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SEMI-ITERATIVE METHODS ON DISTRIBUTED MEMORY MULTIPROCESSOR ARCHITECTURES

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ABSTRACT

In the parallel ELLPACK (//ELLPACK) project [Hous 89a] we are developing a library of parallel iterative methods for distributed memory multiprocessor systems and software tools for partitioning and allocation of the underlying computations. In this paper we report the formulation, implementation and performance of eight adaptive semi-iterative methods on three hypercube based architectures: NCUBE, iPSC/1 and iPSC/2. Preliminary experimental results indicate that these methods are capable of delivering close to optimal scaled speed ups while the combination of concurrent/vector processing can lead to sizeable improvements of the overall performance. These experiments have shown that distributed memory systems are capable of solving significantly larger problems than cost equivalent shared memory multiprocessor systems.

AMS (MOS) subject classification. 65N35, 65N05.

Key words. iterative methods, parallel computation, hypercubes, elliptic partial differential equations.

Abbreviation of the title. Iterative Methods on Hypercubes.

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1. INTRODUCTION

The main objective of this research is the development of an efficient general purpose library of parallel iterative methods (//ITPACK) for the solution of large algebraic linear systems on distributed memory multiprocessor systems. Currently, the //ITPACK library consists of 12 modules described as follows

<table>
<thead>
<tr>
<th>//ITPACK module</th>
<th>Ordering Scheme</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jacobi-CG</td>
<td>block, arrow-head</td>
<td>Jacobi conjugate gradient</td>
</tr>
<tr>
<td>Jacob-SI</td>
<td>block, arrow-head</td>
<td>Jacobi with Chebyshev acceleration</td>
</tr>
<tr>
<td>SOR</td>
<td>block, arrow-head</td>
<td>Successive Over Relaxation</td>
</tr>
<tr>
<td>SSOR CG</td>
<td>block, arrow-head</td>
<td>Symmetric SOR conjugate gradient</td>
</tr>
<tr>
<td>SSOR SI</td>
<td>block, arrow-head</td>
<td>Symmetric SOR with Chebyshev acceleration</td>
</tr>
<tr>
<td>Jacobi Schwarz</td>
<td>block</td>
<td>Schwarz splitting with Jacobi iterations</td>
</tr>
<tr>
<td>GS Schwarz</td>
<td>block</td>
<td>Schwarz splitting with Causs-Seidel iterations</td>
</tr>
</tbody>
</table>

We plan to add several multicolor iterative schemes in the future.

The block semi-iterative modules in //ITPACK are based on the ITPACK [Kinc 82] implementations of the corresponding modules in the ELLPACK environment [Rice 85]. In this first version of the paper we describe the parallel Jacobi CG and SI modules on three distributed memory multiprocessor systems with hypercube interconnection. The final paper will include the discussion of the rest. Specifically we measure the performance of the //ITPACK modules on the NCUBE (128 processors), iPSC/1 (32 processors) and iPSC/2 (32 processors). The //ITPACK modules have been implemented in the parallel ELLPACK (//ELLPACK) system and are driven by a domain decomposition tool [Hous 89b].

The rest of the paper is organized as follows. Section 2 contains a brief description of the corresponding sequential methods. In Section 3 we present the parallel implementation strategies used and analyze their communication complexity. Performance results obtained on Ncube, iPSC/1 and iPSC/2 hypercube machines are presented and discussed in Section 4. The conclusions and discussion of our future plans are in Section 5.

2. SEQUENTIAL SEMI-ITERATIVE ALGORITHMS.

It is well known that the basic iterative methods (such as Jacobi, SOR) can be accelerated by using appropriate linear combinations of consecutive iterants of the basic methods. These acceleration techniques lead to the so-called semi-iterative methods. We consider two such methods based on the Jacobi iteration and Chebyshev (Jacobi-SI) or conjugate gradient (Jacobi-CG) acceleration. A detailed description of these methods can be found in [Rice 85] and [Kinc 82]. If \( G \) is the Jacobi iteration matrix then both methods are defined by the iteration equation

\[
u^{(n+1)} = \rho_n + 1 (\gamma_n + 1 (Gu^{(n)} + k) + (1 - \gamma_n + 1)u^{(n)}) + (1 - \rho_n + 1)u^{(n-1)}
\]

where \( \rho_n \) and \( \gamma_n \) are appropriate acceleration parameters. These parameters are given in
terms of the $M(G)$ largest and $m(G)$ smallest eigenvalues of $G$. In the absence of their values adaptive procedures can be used to estimate them. For the description of their parallel implementation we present the Jacobi–SI/ELLPACK version.

INPUT: $f$ the right hand side vector $f$
A the coefficient matrix
$u$ the initial estimation of the unknown vector

scale(A) scaling of $A$

$d := f$ ; $d := d+(I-A)u$ ; $d := d-u$ compute pseudo residuals

dnorm = $d \times d^T$ ; unorm = $u \times u^T$ compute norms of $d$ and $u$

if conv_test(dnorm,unorm) then stop stopping test based on $d_{norm}$ and $u_{norm}$
if adapt_test(dnorm) then test for recomputation of parameters

dtnrm = $d \times A \times d^T$
if cme_test(dnorm,unorm) then test for recomputing $M(G)$
cme = accel(dtnrm) compute $M(G)$
else if sme_test(dnorm,unorm) then test for recomputing $m(G)$
sme = accel(dtnrm) compute $m(G)$
endif
endif

$u :=$ compute(sme,cme,u) compute new estimation of $u$

unscale(A) unscaling of $A$

Algorithm 2.1 The sequential adaptive Jacobi–SI algorithm.

3. PARALLEL SEMI-ITERATIVE METHODS.

Now we describe the reorganization of the computation in the above algorithms so they can run efficiently on hypercube architectures while preserving the convergence properties of the original sequential schemes. This reorganization is based on two partition schemes of the algebraic data structures while the reordered computation consist primarily by vector/vector and matrix/vector operations. It has been recognized ([Keye 87], [Ayka 88], [Duni 88], [Gust 88]) that these type of operations can be implemented very efficiently on distributed memory architectures using fanin/fanout algorithms or bidirectional exchanges. Next we present two parallel implementations of the adaptive Jacobi–SI algorithm.
3.1 Block Jacobi–SI method.

In this implementation the algebraic data structures of the system $Au = f$ are partitioned rowwise. Each processor $i$ is assigned the computation associated with $r_i$ consecutive rows of the matrix $A$ and the corresponding slice of the unknown and the right hand side $f$. Depending on the bandwidth of the matrix $A$ and the hardware configuration (number of processors) selected this can be achieved by mapping the block structure onto a ring (see Figure 3.1a) or grid (see Figure 3.1b) interconnections which can be embedded into a hypercube ensemble of processors.

![Figure 3.1 Block partitions used for parallel accelerated Jacobi.](image)

We denote by $A^{(i)}$, $u^{(i)}$ and $f^{(i)}$ the linear system blocks assigned to processor $i$ and assume they reside in its local memory. According to the description of Algorithm 2.1, each processor needs to broadcast its own diagonal entries of $A$ and receive appropriate diagonal entries of other processors for scaling and unscaling the matrix $A$. This can be done by means of fanout/fanin algorithms. The computation of the inner products required for the calculation of the norms of $u$ and $d$ are done by first computing on each processor $i$, the local part of the inner product and then use additive bidirectional exchanges to calculate the inner product as the sum of all partial sums. An inner product like expression $d \times A \times d^T$ can be treated similarly and only some indexing overhead is involved to get the appropriate locations of the matrix elements. The calculation of the new estimation of $u$ within each iteration is done locally after receiving appropriate values of the old estimation from neighbor processors. From the above discussion one concludes that the only additional computation required to parallelize the original algorithm has to do only with indexing. In addition interprocessor communication involves mostly nearest neighbor exchanges of one dimensional arrays and global exchanges of scalars. This parallel implementation gives a good aspect ratio and efficient performance.

3.2 Domain–Decomposition Jacobi–SI Method.

Many scientific/engineering applications involve computations associated with geometrical objects. Very often these computations require the solution of large linear systems. Domain decomposition or substructuring methods are based on some
decomposition or splitting of the associated discrete geometric data structures in non-overlapping subdomains. They conceptually treat each subdomain as a separate computation. In [Hous 89c] we study this partition problem while in [Chri 89] we are developing software tools that assist the user in obtaining nearly optimal domain decompositions. The algebraic data structures obtained using this partitioning strategy depends very much on the ordering of the unknowns and equations. Here we formulate the semi-iterative methods which assume that equations associated with subdomain interfaces are ordered last while the rest of them are ordered first, this is the Arrow-Head ordering. Figure 3.2 indicates the data structures obtained by this scheme.

![Data Structure](image)

**Figure 3.2** Data structure obtained from the Arrow-Head ordering scheme for linear equations.

4. PERFORMANCE RESULTS AND DISCUSSION

In this section we present the performance data of the Jacobi-SI and CG methods on the Ncube, iPSC/1 and iPSC/2 hypercubes multiprocessors. Table 4.1 indicates the specific hardware configurations of these machines used in our experiments. Extensive performance comparison of these machines together with a detailed description of their hardware and software characteristics can be found in [Duni 88]. All computations presented in this paper were carried out in single precision FORTRAN.

<table>
<thead>
<tr>
<th></th>
<th>Ncube</th>
<th>iPSC/2</th>
<th>iPSC/1</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU-Node</td>
<td>custom 32-bit</td>
<td>80386/387</td>
<td>80286/287</td>
</tr>
<tr>
<td>Memory-Node</td>
<td>512K</td>
<td>4M</td>
<td>512K</td>
</tr>
<tr>
<td>Clock Rate</td>
<td>6 MHZ</td>
<td>16 MHZ</td>
<td>8 MHZ</td>
</tr>
<tr>
<td>Number of Nodes</td>
<td>128</td>
<td>32</td>
<td>32</td>
</tr>
</tbody>
</table>

Table 4.1 Hypercube configurations used for the implementation of semi-iterative methods.
The linear systems considered are obtained by discretizing linear second order elliptic partial differential equations on rectangular and non-rectangular domains. The timings reported here do not include the cost of the discretization phase, this time is at most 10% of the total solution cost. The solution time includes the time per iteration and the cost of adaptive and the convergence test procedures. The FORTRAN implementation of the algorithms is almost identical for the three machines. Specifically, they differ in the timing and communication routines used.

4.1 Performance of Block Jacobi-SI and Jacobi-CG

In this experiment we consider the solution of the elliptic equation \( u_{xx} + u_{yy} - 100u = f \) on the domain \( \Omega = [0,10] \times [0,10] \) with solution \( u = 1 \) on the boundary of \( \Omega \). We apply the 5 point star finite difference method with fixed and scaled grids. Figure 4.1 shows the scaled performance of the Jacobi-SI and CG semi-iterative methods. The data indicate almost perfect scaled speed up for both methods. It is apparent that Jacobi-CG is faster than Jacobi-SI since it requires less iterations (42) compared to the Jacobi-SI (55).

![Figure 4.1 Scaled speed up of parallel Jacobi-SI (J-SI) and Jacobi-CG (J-CG) on the NCUBE multiprocessor. Each processor is assigned 400 equations and the assumed iteration tolerance is \( 10^{-6} \).](image)

In Table 4.2 we give the fixed size speed ups achieved by the parallel Jacobi-SI on the NCUBE after 400 iterations. Table 4.3 lists the numerical values of the scaled performance of the Jacobi-SI for the NCUBE and iPSC/2 machines. These data suggest that iPSC/2 is a faster machine while the speed up of the method is identical.
Table 4.2  Fixed speed up of Jacobi-SI on NCUBE after 400 iterations.

<table>
<thead>
<tr>
<th>Processors</th>
<th>Grid</th>
<th>Speed up</th>
<th>Grid</th>
<th>Speed up</th>
<th>Grid</th>
<th>Speed up</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3200 x 4</td>
<td>1.12</td>
<td>Grid</td>
<td>1.23</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>8</td>
<td>1600 x 8</td>
<td>2.08</td>
<td>Grid</td>
<td>2.17</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>16</td>
<td>800 x 16</td>
<td>4.19</td>
<td>Grid</td>
<td>4.52</td>
<td>256 x 256</td>
<td>4.38</td>
</tr>
<tr>
<td>32</td>
<td>400 x 32</td>
<td>7.93</td>
<td>128 x 128</td>
<td>8.52</td>
<td>—</td>
<td>9.10</td>
</tr>
<tr>
<td>64</td>
<td>200 x 64</td>
<td>14.93</td>
<td>Grid</td>
<td>15.90</td>
<td>—</td>
<td>17.45</td>
</tr>
<tr>
<td>128</td>
<td>100 x 128</td>
<td>13.60</td>
<td>Grid</td>
<td>26.74</td>
<td>—</td>
<td>33.15</td>
</tr>
</tbody>
</table>

Table 4.3  Scaled speed up of Jacobi-SI on NCUBE and iPSC/2 for 4000 equations per processor.

<table>
<thead>
<tr>
<th>Processors</th>
<th>NCUBE</th>
<th>iPSC/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Finally, Figure 4.2 illustrates the effect of vector processors in the iPSC/2. The results indicate speed up by a factor of four is obtained from vectorization. The per processor implementation of the Jacobi-SI was achieved by using the vector BLAS, fill in, gather and scatter routines.
4.2 The performance of domain decomposition Jacobi-SL

In this experiment we consider the partial differential equation $u_{xx} + u_{yy} - (1+x)u = f(x)$ defined on the L-shaped domain depicted in Figure 4.4. The function $f$ selected so that $u = e^{(x+y)}$ and the rectangular grid is defined by an overlay grid of $64 \times 64$ lines.
The domain decomposition is done heuristically using the Domain Decomposition Tool (DecTool) of ELLPACK and the automatic load partitioning strategies developed in [Hous 89c]. We have used the ELLPACK–NCUBE 5 point star discretization module to generate linear systems of equations. In this environment the host processor gets the domain’s decomposition from DecTool, then applies the specified ordering of the algebraic data structures and distributes this information to processor nodes where the generation of the discrete equations take place. Figure 4.5 shows the per iteration scaled and fixed speed up achieved in the case of Jacobi–CG on NCUBE. For these measurements we used 100 equations per processor to compute the scaled speed up and 64 x 64 overlay grid for the estimation of the fixed speed up. It is worth pointing out that the performance of this method depends on the decomposition. The final paper will include experimental data indicating the effect of load balancing in the speed up of domain decomposition semi-iterative methods.
5. CONCLUSIONS AND FUTURE GOALS

Iterative methods have been shown [Hous 88] to be effective alternatives for solved well behaved sparse large linear systems of equations with "realistic" accuracy requirements. Their potential is even greater in parallel computation environments. We are developing a library of parallel iterative methods which is an extension of the ITPACK package for distributed memory machines. In this paper we present performance of some of them on commercially available message passing MIMD (hypercube) machines. The preliminary experimental results indicate that they are capable of exploiting the parallel processing power of these machines and delivering close to optimal scaled speed ups. These data also indicate that the combination of concurrent/vector processing can lead to significant speed ups. Many studies have overlooked the space complexity of parallel algorithms/architecture pairs. Our experiments show that distributed memory systems are capable of solving significantly larger problems than cost equivalent shared memory multiprocessor systems. Specifically, we were able to solve close to 1/2 million finite difference equations in a reasonable time on NCUBE with 128 processors.
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REFERENCES


