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LINEAR ALGEBRA ON HIGH-PERFORMANCE COMPUTERS

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Linear Algebra on High-Performance Computers*

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ABSTRACT

This paper surveys work recently done at Argonne National Laboratory in an attempt to discover ways to construct numerical software for high-performance computers. The numerical algorithms are taken from several areas of numerical linear algebra. We discuss certain architectural features of advanced-computer architectures that will affect the design of algorithms. The technique of restructuring algorithms in terms of certain modules is reviewed. This technique has proved successful in obtaining a high level of transportability without severe loss of performance on a wide variety of both vector and parallel computers.

The module technique is demonstrably effective for dense linear algebra problems. However, in the case of sparse and structured problems it may be difficult to identify general modules that will be as effective. New algorithms have been devised for certain problems in this category. We present examples in three important areas: banded systems, sparse *QR* factorization, and symmetric eigenvalue problems.

1. Introduction

This paper surveys work recently done at Argonne National Laboratory in an attempt to discover ways to construct numerical software for high-performance computers. We have focused on numerical linear algebra problems involving dense matrices since the algorithms for these problems are well understood in most cases. This focus has allowed us to concentrate on utilization of the new hardware rather than on development of new algorithms for many of the standard problems. Nevertheless, there are instances when efficient use of the architecture begs for new algorithms, and we give examples of such instances here.

Within the last ten years many who work on the development of numerical algorithms have come to realize the need to get directly involved in the software development process. Issues such as robustness, ease of use, and portability are now standard in any discussion of numerical algorithm design and implementation. New and exotic architectures are evolving that

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depend on the technology of concurrent processing, shared memory, pipelining, and vector components to increase performance capabilities. Within this new computing environment the portability issue, in particular, can be very challenging. To exploit these new capabilities, one feels compelled to structure algorithms that are tuned to particular hardware features, yet the sheer number of different machines appearing makes this approach intractable. It is tempting to assume that an unavoidable by-product of portability will be an unacceptable degradation in performance on any specific machine architecture. Nevertheless, we contend that it is possible to achieve a reasonable fraction of the performance on a wide variety of different architectures through the use of certain programming constructs.

Complete portability is an impossible goal at this time, but a level of transportability can be achieved through the isolation of machine-dependent code within certain modules. Such an approach is essential, in our view, even to begin to address the portability problem. To illustrate the immensity of the problem, we list in Table 1 thirty-three commercial high-performance computers. Most of these machines are already in use; all are projected to be available in 1986. They are categorized here with respect to the levels of parallelism they exploit and with respect to their memory access schemes. It is particularly noteworthy that each of the parallel machines offers different synchronization schemes with different software primitives used to invoke synchronization.

2. Advanced Computer Architectures

The machines listed above are representative implementations of advanced computer architectures. Such architectures involve various aspects of vector, parallel, and parallel-vector capabilities. These notions and their implications on the design of software are discussed briefly in this section. We begin with the most basic: vector computers.

The current generation of vector computers exploit several advanced concepts to enhance their performance over conventional computers:

- Fast cycle time,
- Vector instructions to reduce the number of instructions interpreted,
- Pipelining to utilize a functional unit fully and to deliver one result per cycle,
- Chaining to overlap functional unit execution, and
- Overlapping to execute more than one independent vector instruction concurrently.

Table 1

High-Performance Computers

scalar parallel pipelined microcoded	parallel - global memory
FPS 164	Elxsi
FPS 264	Encore
STAR ST-100	Flex
	IP1
	Sequent
vector	Denelcor HEP
CDC CYBER 205	
American Supercomputer	parallel - global memory - vector
CRAY-1	
CRAY X-MP-1	ETA 10
Fujitsu VP (Amdahl 1000)	Alliant FX/8
Galaxy YH-1	CRAY-2
Hitachi S-810	CRAY-3
NEC SX	CRAY X-MP-2/4
Scientific Computer Systems	
Alliant FX/1	
Convex C-1	
parallel - local memory	
Ametek	
Intel iPSC	
NCUBE	
Connection Machine	
BBN Butterfly	
CDC Cyberplus	
Myrias 4000	
ICL DAP	
Loral Instruments	

Current vector computers typically provide for "simultaneous" execution of a number of elementwise operations through pipelining. Pipelining generally takes the approach of splitting the function into smaller pieces or stages and allocating separate hardware to each of these stages. With this mechanism several instances of the same operation may be executed simultaneously, with each instance being in a different stage of the operation.

The goal of pipelined functional units is clearly performance. After some initial startup time, which depends on the number of stages (called the length of the pipeline, or pipe length), the functional unit can turn out one result per clock period as long as a new pair of operands is supplied to the first stage every clock period. Thus, the rate is independent of the length of the pipeline and depends only on the rate at which operands are fed into the pipeline. Therefore, if two vectors of length k are to be added, and if the floating-point adder requires 3 clock periods to complete, it would take $3 + k$ clock periods to add the two vectors together, as opposed to $3 * k$ clock periods in a conventional computer.

Another feature used to achieve high rates of execution is chaining. *Chaining* is a technique whereby the output register of one vector instruction is the same as one of the input registers for the next vector instruction. If the instructions use separate functional units, the hardware will start the second vector operation during the clock period when the first result from the first operation is just leaving its functional unit. A copy of the result is forwarded directly to the second functional unit, and the first execution of the second vector is started. The net result is that the execution of both vector operations takes only the second functional unit startup time longer than the first vector operation. The effect is like having a new instruction that performs the combined operations of the two functional units chained together. On the CRAY, in addition to the arithmetic operations, vector loads from memory to vector registers can be chained with other arithmetic operations.

It is also possible to overlap operations if the two operations are independent. If an addition and an independent multiplication operation are to be processed, the execution of the second independent operation will begin one cycle after the first operation has started.

The key to utilizing a high-performance computer effectively is to avoid unnecessary memory references. In most computers data flows from memory into and out of registers, and from registers into and out of functional units, which perform the given instructions on the data. Performance of algorithms can be dominated by the amount of memory traffic, rather than the number of floating-point operations involved. The movement of data between memory and registers can be as costly as arithmetic operations on the data. This situation provides considerable motivation to restructure existing algorithms and to devise new algorithms that minimize data movement.

Many of the algorithms in linear algebra can be expressed in terms of a SAXPY operation, $y \leftarrow y+\alpha x$, i.e., adding a multiple α of a vector x to another vector y. This would result in three vector memory references for each two vector floating-point operations. If this operation comprises the body of an inner loop that updates the same vector y many times, then a considerable amount of unnecessary data movement will occur. Usually, a SAXPY occurring in an inner loop will indicate that the algorithm may be recast in terms of some matrix vector operation, such as $y \leftarrow y+M*x$, which is just a sequence of SAXPYs involving the columns of the matrix M and the corresponding components of the vector x. The advantage of this is that the y vector and the length of the columns of M are a fixed size throughout. Thus, it is relatively easy to automatically recognize that only the columns of M need be moved into registers while accumulating the result y in a vector register, avoiding two of the three memory references in the innermost loop. This also allows chaining to occur on vector machines, and results in a factor of three increase in performance on the CRAY-1. The cost of the algorithm in these cases is determined not by floating-point operations, but by memory references.

Programs that properly use all of the features mentioned above will fully exploit the potential of a vector machine. These features, when used to varying degrees, give rise to three basic modes of execution: scalar, vector, and super-vector [4]. To provide a feeling for the difference in the modes, we give in Table 2 the execution rates on a CRAY-1:

Table 2

Execution Rates on a CRAY-1

Mode of Execution	Rate of Execution
Scalar	0-10 MFLOPS
Vector	10-50 MFLOPS
Super-Vector	50-160 MFLOPS

These rates represent, more or less, the upper end of their range. We define the term MFLOPS to be a rate of execution representing millions of floating point operations (additions or multiplications) performed per second.

The basic difference between scalar and vector performance is the use of vector instructions. The difference between vector and super-vector performance hinges on avoiding unnecessary movement of data between vector registers and memory. The CRAY-1 is limited in the sense that there is only one path between memory and the vector registers. This creates a bottlen ^k if a program loads a vector from memory, performs some arithmetic operations, and then stores the results. While the load and arithmetic can proceed simultaneously as a chained operation, the store is not started until that chained operation is fully completed.

Most algorithms in linear algebra can be easily vectorized. However, to gain the most out of a machine like the CRAY-1, such vectorization is usually not enough. For top performance, the scope of the vectorization must be expanded to facilitate chaining and minimization of data movement in addition to using vector operations. Recasting the algorithms in terms of matrix-vector operations makes it easy for a vectorizing compiler to achieve these goals. This is primarily due to the fact that the results of the operation can be retained in a register and need not be stored back to memory, thus eliminating the bottleneck. Moreover, when the compiler is not successful, it is reasonable to hand tune these operations, perhaps in assembly language, since there are so few of them and since they involve simple operations on regular data structures. These modules and their use in recasting algorithms for linear algebra are discussed in detail in the next section. The resulting codes achieve super-vector performance levels on a wide variety of vector architectures. Moreover, the modules have also proved effective on parallel architectures.

Vector architectures exploit parallelism at the lowest level of computation. They require very regular data structures (i.e., rectangular arrays) and large amounts of computation to be effective. The next level of parallelism that may be effective is to have individual scalar processors execute serial instruction streams simultaneously on a shared data structure. A typical example would be the simultaneous execution of a loop body for various values of the loop index. This is the capability provided by a parallel processor. Unfortunately, along with this increased functionality comes a burden. If independent processors are to work together on the same computation, they must be able to communicate partial results to each other, and this requires a synchronization mechanism. Synchronization introduces overhead (in terms of machine use) that is unrelated to the primary computation. It also requires new programming techniques that are not well understood at the moment. While this situation is obviously more general than that of a vector processor, many of the same principles apply.

Typically, a parallel processor with globally shared memory must employ some sort of interconnection network so that all processors may access all of the shared memory. There must also be an arbitration mechanism within this memory access scheme to handle cases where two processors attempt to access the same memory location at the same time. These two requirements obviously have the effect of increasing the memory access time over that of a single processor accessing a dedicated memory of the same type. Usually, the increase is substantial, especially if the processor and memory are at the high end of the performance spectrum.

Again, memory access and data movement dominate the computations in these machines. Achieving near-peak performance on such computers relies upon the same principle. One must devise algorithms that minimize data movement and reuse data that has been moved from globally shared memory to local processor memory. The effects of efficient data management on the performance of a parallel processor can be dramatic. For example, performance of the Denelcor HEP computer may be increased by a factor of 10 through efficient use of its very large (2-Kword) register set [31]. The modules again aid in accomplishing this memory management. Moreover, they provide a way to make effective use of the parallel processing capabilities in a manner that is transparent to the software user. Thus, the user does not need to wrestle with the problems of synchronization to use the parallel processor effectively.

The two types of parallelism we have just discussed are combined when vector rather than serial processors are used to construct a parallel computer. These machines are able to execute independent loop bodies that employ vector instructions. The most powerful computers today are of this type; they include the CRAY X-MP line and a new, high-performance "mini-super" FX/8 computer manufactured by Alliant. The problems with using such computers efficiently are, of course, more complex than those encountered with each type individually: synchronization overhead becomes more significant when compared to a vector operation rather than a scalar operation, blocking loops to exploit outer-level parallelism may conflict with vector length, etc.

Finally, a third level of complication is added when parallel-vector machines are interconnected to achieve yet another level of parallelism. This is the case for the CEDAR architecture being developed at the Center for Supercomputer Research and Development at the University of Illinois at Urbana. Such a computer is intended to solve large applications problems that split naturally into loosely coupled parts which may be solved efficiently on the *cluster* of parallel-vector processors.

3. Performance of Software for Dense Matrix Factorization

We are interested in examining the performance of linear algebra algorithms on large-scale scientific vector processors and on emerging parallel processors. In many applications, linear algebra calculations consume large quantities of computer time. If substantial improvements can be found for the linear algebra part, a significant reduction in the overall performance will be realized. We are motivated to look for alternative formulations of standard algorithms, as implemented in software packages such as LINPACK [8] and EISPACK [12, 29], because of their wide use in general and their poor performance on vector computers. As mentioned earlier, we are also motivated to restructure the algorithms in a way that will allow these packages to be easily transported to new computers of radically different design, provided this can be achieved without serious loss of efficiency.

In this section we report on some experience with restructuring these linear algebra packages in terms of the high-level modules proposed by Dongarra et al. [6]. This experience verifies that performance increases are achieved on vector machines and that the modular approach offers a viable solution to the transportability issue. Restructuring often improves performance on conventional computers and does not degrade the performance on any computer we are aware of.

Both of the packages have been designed in a portable, robust fashion, so they will run in any Fortran environment. The LINPACK routines use a set of vector subprograms called the BLAS [22] to carry out most of the arithmetic operations. The EISPACK routines do not explicitly refer to vector routines, but the routines do have a high percentage of vector operations which most vectorizing compilers detect. The routines from both packages should be well suited for execution on vector computers. As we shall see, however, the Fortran programs from LINPACK and EISPACK do not attain the highest execution rate possible on a CRAY-1 [4]. Although these programs exhibit a high degree of vectorization, the construction that leads to super-vector performance is, in most cases, not present. We shall examine how the algorithms can be constructed and modified to enhance performance without sacrificing clarity or resorting to assembly language.

To give a feeling for the difference between various computers, both vector and conventional, Dongarra [4] carried out a timing study on many different computers for the solution of a 100×100 system of equations. The LINPACK routines were used in the solution without modification. The results are shown in Table 3.

The LINPACK routines used to generate the timings in Table 3 do not reflect the true performance of "high-performance computers." A different implementation of the solution of linear equations, presented in a report by Dongarra and Eisenstat [7], better reflects the performance on such machines. That implementation is based on matrix-vector operations rather than just vector operations. The restructuring allows the various compilers to take advantage of the features described in Section 2. It is important to note that the numerical properties of the algorithm have not been altered by this restructuring. The number of floating-point operations required and the roundoff errors produced by both algorithms are exactly the same; only the way in which the matrix elements are accessed is different.

The results are shown in Table 4. As before, a Fortran program was used, and all runs were for full precision. The table shows the time to complete the solution of equations for a matrix of order 300.

Table 3

Solving a System of Linear Equations with LINPACK[a] in Full Precision [b]

Computer	OS/Compiler[c]	Ratio[d]	MFLOPS[e]	Time, s
CRAY X-MP-1	CFT (Coded BLAS)	.36	33	.021
CDC CYBER 205	FTN (Coded BLAS)	.48	25	.027
CRAY 1-S	CFT (Coded BLAS)	.54	23	.030
CRAY X-MP-1	CFT (Rolled BLAS)	.57	21	.032
Fujitsu VP-200	Fortran 77 (Comp. Directive)	.64	19	.040
Fujitsu VP-200	Fortran 77 (Rolled BLAS)	.72	17	.040
Hitachi S-810/20	FORT77/HAP (Rolled BLAS)	.74	17	.042
CRAY 1-S	CFT (Rolled BLAS)	1	12	.056
CDC CYBER 205	FTN (Rolled BLAS)	1.5	8.4	.082
NAS 9060 w/VPF	VS opt=2 (Coded BLAS)	1.8	6.8	.101

[a] LINPACK routines *SGEFA* and *SGESL* were used for single precision, and routines *DGEFA* and *DGESL* were used for double precision. These routines perform standard *LU* decomposition with partial pivoting and back substitution.

[b]*Full Precision* implies the use of (approximately) 64-bit arithmetic, e.g., CDC single precision or IBM double precision.

[c]*OS/Compiler* refers to the operating system and compiler used: (*Coded BLAS*) refers to the use of assembly language coding of the BLAS; (*Rolled BLAS*) refers to a Fortran version with single-statement, simple loops; and *Comp. Directive* refers to the use of compiler directives to set the maximum vector length.

[d]*Ratio* is the number of times faster or slower a particular machine configuration is when compared to the CRAY 1-S using Fortran coding for the BLAS.

[e] For solving a system of n equations, approximately $2/3n^3 + 2n^2$ operations are performed (we count both additions and multiplications).

Table 4

Solving a System of Linear Equations Using the Vector Unrolling Technique

Computer	OS/Compiler	MFLOPS	Time, s
CRAY X-MP-4 [a]	CFT (Coded ISAMAX)	356	.051
CRAY X-MP-2 [b]	CFT (Coded ISAMAX)	257	.076
Fujitsu VP-200	Fortran 77 (Comp. Directive)	220	.083
Fujitsu VP-200	Fortran 77	183	.099
CRAY X-MP-2 [b]	CFT	161	.113
Hitachi S-810/20	FORT77/HAP	158	.115
CRAY X-MP-1 [c]	CFT (Coded ISAMAX)	134	.136
CRAY X-MP-1 [c]	CFT	106	.172
CRAY 1-M	CFT (Coded ISAMAX)	83	.215
CRAY 1-S	CFT (Coded ISAMAX)	76	.236
CRAY 1-M	CFT	69	.259
CRAY 1-S	CFT	66	.273
CDC CYBER 205	ftn 200 opt=1	31	.59
NAS 9060 w/VPF	VS opt=2 (Coded BLAS)	9.7	1.9

[a] These timings are for four processors, with manual changes to use parallel features.

[b] These timings are for two processors, with manual changes to use parallel features.

[c] These timings are for one processor.

Similar techniques of recasting matrix decomposition algorithms in terms of matrix-vector operations have provided significant improvements in the performance of algorithms for the eigenvalue problem. In a paper by Dongarra, Kaufman, and Hammarling [8] many of the routines in the EISPACK collection were restructured to use matrix-vector primitives, resulting in improvements by a factor of two to three in performance over the standard implementation on vector computers such as CRAY X-MP, Hitachi S-810/20, and Fujitsu VP-200.

Using the matrix-vector operations as primitives in constructing algorithms can also play an important role in achieving performance on multiprocessor systems with minimal recoding effort. Again, the recoding is restricted to the relatively simple modules, and the numerical properties of the algorithms are not altered as the codes are retargeted for a new machine. This feature takes on added importance as the complexity of the algoritnms reach the level required for some of the more difficult eigenvalue calculations. A number of factors influence the performance of an algorithm in multiprocessing. These include the degree of parallelism, process synchronization overhead, load balancing, interprocessor memory contention, and modifications needed to separate the parallel parts of an algorithm.

To exploit the computational advantages offered by a parallel computer, a parallel algorithm must partition the work into tasks, or processes, that can execute concurrently. These cooperating processes usually have to communicate with each other, to claim a unique identifier or follow data dependency rules, for example. Communication takes place at synchronization points within the instruction streams defining the process. The amount of work in terms of number of instructions that may be performed between synchronization points is referred to as the granularity of a task. The need to synchronize and to communicate before and after parallel work will greatly affect the overall execution time of the program. Since the processors have to wait for one another instead of doing useful computation, it is obviously better to minimize that overhead. In the situation where segments of parallel code are executing in vector mode, typically at ten to twenty times the speed of scalar mode, granularity becomes an even more important issue, since communication mechanisms are implemented in scalar mode.

Granularity is also closely related to the degree of parallelism, which is defined to be the percentage of time spent in the parallel portion of the code. Typically, a small-granularity job means that parallelism occurs in an inner-loop level (although not necessarily the innermost loop). In this case, even the setup time in outer loops will become significant (not to mention the frequent task synchronization needs).

Matrix-vector operations offer the proper level of modularity for achieving both performance and transportability across a wide range of computer architectures. Evidence has already been given for a variety of vector architectures. In the following sections, we shall present evidence supporting their suitability for parallel architectures.

In addition to computational evidence, several factors support the use of these modules. First, we can easily construct the standard algorithms in linear algebra out of these types of modules. Also, the matrix-vector operations are simple and yet encompass enough computation that they can be vectorized and also parallelized at a reasonable level of granularity [4, 7, 10, 31]. Finally, the modules can be constructed in such a way that they hide all of the machine-specific intrinsics required to invoke parallel computation, thereby shielding the user from being concerned with any machine-specific changes to the library.

4. Structure of the Algorithms

In this section we discuss the way algorithms may be restructured to take advantage of the modules introduced above. Typical recasting that occurs within LINPACK and EISPACK subroutines is discussed here. We begin with definitions and a description of the efficient implementation of the modules themselves.

4.1 The Modules

Only three modules are required for recasting LINPACK in a way that achieves super-vector performance.

$$z = Mw \qquad (\textit{matrix} \times \textit{vector}),$$

$$\hat{M} = M - wz^T \qquad (\textit{rank one modification}), \text{ and}$$

$$z = Tz \qquad (\textit{solve a triangular system}).$$

Efficient coding of these three routines is all that is needed to transport the entire package from one machine to another while retaining close to top performance.

We shall describe some of the considerations that are important when coding the matrix-vector product module. The other modules require similar techniques. For a vector machine such as the CRAY-1, the vector times matrix operation should be coded in the form

(4.1.1) $$y(*) \leftarrow y(*) + M(*,j)x(j) \quad \text{for } j = 1,2,\ldots,n \;.$$

In (4.1.1) the * in the first entry implies this is a column operation. The intent here is that a vector register is reserved for the result while the columns of M are successively read into vector registers, multiplied by the corresponding component of x, and then added to the result register in place. In terms of ratios of data movement to floating-point operations, this arrangement is most favorable: it involves one vector move for two vector floating-point operations (compared to the three vector moves needed to get the same two floating-point operations when a sequence of SAXPY operations are used).

This arrangement is perhaps inappropriate for a parallel machine because one would have to synchronize the access to y by each of the processes, and this would cause busy waiting to occur. One might do better to partition the vector y and the rows of the matrix M into blocks

$$\begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_k \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_k \end{bmatrix} + \begin{bmatrix} M_1 \\ M_2 \\ \cdot \\ \cdot \\ \cdot \\ M_k \end{bmatrix} x$$

and self-schedule individual vector operations on each of the blocks in parallel:

$$y_i \leftarrow y_i + M_i x \quad \text{for } i = 1,2,\ldots,k \;.$$

That is, the subproblem indexed by i is picked up by a processor as it becomes available, and the entire matrix-vector product is reported done when all of these subproblems have been completed.

If the parallel machine has vector capabilities on each of the processors, this partitioning introduces short vectors and defeats the potential of the vector capabilities for small- to medium-size matrices. A better way to partition in this case is

$$y \leftarrow y + (M_1 , M_2 , \cdots , M_k) \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_k \end{bmatrix} .$$

Again, subproblems are computed by individual processors. However, in this scheme, we must either synchronize the contribution of adding in each term $M_i x_i$ or write each of these into temporary locations and hold them until all are complete before adding them to get the final result. This scheme does prove to be effective for increasing the performance of the factorization subroutines on the smaller (order less than 100) matrices. From the data access scheme for *LU* decomposition shown in Figure 4.1, we see that during the final stages of the factorization, vector lengths become short regardless of matrix size. For the smaller matrices, subproblems with vector lengths that are below a certain performance level represent a larger percentage of the calculation. This problem is magnified when the row-wise partitioning is used.

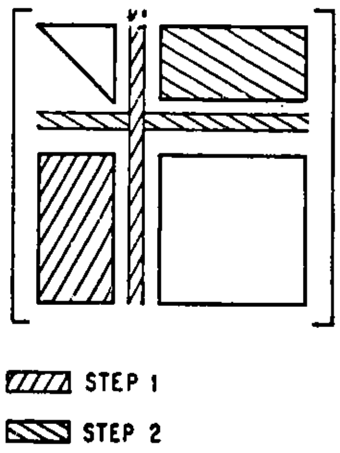


Figure 4.1 *LU* Data References

4.2 Recasting LINPACK Subroutines

We now turn to some examples of how to use the modules to obtain various standard matrix factorizations. We begin with the *LU* decomposition of a general nonsingular matrix. Restructuring the algorithm in terms of the basic modules described above is not so obvious in the case of *LU* decomposition. The approach described here is inspired by the work of Fong and Jordan [11], who produced an assembly language code for *LU* decomposition for the CRAY-1. That code differed significantly in structure from those commonly in use because it did not modify the entire *k*-th reduced submatrix at each step but only the *k*-th column of that matrix. This step was essentially a matrix-vector multiplication operation.

Dongarra and Eisenstat [4] showed how to restructure the Fong and Jordan implementation explicitly in terms of matrix-vector operations and were able to achieve nearly the same performance from a Fortran code as Fong and Jordan had done with their assembly language implementation. The pattern of data references for factoring a square matrix A into $PA = LU$ (with P a permutation matrix, L a unit lower triangular, and U an upper triangular) is shown in Figure 4.1. At the k-th step of this algorithm, a matrix formed from columns 1 through k–1 and rows k through n is multiplied by a vector constructed from the k-th column, rows 1 through k–1, with the results added to the k-th column, rows k through n. The second part of the k-th step involves a vector-matrix product, where the vector is constructed from the k-th row, columns 1 through k–1, and a matrix constructed from rows 1 through k–1 and columns k+1 through n, with the results added to the k-th row, columns k+1 through n.

One can construct the factorization by analyzing the way in which the various pieces of the factorization interact. Let us consider decomposition of the matrix A into its LU factorization, with the matrix partitioned in the following way:

$$\begin{bmatrix} L_{11} & & \\ l_{21}^T & 1 & \\ L_{31} & l_{32} & L_{33} \end{bmatrix} \begin{bmatrix} U_{11} & u_{12} & U_{13} \\ & u_{22} & u_{23}^T \\ & & U_{33} \end{bmatrix}.$$

Multiplying L and U together and equating terms with A, we have

$$\begin{array}{lll} A_{11} = L_{11}U_{11} & a_{12} = L_{11}u_{12} & A_{13} = L_{11}U_{13} \\ a_{12}^T = l_{21}^T U_{11} & a_{22} = l_{21}^T u_{12} + u_{22} & a_{23}^T = l_{21}^T U_{13} + u_{23}^T \\ A_{31} = L_{31}U_{11} & a_{32} = L_{31}u_{12} + u_{22}l_{32} & A_{33} = L_{31}U_{13} + l_{32}u_{23}^T + L_{33}U_{33} \end{array}$$

We can now construct the various factorizations for LU decomposition by determining how to form the unknown parts of L and U, given various parts of A, L, and U. For example,

> Given the triangular matrices L_{11} and U_{11}, to construct vectors l_{12}^T and u_{12} and scalar u_{22} we must form $u_{12} = L_{11}^{-1}a_{12}$, $l_{21}^T = U_{11}^{-1}a_{12}^T$, $u_{22} = a_{22} - l_{21}^T u_{12}$.

Since these operations deal with triangular matrix L_{11} and U_{11}, they can be expressed in terms of solving triangular systems of equations.

> Given the rectangular matrices L_{31} and U_{13}, and the vectors l_{21}^T and u_{12}, we can form vectors l_{32} and u_{23}^T and scalar u_{22} by forming $u_{23} = a_{23}^T - l_{21}^T U_{13}$, $u_{22} = a_{22} - l_{21}^T u_{12}$, and $l_{32} = (a_{23} - L_{31}u_{12})/u_{22}$,

Since these operations deal with rectangular matrices and vectors, they can be expressed in terms of simple matrix-vector operations.

> Given the triangular matrix L_{11}, the rectangular matrix L_{31}, and the vector l_{21}^T, we can construct vectors u_{12} and l_{32} and scalar u_{22} by forming $u_{12} = L_{11}^{-1} a_{12}$, $u_{22} = a_{22} - l_{21}^T u_{12}$, $l_{32} = (a_{32} - L_{31} u_{12})/u_{22}$.

These operations deal with a triangular solve and a matrix-vector multiply.

The same ideas for use of high-level modules can be applied to other algorithms, including matrix multiply, Cholesky decomposition, and QR factorization.

For the Cholesky decomposition the matrix is symmetric and positive definite. The factorization is of the form

$$A = LL^T \ ,$$

where $A = A^T$ and is positive definite. If we assume the algorithm proceeds as in LU decomposition, but references only the lower triangular part of the matrix, we have an algorithm based on matrix-vector operations that accomplishes the desired factorization.

The final method we shall discuss is the QR factorization using Householder transformations. Given a real $m{\times}n$ matrix A, the routine must produce an $m{\times}m$ orthogonal matrix Q and an $n{\times}n$ upper triangular matrix R such that

$$A = Q\begin{bmatrix} R \\ 0 \end{bmatrix} .$$

Householder's method consists of constructing a sequence of transformations of the form

$$(4.2.1) \qquad I - \alpha w w^T, \ \text{ where } \alpha\, w^T w = 2.$$

The vector w is constructed to transform the first column of a given matrix into a multiple of the first coordinate vector e_1. At the k-th stage of the algorithm one has

$$Q_{k-1}^T A = \begin{bmatrix} R_{k-1} & S_{k-1} \\ 0 & A_{k-1} \end{bmatrix},$$

and w_k is constructed such that

$$(4.2.2) \qquad \left[I - \alpha_k w_k w_k^T \right] A_{k-1} = \begin{bmatrix} \rho_k & s_k^T \\ 0 & A_k \end{bmatrix} .$$

The factorization is then updated to the form

$$Q_k^T A = \begin{bmatrix} R_k & S_k \\ 0 & A_k \end{bmatrix},$$

with

$$Q_k^T = \begin{bmatrix} I & 0 \\ 0 & I - \alpha_k w_k w_k^T \end{bmatrix} Q_{k-1}^T .$$

However, this product is not explicitly formed, since it is available in product form if we simply record the vectors w in place of the columns they have been used to annihilate. This is the basic algorithm used in LINPACK [5] for computing the QR factorization of a matrix.

The algorithm may be coded in terms of two of the modules. To see this, note that the operation of applying a transformation shown on the left-hand side of (4.2.2) above may be broken into two steps:

(4.2.3) $$z^T = w^T A \qquad (\textit{vector} \times \textit{matrix})$$

and

$$\hat{A} = A - \alpha w z^T \qquad (\textit{rank–one modification}).$$

4.3 Restructuring EISPACK Subroutines

As we have seen, all of the main routines of LINPACK can be expressed in terms of the three modules described in Section 4.1. The same type of restructuring may be used to obtain efficient performance from EISPACK subroutines. A detailed description may be found in Ref. 8. In the following discussion we outline some of the basic ideas used there.

Many of the algorithms implemented in EISPACK have the following form:

```
Algorithm (4.3.1):
For i = 1,....
   Generate matrix $T_i$
   Perform transformation $A_{i+1} \leftarrow T_i A_i T_i^{-1}$
End .
```

Because we are applying similarity transformations, the eigenvalues of A_{i+1} are those of A_i. Since the application of these similarity transformations represents the bulk of the work, it is important to have efficient methods for this operation. The main difference between this situation and that encountered with linear equations is that these transformations are applied from both sides. The transformation matrices T_i used in (4.3.1) are of different types depending on the particular algorithm.

The simplest are the stabilized elementary transformation matrices of the form $T = LP$, where P is a permutation matrix required to maintain numerical stability [12, 29, 32] and L has the form

$$\begin{bmatrix} 1 & & & & & \\ & \cdot & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & * & 1 & \\ & & & \cdot & & \cdot \\ & & & * & & & 1 \end{bmatrix}.$$

The inverse of L has the same structure as L and may be written in terms of a rank-one modification of the identity as follows:

$$L^{-1} = \begin{bmatrix} I & 0 \\ 0 & I - we_1^T \end{bmatrix},$$

with $e_1^T w = 0$. If we put

$$PAP^T = \begin{bmatrix} \hat{A} & B \\ C & D \end{bmatrix},$$

then

$$TAT^{-1} = \begin{bmatrix} I & 0 \\ 0 & I + we_1^T \end{bmatrix} \begin{bmatrix} \hat{A} & B \\ C & D \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & I - we_1^T \end{bmatrix}$$

$$= \begin{bmatrix} \hat{A} & B - b_1 w^T \\ C + wc_1^T & D + wd_1^T - f_1 w^T - \delta_{11} ww^T \end{bmatrix},$$

where $c_1^T = e_1^T C$, $d_1^T = e_1^T D$, $b_1 = Be_1$, $f_1 = De_1$, $\delta_{11} = d_1^T e_1$ and e_1 is the first coordinate vector (of appropriate size). The appropriate module to use, therefore, is the rank-one modification. However, more can be done with the rank-two correction that takes place in the modification of the matrix D above.

In most of the algorithms, the transformation matrices T_i are Householder matrices of the form (4.2.1). This results in a rank-two correction that might also be expressed as a sequence of two rank-one corrections. Thus, it would be straightforward to arrange the similarity transformation as two successive applications of the scheme (4.2.3). However, more can be done with a rank-two correction, as we now show.

First, suppose that we wish to form $(I-\alpha ww^T)A(I-\beta uu^T)$, where for a similarity transformation $\alpha = \beta$ and $w = u$. We may replace the two rank-one updates by a single rank-two update using the following algorithm:

```
Algorithm 4.3.2:
1. $v^T = w^T A$
2. $x = Au$
3. $y^T = v^T - (\beta w^T x) u^T$
4. Replace $A$ by $A - \beta x u^T - \alpha w y^T$
```

As a second example applicable to the linear equation setting, suppose that we wish to form $(I-\alpha ww^T)(I-\beta uu^T)A$. Then, as with Algorithm 4.3.2, we might proceed as follows:

```
Algorithm 4.3.3:
1. $v^T = w^T A$
2. $x^T = u^T A$
3. $y^T = v^T - (\beta w^T u) x^T$
4. Replace $A$ by $A - \beta u x^T - \alpha w y^T$
```

In both cases we can see that Steps 1 and 2 can be achieved by calls to the matrix-vector and vector-matrix modules. Step 3 is a simple vector operation, and Step 4 is now a rank-two correction, and one gets four vector memory references for each four vector floating-point operations (rather than three vector memory references for every two vector floating-point operations, as in Step 2 of Algorithm 4.2.3).

These techniques have been used successfully to increase the performance of EISPACK on various vector and parallel machines. The results of these modifications are reported in full detail in Ref. 8. Table 5 gives a typical example of the performance increase possible with these techniques.

5. Sparsity and Structured Problems

Modules work well for full dense-matrix problems, but different constructs may be needed for sparse or special structures. These constructs are likely to be specific to parallel machines, which typically cannot be based on the modules described above. We give three examples of such algorithms here. These algorithms all have portions that might take advantage of certain vector constructs, but the primary gain in all of them is through the explicit use of parallel computation. Each example has requirements for synchronization, and in some cases additional computation may be present that would not be needed for the serial algorithm. Nevertheless, all of these have proved effective in terms of speedup over the corresponding serial algorithm. One of the algorithms has actually proved faster than the corresponding serial code even when it is run on a serial machine.

Table 5

Comparison of EISPACK to the Matrix-Vector Version

Routine[a]	Order 50	100	Machine
ELMHES	1.5	2.2	CRAY-1
ORTHES	2.5	2.5	CRAY-1
ELMBAK	2.2	2.6	CRAY-1
ORTBAK	3.6	3.3	CRAY-1
TRED1	1.5	1.5	CRAY X-MP-1
TRBAK1	4.2	3.7	CRAY X-MP-1
TRED2	1.6	1.6	CRAY X-MP-1
SVD (no vectors)	1.7	2.0	Hitachi S-810/20
SVD (vectors)	1.6	1.7	Hitachi S-810/20
REDUC	1.8	2.2	Fujitsu VP-200
REBAK	4.4	5.8	Fujitsu VP-200

[a]All versions are in Fortran.

5.1 Banded Systems

An important structured problem that arises in many applications such as numerical solution of certain PDE problems is the solution of banded systems of linear equations. We consider algorithms for solving narrow-banded, diagonally dominant linear systems which are suitable for multiprocessors.

Let the linear system under consideration be denoted by

(5.1.1) $Ax = f$,

where A is a banded diagonally dominant matrix of order n. We assume that the number of superdiagonals $m \ll n$ is equal to the number of subdiagonals. On a sequential machine such a system would be solved with Gaussian elimination without pivoting, at a cost of $O(m^2n)$ arithmetic operations. We describe here an algorithm for solving this system on a multiprocessor of p processing units. Each unit may be a sequential machine, a vector machine, or an array of processors. In this paper, however, we consider only p sequential processing units.

Let the system (5.1.1) be partitioned into the block-tridiagonal form

(5.1.2)
$$\begin{bmatrix} A_1 & B_1 & & & \\ C_2 & A_2 & B_2 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & C_{p-1} & A_{p-1} & B_{p-1} \\ & & & C_p & A_p \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ f_{n-1} \\ f_n \end{bmatrix},$$

where A_i, $1 \le i \le p-1$, is a banded matrix of order $q = \lceil n/p \rceil$ and bandwidth $2m + 1$ (same as A),

(5.1.3a)
$$B_i = \begin{bmatrix} 0 & 0 \\ \hat{B}_i & 0 \end{bmatrix}, \quad 1 \le i \le p-1 ,$$

and

(5.1.3b)
$$C_{i+1} = \begin{bmatrix} 0 & \hat{C}_{i+1} \\ 0 & 0 \end{bmatrix},$$

in which $\hat{B}_i$ and $\hat{C}_{i+1}$ are lower and upper triangular matrices, respectively, each of order m. The algorithm consists of four stages.

5.1.1 Stage 1

Obtain the *LU* factorization

(5.1.4) $A_i = L_iU_i$, $\quad 1 \le i \le p$,

using Gaussian elimination without pivoting, one processor per factorization. Here L_i is unit lower triangular matrix, and U_i is a nonsingular upper triangular matrix. Note that each A_i is also diagonally dominant.

The cost of this stage is $O(m^2n/p)$ arithmetic operations; no interprocessor communication is required.

5.1.2 Stage 2

If we premultiply both sides of (5.1.2) by

$diag(A_1^{-1}, A_2^{-1}, \cdots, A_p^{-1})$, we obtain a system of the form

$$(5.1.5)\qquad \begin{bmatrix} I_q & E_1 & & & \\ F_2 & I_q & E_2 & & \\ & \cdot & \cdot & & \\ & & \cdot & \cdot & \\ & & F_{p-1} & I_q & E_{p-1} \\ & & & F_p & I_q \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ \cdot \\ \cdot \\ g_{n-1} \\ g_n \end{bmatrix},$$

where $E_i = (\hat{E}_i, 0)$, $F_i = (0,$ *F.if 1152>.5v .nr T.* $0_i)$, in which $\hat{E}_i$ and $\hat{F}_i$ are matrices of m columns given by

$$\hat{E}_i = A_i^{-1} \begin{bmatrix} 0 \\ \hat{B}_i \end{bmatrix}$$

and

$$\hat{F}_i = A_i^{-1} \begin{bmatrix} \hat{C}_i \\ 0 \end{bmatrix}$$

and will, in general, be full. In other words, $\hat{E}_i$, $\hat{F}_i$, and g_i are obtained by solving the linear systems

$$L_j U_j [\hat{F}_j, \hat{E}_j, g_j] = [\begin{bmatrix} 0 \\ \hat{B}_i \end{bmatrix}, \begin{bmatrix} \hat{C}_i \\ 0 \end{bmatrix}, f_i]$$

for $1 \le i \le p$; here, $\hat{C}_1 = 0$ and $\hat{B}_p = 0$. Each processor $2 \le k \le p-1$ handles $2m + 1$ linear systems of the form $L_k U_k v = r$, while processors 1 and p each handle $m+1$ linear systems of the same form.

The cost at this stage is $O(m^2 n/p)$ arithmetic operations; no interprocessor communications are needed.

5.1.3 Stage 3

Let $\hat{E}_i$ and $\hat{F}_i$ be partitioned, in turn, as follows:

$$\hat{F}_i = \begin{bmatrix} P_i \\ M_i \\ Q_i \end{bmatrix}, \text{ and } \hat{E}_i = \begin{bmatrix} S_i \\ N_i \\ T_i \end{bmatrix},$$

where P_i, Q_i, S_i, and $T_i \in R^{m \times m}$. Also, let g_i and x_i be conformally partitioned:

$$g_i = \begin{bmatrix} h_{2i-2} \\ w_i \\ h_{2i-1} \end{bmatrix}, \text{ and } x_i = \begin{bmatrix} y_{2i-2} \\ z_i \\ y_{2i-1} \end{bmatrix}.$$

As an illustration we show the system (5.1.5) for p=3.

$$
\left|\begin{array}{ccccccccc}
I_m & & & S_1 & & & & & \\
& I_v & & N_1 & & & & & \\
& & I_m & T_1 & & & & & \\
& & P_2 & I_m & & & S_2 & & \\
& & M_2 & & I_v & & N_2 & & \\
& & Q_2 & & & I_m & T_2 & & \\
& & & & & P_3 & I_m & & \\
& & & & & M_3 & & I_r & \\
& & & & & Q_3 & & & I_m
\end{array}\right|
\left|\begin{array}{c} y_0 \\ z_1 \\ y_1 \\ y_2 \\ z_2 \\ y_3 \\ y_4 \\ z_3 \\ y_5 \end{array}\right|
=
\left|\begin{array}{c} h_0 \\ w_1 \\ h_1 \\ h_2 \\ w_2 \\ h_3 \\ h_4 \\ w_3 \\ h_5 \end{array}\right|
$$

Observe that the unknown vectors y_1, y_2, y_3, and y_4 (each of order m) are disjoint from the rest of the unknowns. In other words, the m equations above and the m equations below each of the p–1 partitioning lines form an independent system of order $2m(p-1)$. We shall refer to this system as the "reduced system" Ky=h, which is of the form

$$
\left|\begin{array}{cccccccccc}
I_m & T_1 & 0 & 0 & & & & & & \\
P_2 & I_m & 0 & S_2 & & & & & & \\
Q_2 & 0 & I_m & T_2 & 0 & 0 & & & & \\
& & P_3 & I_m & 0 & S_3 & & & & \\
& & Q_3 & 0 & I_m & T_3 & & & & \\
& & & & P_4 & I_m & & & & \\
& & & & & & & & & \\
& & & & & & I_m & T_{p-2} & 0 & 0 \\
& & & & & & P_{p-1} & I_m & 0 & S_{p-1} \\
& & & & & & Q_{p-1} & 0 & I_m & T_{p-1} \\
& & & & & & & & P_p & I_m
\end{array}\right|
\left|\begin{array}{c} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ \cdot \\ y_{2p-5} \\ y_{2p-4} \\ y_{2p-3} \\ y_{2p-2} \end{array}\right|
=
\left|\begin{array}{c} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \\ \cdot \\ h_{2p-5} \\ h_{2p-4} \\ h_{2p-3} \\ h_{2p-2} \end{array}\right|
\qquad (5.1.6)
$$

The cost of the algorithm to be used for solving (5.1.6) depends on the interconnection network. Processor 1 contains T_1 and h_1; processor j, $2 \le j \le p-1$, contains P_j, Q_j, S_j, T_j, and h_{2j-2}, h_{2j-1}; and processor p contains P_p and h_{2p-2}. Hence, if the processors are linearly connected, we can only solve (5.1.6) sequentially at the cost of $O(m^3p)$ steps, where a step is the cost of an arithmetic operation or the cost of transmitting a floating-point number from one processor to either of its immediate neighbors. We should add here that since A is diagonally dominant, it can be shown that (5.1.6) is also diagonally dominant and hence can be solved with Gaussian elimination without pivoting.

5.1.4 Stage 4

Once the y_i's are obtained, with y_1 in processor 1, y_{2j-2} and y_{2j-1} in processor j $(2 \le j \le p-1)$, and y_{2p-2} in processor p, the rest of the components of the solution vector of (5.1.5) may be computed as follows. Processor k, $1 \le k \le p$, evaluates

(5.1.7) $$z_k = w_k - M_k y_{2k-3} - N_k y_{2k}$$

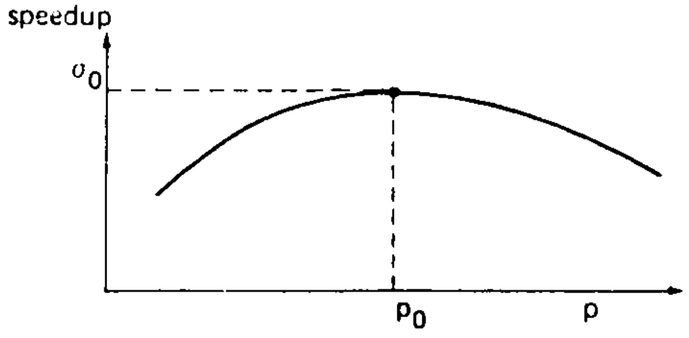
with processors 1 and p performing the additional tasks

$$y_0 = h_0 - S_1 y_2,$$

(5.1.8) $$y_{2p-1} = h_{2p-1} - Q_p y_{2p-3},$$

respectively (M_1 and N_p are nonexistent and are taken to be zero in this equation). The cost of this stage is $O(mn/p)$ steps, with no interprocessor communication.

For a linear array of processors, the speedup of this algorithm over the classical sequential algorithm behaves as follows:



where p_0 and σ_0 are $O(\sqrt{n/m})$. Stage 2 dominates the computation until p_0; then the communication costs affect the performance, and Stage 3 has a greater influence.

5.2 *QR* Factorization of a Sparse Matrix

The version of Householder's method for the *QR* factorization of a dense matrix given in Section 4.2 is well suited to vector and parallel-vector architectures. However, for parallel processors without vector capabilities, this may not be the algorithm of choice. An alternative is to use a parallel version of Givens method. There are many papers on this subject especially within the study of systolic arrays of processors [13, 14, 28]. Here we present a variant of these techniques that is suitable for parallel processors with far more computing power in a single processor than considered in the systolic array case. This method, first presented by Dongarra, Sameh, and Sorensen [9], is called the Pipelined Givens method.

The Pipelined Givens method is well suited to the architecture and synchronization mechanism of the Denelcor HEP computer. However, any parallel computer with globally shared memory and a relatively inexpensive synchronization primitive could take advantage of this method.

Two factors explain why this algorithm is more successful than Householder's method on such a parallel computer. As demonstrated by the computational results presented in Ref. 9, memory references play a far more important role in determining algorithm performance on a parallel machine such as the HEP than they do on serial machines. The Givens algorithm requires half as many array references as the Householder method. In addition, the Pipelined Givens method offers a greater opportunity to keep many (virtual) processors, busy because it does not employ a fork-join synchronization mechanism and does not have the inherent serial bottlenecks present in the Householder method. Moreover, there is an opportunity to adjust the level of granularity through the specification of a certain parameter (discussed below), to mask synchronization costs with computation.

The serial variant of the Givens method that we consider is as follows. Given a real $m \times n$ matrix A, the goal of the algorithm is to apply elementary plane rotations G_{ij} that are constructed to annihilate the ji-th element of the matrix A. Such a matrix may be thought of as a 2×2 orthogonal matrix of the form

$$G = \begin{bmatrix} \gamma & \sigma \\ -\sigma & \gamma \end{bmatrix},$$

where $\sigma^2 + \gamma^2 = 1$. If

$$\begin{bmatrix} \alpha & a^T \\ \beta & b^T \end{bmatrix}$$

represents a $2 \times n$ matrix, then, with proper choice of γ and σ, a zero can be introduced into the β position with left multiplication by G. When embedded in the $n \times n$ identity, the matrix G_{ij} is of the form

$$G_{ij} = I + D_{ij},$$

where all elements of D_{ij} are zero except possibly the ii, ij, ji, and jj entries. The matrices G_{ij} are used to reduce A to upper triangular form in the following order:

$$\left[G_{n,m} \cdots G_{2m} G_{1m}\right] \cdots \left[G_{n-1,n} \cdots G_{2n} G_{1n}\right]\left[G_{n-2,n-1} \cdots G_{2,n-1} G_{1,n-1}\right] \cdots \left[G_{12}\right] A = \begin{bmatrix} R \\ 0 \end{bmatrix}.$$

The order of the zeroing pattern may be seen in the 6×5 example:

$$\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\otimes_1 & \times & \times & \times & \times \\
\otimes_2 & \otimes_3 & \times & \times & \times \\
\otimes_4 & \otimes_5 & \otimes_6 & \times & \times \\
\otimes_7 & \otimes_8 & \otimes_9 & \otimes_{10} & \times \\
\otimes_{11} & \otimes_{12} & \otimes_{13} & \otimes_{14} & \otimes_{15}
\end{array}$$

Figure 5.2.1 Zeroing Pattern of the Givens Method

In Figure 5.2.1 the symbol $\times$ denotes a nonzero entry of the matrix, and the symbol $\otimes_k$ means that entry is zeroed out by the k-th transformation. This order is important if one wishes to "pipeline" the row reduction process. Pipelining may be achieved by expressing R as a linear array in packed form by rows and then dividing this linear array into equal-length pipeline segments. A process is responsible for claiming an unreduced row of the original matrix and reducing it to zero by combining it with the existing R matrix using Givens transformations. A new row may enter the pipe immediately after the row ahead has been processed in the first segment. Each row proceeds one behind the other until the entire matrix has been processed. However, because of data dependencies, these rows must not be allowed to get out of order, once they have entered the pipe.

The synchronization required to preserve this order is accomplished using an array of locks, with each entry of the array protecting access to a segment of the pipe. A process gains access to the next segment by locking the corresponding entry of the lock array before unlocking the entry protecting the segment it currently occupies. Granularity may be adjusted to hide the cost of this synchronization by simply altering the length of a segment. Segment boundaries do not correspond to row boundaries in R. This feature has the advantage of balancing the amount of work between synchronization points, but the disadvantage of having to decide on one of two possible computations at each location within a segment: compute a transformation or apply one.

The method is more easily grasped if one considers the following three diagrams. In Figure 5.2.2 we represent the matrix A in a partially decomposed state. The upper triangle of the array contains the current state of the triangular matrix R. The entries ($\alpha\ \alpha\ \alpha\ \alpha\ \alpha$) and the entries ($\beta\ \beta\ \beta\ \beta\ \beta$) represent the nonzero components of the next two rows of A that must be reduced.

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \\ & & & & \times \\ & & & & \\ & & & & \\ & & & & \\ \alpha & \alpha & \alpha & \alpha & \alpha \\ \beta & \beta & \beta & \beta & \beta \end{bmatrix}$$

Figure 5.2.2 Partially Reduced Matrix

A natural way to pipeline this reduction process is shown in Figure 5.2.3. There we see the row ($\alpha\ \alpha\ \alpha\ \alpha\ \alpha$) being passed through the triangle R during the reduction process, with the row ($\beta\ \beta\ \beta\ \beta\ \beta$) flowing immediately behind it. The position of the β row and the α row interleaved within the rows of R is meant to indicate that they are ready to be combined with the first and second rows of R, respectively. The first entry of the α row has been zeroed by computing and applying the appropriate Givens transformation as described above, and we are ready to zero out the second entry. In a serial algorithm this α row would be completely reduced to zero before beginning to reduce the β row. However, this process may be pipelined by beginning to combine the β row with the first row of R as soon as the α row is ready to be combined with the second row of R. Since the first row of R is modified during the introduction of a zero in the first position of the α row, it is important that the processing of the β row be suitably synchronized with the processing of the α row. In practice, after initial startup, there would be n rows in the pipe throughout the course of the computation.

$$\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\beta & \beta & \beta & \beta & \beta \\
 & \times & \times & \times & \times \\
\alpha & \alpha & \alpha & \alpha & \alpha \\
 & & \times & \times & \times \\
 & & & \times & \times \\
 & & & & \times
\end{array}$$

Figure 5.2.3 Pipelined Row Reduction

A disadvantage of the scheme just described is that the granularity becomes finer as the process advances, because the length of the nonzero entries in a row of R decreases. A better load balance and a natural way to adjust the granularity may be achieved by considering the matrix R as a linear array divided into segments of equal length.

$$(\rho_{11}\ \rho_{12}\ \rho_{13} | \rho_{14}\ \rho_{15}\ \rho_{22} | \rho_{23}\ \rho_{24}\ \rho_{25} | \rho_{33}\ \rho_{34}\ \rho_{35} | \rho_{44}\ \rho_{45}\ \rho_{55})$$

Figure 5.2.4 R as a Segmented Pipe

In Figure 5.2.4 we depict the nonzero elements of R as ρ_{ij} and note that in this linear array the natural row boundaries occur at entries ρ_{i5}. The length of a segment is 3 in this example, and we denote pipe segment boundaries with |. In general, we specify the number of segments desired. Then the length of a segment is

$$\left\lceil \frac{n(n+1)/2}{\textit{number of segments}} \right\rceil .$$

The number of segments is an adjustable parameter in the program. The α row and β row are represented as in Figure 5.2.3, with the α row entering the second segment and the β row entering the first segment. The difference between this scheme and the one depicted in Figure 5.2.3 is that the α row is not fully combined with the first row of R before processing of the β row is begun. To keep the rows in order, a row must gain entry to the next segment before releasing the current segment. If the number of segments is equal to the number of nonzero elements of R, then this algorithm reduces to a variant of the more traditional dataflow algorithm presented in Refs. 13, 14, and 28. Computational experience reported in Ref. 9 indicates that performance is not extremely sensitive to this parameter. The optimal length of a segment appeared to be approximately n, but performance degraded noticeably only with extremely large or extremely small segment lengths.

We now turn to the main point of interest in this discussion, the case when the matrix A is large and sparse. The algorithm we present was developed by Heath and Sorensen [21] as an generalization of the Pipelined Givens method to the sparse case. Specifically, we assume that the matrix

$$A^TA$$

is suitably sparse. In this case there are well-established techniques [17] for determining a permutation matrix P such that

$$P^TA^TAP = R^TR$$

has a sparse Cholesky factor R. This permutation is obtained from the symbolic nonzero structure of the matrix A and is designed to reduce the number of nonzeros in the factor R as much as possible. It is of considerable interest to parallelize this symbolic step, but for this discussion we have concentrated only on parallelizing the numerical portion of the algorithm, which involves applying Givens transformations to the matrix AP to produce R.

$$R = \begin{bmatrix} r_{11} & r_{12} & & r_{14} & & & \\ & r_{22} & & r_{24} & & & \\ & & r_{33} & & r_{35} & r_{36} & \\ & & & r_{44} & r_{45} & & \\ & & & & r_{55} & r_{56} & r_{57} \\ & & & & & r_{66} & r_{67} \\ & & & & & & r_{77} \end{bmatrix}$$

DIAG	r_{11}	r_{22}	r_{33}	r_{44}	r_{55}	r_{66}	r_{77}		
RNZ	r_{12}	r_{14}	r_{24}	r_{35}	r_{36}	r_{45}	r_{56}	r_{57}	r_{56}
XRNZ	1	3	4	6	7	9	10		
NZSUB	2	4	5	6	5	6	7		
XNZSUB	1	2	3	5	6	6			

Figure 5.2.5 Sparse Data Structure of R

The algorithm is virtually identical to the serial algorithm. There are some notable exceptions, however, an explanation of which requires an understanding of the data structure for R as illustrated in Figure 5.2.5. The *RNZ* array contains the off-diagonal nonzero entries of R in packed form. It is evident that the *RNZ* array lends itself to the same segmentation and that the row reduction process may be pipelined in almost exactly the same way as the R array in the dense case. The natural row boundaries are determined by the array *XRNZ*. The i-th entry of this array points to the location of the first nonzero in the i-th row of the full array R. The arrays *NZSUB* and *XNZSUB* are used to determine the column indices of entries in *RNZ* as described in Ref. 15. The *RNZ* array is divided into equal length segments as shown in Figure 5.2.6.

$$\text{RNZ} \quad r_{12} \; r_{14} \mid r_{24} \; r_{35} \mid r_{36} \; r_{45} \mid r_{56} \; r_{57} \mid r_{56} \mid$$

Figure 5.2.6 *RNZ* as a Segmented Pipe

Just as in the dense case, a process is responsible for claiming a row and then combining it with the current R array using Givens transformations. These processes synchronize as before: The first nonzero of the unreduced row is determined, the location of the segment containing the corresponding row boundary in *RNZ* is determined, entry is gained to that segment (by reading an asynchronous variable on the HEP), and then the row reduction is started. To preserve the correctness of the factorization, once the pipeline has been entered by a process, it must stay in proper order. A process keeps itself in proper order by gaining access to the next segment before releasing the segment it currently owns. In the dense case, every process has work to do in every segment. In the sparse case, however, there may be segments where no work is required because the sparsity pattern of the row currently being reduced allows it to skip several rows of R .

This phenomenon is best understood when illustrated by example. Consider a row which has the initial nonzero structure

$$a = (\; 0 \;\; \alpha \;\; 0 \;\; \alpha \;\; 0 \;\; 0 \;\; 0 \;) ,$$

and suppose this row is to be reduced to zero against the nonzero R structure shown in Figure 5.2.5 with *RNZ* segmented as shown in Figure 5.2.6. The first nonzero of the row a is in position 2, so it is first combined with row number 2. This row starts at position 3, as indicated by the second entry of *XRNZ*, and position 3 is in segment number 2 in *RNZ*. The diagonal entry r_{22} is used together with the first nonzero in a to compute the Givens transformation, and then this transformation is applied to element r_{24} together with the entry in position 4 of a. No fill is created in a, so after the application there is one nonzero at position 4. Thus, row 3 may be skipped. Row 4 begins in position 6 of *RNZ*, which is in segment 3. Entry is gained to segment 3, and then segment 2 is released and the factorization proceeds. In this example the next row boundary required happens to be in the adjacent segment. In general, however, there might be several segments between the relevant row boundaries. In that case, entry into each of the intervening segments must be gained and released to ensure that the proper order is maintained between the various rows being processed.

Computational results reported by Heath and Sorensen [21] show that this scheme achieves near-perfect speedup on typical problems such as those found in Refs. 16 and 20. The scheme has the advantage of using existing data structures that are found in SPARSPAK and thus does not require modification of the user interface in existing codes that rely on this package. Such routines can take advantage of this speedup without modification.

5.3 Eigensystems of Tridiagonal Matrices

The final problem we consider is that of determining the eigensystem of a real $n \times n$ symmetric matrix A, finding all of the eigenvalues and corresponding eigenvectors of A. It is well known [30, 32] that under these assumptions

(5.3.1) $$A = QDQ^T \,, \quad \text{with } Q^TQ = I \,,$$

so that the columns of the matrix Q are the orthonormal eigenvectors of A and $D = diag(\delta_1, \delta_2, \ldots, \delta_n)$ is the diagonal matrix of eigenvalues. The standard algorithm for computing this decomposition is first to use a finite algorithm to reduce A to tridiagonal form using a sequence of Householder transformations, and then to apply a version of the QR algorithm to obtain all the eigenvalues and eigenvectors of the tridiagonal matrix [12, 29, 30, 32]. In Section 4.3 we discussed a method for parallelizing the initial reduction to tridiagonal form. We now describe a method for parallelizing the computation of the eigensystem of the tridiagonal matrix.

The method is based on a divide-and-conquer algorithm suggested by Cuppen [3]. A fundamental tool used to implement this algorithm is a method developed by Bunch, Nielsen, and Sorensen [2] for updating the eigensystem of a symmetric matrix after modification by a rank-one change. This rank-one updating method was inspired by some earlier work of Golub [19] on modified eigenvalue problems. The basic idea of the new method is to use rank-one modifications to tear out selected off-diagonal elements of the tridiagonal problem in order to introduce a number of independent subproblems of smaller size. The subproblems are solved at the lowest level using the subroutine TQL2 from EISPACK. Results of these problems are successively glued together using the rank-one modification routine SESUPD that we have developed based upon the ideas presented in Ref. 2.

In the following discussion we describe the partitioning of the tridiagonal problem into smaller problems by rank-one tearing. Then we describe the numerical algorithm for gluing the results back together. The organization of the parallel algorithm is laid out, and finally some preliminary computational results are presented.

5.3.1 Partitioning by Rank-One Tearing

The crux of the algorithm is to divide a given problem into two smaller subproblems. To do this, we consider the symmetric tridiagonal matrix

$$(5.3.2)\quad T = \begin{bmatrix} T_1 & \beta e_k e_1^T \\ \beta e_1 e_k^T & T_2 \end{bmatrix} = \begin{bmatrix} \hat{T}_1 & 0 \\ 0 & \hat{T}_2 \end{bmatrix} + \beta \begin{bmatrix} e_k \\ e_1 \end{bmatrix} (e_k^T , e_1^T) \ ,$$

where $1 \le k \le n$ and e_j represents the j-th unit vector of appropriate dimension. The k-th diagonal element of T_1 has been modified to give $\hat{T}_1$, and the first diagonal element of T_2 has been modified to give $\hat{T}_2$. There are some numerical difficulties here concerning possible cancellation. A way to overcome these difficulties is discussed fully in Ref. 5.

Now we have two smaller tridiagonal eigenvalue problems to solve. According to Equation (5.3.2) we compute the two eigensystems

$$\hat{T}_1 = Q_1 D_1 Q_1^T \, , \quad \hat{T}_2 = Q_2 D_2 Q_2^T \, .$$

This gives

$$(5.3.3)\quad T = \begin{bmatrix} Q_1 D_1 Q_1^T & 0 \\ 0 & Q_2 D_2 Q_2^T \end{bmatrix} + \beta \begin{bmatrix} e_k \\ e_1 \end{bmatrix} (e_k^T , e_1^T) = \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \left[\begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} + \beta \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} (q_1^T , q_2^T) \right] \begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix} \ ,$$

where $q_1 = Q_1^T e_k$ and $q_2 = Q_2^T e_1$. The problem now is to compute the eigensystem of the interior matrix in Equation (5.3.3). A numerical method for solving this problem has been provided in Ref. 2, and we shall discuss this method in the next section.

It should be fairly obvious how to proceed from here to exploit parallelism. One simply repeats the tearing on each of the two halves recursively until the original problem has been divided into the desired number of subproblems; then the rank-one modification routine may be applied from bottom up to glue the results together again.

5.3.2 The Updating Problem

The general problem we are required to solve is that of computing the eigensystem of a matrix of the form

$$(5.3.4)\qquad \hat{Q}\hat{D}\hat{Q}^T = D + \rho z z^T ,$$

where D is a real $n \times n$ diagonal matrix, α is a scalar, and z is a real vector of order n. It is assumed without loss of generality that z has Euclidian norm 1.

As shown in Ref. 2, if $D = diag(\delta_1, \delta_2, \cdots, \delta_n)$, with $\delta_1 < \delta_2 < \cdots < \delta_n$ and no component ζ_i of the vector z is zero, then the updated eigenvalues $\hat{\delta}_i$ are roots of the equation

(5.3.5)
$$f(\lambda) \equiv 1 + \rho \sum_{j=1}^{n} \frac{\zeta_j^2}{\delta_j - \lambda} = 0.$$

Golub [19] refers to this as the secular equation. The behavior of its roots is completely described by the graph in Figure 5.3.1.

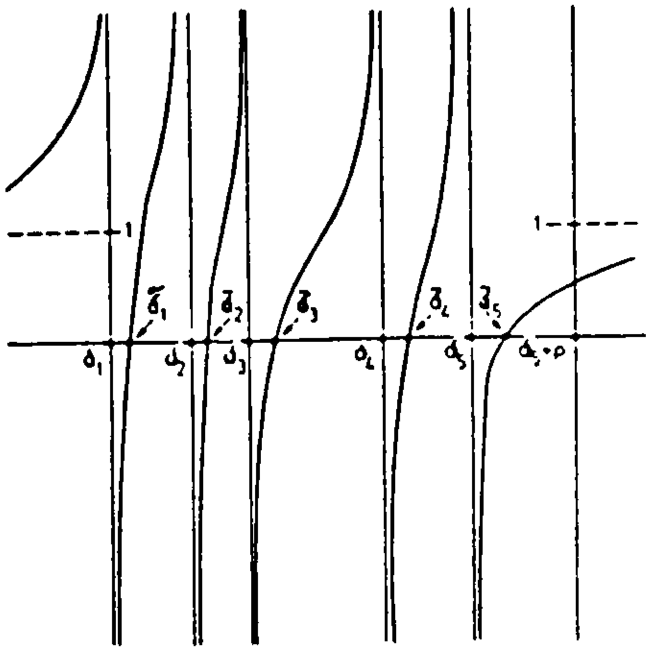


Figure 5.3.1 The Secular Equation

Moreover, as shown in Ref. 2, the eigenvectors (i.e., the columns of $\hat{Q}$ in (5.3.4)) are given by the formula

(5.3.6)
$$\hat{q}_i = \gamma_i \Delta_i^{-1} z,$$

with γ_i chosen to make $\|\hat{q}_i\| = 1$, and with $\Delta_i = diag(\delta_1 - \hat{\delta}_i, \delta_2 - \hat{\delta}_i, \cdots, \delta_n - \hat{\delta}_i)$. Because of this structure, an excellent numerical method may be devised to find the roots of the secular equation and, as a by-product, to compute the eigenvectors to full accuracy.

In the following discussion we assume that $\rho > 0$ in (5.3.5). A simple change of variables may always be used to achieve this, so there is no loss of generality. The method we shall describe was inspired by the work of More' [25] and Reinsch [26, 27] and relies on the use of simple rational approximations to construct an iterative method for the solution of Equation (3.2). Given that we wish to find the i-th root $\hat{\delta}_i$ of the function f in (3.2), we may write this function as

$$f(\lambda) = 1 + \phi(\lambda) + \psi(\lambda),$$

where

$$\psi(\lambda) = \rho \sum_{j=1}^{i} \frac{\zeta_j^2}{\delta_j - \lambda}$$

and

$$\phi(\lambda) \equiv \rho \sum_{j=i+1}^{n} \frac{\zeta_j^2}{\delta_j - \lambda} .$$

From the graph in Figure 5.3.1 it is seen that the root $\hat{\delta}_i$ lies in the open interval (δ_i, δ_{i+1}). For λ in this interval, all of the terms of ψ are negative and all of the terms of ϕ are positive. We may derive an iterative method for solving the equation

$$-\psi(\lambda) = 1 + \phi(\lambda)$$

by starting with an initial guess λ_0 in the appropriate interval and then constructing simple rational interpolants of the form

$$\frac{p}{q-\lambda} , \quad r + \frac{s}{\delta - \lambda} ,$$

where the parameters p, q, r, and s are defined by the interpolation conditions

(5.3.7)
$$\frac{p}{q-\lambda_0} = \psi(\lambda_0) , \quad r + \frac{s}{\delta - \lambda_0} = \phi(\lambda_0)$$

$$\frac{p}{(q-\lambda_0)^2} = \psi'(\lambda_0) , \quad \frac{s}{(\delta - \lambda_0)^2} = \phi'(\lambda_0) .$$

The new approximate λ_1 to the root $\hat{\delta}_i$ is then found by solving

(5.3.8)
$$\frac{-p}{q-\lambda} = 1 + r + \frac{s}{\delta - \lambda} .$$

It is possible to construct an initial guess that lies in the open interval $(\delta_i, \hat{\delta}_i)$. A sequence of iterates $\{\lambda_k\}$ may then be constructed as we have just described, with λ_{k+1} being derived from λ_k as λ_1 was derived from λ_0 above. It is proved in Ref. 3 that this sequence of iterates converges quadratically from one side of the root and does not need any safeguarding.

During the course of this iteration, the quantities $\delta_j - \lambda_k$ are maintained, and the iterative corrections to λ_k are added to these differences directly. As the iteration converges, the lower order bits of these quantities are corrected to full accuracy. Since these differences make up the diagonal entries of the matrix Δ_i appearing in (5.3.6), this allows computation of the updated eigenvectors to full accuracy and avoids cancellation that would occur if we first computed the roots and then formed the differences.

Another important numerical aspect of the updating problem is "deflation." There are two cases where such deflation occurs: when two given roots are nearly equal, and when certain components of the vector z are "small." The effects of such deflation can be dramatic, for the amount of computation required to perform the updating is greatly reduced. We shall not present here the details nor the numerical motivation for deflation. We simply remark that the result of deflation is to replace the updating problem (5.3.4) with one of smaller size. This is accomplished by applying similarity transformations consisting of several Givens transformations. If G represents the product of these transformations, the result is

$$G(D + \rho zz^T)G^T = \begin{bmatrix} D_1 - \rho z_1 z_1^T & 0 \\ 0 & D_2 \end{bmatrix} + E ,$$

where

$$\| E \| \le \varepsilon \| D + \rho zz^T \| ,$$

with ε roughly the size of machine precision. The cumulative effect of such errors is additive, and thus the final computed eigensystem $\hat{Q}\hat{D}\hat{Q}^T$ satisfies

$$\| A - \hat{Q}\hat{D}\hat{Q}^T \| \le \varepsilon\eta \| A \|,$$

where η is order 1 in magnitude. The reduction in size of $D_1 - \rho z_1 z_1^T$ over the original rank-one modification can be spectacular in certain cases. The details of deflation, as well as further numerical results, may be found in Ref. 5; we indicate the potential in Table 6.

In this table we report the results of this algorithm on a tridiagonal matrix with pseudo-random nonzero entries in the interval [−1,1]. The table entries show ratios of execution time required by TQL2 (from EISPACK) to that required by the parallel algorithm on the same machine with the same compiler options and the same environment. In all cases the time reported by TQL2 was obtained by executing it as a single process. It should be emphasized that in all cases the computations were carried out as though the tridiagonal matrix had come from Householder's reduction of a dense symmetric matrix to tridiagonal form. The identity was passed in place of the orthogonal basis that would have been provided by this reduction, but the arithmetic operations performed were the same as those that would have been required to transform that basis into the eigenvectors of the original symmetric matrix.

Table 6

Results of Algorithm on Random Matrix (order = 150)

Ratio of Execution Time $\frac{\textit{TQL2 time}}{\textit{parallel time}}$

VAX 785/FPA	Denelcor HEP	Alliant FX/8	CRAY X-MP-1	CRAY X-MP-4
2.6	12	15.2	1.8	4.5

These results are remarkable because speedups greater than the number of physical processors were obtained in all cases. The gain is due to the numerical properties of the deflation portion of the parallel algorithm. In all cases the word length was 64 bits, and the same level of accuracy was achieved by both methods. The measurement of accuracy used was the maximum 2-norm of the residuals $Tq - \lambda q$ and of the columns of $Q^TQ - I$. The results are typical of the performance of this algorithm on random problems. Indeed, speedups become more dramatic as the matrix order increases. In problems of order 500, speedups of 15 have been observed on the CRAY-XMP-4 (a four-processor machine); and speedups over 50 have been observed on the Alliant FX/8 (an eight-processor machine). The CRAY results can actually be improved because parallelism at the root finding level was not exploited in the implementation run on the CRAY but was fully exploited on the Alliant. Finally, we remark that deflation does not occur for all matrices; examples are given in Ref. 5.

5.3.2 The Parallel Algorithm

Although it is fairly straightforward to see how to obtain a parallel algorithm, certain details are worth discussing further. We begin by describing the partitioning phase. This phase amounts to constructing a binary tree with each node representing a rank-one tear and hence a partition into two subproblems. A tree of level 3 therefore represents a splitting of the original problem into eight smaller eigenvalue problems. Thus, there are two standard symmetric tridiagonal eigenvalue problems to be solved at each leaf of the tree. Each of these problems may be spawned independently without fear of data conflicts. The tree is then traversed in reverse order, with the eigenvalue updating routine SESUPD applied at each node joining the results from the left-son and right-son calculations. The leaves each define independent rank-one updating problems, and again there is no data conflicts between them. The only data dependency at a node is that the left- and right-son calculations must have been completed. As this condition is satisfied, the results of two adjacent eigenvalue subproblems are ready to be joined through the rank-one updating process, and this node may spawn the updating process immediately. Information required at a node to define the problem consists of the index of the element torn out, together with the dimension of the left- and right-son problems. For example, if $n = 50$ with a tree of level 3, we have the computational tree shown in Figure 5.3.2.

The tree defines eight subproblems at the lowest level. The beginning indices of these problems are 1, 7, 13, 19, 26, 32, 38, and 44. The dimension of each of them may be read off from left to right at the lowest level as 6, 6, 6, 7, 6, 6, 6, and 7, respectively. As soon as the calculation for the problems beginning at indices 1 and 7 has been completed, a rank-one update may proceed on the problem beginning at index 1 with dimension 12. The remaining updating problems at this level begin at indices 13, 26, and 38. There are then two updating problems at indices 1 and 26, each of dimension 25, and a final updating problem at index 1 of dimension 50.

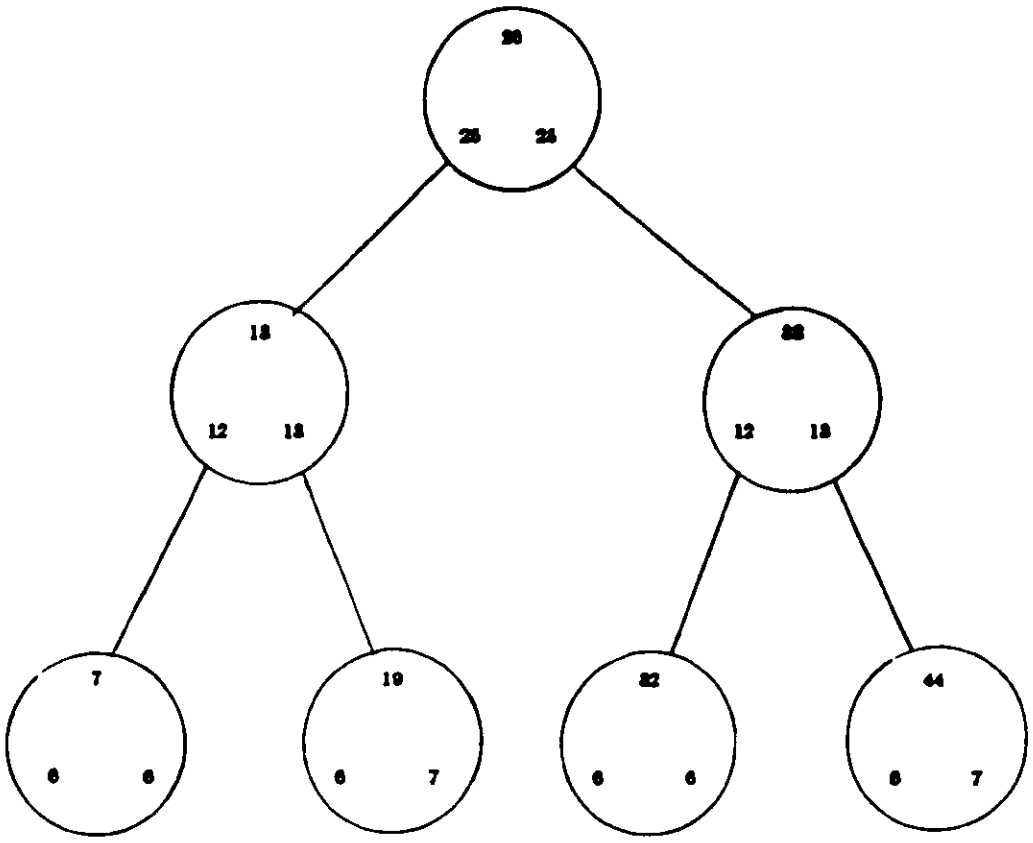


Figure 5.3.2 The Computational Tree

Evidently, we lose a degree of large-grain parallelism as we move up the tree. However, more parallelism is to be found at the root-finding level; and the amount of this increases as we travel up the tree, so there is ample opportunity for load balancing in this scheme. The parallelism at the root-finding level stems from the fact that each of the root calculations is independent and requires read-only access to all but one array — the array that contains the diagonal entries of the matrix Δ_i described above. For computational efficiency we may decide on an advantageous number of processes to create at the outset. In the example above, that number was 8. Then, as we travel up the tree, the root-finding procedure is split into 2, 4, and finally 8 parallel parts in each node at level 3, 2, and 1, respectively. As these computations are roughly equivalent in complexity on a given level, it is reasonable to expect to keep all processors devoted to this computation busy throughout.

6. Implementation and Library Issues

The notion of introducing parallelism at the level of the modules as detailed in Section 4 presents an unpleasant situation. All of the algorithms are properly considered low-level library subroutines when taken in the context of a large-scale applications code. If properly designed, such codes rely on software libraries to perform calculations of the type discussed here. When designing a library, one wishes to conceal machine dependencies as much as possible from the user. Also, in the case of transporting existing libraries to new machines, one wishes to preserve user interfaces in order to avoid unnecessary modification of existing code that references library subroutines. These important considerations seem to be difficult to accommodate if we are to invoke parallelism at the level described above. It would appear that the user must be conscious of the number of parallel processes required by the library subroutines throughout his program. This situation is the result of physical limitations on the total number of processes allowed to be be created. Should the library routines be called from multiple branches of a parallel program, the user could inadvertently attempt to create many more processes than allowed.

A second issue arises within the context of merely programming the more explicitly parallel algorithms discussed in Section 5. These algorithms present far more challenging synchronization requirements than the simple fork-join construct used to implement the modules on a parallel machine. How can these routines be coded in a transportable way?

A possible solution that will have impact on both situations has been inspired by work of Lusk and Overbeek on methodology for implementing transportable parallel codes. We have adapted the "pool of problems" approach they present [23, 24] to the problem of constructing and implementing transportable software libraries. We use a package called SCHEDULE, which we have designed for the user familiar with a Fortran programming environment. The approach relies upon the user's adopting a particular style of expressing a parallel program. Once this has been done, the subroutines and data structure provided by SCHEDULE will allow implementation of the parallel program without dependence on specific machine intrinsics. The user is required to fully understand the data dependencies, parallel structure, and shared memory requirements of the program.

The basic philosophy taken here is that Fortran programs are naturally broken into subroutines that identify self-contained units of computation and that operate on shared data structures. Typically, these data structures are rectangular arrays; and the portion of the data structure to be operated on is often identified by passing an element of the array that is treated within the subroutine as the first element of the array to be operated on. This standard technique is extremely useful in implementing a parallel algorithm in the style adopted in SCHEDULE. Morever, it allows one to call upon existing library subroutines without any modification, and without having to write an envelope around the library subroutine call in order to conform to some unusual data-passing conventions imposed by a given parallel programming environment. One defines a shared data structure and subroutines to operate on this data structure. Then a parallel(izable) program is written in terms of calls to these subroutines, which in principle may be performed independently or according to data-dependency requirements which the user is responsible for defining. The result is a serial program that could run in parallel if there was a way to schedule the units of computation on a system of parallel processors while obeying the data dependencies.

SCHEDULE works in a manner similar to an operating system to schedule processes that are ready to execute. It consists of two queues: a process queue and a ready queue. A process identifies a subroutine call and pointers to addresses needed to make the call. A process tag is placed on the ready queue when its data dependencies have been satisfied. In addition, work routines are constructed that are capable of assuming the identity of any process appearing on the queue. A fixed number of these routines are devoted to the library. They are activated (created, forked, etc.) at the outset of the computation and remain activated throughout the course of this computation. Within this scheme, calls to matrix vector routines (for example) are not made explicitly. Instead, they are put on the process queue to be performed as soon as they can be picked up by one of the workers through the scheduler mechanism. Transportability is achieved because the actual references to machine-specific synchronization primitives are few in number and are isolated in two low-level SCHEDULE routines. These, together with the specific means for creating or forking processes, are the only items that need to be changed when moving from one machine to another. A schematic of the abstract idea behind the scheduler is represented in Figure 6.1.

7. Conclusions

We have presented a sampling of the ideas for algorithms and implementation techniques that we have been considering recently in the Mathematics and Computer Science Division at Argonne National Laboratory. Traditionally, our activities have involved the development of algorithms and techniques for implementing these algorithms in a transportable manner. We view the work presented here as an extension of these activities, an extension that will help us address similar problems that are arising with the advent of exotic computer architectures. We find the subject challenging and rewarding in terms of its potential. We encourage others to join us in pursuing methodologies and software techniques that will enable effective use of the developing hardware.

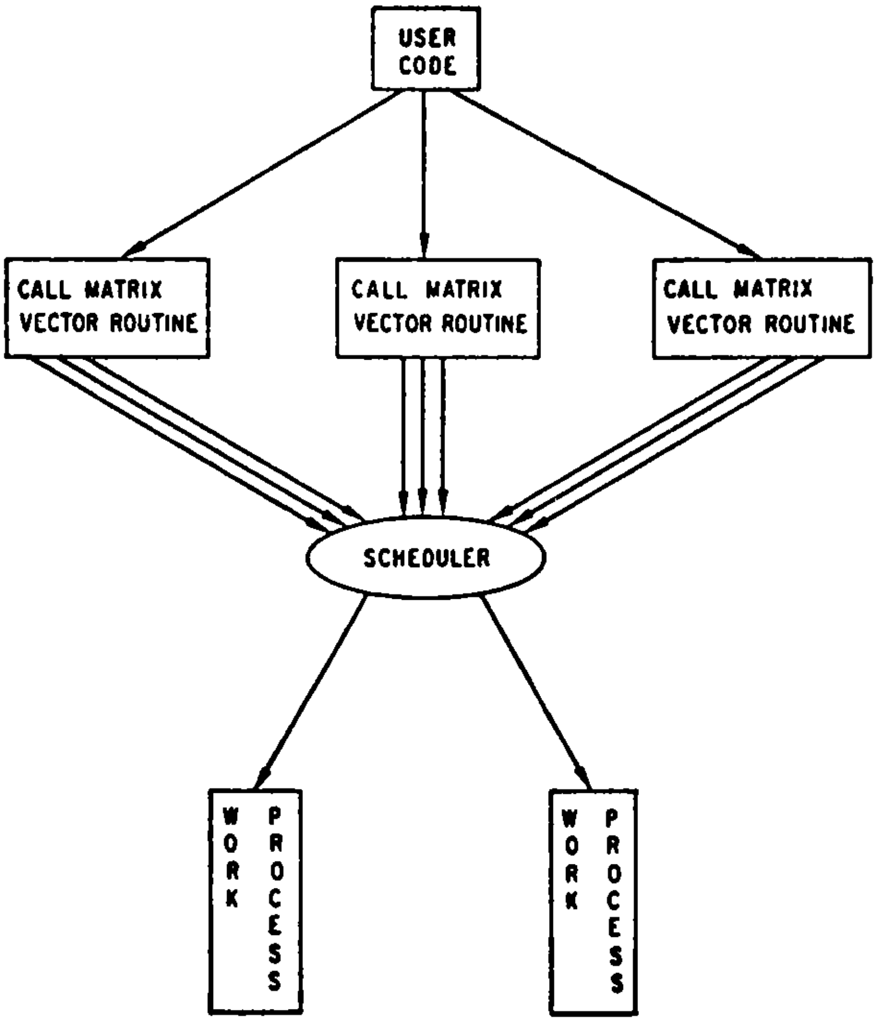

USER CODE
CALL MATRIX VECTOR ROUTINE
CALL MATRIX VECTOR ROUTINE
CALL MATRIX VECTOR ROUTINE
SCHEDULER
WORK PROCESS
WORK PROCESS

Figure 6.1 Library Scheduler

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