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Multitasking the conjugate gradient on the CRAY X-MP/48

by

Gérard Meurant

Numerical Analysis Project Computer Science Department Stanford University Stanford, California 94305

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Gerard MEURANT

Centre d'Etudes de Limeil-Valenton

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BP 27

94190 Villeneuve St Georges, France

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Abstract

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We showhow to efficiently implement the preconditioned conjugate gradient method on a four processors computer CRAY X-MP/48.

We solve block tridiagonal systems using block **preconditioners** well suited to parallel computation.

Numerical results are presented that exhibit nearly optimal speed up and high Mflops rates.

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1. - i o n

In this paper we show how to efficiently implement the preconditioned conjugate gradient method on the CRAY X-MP/48 using the four processors in parallel. We considerblocktridiagonallinearsystemsthatarise from the discretization of partial differential equations.

Let

be such a linear system, where



A being a symmetric M-matrix.

In the prototype two dimensional model problem matrices D_i , i=1,...,n are tridiagonal and matrices A_i , i=2,...,n are diagonal.

We use the preconditioned conjugate gradient (PCG) method to solve this linear system But if this method has been used successfullyon vector computers, see for instance /10/, it is not well suited to parallel computation because of the data dependancies in the algorithm. Wewillshow, in a similar way than /12/,/13/ how PCG canbemodified to reduce the dependancies and how to get a more parallel algorithm. Anotherproblemistodevise a preconditioner well adapted to parallel computation.

To solve this problem we will use modifications of the block preconditioners introduced in /4/, as vectorized in /10/.

THe outline of the paper is as follows:

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-insection 2 we briefly recall the main features of the CRAY X-MP/48 and showhow to synchronize the processors.

- section 3 gives acomputationalvariantofthemethod introducedin /12/,/13/ to reduce data dependancies in PCG.

- section 4 defines, firstly for two and then for four processors, parallel block preconditioners well adapted to the X-MP/48.

- in section 5 we present numerical results for a model problem. With two processors we get a nearly optimal speed up but with four processors memory conflicts reduce the potential speed up.

2. Overview of CRAY X-MP/48

CRAY X-MP/48 is apowerfulcomputer with fourtightly coupled processors sharing a large memory. Each processor is a vector machine with a CRAY 1 like architecture, but many improvements have been done that give a much more efficient computer. Each processor has four accesses to memory including two for vector loads and an Improved chaining mechanism allowing to exploit the full potential of the functional units.

On many vectorized codes one CRAY X-MP processor is twotothreetimes fasterthan the CRAY 1 although the clock period is only 1.33 times faster. The maximum performance of the four processors altogether is 840 Mflops.

The most **novel_feature** of CRAY **X-MP** is that the four processors can be used **simultaneously in a single job. Expression of parallelism is done inside the Fortran** codes through **calls to a multitasking** library.

There are some low level primitives that allow

1)to start a task and eventually to wait for its completion (TSKSTART,TSKWAIT)
2)todefine criticalregionsthatmustbe executed by only one processor at a time
(LOCKON,LOCKOFF)

3) to synchronize processors waiting for **some** events **to happen** (EVPOST, EVWAIT, EVCLEAR).

For a more detailed description of these routines see /6/,/2/,/11/. Here we justwanttodescribehowwe cansynchronize severalprocessors usingthese primitives.

The Fortran list of subroutine SYNC is given in figure 1 below, /2/.

SUBROUTINE SYNC(ID)

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DIMENSION ID(6)

CALL LOCKON(ID(3))

NEVN=ID(6)

ID(5)=ID(5)-1

IF(ID(5).EQ.0)THEN

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~ID(5)=ID(4)

NEXEVN=3-NEVN

ID(6)-NEXEVN

CALL EVCLEAR(ID(NEXEVN))

CALL EVPOST(ID(NEVN))

CALL LOCKOFF(ID(3))

ELSE

CALL LOCKOFF(ID(3))

CALL EVWAIT(IDNEVN))

ENDIF

END

Pigure **1**

ID is a 6 words arraythathas been initialized before. ID(1) and ID(2) are events whichareusedinturn, ID(3) is the lock of the critical region, ID(4) is the number of tasks to be synchronized, ID(5) is the number of tasks not yet arrived at the synchronization point and ID(6) is the event used for synchronizing.

We used two events in turn because it is safer to have different events used in consecutive synchronization points, see /2/.

A synchronizationbarrier on the X-MP/48 is done by n processors, $2 \le n \le 4$, calling SYNC with the same array ID (which must be in common in the calling program). There is anoverheadthatcomeswiththe synchronization, thisimpliesthatthecode **must be large enough between two synchronization barriers for the computation not to** be overhead **dominated**, **see /3/. Previous** attempts to **use PCG** on the **CRAY X-MP were** partly unsuccessfull because of that problem /11/.

3. The conjugate gradient algorithm

The preconditioned conjugate gradient (PCG) method for solving a linear system of equations is as follows :

Algorithm PCG

Let \mathbf{x}^0 be given, $\mathbf{r}^0 = \mathbf{b} - \mathbf{A} \mathbf{x}^0$ and \mathbf{p}^{-1} arbitrary. For k=0,1,... until convergence, perform the steps

 $M z^{k} = r^{k}$ $\beta_{k} = (M z^{k}, z^{k}) / (M z^{k-1}, z^{k-1}), \quad \beta_{0}=0$ $p^{k} = z^{k} + \beta_{k} p^{k-1}$ $\alpha_{k} = (M z^{k}, z^{k}) / (A p^{k}, p^{k})$ $x^{k+1} = x^{k} + \alpha_{k} p^{k}$ $r^{k+1} = r^{k} - \alpha_{k} A p^{k}$

M is a positive definite preconditioning matrix.

PCG is very well suited for vector computers if the **preconditioner M** is *chosen* carefully, see /10/ and the references therein (see also /1/). Previous workontheuse of **PCG** on **parallel computers was** done in /9/. Unfortunately there is a very low degree of parallelism in PCG as all the steps arise in a very sequentialway, leading to many synchronization points and a large overhead. The two scalar products cannot be done in parallel and we need p^k to commpute a_k . Regardless of M $z^k = r^k$ the only things that can be done in parallel (at least with an acceptable granularity for the given computer) are the computations of x^{k+1} and r^{k+1} . Of courseitcanbe said that usually, most of thetime is spent in the solution of M $z^k = r^k$ and that is does not really matter that the remaining parts are done in sequential mode. But remember that if only 10% of the algorithm is not parallel then the speed up cannot be greater than 1.82 with two processors and 3.1 with four processors. Hence it is interesting to try to increase the parallelism of PCG. Some proposals in this way have been made by Saad /12/ and Van Rosendale /13/ without numerical results. The idea is based on the following remark : in exact arithmetic we have, see /5/

 $(M z^i, z^j) = 0$ Vi, ji \neq j

But

$$z^{k+1} - z^k = -\alpha_k M^{-1} A p^k$$

SO

$$M z^{k+1} - M z^{k} = -\alpha_{k} A p^{k}$$

therefore using orthogonality

$$(M z^{k+1}, z^{k+1}) = \alpha_k^2 (M^{-1} A p^k, A p^k) - (M z^k, z^k)$$

This implies that (theoretically), we can **compute** (M z^{k+1} , z^{k+1}) before computing . z^{k+1} . The algorithm can then be conveniently recast in the following form :

Let \mathbf{x}^0 be given, $\mathbf{r}^0 = \mathbf{b} - \mathbf{A} \mathbf{x}^0$, $\mathbf{M} \mathbf{z}^0 = \mathbf{r}^0$, $\mathbf{p}^0 = \mathbf{z}^0$, $\mathbf{s}_0 = (\mathbf{r}^0, \mathbf{z}^0)$. For k=0,1,... until convergence perform the steps

1)
$$M v^{k} = A p^{k}$$

2) compute $(v^{k}, A p^{k}), (A p^{k}, p^{k})$
3) $\alpha_{k} = s_{k} / (A p^{k}, p^{k})$
 $s_{k+1} = \alpha_{k}^{2} (v^{k}, A p^{k}) - s_{k}$
 $\beta_{k+1} = s_{k+1} / s_{k}$
4) $x^{k+1} = x^{k} + \alpha_{k} p^{k}$
 $r^{k+1} = r^{k} - \alpha_{k} A p^{k}$
 $z^{k+1} = z^{k} - \alpha_{k} v^{k}$

$$p^{k+1} = (z^k - \alpha_k v^k) + \beta_{k+1} p^k$$

In this algorithm there is one more vector to store but the parallelism has been greatly increased. Regardless of step 1), both scalarproducts can be computed in parallel and after the scalar step 3) the four vectors x, r, z, pcan be split in as many subvectors as the number of available processors, so step 4) is fully parallel. One may ask why we do not make the change of variable A'=M⁻¹A and b'=M⁻¹b. This can savetheneedtocomputevectorz. We arekeepingzbecausetheconvergencecriteria we used in PCG is $(M z^k, z^k) / (M z^0, z^0) \le \epsilon$ andwewanttokeepexactly the same one in the modified algorithm.

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Themaindrawbackofthelastalgorithmisits numericalinstability. S_k is supposed totendto zero as does α_k and rounding errors frequently give a negative value of s_{k+1} for some k. Then the **algorithm** breaks down.

However there is a way to fix this problem, the trick being to use s_{k+1} as a predictor for the true value of the scalar product and to correct it, recomputing (r^{k+}, z^{k+1}) , at the end of the iteration.

The modified algorithm MPCG becomes :

Let x^0 be given, $r^0 = b - A x^0$, $M z^0 = r^0$, $p^0 = z^0$. For k=0,1,... until convergence perform the steps

$$1) \qquad M \dot{v}^{k} = A p^{k}$$

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2) compute
$$(v^k, A p^k)$$
, $(A p^k, p^k)$, (r^k, z^k)

3)
$$\alpha_{k} = (r^{k}, z^{k}) / (A p^{k}, p^{k})$$

$$\mathbf{s}_{k+1} = \alpha_k^2 (\mathbf{v}^k, \mathbf{A} \mathbf{p}^k) - (\mathbf{r}^k, \mathbf{z}^k)$$

$$\beta_{k+1} = s_{k+1} / (r^k, z^k)$$

4)
$$x^{k+1} = x^k + \alpha_k p^k$$

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$$r^{k+1} = r^k - \alpha_k \wedge p^k$$

$$z^{k+1} = z^k - \alpha_k v^k$$

$$p^{k+1} = (z^k - \alpha_k v^k) + \beta_{k+1} p^k$$

There is only one **more** scalar product in this algorithm.

Although we are not able to theoretically proveits stability, it work quite well for

all the examples we tried.

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We usually get the same **number** of iterations as for the standard algorithm. We will see later on how the computations are organized.

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4. Parallel preconditioning

In /4/ block preconditioning was introduced (see also /1/) in which M was chosen as follows :

let A be a block diagonal matrix with diagonal blocks Δ_i i=1,...,n then

 $\mathbf{M} = (\mathbf{A} + \mathbf{L}) \Delta^{-1} (\mathbf{A} + \mathbf{L}^{\mathrm{T}})$

where L is the block lower triangular part of A.

Tridiagonal matrices Δ_i are computed recursively by

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 $\Delta_{i} = D_{i} - A_{i} \Omega_{i-1}(1) A_{i}^{T} \qquad 2 \leq i \leq n$

 $\Omega_{i}(j)$ is a symmetric banded matrix with 2j+1 diagonals whose elements within the band are the same as those of Δ_{i}^{-1} .

This preconditioner is not vectorizable, therefore in /10/ when solving My = c, Δ_1^{-1} was replaced by $\Omega_1(3)$. But even if now completely in vector mode, this preconditioneris not parallel as there remains two block recursions when solving M z-r. We now show how to modify this preconditioner for use on a parallel computer with a few vector processors. For the sake of simplicity let us begin with two processors and assume **n** is even (but there is no loss of generality).

We use the so called "twisted factorization*, see /7/, /8/.

Mistaken in the form

$$\mathbf{M} = \mathbf{\Pi} \quad \Delta^{-1} \quad \mathbf{\Pi}^{\mathbf{T}}$$

where



When doing the **product** one can easily see that the resulting matrix is block tridiagonal, that is to say there is no block fill in. Matrices Δ_i are computed by

> $\Delta_{1} = D_{1}$ $\Delta_{i} = D_{i} - A_{i} \Omega_{i-1}(1) A_{1}^{T}, \quad 2 \le i \le n/2$

 $\Delta_n = D_n$

$\Delta_i = D_i - A_{i+1}^T \Omega_{i+1}(1) A_{i+1}, i=n,..., n/2-1$

One can remark that we do not get these formulas by direct identification, in fact we neglect a coupling term in the computation of $\Delta_{n/2}$, but as we only need an **approximation and** as the numerical examples will show, this has no influence on the results. Hence the computation of Δ_i can be done in two completely independent pieces.

The existence of the decomposition may be proven using the same techniques as in /4/and /10/.

The solve of M y -c is parallel as well. In order to vectorize, each time we have to solve a tridiagonal system, we replace Δ_1^{-1} by $\Omega_1(3)$ as in /10/. Hencewithobvious block notations, the solution y is given by

1)
$$W_1 = \Omega_1(3) c_1$$

$$w_i = \Omega_i(3) (c_i - A_i w_{i-1}), i=2, ..., n/2-1$$

2) $w_n = \Omega_n(3) c_n$

 $w_i = \Omega_i(3)(c_i - A_{i+1}^T w_{i+1}), \quad i=n-1, \dots, n/2+1$

3)
$$w_{n/2} = \Omega_{n/2}(3) (c_n - A_{n/2} w_{n/2} - A_{n/2+1}^T w_{n/2+1})$$

4)
$$y_i = w_i - \Omega_i(3) A_{i+1}^T Y_{i+1}, \quad i=n/2-1,...,1$$

$$y_i = w_i - \Omega_i(A_i y_{i-1}, i=n/2+1, ..., n)$$

It is obvious that steps 1) and 2) can be executed in parallel as well as 4) and 5). Only step 3) requires the synchronization of both processors.

This method is similar to the dissection techniques used in **/9/, except** we are considering block methods instead of point ones.

Let us now look at how we can organize the computation in MPCG. Suppose that both processors are synchronized at the beginning of 1) (although this requirement can be weakened).

weakened).

Processor 1 computes :

$$c_i = CA p^k l_i, i=1,...,n/2$$

$$s_{1}^{1} = \sum_{i=1}^{n/2} ([A p^{k}]_{i}, [p^{k}]_{i})$$
$$s_{1}^{2} = \sum_{i=1}^{n/2} ([r^{k}]_{i}, [z^{k}]_{i})$$

Processor 2 computes in parallel :

$$C_i = [A p^k]_i, \quad i=n/2+1,...,n$$

$$w_{i}, \quad i=n, \dots, n/2+1$$

$$\int_{2}^{1} = \sum_{i=n/2+1}^{n} ([A p^{k}]_{i}, [p^{k}]_{i})$$

$$\int_{2}^{2} = \sum_{i=n/2+1}^{n} ([r^{k}]_{i}, [z^{k}]_{i})$$

Then both processors are synchronized, each one calling routine SYNC of section 2 and processor 1 computes $[v^k]_{n/2}$ (note that in a more refined organization, after synchronization, each processor may compute one half of $[v^k]_{n/2}$). After this sequential step, processor 1 computes :

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$$\mathbf{s}_{1}^{3} = \sum_{i=1}^{n/2} ([\mathbf{v}^{k}]_{i}, [p^{k}]_{i})$$

Processor 2 computes in parallel : .

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$$\mathbf{s}_{2}^{3} = \sum_{i=n/2+1}^{n} ([\mathbf{v}^{k}]_{i}, [\mathbf{p}^{k}]_{i})$$

Then both processors are synchronized and afterthebarrier each processor is able to compute its own copy of :

$$s^{1} = s_{1}^{1} + s_{2}^{1}$$

 $s^{2} = s_{1}^{2} + s_{2}^{2}$
 $s^{3} = s_{1}^{3} + s_{2}^{3}$

$$\alpha_k, s_{k+1}, \beta_{k+1}$$

This is done to avoid one useless barrier and more overhead.

Having computed the scalars, Processor 1 computes

$$[x^{k+1}]_{i}, [r^{k+1}]_{i}, [z^{k+1}]_{i}, [p^{k+1}]_{i}, i=1, \dots, n/2$$

and Processor 2 computes

 $[x^{k+1}]_i, [r^{k+1}]_i, [z^{k+1}]_i, [p^{k+1}]_i, i=n/2+1,...,n$ This ends one iteration.

As the stopping criteria is $(r^k, z^k) / (r^0, z^0) \le \epsilon$, the test can be donebyboth processors, if the test is **satisfied Processor** 2 executes a return, Processor 1 waits for Processor 2 doing a **TSKWAIT**.

One can see that except for **solving** for $[v^k]_{n/2}$ everything is done in parallel and there is only 3 synchronization barriers in one 'iteration.

We will denote thismethod using two processors by INV2P.

Let us now look at what we can achieved with four processors.

The **preconditioner** is taken as

$$\mathbf{M} = \mathbf{\Theta} \quad \Delta^{-1} \quad \mathbf{\Theta}^{\mathrm{T}}$$

where O has the following structure









Matrices Δ_i are computed by :

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 $A_{1} = D_{1}$ $\Delta_{i} = D_{i} - A_{i} \Omega_{i-1}(1) A_{1}^{T}, \qquad 2 \le i \le n/4$ $\Delta_{n/2} = D_{n/2}$ $\Delta_{i} = D_{i} - A_{i+1}^{T} \Omega_{i+1}(1) A_{i+1}, \qquad i=n/2-1, \dots, n/4+1$

$$\Delta_{i} = D_{i} - A_{i} \Omega_{i-1}(1) A_{1}^{T}, \quad n/2+1 \le i \le 3n/4$$

$$\Delta_{n} = D_{n}$$

$$\Delta_{i} = D_{i} - A_{i+1}^{T} \Omega_{i+1}(1) A_{i+1}, \quad i=n-1, \dots, 3n/4+1$$

A system M y = c is solved in the following obvious way

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1)
$$w_{n/2} = \Omega_{n/2}(3) c_{n/2}$$

2) $w_1 = \Omega_1(3) c_1$
 $w_i = \Omega_i(3)(c_i - A_i w_{i-1}), \quad i^{-2}, \dots, n/4^{-1}$
3) $w_i = \Omega_i(3) (c_i - A_{i+1}^T w_{i+1}), \quad i^{-n/2-1}, \dots, n/4^{+1}$
4) $w_i = \Omega_i(3) (c_i - A_i w_{i-1}), \quad i^{-n/2+1}, \dots, 3n/4^{-1}$
5) $w_n = \Omega_n(3) c_n$
 $w_i = \Omega_i(3) (c_i - A_{i+1}^T w_{i+1}), \quad i^{-n-1}, \dots, 3n/4^{+1}$
6) $w_{n/4} = \Omega_{n/4}(3)(c_{n/4} - A_{n/4} w_{n/4-1} - A_{n/4+1}^T w_{n/4+1})$
7) $w_{3n/4} = \Omega_{3n/4}(3) (c_{3n/4} - A_{3n/4} w_{3n/4-1} - A_{3n/4+1}^T w_{3n/4+1})$

8)
$$y_{n/4} = w_{n/4}, y_{3n/4} = w_{3n/4}$$

9) $y_i = w_i - \Omega_i(3) A_{i+1}^T y_{i+1}, \quad i=n/4-1, ..., 1$
10) $y_i = w_i - \Omega_i(3) A_i y_{i-1}, \quad i=n/4+1, ..., n/2-1$
11) $y_i = w_i - \Omega_i(3) A_{i+1}^T y_{i+1}, \quad i=3n/4-1, ..., n/2+1$
12) $y_i = w_i - \Omega_i(3) A_i y_{i-1}, \quad i=3n/4+1, ..., n$
13) $y_{n/2} = w_{n/2} - \Omega_{n/2}(3) (A_{n/2} y_{n/2-1} + A_{n/2+1}^T y_{n/2+1})$

Evidently when step 1) is completed, steps 2), 3), 4) and 5) can proceed in parallel, then steps 6) and 7) and again steps 9), 10), 11) and 12). solving is completed by sequential step 13).

As with two processors, parts of the scalar products can be computed during steps 9), 10), 11) and 12).

There are two synchronizations of two processors and one global synchronization of the four processors at the end.

Note that when doing the product $\Theta \Delta^{-1} \Theta^{T}$, the resulting matrix is block tridiagonal except for two block fills in that we have neglected in the computation, therefore we must be prepared to have a larger number of iterations than in the standard algorithm. We denote this method with four *processors by* INV4P. Note that here the method is different of the one in /9/, apart from the fact that we

use block **algorithms**, because the blocks are not **numbered** in the same way.

5. Numerical results

In this section we give numerical results for the **model** problem viz. the **discretization** by a five point finite difference scheme of the Poisson equation

 $-\Delta u = f in n =]0, 1[x]0, 1[$ u - 0 on 80

Let h = 1/(n+1) be the **stepsize.** The matrices D_i of order n are



and A_i = -1, I being the identity matrix.

The chosen stopping criteria was 10⁻⁶.

We give detailed results for two cases, a small one with n=50 and a large one with n=150. Further results can be seen on Figures 2, 3, 4 and 5.

For each case we give results for the standard algorithm **INV** and the two **parallel** ones **INV2P** and **INV4P**. Results include the computer time (CRAY X-MP) in seconds, the number of iterations to reach the given criteria, the **Megaflops** rates and for **parallel methods two different values** of the **speed up**. The **first one Sl** is the ratio of times for the execution of *the parallel code* on *one processor and on several*

processors, the second one S2 is the ratio of the time for the standard algorithm INV to the time of the parallel algorithm. It is clear that S1 measures the ability of the computer (both hardware and software) to execute a code on several processors. S2 is more algorithm oriented and measures what we can gain over what was thought to be the best sequential algorithm.

method	1	time	Ι	Mflops	iter	S1	s2
INV 🛸		0.0199		108.86	17	-	-
INV2P		0.0115		187.55	19	1.86	. 1.73
INV4P	ł	0.0127	1	220.7	22	2.75	1.56

n-50

Table 1

All time measurements have been done in dedicated, mode using the real clock time. They do not Include the computation of the preconditioner.

The first thing to note in this **small** problem is that it pays more to use two processors. The loss due to the increasing number of iterations and the larger overhead (as the vector lengthes are two times shorter and there are four processors to synchronize) give a poor result with fourprocessors, but note that the situation changes rapidly as n grows.

method	ļ	time	1	Mflops	I	iter	S1	S2
INV	ł	0.3185	ł	136.9		38	-	
INV2P		0.1859	1	246.9		40	1.92	-1.71
INV4P	•	0.131	ł	401.8	ł	46	3.29	2.43

n=150

Table 2

Table 2 shows that for large problems it does pay to use four processors although the speed up is not as great as we have expected. From different experiments see /2/, we think that this problem comes from memory contention during vector operations. When we run INV4P on two processors we get a speed up larger than 1.9 indicating that the algorithm is well parallelized, but the contention between processors is larger with four processors than with two.

Figures 2, 3 4 and 5 give the Mflops rate, the speed up S1, the computing time and the number of iterations versus n (the order of A being n^2).

It is clear that with four processors we have not reach the full potential of the machine and that with larger problems we can go beyond 420 Mflops but clearly the speed up is bounded. The situation for computing time is not as good because of the increase in the number of iterations going from two to four processors.

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6. Conclusions

We have shown how to efficiently use the preconditioned conjugate gradient method on the CRAY X-MP/48.

With two processors we reach almost the maximum efficiency we can.

Using the four processors the situation is a little bit worst, firstly speed up is bounded by memory contention and secondly we need parallel preconditioners giving a better rate of convergence as it seems difficult to generalize INV4P to more than four processors.

Despite these facts, for large problems, we get interesting improvements over the sequential approach

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