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Publication Date

1989-07-01

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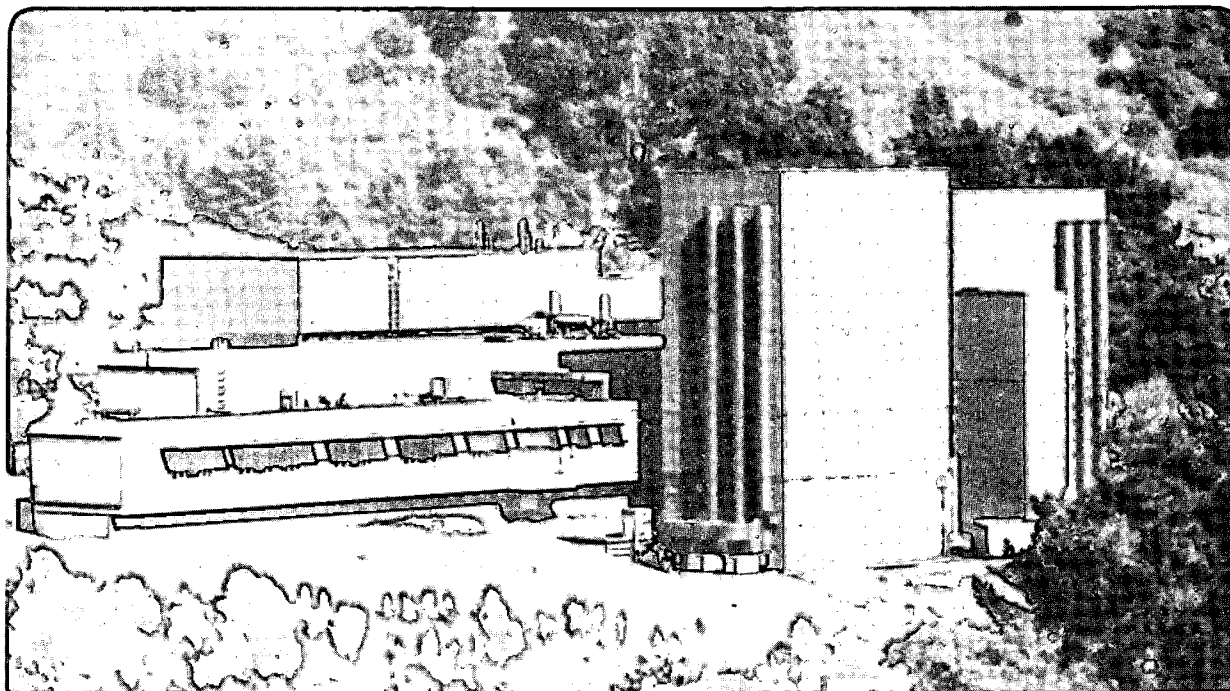
National Center for Electron Microscopy

Presented at the Symposium on Computer Simulation of
Electron Microscope Diffraction and Images, Las Vegas, NV,
February 28–March 3, 1989, and to be published in the Proceedings

The Design of a Computer System for Image Simulation and Image Processing of High Resolution Electron Micrographs

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July 1989



Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

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THE DESIGN OF A COMPUTER SYSTEM FOR IMAGE SIMULATION AND IMAGE
PROCESSING OF HIGH RESOLUTION ELECTRON MICROGRAPHS

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Abstract

The task of assembling a system for simulation and processing of High Resolution Transmission Electron Microscope images is discussed with attention paid to both hardware and software. Two separate systems are presented, one optimized for low cost, the other for performance. In both systems, the emphasis is on compatibility between the separate components making up the system. Finally a third system is presented, adding the functionality of real time data acquisition and processing.

Introduction

High Resolution Electron Microscopy is no longer associated only with the state of the art microscope, but also increasingly with the latest and fastest in high speed computers, array processors, image processors and appropriate software. Scientists setting up new research centers for electron microscopy will, in addition to deciding on microscope equipment, also need to choose computer hardware and software from a large selection of available components. Terms which one could safely omit from the vocabulary, unless by choice being preoccupied with computers, such as buses, backplanes, I/O devices, CPU, RAM, MIPS, MFLOPS, requires attention and an understanding. The selection process would be simpler if the choice could be made from specification sheets alone. However, one soon finds out that the hardware from vendor A will not work with that from B and the software available from C will not work with either. Choosing the correct components becomes a confusing task and even the experienced will from time to time make a choice only to later find out that the different components will not work together.

There are three separate operations that may be required by a computer system installed in the High Resolution TEM facility.

- 1) Image Simulation from hypothesized models.
- 2) Image Processing of previously recorded images.
- 3) Real time data acquisition/processing of images from the microscope.

It turns out that the third operation is best controlled by a separate host cpu loosely coupled to the remaining computer system over a communication network. While performing real time operations, the cpu is required to respond on demand which may not be possible if simulation and/or processing is performed on the cpu at the same time. Real time processes are also served best by a real time operating system rather than a multi-tasking operating system. The "real time" part of the computer setup should have its own image-processor for recursive averaging, background subtraction etc., and an array processor for on line diffractogram calculations. The scope of this paper will deal primarily with image simulation and image processing, only touching briefly upon real time requirements.

This paper is an attempt to provide some information to the uninitiated in order to ease the process of assembling the computer part of the electron microscope facility. It must be understood that it is impossible to cover all available hardware and software and that the options change from month to month. Two computer setups will be given, falling in two different price categories. In addition a system for real time data-acquisition has been included. The choice of a component does not necessarily mean it is the fastest and newest one available, but that it, to the authors knowledge, will provide a good solution from both a performance and compatibility point of view. It must be made perfectly clear that alternatives exist.

The Alternatives

The first problem in deciding what to purchase, is finding out what is available. Since the end goal is to obtain a system that works harmoniously together, selecting a CPU is not independent from selecting the software and peripheral equipment. In spite of this, the different components have been split up into their respective categories below. The question of compatibility will be deferred until later.

1) Hardware

a) Host Computer

Mainframes Nobody buys a mainframe computer for the specific task of running image simulation and/or processing. Mainframes are used because there already is access to one. The main advantage to using a mainframe, apart from the fact that one doesn't have to spend money on a new CPU is that it is a powerful and fast computer. The disadvantage is that most of the time the machines are used by many others and the performance often is not what would be expected. The second problem is being able to manipulate images and output the results. Most mainframes will not have suitable display devices attached, and since mainframes are generally maintained by a central computing department, attaching a peripheral device can be a complicated task.

Giving a list of available mainframe computers makes very little sense, since in most case the choice has already been made by the central computing division.

Mini, Micro-mini Computers These computers are designed to be multi user machines and should be considered when more than one user is expected to be carrying out calculations at the same time. The machines are all-purpose machines and can serve the computing needs for an entire group. In general they do not have a graphics output device for displaying images, and one would need to be added. The cost of these computers range from tens of thousands of dollars to hundreds of thousands of dollars. The performance in general is proportional to the price. The lower priced computers, such as the MicroVax II and III computers made by the Digital Equipment Corporation, are also available as workstation models. While they cannot compete with mainframes in overall performance, the addition of a relatively inexpensive array-processor or high speed math co-processors allows some calculations to be performed at speeds comparable to those of a supercomputer. Parts of the calculations performed in image simulation and processing fall within this category.

Workstations Workstations are generally single user machines equipped with a large graphics screen. Versions will vary, with the less expensive capable of displaying the output in black and white and the most expensive capable of displaying images in 24 bit color. In order to be suitable for display of images, the system should be able to display the image in 64 levels of grey or more. The category workstation spans computers that vary in performance by an order of magnitude, the common theme being a single user machine with a graphic screen, an interactive input device and special windowing software. Some manufacturers will sell both a workstation and a general purpose multi user computer built around the same parts. The integration of the graphics display with interactive input makes the workstation suitable as a turn-key system for image simulation and processing. In order to take full advantage of the workstation, the software is customized to the particular features of the workstation. While the workstation can easily be made into an image simulation and/or processing machine, it is not well suited to handle the general purpose computing needs of a large group. Although some workstations will allow additional terminals to be connected, users connected to these terminals would not be able to run software written for the

workstation screen. However the prices of workstations have been coming down and inexpensive models designed to be connected together over a network have been introduced. Thus it is possible to configure a system with a fileserver and other centralized peripheral hardware with individual workstations taking the place of conventional terminals. In terms of performance, the workstation would also benefit from the addition of an array processor or some other accelerator board to handle floating point intensive calculations.

Workstations are offered by a large number of manufacturers that all compete to bring out the fastest product for the lowest price. Digital Equipment Corporation has several models based upon the Q-bus and the BI-bus. Others like SUN microcomputers, Apollo (now owned by Hewlett Packard), Integrated Solutions and Silicon Graphics offer VME based versions. The choice again will depend on the preferred software and available peripheral hardware.

Personal computers The distinction between a personal computer and a workstation is blurring, with the more costly personal computers claiming to be the latter. While traditionally, workstations offered much higher performance at a greater cost, many personal computers now use components previously used only in workstations. With "personal" referring to cost, meaning that individuals should be able to afford one, and workstations referring to a certain level of performance, traditional workstation manufacturers are now offering "personal workstations" and personal computer manufacturers are offering personal computers with workstation performance. Until recently the personal computer did not possess the power to serve as a good choice for an image processing and simulation computer. Although it is possible to get reasonable performance for some operations by the addition of accelerator boards, the overall design of the computer; limited amount of directly addressable memory, slow cpu and low data transfer rates made it unsuitable as the heart of a sophisticated image processing computer setup. Nevertheless the personal computer was used in many laboratories, mainly as the traffic controller for more powerful add-on equipment.

As mentioned previously, the newer personal computers fall more in the workstation category. They have an interactive input device, usually a mouse, and graphics screens capable of displaying images in color. Because they are still relatively new, the selection of available add-on peripherals is limited, but growing by the day. The personal computer is a true single user machine and few would use it as a general purpose scientific computer. Even today, the personal computer does not deliver the performance that is desired for such number crunching intensive calculations as image simulations. However, with the addition of such hardware as array processors and transputers, the performance can become quite outstanding.

The personal computer arena used to be dominated by the IBM PC-AT and its clones. The development of the 80386 chip introduced faster versions, and lately IBM introduced the new PS-2 personal system. Apple computer produced the Macintosh II computer based around the 68020 chip and has introduced models running the 68030. The current trend in personal computers seem to favor the Macintosh, at least in the US and the IBM PS-2 system is only slowly gaining acceptance. The new NEXT machine (the brainchild of Steve Jobs, formerly with Apple Computers) ,which offers outstanding performance at a low price currently suffers from a lack of available software and is not a contender for the time being.

b) Auxiliary equipment

Image-processors The need for an image processor varies with the type of host computer in use and the application. The general image processor consists of several parts: a digitizing board for input of images from an external source such as a video camera; a framestore section to store images as 8,16 or 32 bit images; an image processing section equipped with Arithmetic Logic Units (ALU's) that can perform real time operations on images, such as addition, multiplication, division etc.;

and a digital to analog converter to display the content of one of the frame stores on a tv monitor. Image processors vary from inexpensive board sets designed to plug into the host computer to expensive multi-user units costing up to \$100,000. The three areas that we are concerned with; image simulation, processing and data acquisition/processing have different needs. In the simplest case image simulation requires only an output display, which may be taken care of by the proper choice of host computer. Image processing requires an output display and a means of getting the experimental images into the system and real time acquisition/processing additionally requires the ALU section in order to perform real time averaging over several incoming images. While all available image processors can handle the input/output functions with ease, not all can perform the necessary mathematical operations on images in the required sequence and in the required time to perform the desired real time image processing tasks.

There is a large number of companies making frame-grabbers and image processing boards for a large number of host computers. The most popular board sets in the low to mid price range seem to be those from Datacube and Imaging Technology. While Datacube's newer products are manufactured for the VME bus, Imaging Technology produces cards for both the VME and the Q-bus. Data Translation produces cards for the IBM's and the Macintoshes, however most are frame-grabbers and won't do recursive averaging. Recursive averaging requires a particular sequence of multipliers, adders and dividers which are not found in boards designed only to grab images from a video camera, see appendix A.

Array processors The array processor is a specialized piece of hardware architecture that is optimized for calculations of a type where the same mathematical operation is repeatedly performed on every element in a large set of numbers, such as squaring each element in an array. The need for an array processor depends on the performance of the host computer, but the addition of an array processor will greatly improve the overall performance of the system for anything but a supercomputer. It should be kept in mind that not all of the calculations are well suited for the array processor and that these will be limited by the performance of the host cpu. In order to take full advantage of the array processor it is necessary to minimize data transfer between the host memory and the array processor memory. For the multislice calculation this means that the array processor should be equipped with a minimum of 6MB of memory. This will allow a calculation of an image of up to 512*512 points to be performed entirely in the array processor. Array processors are rated in MFLOPS (Million Floating point Operations Per Second) which often is an artificial way of measuring the actual performance of the unit. Manufacturers of array processors like to give benchmark times for a 1024 complex FFT which can be used to estimate the time to perform a multislice calculation since the FFT formalism requires 2 FFT's and 2 complex vector multiplications per slice. A typical array processor runs at about 20 MFLOPS and cost in the range of \$14,000 - \$20,000 with the necessary amount of memory. The typical calculation time for a 512 by 512 point image is about 2-3 sec. per slice. The selection of array processors include Mercury Computer's MC3200 and Zip3200 series, SKY Computer's Warrior and Vortex and CSPI's QuickCard. The most important factors are the amount of memory attached to the array processor and the availability for the particular backplane of the intended host computer.

2) Software

There is no single piece of software that is capable of handling both image simulation and processing to the knowledge of the authors. From a practical point of view, simulation and processing represent two quite different calculational problems and are served best by two separate applications. Instead of trying to cover too many things, specializing on a smaller area usually produces a better product.

Image Simulation There are several software packages available for image simulation. SHRLI (1) (Simulation of High Resolution Lattice Images) developed by Dr. M.A. O'Keefe was the first to be made available and has undergone several revisions since the first version. SHRLI was designed to run on mainframe computers with output of images onto computer paper using overprinted characters. The design of SHRLI still reflects the shortage of memory associated with the older computers and takes very little advantage of the new interactive input/output devices available today. However, as a result it is highly portable and can easily be ported to most machines. The most severe limitation is the limitation on the size of the unit cell that SHRLI can calculate. Lately a new breed of software packages have become available which try to take advantage of recent advances in interactive hardware. EMS written by Dr. P. Stadelmann (2) is a software package which will run on a variety of host computers including the IBM PC-AT. This software package is not specifically a simulation software package, but includes the possibility to compute images using both the multislice formalism and the Block wave formalism. A highly interactive mouse driven software package has been developed by Dr. R.Kilaas (3). There are several versions of this software, including one for the Macintosh II/IIx/IIcx personal computers. Specifically, a version written for the DEC Workstation GPX and equivalent DEC models will be supported and distributed by the National Center for Electron Microscopy (4), Lawrence Berkeley Laboratory, free of charge. Other software packages have been written, including ones written by Dr. K. Ishizuka, Dr. D.Van Dyck, Dr. J. Skarnulis and Dr. W. Krakow.

Image Processing While there are several software packages available that claim to be image processing software, not all of them are suitable for the type of image processing most commonly employed in High Resolution Electron Microscopy. Many of these software packages will perform small block convolution, high and low pass filtering, edge detection, histogram equalization, line traces etc., but do not include real space lattice averaging and various window filtering techniques in frequency space which are often used to enhance images obtained from crystalline structures. An understanding of the techniques that are likely to be used is essential when deciding what image processing software to acquire. One image processing software package designed for electron microscopy is SEMPER written by W.O Saxton (5), which will run on a large number of computers. No version of SEMPER currently exists for the Macintosh. A software package written by Dr. J. Frank offers much of the functionality of SEMPER and is available as public domain software. Two pieces of software recently made available for the Macintosh II computer are Ultimage from GTFIS and NuVision by Perceptics. Both will work with the Quickcard frame-grabber from Data Translation. In addition there are a few software/hardware combinations sold as image processing turn-key systems. One such system is the Temdips system produced by H.R. Tietz of West Germany, integrating the software with both a powerful image processor and array processor. A similar system is Imagine which uses the SEMPER software combined with a fast image processor and a FFT board. A system for the Apple Macintosh is NuVision by Perceptics.

Image data acquisition/processing and analysis Compared to image simulation and *a posteriori* image processing, real time image processing, analysis of data for adjustment of astigmatism and automatic control of the microscope is a less mature field, in particular from a software point of view. Several image processing packages running on personal computers and workstations and which are designed to grab images from a video camera connected to a particular frame-grabber usually have built in menu-commands for items like *grab*, *straight average*, *freeze*, *store*, etc., while items like *recursive average* and *diffractiongram* are likely to be absent. The field of automatic microscope control is still under development and one will probably need to write one's own software. To the knowledge of the authors, no turn-key system which does all the above functions currently exists.

Image Simulation/Processing Systems

System 1

The first system for image simulation and image processing is centered around an Apple Macintosh II (or IIx/IIcx) personal computer. The Macintosh II(x) runs the same cpu as many popular workstations, namely the 68020/68030 processor from Motorola. Besides being relatively inexpensive, the Macintosh is a favorite among many for performing such tasks as writing letters, creating illustrations, preparing exams, etc. Thus many scientists already own one of these computers, and would like to do calculations previously associated with big and expensive computers at their own desks. The Macintosh's strong feature is its graphical interface and the presentation of images is a perfect use of this computer. It should be emphasized that image simulation and processing are floating point intensive calculations that can make use of as much speed and memory as possibly available. A 68020 processor coupled with the 68020 math coprocessor will perform a 128^2 Fast Fourier Transform in about 12 seconds., which means that simulating an image from a model of the size 1.6 by 1.6nm will take about 30 seconds. A typical calculation may require 50 slices, thus taking 25 minutes. This does not include the time required to set up the potential from the atoms within the model, nor forming the images by including the effects of the conditions of the microscope. A calculation of this size is considered a medium size calculation, and many calculations involving defects would require a larger unit cell and consequently take longer to compute. As mentioned previously, a typical array processor can perform the same calculation in a few seconds and would require about 2-3 seconds/slice for a unit cell measuring 6.4 by 6.4 nm (512^2 points). Thus in order to increase the performance of the system, an array processor has been added. Since the Macintosh II/IIx/IIcx is a new product, compatible array processors are only starting to appear. One such array processor has been integrated into this system, namely the MC3200 from Mercury Computer Inc. It occupies a single slot on the NuBus and houses 8MB of memory, enough to do a 512^2 calculation entirely within the AP without the need to transfer data between the host and the cpu except for at the start and finish of the calculation.

In order to get experimental data into the computer, a video camera is connected to a Data Translation QuickCard frame grabber and hardcopy output of images is accomplished through a Postscript Laser printer.

The image processing software chosen for this system is the Ultimage software package and image simulation is carried out using MacTempas image simulation software. The system can easily be extended to include a more sophisticated CCD camera for input of images and a film writer for output of images onto 35mm film.

MACINTOSH II

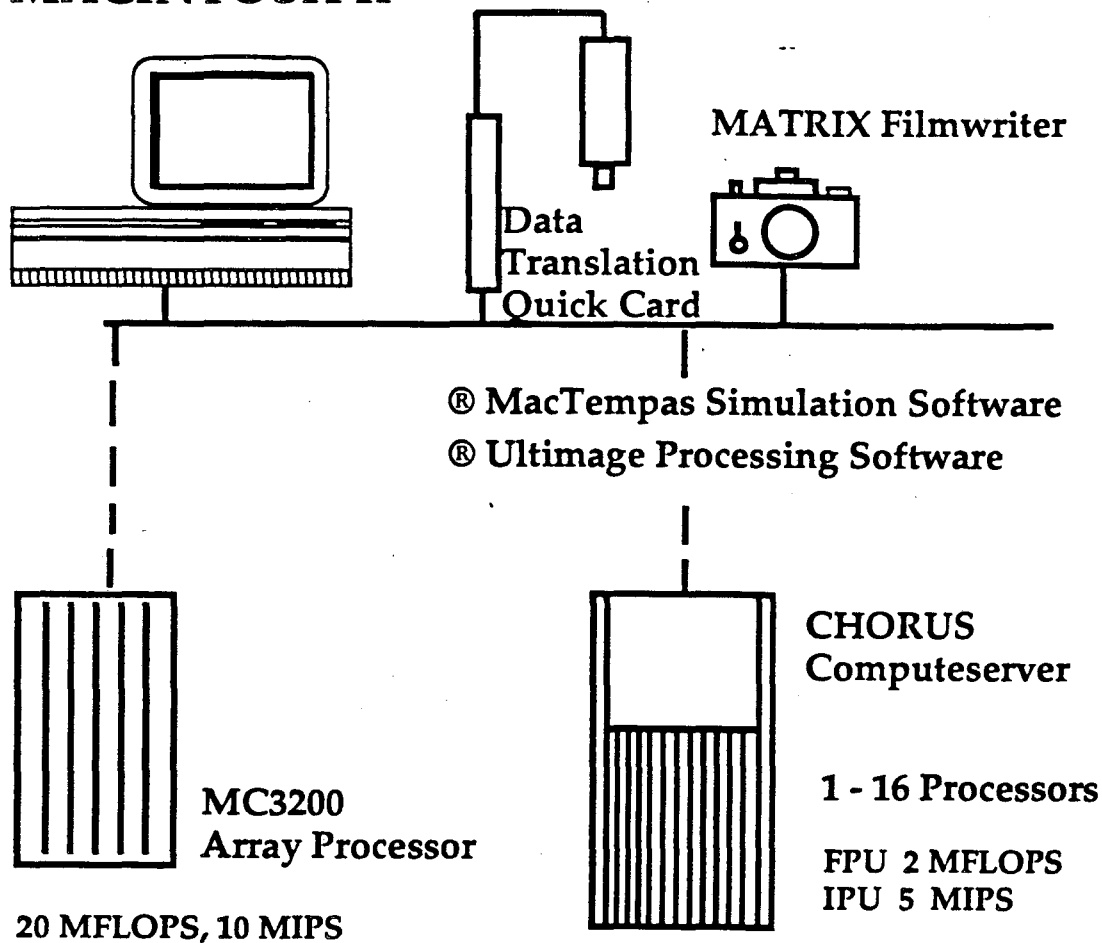


Figure 1 - An integrated image simulation and processing workstation based around the Macintosh II personal computer

System 2

The next system differs from the first by using a more powerful workstation as the heart of the image simulation/processing system. There are a number of available workstations to choose from. The VAXStation 3500 is not the fastest available, but runs the familiar VMS operating system and integrates well into a network of other DEC products. The VAXStation 3500 is capable of displaying images in shades of grey or in color and doesn't need an additional framestore for display of images. The input of experimental images is through the Eikonix Series 78/99 camera. The camera consists of a linear array of 2048 diodes which digitizes up to 2048 rows of 2048 pixels. Each pixel is digitized into either 8 bits or 12 bits. Output of images, processed, experimental or calculated, is through either the postscript laser printer or through the Matrix film recorder. The Matrix film recorder captures images up to 4096 x 2700 pixels onto a 35 mm negative. In order to speed up the calculations, a suitable array processor is integrated into the system. The Mercury Zip 3232+ is a Q-bus compatible product rated at 16MFLOPS and a 512² multislice calculation can be done in 2.5sec/slice. Picking software becomes a personal choice, but this particular system has been equipped with the National Center for Electron Microscopy Simulation Software (NCEMSS). This version of NCEMSS running on DEC VAXStations is distributed in executable form by NCEM/MCSD, Lawrence Berkeley Lab. free of charge. SEMPER is used as the image processing

software. SEMPER is particularly suited for the type of image processing techniques commonly employed in HRTEM and versions written for the VAX-Workstations are available.

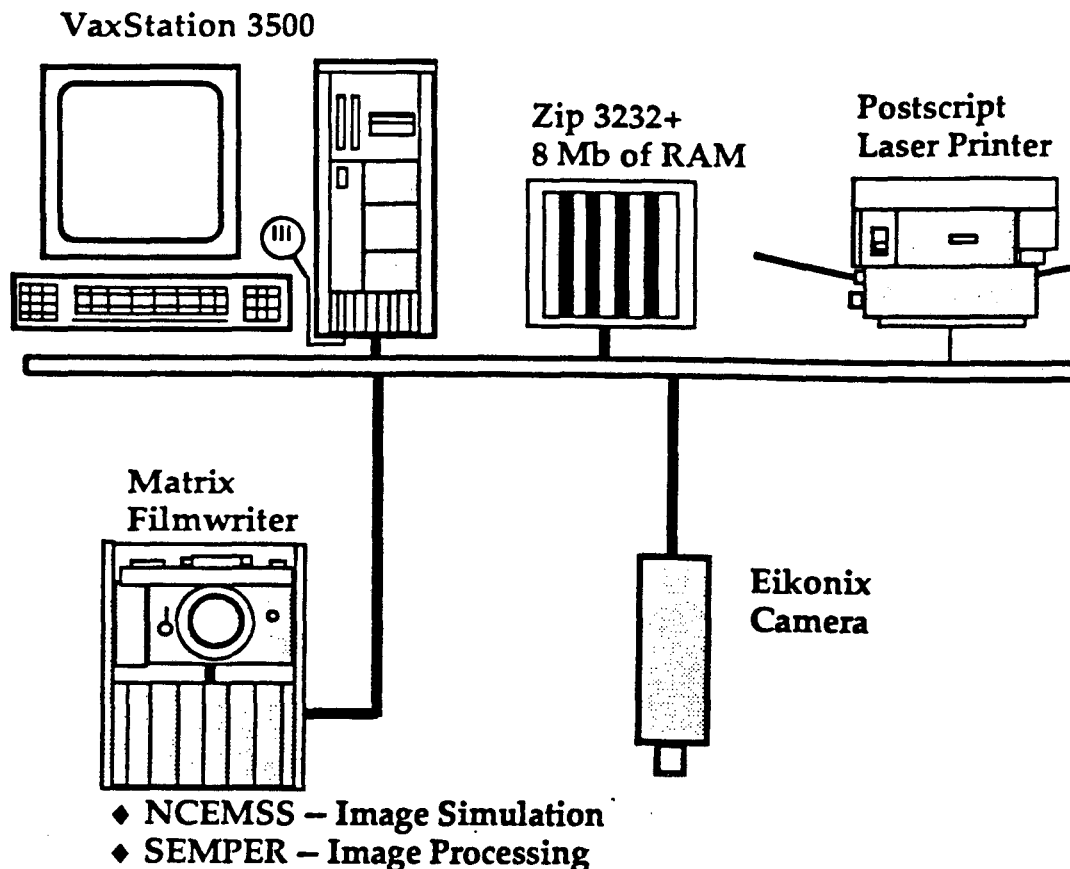


Figure 2 - A more powerful and expensive setup based around the DEC VaxStation 3500

System 3

In order to cover the task of real time data acquisition, a final system is shown. This system uses a SUN workstation connected to independent modules each of which can handle input from one microscope. Each module contains a Control Processor Unit, Ethernet card, array processor cards and a set of image processing cards and is capable of recursive average on incoming frames, grabbing and storing images, calculation of diffractograms, etc. Each unit could also be used to control microscope alignment and correct for astigmatism. The CPU runs the real time operating system VxWorks (of Wind River Systems, Inc.), and application software is developed on the SUN and downloaded into each module. Flow of data to and from the SUN is through the ethernet connection. The SUN is left to perform image simulation and processing of recorded images without having to service interrupts from the real time stations. The choice of the host computer (SUN) is based upon the need to develop the application software to run in the real time modules. As the system grows and new microscopes are added, only a new hardware module needs to be added to the system; no new software is required.

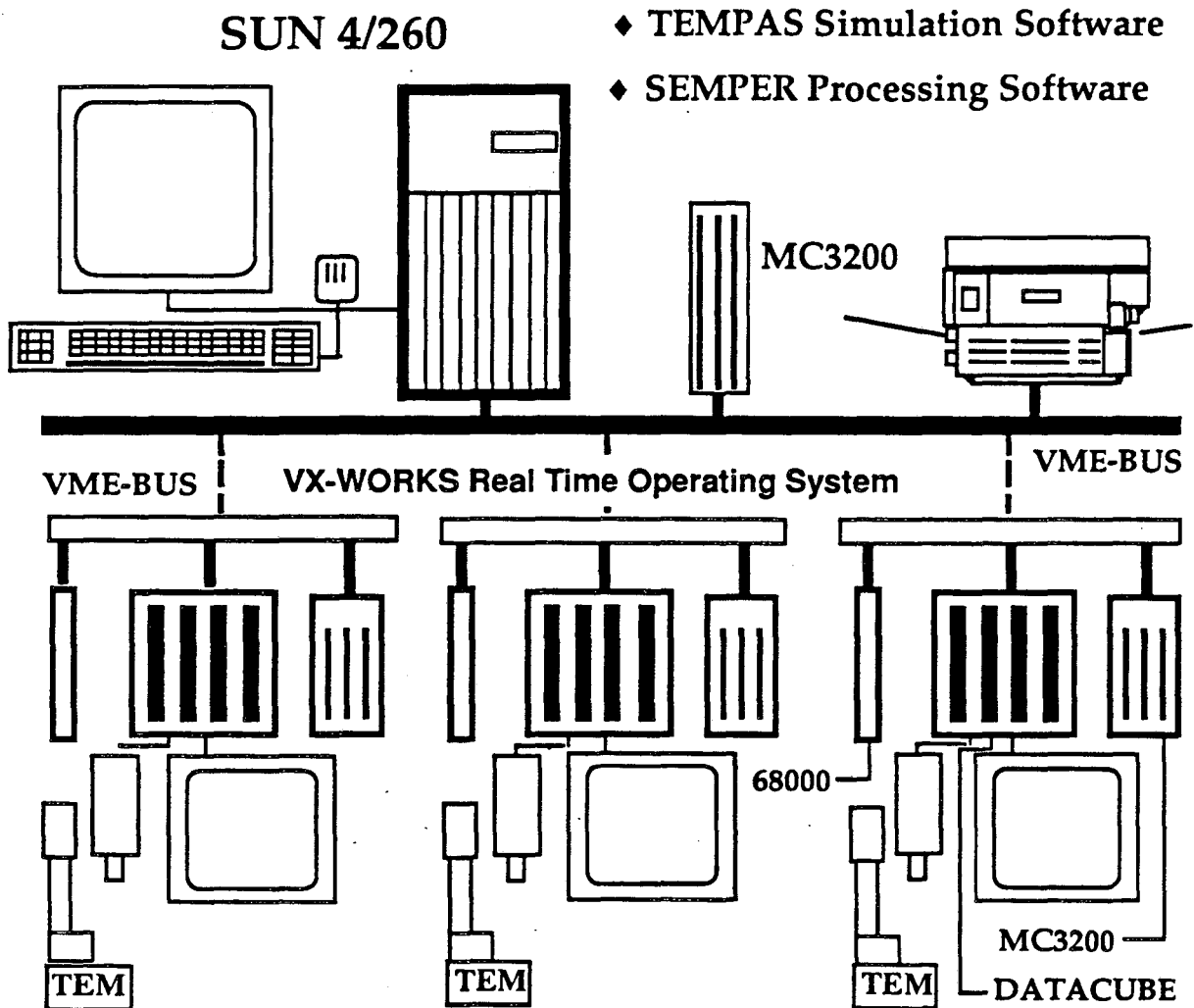


Figure 3 - A system capable of handling both *a posteriori* image simulation and processing of TEM images in addition to real time enhancement and data acquisition. Each microscope is serviced by its own cpu, framestore and array processor. A new microscope can be added by adding a new module. No new software is required.

APPENDIX A

Recursive Averaging

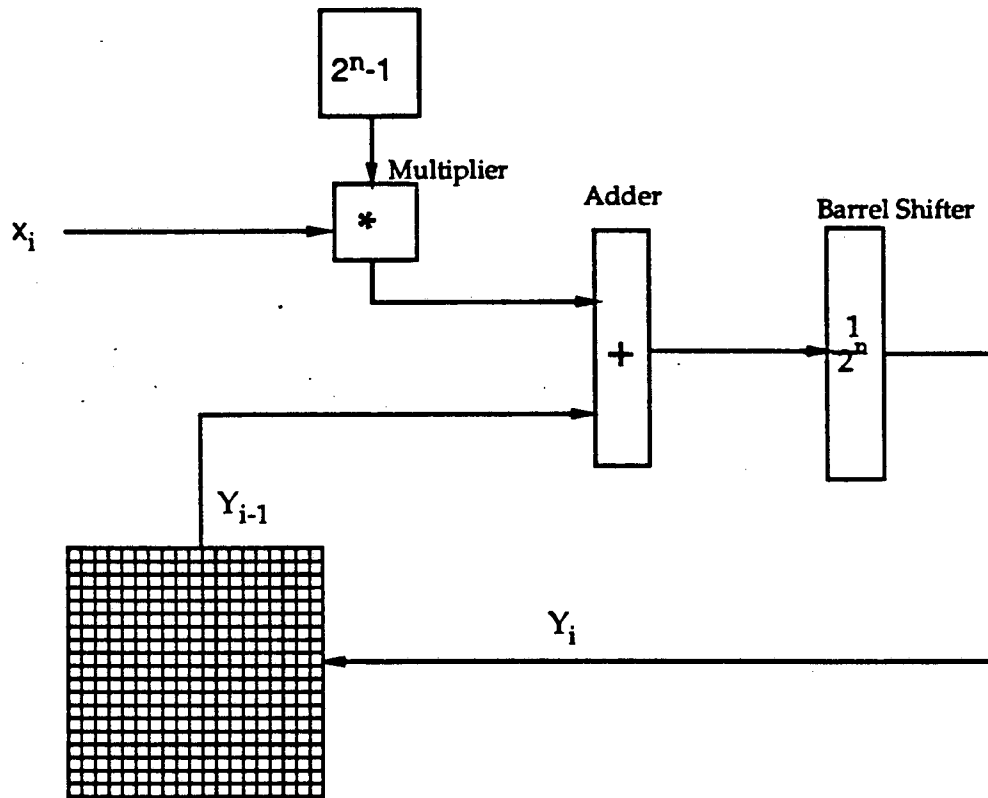
The recursive average or running average is often used in image enhancement since it provides a continuously viewable image. The image on the screen y_i can be written in terms of the incoming image x_i and the previous image on the screen y_{i-1} in the following way:

$$Y_i = \alpha X_i + (1-\alpha)Y_{i-1} \quad 0 \leq \alpha \leq 1 \quad \text{A1}$$

Usually the coefficient α is written as $1/2^n$ since a division by 2^n is easily accomplished by shifting each pixel in the image down by n bits. One way to write the above expression is now:

$$[(2^n - 1)Y_{i-1} + X_i] / 2^n \quad \text{A2}$$

Thus the above operation could be carried out by the following sequence:



There are ways to rewrite eq. A1 such that the sequence of the multiplier, adder and shifter would be different, but the hardware should be capable of implementing equation A1 in a frame time for proper recursive averaging. Attention also needs to be paid to the number of bits representing each pixel at every step of the calculation in order to ensure enough accuracy in the result.

Appendix B

Sources of Hardware and Software referred to in text

Hardware

Apollo Workstations	Hewlett Packard, 3000 Hanover St., Palo Alto, CA 94303, USA (415-857-1501)
CSPI Array Processors	CSPI 40 Linnell Circle, MA 01821, USA (508-272-6020)
Chorus ComputeServer	Human Devices, Inc. 100 Varick St. NYC, NY 10013, USA (212-925-1715)
Data Translation Image Proc.	Data Translation, Inc. 100 Locke Drive, Marlboro, MA 01752, USA (508-481-3700)
FPS Array Processors	Floating Point Systems, Inc. P.O. Box 23489, Portland Oregon 97223 (800-547-1445)
IBM Computers	IBM Corporation, Old Orchard Rd. Armonk, NY 10504, USA (914-765-1900)
Imagine Image Processor	Synoptics Ltd. 15, The Innovation Centre, Cambridge Science Park, Milton Road, Cambridge, CB4 4BN England (44-223-863223)
Imaging Tech. Image Proc.	Imaging Technology, Inc. 600 W. Cummings Park, Woburn, MA 01801, USA (508-938-8444)
Macintosh Computers	Apple Computer, 20525 Mariani Ave., Cupertino, CA 95014 USA (408-996-1010)
MaxVideo Image Processor	Datacube Inc., 4 Dearborn Road, Peabody, MA 01960, USA (508-535-6644)
MicroVax and Vax Computers	Digital Equipment Corporation, 146 Main Street, Maynard, MA 01754-2571
Next	Next Inc. 3475 Deer Creek Rd. Palo Alto, CA 94304 USA (415-424-8500)
NuVision Image Processor	Perceptics Corporation Pellissippi Center P.O. Box 22991, Knoxville, TN 37933, USA (615-966-9200)
Silicon Graphics Workstations SKY Warrior, Vortex APs	Silicon Graphics SKY Computers, Inc. Foot of John Street, Lowell, MA 01852, USA (508-454-6200)
Sun Workstations	Sun Microsystems, Inc. 2550 Garcia Ave., Mountain View, CA 94043, USA (415-960-1300)
Temdips	H.R. Tietz, Herbststr. 7, D-8035 Gauting, West Germany (089-8506567)
Zip3200/Mc3200 Array Processors	Mercury Computer Inc. 600 Suffolk Street, Lowell. MA 018543, USA (508-458-3100)

Software

Ems	Pierre Stadelmann, I2M-EPFL, Swiss Federal Institute of Technology, CH-1015 Lausanne, Switzerland.
MacTempas	Total Resolution, 20 Florida Ave., Berkeley, CA 94707, USA
Ncemss	Managing Director, NCEM/MCSD, Lawrence Berkeley Laboratory, Berkeley, CA 94720, USA
NuVision	Perceptics Corporation (see address above)
Semper	Synoptics Inc, (see address above)
Shrli	Total Resolution (see address above)
Ultimage	GTFS Inc. 2455 Bennett Valley Rd, #100C Santa Rosa, CA 95404, USA (707-579-1733)
VxWorks	Wind River Systems 1351 Ocean Ave., Emeryville, CA 94608 (415-428-2623)

General Mac II Image Analysis Systems

Image	Wayne Rasband, National Institutes of Health, Bldg 36, Room 2A-03 Bethesda, MD 20892, USA
Image Analyst	Automatix, 1000 Tech Park Drive, Billerica, MA 01821, USA (505-667-7900)
Prism Image Analysis System	Dapple Systems, Inc. 355 West Olive Ave. Sunnyvale, CA 94086, USA (408-733-3283)
RIMS (Report and Image Management Systems)	MIPS - Medical Image Processing Specialists 6087 Jackson Rd. Ann Arbor, MI 48103, USA (313-655-5400)

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6. This work is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division, U. S. Department of Energy under Contract DE-AC03-76SF00098

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