysis techniques requires multiple experts to convene to develop a sample plan.

New computing techniques are required to assist sample planners[24]. The Environmental Protection Agency (EPA) is studying new computing strategies to assist laboratory managers[8]. Knowledge base techniques to automate portions of the analysis process have been created[3,4,10,11,13,18,19,20]. These computing techniques are known as expert systems. The dynamic nature of analysis, the growing number of work orders, and the lack of comprehensive planning expertise dictates that ASG consider other methods for accurate sample planning. The EPA has developed expert systems in the areas of quality assurance, sampling techniques, selection of laboratories, selection of methods, review of data, diagnosis of sampling techniques, and the evaluation of laboratory analyses.

## DISCUSSION

The ASG requires an **E**xpert **S**ample **A**nalyses **P**lanner (XSAP). The best solution method for this problem is an intelligent reasoning system. This type of system is referred to as an expert system. Problems appropriate for this solution can be identified using seven criteria[15]:

1) The need for the solution justifies the cost and effort of building an expert system,
2) Human expertise is not available in all situations where it is needed,
3) The problem may be solved using symbolic reasoning techniques,
4) The problem domain is well structured,
5) The problem may not be solved using traditional computing methods,
6) Cooperative and articulate experts exist,
7) The problem is of sufficient size and scope.

The need for the solution justifies the cost and effort of building an expert system[24]. The cost savings is in excess of the development costs. A feasibility study for XSAP shows that the system will take 2-4 man-years to develop, and should pay for itself in 1-3 years.

Human expertise is not available in all situations when needed. ASG requires a tool that will allow the customers access to expert advise when the expert is not available. The customer can select sample plans that best suit their specific requirements[25,26].

The problem may be solved using symbolic reasoning techniques. This problem is solved algorithmically using tables, empiricals, and "rules-of-thumb". User queries may be required, but real-time device inputs are not required[26].

The problem domain is well structured. Sample plans are derived from "first-principles" or rules from experts. These decisions can be represented in logical sequences, tables of values, or heuristic measures.

Cooperative and articulate experts exist. We have the planners that are currently performing the function and experts at other DOE laboratories. These individuals will be used for the acquisition of information to program this system. This system will not displace experts - but will be a tool to enhance their productivity.

Because most sample plans are taken from existing plans or created from empiricals, the size of the XSAP problem is well constrained. This program is proposed for the purpose of sample plan production and table displays.

## Constraints

The planner may constrain the sample plan and XSAP must allow the planner to override the suggested plan. Planning with XSAP is interactive and iterative.

The selections by XSAP cannot be arbitrary, so XSAP must be able to describe its rationale for plan development. XSAP describes criterion for plan development, and displays tables, charts, graphs and other empiricals available to the planner for inspection. XSAP includes detailed descriptions for the reasoning process.

XSAP optimizes solutions on best, best local, cheapest, and fastest. XSAP weights sample plans based on cost, time, and quality. These constraints require XSAP to optimize resource allocation. Equipment availability/proximity/cost are factors. XSAP considers equipment available at Savannah River Laboratory, at other SRS labs, at other DOE facilities, and at other commercial labs.

LIMS users/planners can access XSAP for online analytical reference. Charts, graphs, tables, or other depictions of empiricals are available to LIMS users and planners.

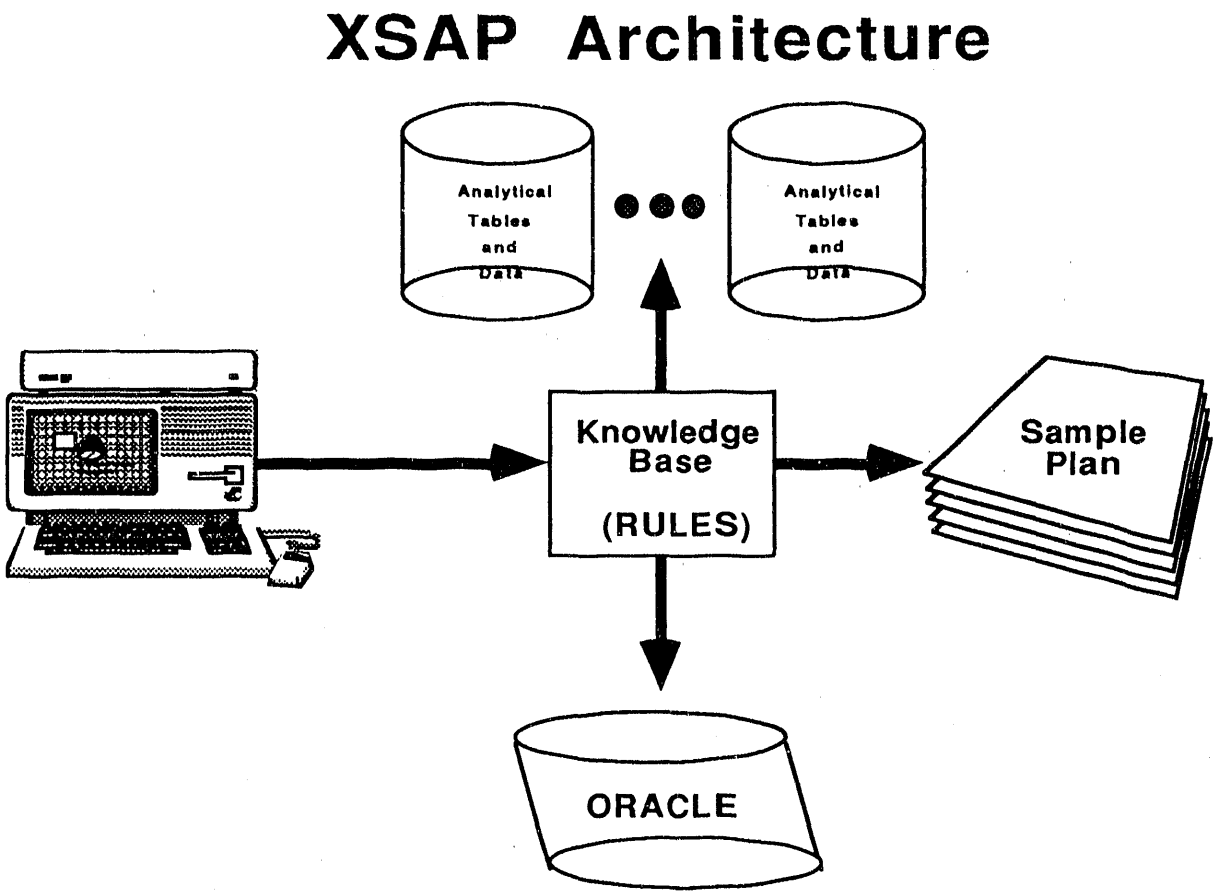
The user interface is a critical design component[6,10]. Presenting data in a format that is familiar to the user is important for the success of the expert system. The interface must be simple so that users will not be required to learn extensive commands and routines, and the data/display must be presented in a manner that is meaningful.

Access to XSAP is partitioned. Initially customers will only have access to features of the online documentation. Customer access to all the features of XSAP will be a future endeavor and must be accounted for in the design.

LIMS compatibility is maintained. XSAP will be developed on the VAX platform so that it can be distributed over the local area network. Other platforms may be considered as technology and markets develop for XSAP[21,24].

## Scope

XSAP architecture will have four functional parts: 1) the knowledge base or rules; 2) the user interface; 3) the ORACLE data base; 4) the tables and analytical data.




*Prototype Hardware/software*

The hardware for the prototype is a MICROVAX II/GPX. The prototype is developed on a stand-alone system running VMS version 5.3. VAX/LISP version 3.0 is the executive controlling the inference engine and frame structure in KEE. KEE (Knowledge Engineering Environment) version 3.1, from Intellicorp, maintains the inference engine and the object system. The LIMS data base is written in ORACLE version 5.0.

*Knowledge base*

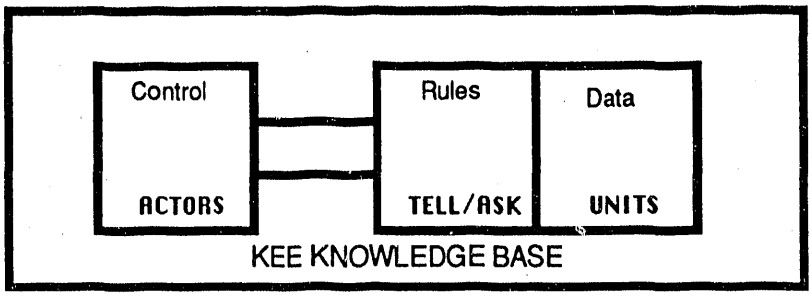
The knowledge base (KB) is the executive that directs program function[20]. The KB contains the rules to combine empirical evidence from the analytical tables, customer information from the ORACLE data base, and user input from the interface to create sample plans.

The KB is divided into control and data/knowledge. Knowledge can be

represented as procedural, qualitative, and semantic[15]. Procedural knowledge is maintained in the KEE TELL/ASK facility. TELL/ASK is the inference mechanism for the system. Qualitative/Semantic knowledge is maintained in the KEE frames.

The KB control is modeled in the ACTOR paradigm[1,6,15]. Each of the functions of the XSAP system is provided by an ACTOR in KEE. The ACTORS are members of the ACTOR knowledge base. Each ACTOR is modeled as a KEE object called a unit. The behavior of the ACTOR is modeled as methods for the KEE objects. The ACTOR methods are written in LISP. The functional description of the code has produced the following ACTORS: Interface Manager, Resource Manager, ORACLE Manager, Table Manager, Knowledge Manager, Executive Manager.

The data/knowledge is maintained in KEE. Static and dynamic entities are modeled in the system. The active entity in the system is called a "request". Each request is modeled as a dynamic object in KEE. Each request has behaviors which are modeled as methods in the dynamic unit. Static knowledge is modeled in KEE objects. Static information includes methods/machines available, and customer information.




*Interface*

The user interface is based on interactive graphics. The interface is iconic and mouseable. The user will direct sample plan construction with mouse and keyboard instructions. The interface is the most visible part of the software, and it must be robust and easy to use[6,18,24].

The interface is controlled by the Interface Manager. The Interface Manager is an ACTOR in the KEE system. The behavior of the interface is controlled by the ACTOR methods. The methods are written in LISP code and DECWindows graphics.

The Interface Manager has the responsibility for user control of XSAP. The Interface Manager reads mouse clicks that dictate program execution. The interface is menu/mouse driven, but may require user data input. The Interface Manager must read data/character input from the keyboard. The Interface Manager assimilates the direction from the user and displays information to the terminal.

*ORACLE Data Base*

The ORACLE data base is ACCESS*LIMS. ACCESS*LIMS is proprietary software developed by PE NELSON. The LIMS system resides on a Digital Equipment Corporation VAX 3800 running VMS[21]. Access to LIMS is distributed over local area nodes and access to data is controlled. Access to LIMS is controlled by the VAX System Manager and the ORACLE Data Base Administrator[22].

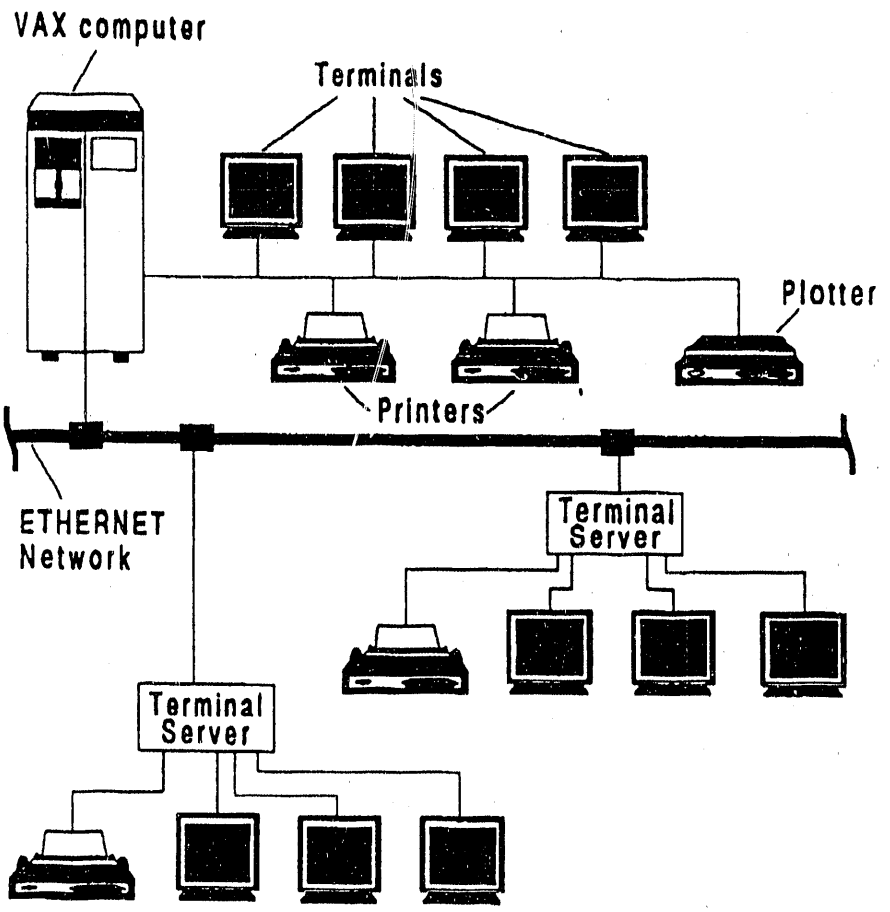
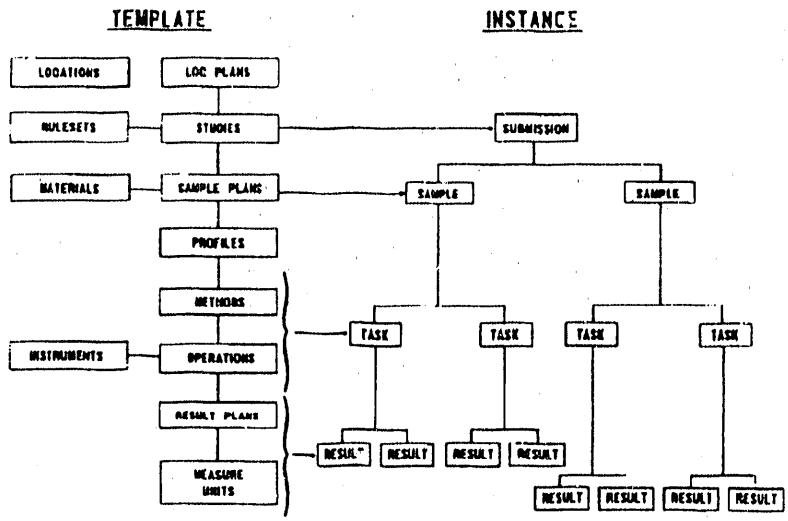



Figure 2-1. Typical ACCESS*LIMS hardware configuration.

ACCESS*LIMS is an object-oriented implementation. A template of the required information is created at installation. The planner fills in the template to create an instance. Each instance is called a submission. XSAP will assist the planner in filling in the template object by supplying the required information.




From template to instance.

## *Analytical tables*

The analytical tables must be developed. These tables contain empirical data. No protocols exist for compilation of these tables. AMES laboratory will assist in the creation of these tables[4].

## Process

The first step in creation of XSAP is completion of Knowledge Acquisition (KA)[15]. Knowledge systems differ from traditional coding regimes in the type of information modeled. KA is the procedure used in the development of knowledge based systems that generates the actual functions of the code. We have stated the general requirement of the system: to be an automated assistant to produce sample plans for the ASG "planner"[25]. The KA function explicitly ferrets out the

information that is required by the system. Once planning information has been identified it can then be codified.

A prototype of the system will be created after KA. The prototype is used for proof-of-correctness[6,17]. This assures both the veracity of the software and the logic processing. Experts will be consulted for the procedures that must be emulated in XSAP. Each planner has an individual planning process; differences will be encountered in the procedures used by the various experts. The prototype is used to identify/rectify the differences before implementation of the system. The prototype is primitive and is intended for incremental development.

Software/hardware is designated for the project. Software/hardware is selected to assure compatibility with the existing LIMS system[6]. XSAP will be developed on a Microvax II/GPX[21], manufactured by Digital Equipment Corporation (DEC). The development platform will be a stand-alone system. Once development, testing and configuration are complete, the code will be ported to the VAX running the PE NELSON LIMS system.

VAX/LISP implements the software executive[11]. VAX LISP is the DEC implementation of Common LISP (the ANSI standard) and is compatible with any ANSI standard LISP implementation[23]. The XSAP executive will be written in LISP and connect to KEE (Knowledge Engineering Environment) from Intellicorp. KEE and VAX/LISP are compatible with the ORACLE software. VAX/LISP can interface to ORACLE with a programmed interface[2]. VAX/LISP interfaces with existing software.

KEE implements the knowledge base. KEE is a powerful tool for developing large expert systems[2,22]. Three major components of KEE are utilized: the inference engine, the truth maintenance system, and the object system. These components comprise most of the software required by an expert system.

## CONCLUSION

The ASG is implementing XSAP to create sample plans. XSAP is an integrated system that interfaces with graphics, ORACLE, and analytical tables. XSAP will take 2 to 4 man-years to develop. The system will provide a considerable cost/benefit savings to ASG. Knowledge acquisition for XSAP is in progress and a prototype is in development. The prototype will be completed in the first quarter of FY91.

## ACKNOWLEDGMENT

The information contained in this article was developed during the course of work done under Contract No. DE-AC09-89SR18035 with the U. S. Department of Energy.

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# Expert Sample Analyses Planner [XSAP]

Presented

by

Scott Parks

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# SRL Provides Analytical Chemistry Analyses

- The mission of the Analytical Services Group
  - R&D analytical support
  - Backup plant processing laboratories
- ASG planners
  - Establish service for customers
  - Program/configure the ASG LIMS for customer support

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# ASG Requires Information Management Support

- Sample planning is not a static function
- Planners are not expert in all areas of analysis

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# The Expert Sample Analyses Planner [XSAP]

- Produces suggested sample plans
- Plans are supported with evidence
- Sample plans are optimized
- Analytical data is available online
- The user interface is mouse-driven
- Access to XSAP is partitioned

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# XSAP is Feasible

- There are currently 800 sample plans in the LIMS data base
- The annual cost savings to ASG is $300,000
- The system pays for itself in 1-3 years

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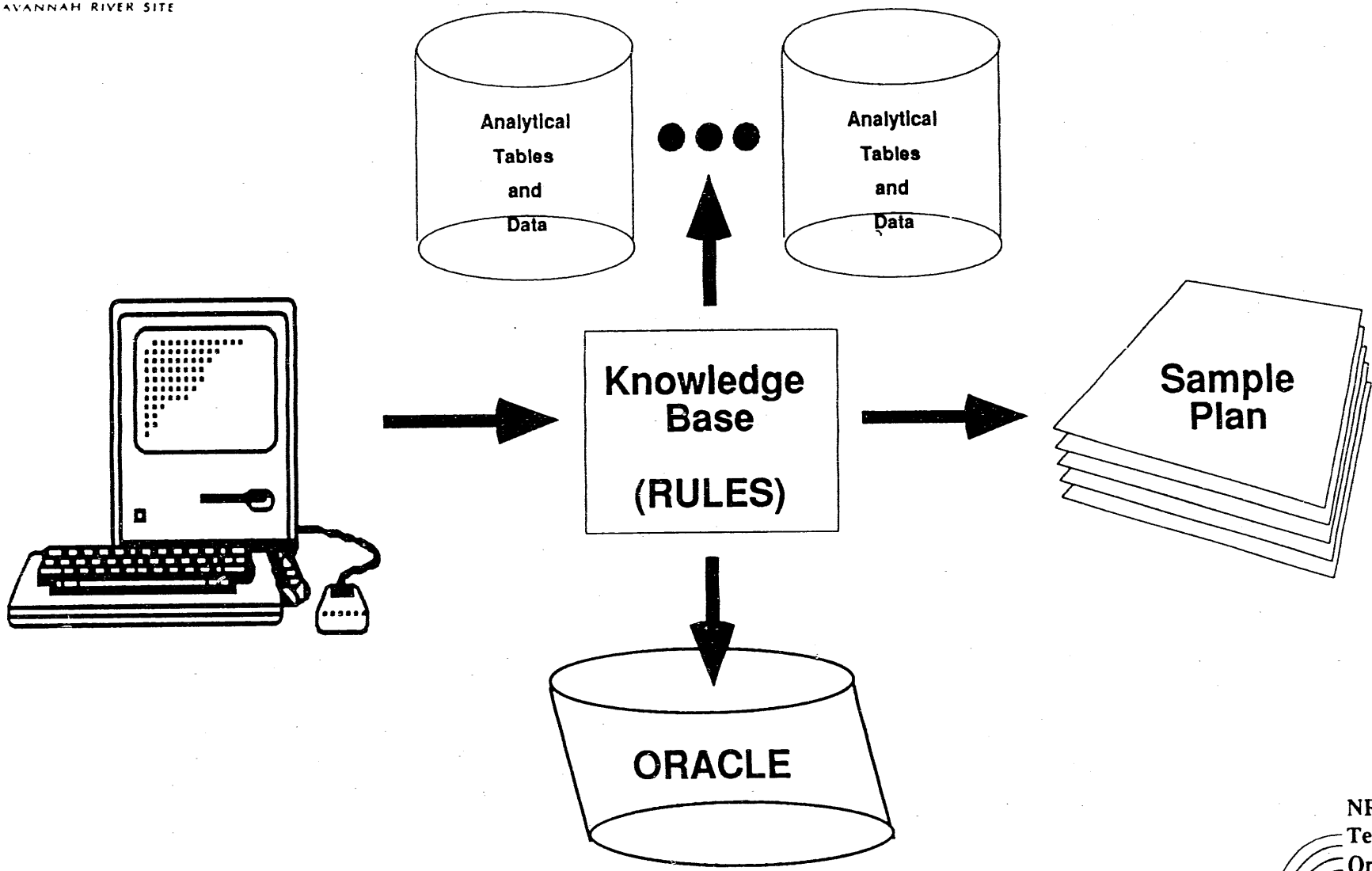
# The XSAP Architecture

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# XSAP Hardware/Software


- MICROVAX II/GPX
- VMS version 5.3

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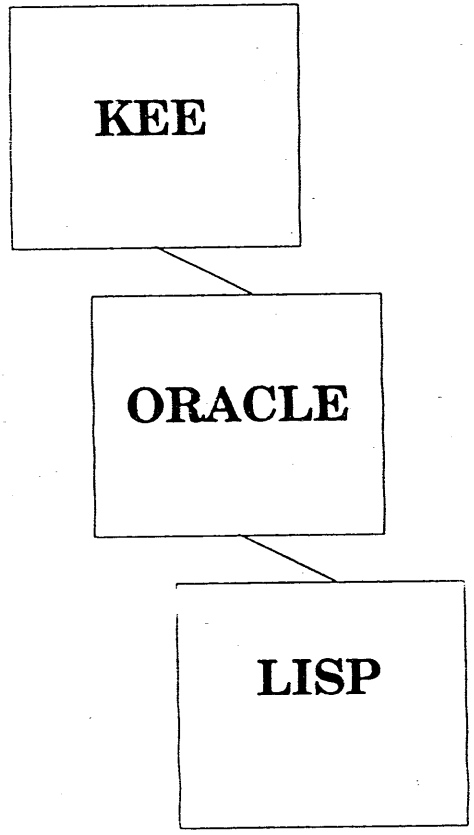
# SOFTWARE




- KEE version 3.1
- ACCESS*LIMS
- ORACLE version 5.0
- LISP version 3.1

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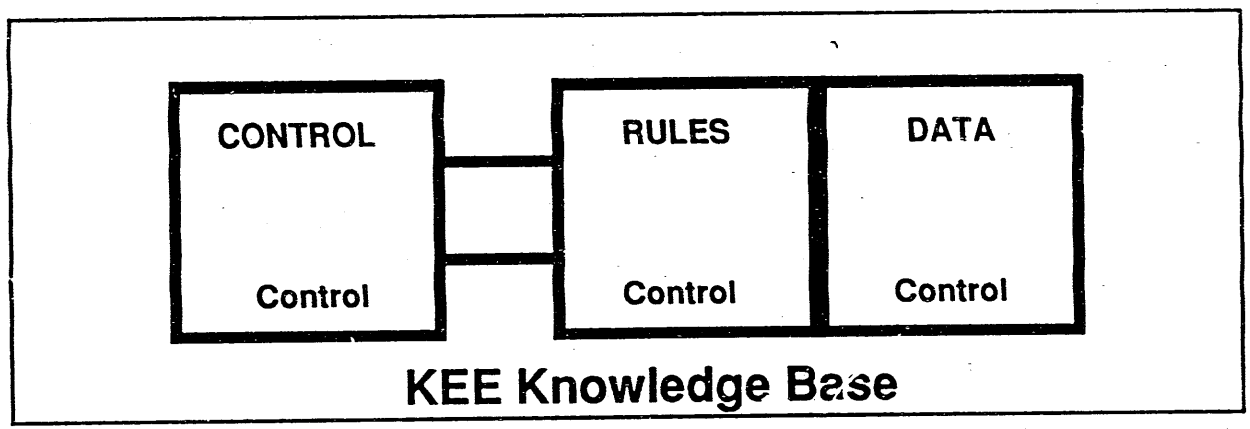
# XSAP Knowledge Base




- Execution is controled by ACTORS
- TELL/ASK generates process control
- Data is stored in KEE units

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# XSAP is Driven by a Mouse

**XSAP functions are control by KEE ACTORS**

- Interface Manager
- Resource Manager
- ORACLE Manager
- Table Manager
- Knowledge Manager
- Executive Manager

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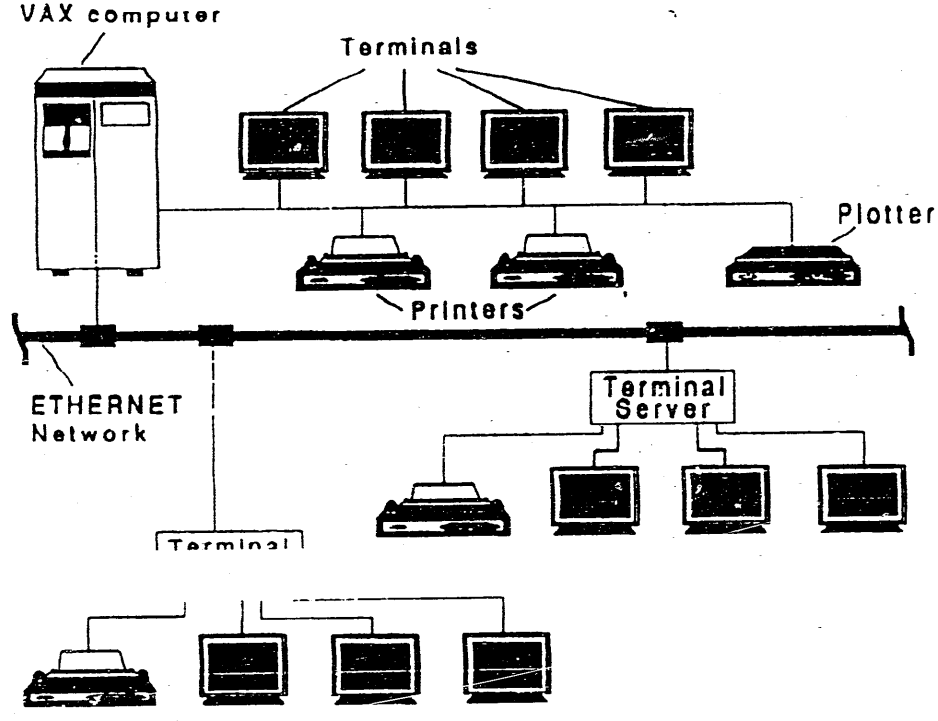
# ACCESS*LIMS

- ORACLE data base
- Access is controlled
- VAX 3800 cluster




Typical ACCESS*LIMS hardware configuration.

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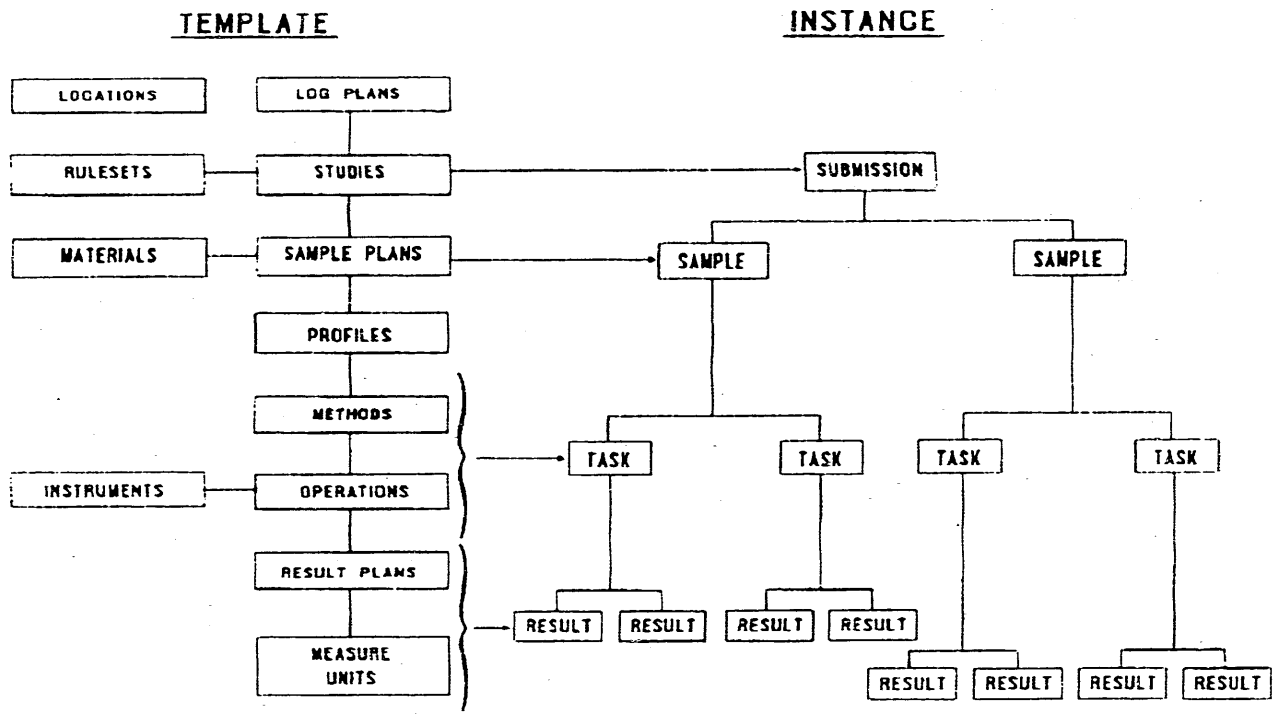
# LIMS is Object-oriented




From template to instance.

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# Summary

- XSAP creates sample plans
- XSAP is an integrated system
- XSAP will take 2-4 man years to develop
- XSAP will pay for its self in 1-3 years
- Knowledge acquisition for XSAP is in progress
- A prototype of XSAP will be completed in 1st quarter FY91

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# END

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