Preconditioned Conjugate Gradient Methods for Serial and Parallel Computers

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Various Preconditioned Conjugate Gradient Methods are investigated for the solution of matrix systems arising from the discretisation of a simple two dimensional partial differential equation of interest to the Oil industry.
Consideration is given to the implementation of these methods on serial computers and efficient parallel implementation on a network of transputers.

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Symbol	Meaning
$\underline{n}$	outward normal vector to region Ω
Ω	region in which problem is being solved
ω	SOR relaxation parameter
p	number of processors/subproblems, pressure of fluid
p_{ij}	approximation to pressure of fluid
p_{BH}	pressure at injection well
$\underline{p}$,$\underline{x}$	solution vector to matrix problem
$\underline{p}$	search direction vector in CG algorithm
ρ	density of fluid, spectral radius of matrix
q	production rate of fluid at production well
$\mathbb{R}$	set of real numbers
s,s_i	block size
S_p,S_p^*	parallel speedup with p processors
U	upper triangular part of matrix
$\underline{u}$	Darcy velocity of fluid
μ	viscosity of fluid
γ	transmissibility at injection well, parameters in polynomial approx.
Γ_{ij}	grid block region
ϕ	porosity of medium, functional to be minimised
λ	mobility of fluid, eigenvalues of matrix
λ_{ij}	approximations to mobilities

There are basically two approaches to obtaining the solution of a matrix system of equations – direct methods or iterative methods. Direct methods solve the system in a known (finite) number of steps, and any errors incurred arise only from the use of finite precision arithmetic. They are often impractical when the matrix is large and sparse, due to fill-in destroying the sparsity. Iterative methods, on the other hand, generate a sequence of approximate solutions that (should) converge to the solution of the problem. These methods are more applicable to large, sparse systems, essentially due to the fact that only a matrix-vector product is required, thus the matrix need not be explicitly stored.

This dissertation deals with the Conjugate Gradient and Preconditioned Conjugate Gradient iterative methods, with respect to large, sparse matrix systems

Chapter 2

Matrix System Generation

2.1 Oil Recovery [2]

Oil reservoirs are beds of porous rock saturated with various fluids and gases. There are three stages to the recovery of the oil. The primary stage involves boring into the rocks and letting the natural pressure of the fluids in the rocks to force the oil to the surface. The secondary stage, reached after the production from the primary stage has decreased substantially, has other fluids injected in an attempt to displace the oil towards the production well. Typical injection fluids are water or steam. There may still be a substantial amount of the original reservoir oil left in the reservoir after secondary recovery, and a tertiary recovery process, such as surfactant flooding [2], can be used to extract some of the remaining oil.

2.1.1 Modelling the Recovery Process

Here, the secondary stage of recovery is investigated, where a fluid is injected into the injection well to keep the pressure constant there. This allows the use

of a single phase (one component) flow model [2]. This model gives the 'mass continuity equation', i.e. the equation representing the fact that the fluid cannot disappear,

$$-\underline{\nabla}.(\rho\underline{u}) = \frac{\partial}{\partial t}(\rho\phi) + \tilde{f} \tag{2.1}$$

where ρ is the density of the fluid, ϕ is the porosity of the medium that the fluid is flowing in, i.e. a representative measure of how much space in the medium is available to hold the fluid, $\tilde{f}$ is the forcing function representing the effect of the injection and production wells, i.e. the rate of the fluid leaving the medium, and $\underline{u}$ is the velocity of the fluid.

As well as the mass continuity equation, a relationship between the flow rate and the pressure gradient is required. Such a relationship, albeit an empirical one, was developed by Darcy (1856) for a single phase flow, i.e.

$$\underline{u} = -\frac{K}{\mu}(\underline{\nabla}p + \rho\underline{g}) \tag{2.2}$$

where $\underline{u}$ is the Darcy velocity, p is the pressure of the fluid, K is the absolute permeability tensor, i.e. the willingness of the medium to allow fluids to flow through it, μ is the viscosity of the fluid, i.e. the internal resistance of the fluid to flow within itself, and $\underline{g}$ is the gravitational acceleration. The permeability tensor has to be determined experimentally. In most practical problems it is possible (or necessary) to assume that K is a diagonal tensor, e.g. in two dimensions

$$K = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix}$$

If $k_x = k_y$, the medium is called isotropic, otherwise it is anisotropic.

By combining (2.1) and (2.2), our fluid flow equation becomes

$$\_\,(\text{—}(\_\ +\ \_)) = \text{—}(\quad) + \tilde{} \tag{2 3}$$

Then, by making some simplifying assumptions; the fluid density remains constant, i.e. there are no temperature dependent changes, there is no gravitational effect, i.e. $\_ = 0$, no time dependence, i.e. steady state version, an isotropic medium, i.e. $=$, and defining the mobility to be $\frac{k}{\mu}$, i.e. the ease with which the fluid moves through the medium, we change equation (2.3) into

$$\_(\ \_\ ) = \tag{2 4}$$

If we assume there is a constant pressure injection well and a constant rate production well, the forcing function can be represented by

$$= \quad (\ _{bh}\quad)\ _I + \quad _P \tag{2 5}$$

where $_I$ and $_P$ are Kronecker Deltas[1] for the injection and production wells respectively, is the transmissibility [2] of the injector, is the production rate

$_{bh}$

– –

[1]If $Q \in \Omega$, then the Kronecker Delta δ_Q is defined by $\forall \underline{x} \in \Omega$, $\delta_Q(\underline{x}) = \begin{matrix} 1 & \underline{x} = Q \\ 0 & \underline{x} \neq Q \end{matrix}$

where _ is the above Darcy velocity (2.2) and _ is the outward normal to the region Ω. With the above assumptions, the boundary condition (2.6) can be written

$$\frac{\partial p}{\partial n}$$

ij

ij

ij

ij ij

ij Γ_{ij} ij

$\frac{1}{2}$ $\frac{1}{2}$

$\frac{1}{2}$ –

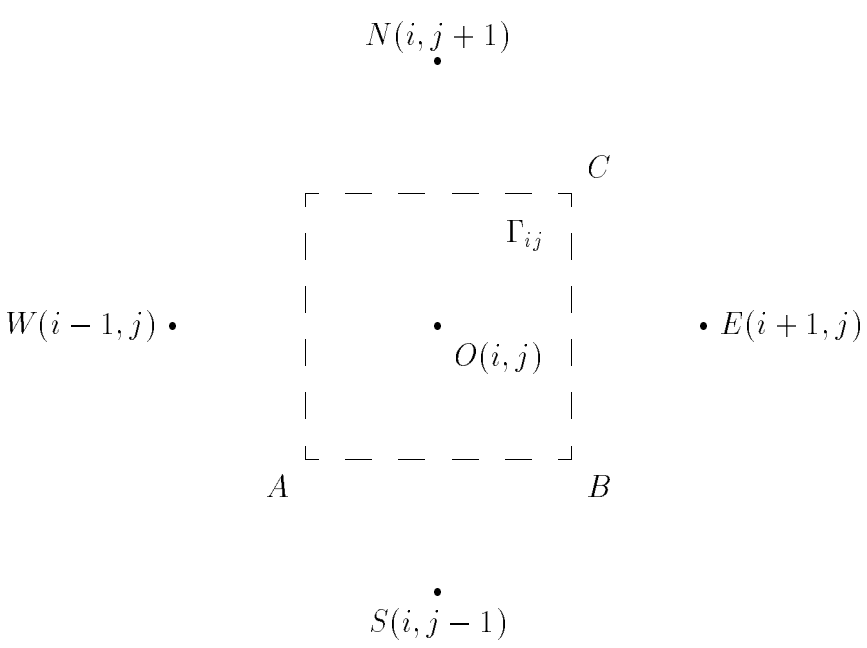


Figure 2.1: Labelling the Grid Block Γ_{ij}

One way approximate the value of a derivative at a point is to use central differences, e.g. the value of $\frac{\partial q}{\partial x}$ at a point C, the midpoint of AB, assuming that AB is in the direction of increasing x, is

$$\frac{\partial q}{\partial x}\,|_C \;=\; \frac{q_B - q_A}{\Delta} \tag{2.11}$$

Thus, by using equations (2.10) and (2.11), we have

$$\begin{array}{rcccl}
\int_A^B \lambda\frac{\partial p}{\partial y}\,dx & \approx & (\lambda\frac{\partial p}{\partial y})|_{i,j-\frac{1}{2}}\Delta x & \approx & \lambda_{i,j-\frac{1}{2}}(\frac{p_O-p_S}{\Delta y})\Delta x \\
\int_C^D \lambda\frac{\partial p}{\partial y}\,dx & \approx & -(\lambda\frac{\partial p}{\partial y})|_{i,j+\frac{1}{2}}\Delta x & \approx & -\lambda_{i,j+\frac{1}{2}}(\frac{p_N-p_O}{\Delta y})\Delta x \\
\int_B^C \lambda\frac{\partial p}{\partial x}\,dy & \approx & (\lambda\frac{\partial p}{\partial x})|_{i+\frac{1}{2},j}\Delta y & \approx & \lambda_{i,j+\frac{1}{2}}(\frac{p_E-p_O}{\Delta x})\Delta y \\
\int_D^A \lambda\frac{\partial p}{\partial x}\,dy & \approx & -(\lambda\frac{\partial p}{\partial x})|_{i-\frac{1}{2},j}\Delta y & \approx & -\lambda_{i,j-\frac{1}{2}}(\frac{p_O-p_W}{\Delta x})\Delta y
\end{array} \tag{2.12}$$

where p_* is the value of p at the point $*$. Combining equations (2.8), (2.9) and (2.12), we obtain

$$\iint_{\Gamma_{ij}} \frac{\partial}{\partial x}(\lambda\frac{\partial p}{\partial x}) + \frac{\partial}{\partial y}(\lambda\frac{\partial p}{\partial y})\,d\Gamma_{ij} \approx \lambda_N p_N + \lambda_E p_E - \lambda_O p_O + \lambda_W p_W + \lambda_S p_S \tag{2.13}$$

where

$$\begin{aligned}
\lambda_N &= \lambda_{i,j+\frac{1}{2}} \frac{\Delta x}{\Delta y} \\
\lambda_E &= \lambda_{i+\frac{1}{2},j} \frac{\Delta y}{\Delta x} \\
\lambda_O &= \lambda_{i,j+\frac{1}{2}} \frac{\Delta x}{\Delta y} + \lambda_{i+\frac{1}{2},j} \frac{\Delta y}{\Delta x} + \lambda_{i-\frac{1}{2},j} \frac{\Delta y}{\Delta x} + \lambda_{i,j-\frac{1}{2}} \frac{\Delta x}{\Delta y} \\
\lambda_W &= \lambda_{i-\frac{1}{2},j} \frac{\Delta y}{\Delta x} \\
\lambda_S &= \lambda_{i,j-\frac{1}{2}} \frac{\Delta x}{\Delta y}
\end{aligned} \tag{2.14}$$

Note that $\lambda_O = \lambda_N + \lambda_E + \lambda_W + \lambda_S$. The right hand side of equation (2.8) is now approximated in a similar manner to that of equation (2.10), i.e. $\iint_{\Gamma_{ij}} f \, d\Gamma_{ij}$ is approximated by the area of Γ_{ij} multiplied by f evaluated at the midpoint of Γ_{ij},

$$\iint_{\Gamma_{ij}} f \, d\Gamma_{ij} \approx \Delta x \Delta y \, f_{ij} \tag{2.15}$$

The equations (2.13), (2.14), and (2.15) are then combined into a matrix equation of the form $A\underline{p} = \underline{f}$ by writing all the equations simultaneously, mapping p_{ij} onto p_n and f_{ij} to f_n where $n = i + (j-1)\,nx$ (this is the natural ordering of the nodes p_{ij}), and then letting $\underline{p}$ be the vector of the p_n's and $\underline{f}$ be the vector of the $\Delta x \Delta y \, f_n$'s.

By negating equations (2.13) and (2.15), we obtain the relation

$$-\lambda_N p_N - \lambda_E p_E + \lambda_O p_O - \lambda_W p_W - \lambda_S p_S = -\Delta x \Delta y \, f_O \tag{2.16}$$

with the λ's as before in (2.14). The above mapping for the p's and the f's leads to a matrix A whose diagonal entries are positive.

2.2.3 Boundary Conditions

quation (2.7) shows that the boundary conditions can be satisfied by letting $\frac{\partial p}{\partial n}$ and/or λ be zero on the boundary $\partial\Omega$.

At a boundary, the working of Section 2.2.2 goes ahead exactly as before, except if, for example, the line A is on the boundary, then

$$\int_D^A \lambda \frac{\partial p}{\partial x}\, dy = \int_D^A \lambda \frac{\partial p}{\partial n}\, dy = 0$$

is substituted directly into equation (2.9), knocking out a term of the approximation.

An equivalent, but easier to implement, effect is obtained by setting $\lambda = 0$ on the boundary, since this also knocks out the same term in the approximation.

2.2.4 Forcing Term

As mentioned in Section 2.2.2, the f term is approximated by (2.15). At everywhere except the injection and production well, the forcing function

$$f = -\gamma(p_{BH} - p)\delta_I + q\delta_P$$

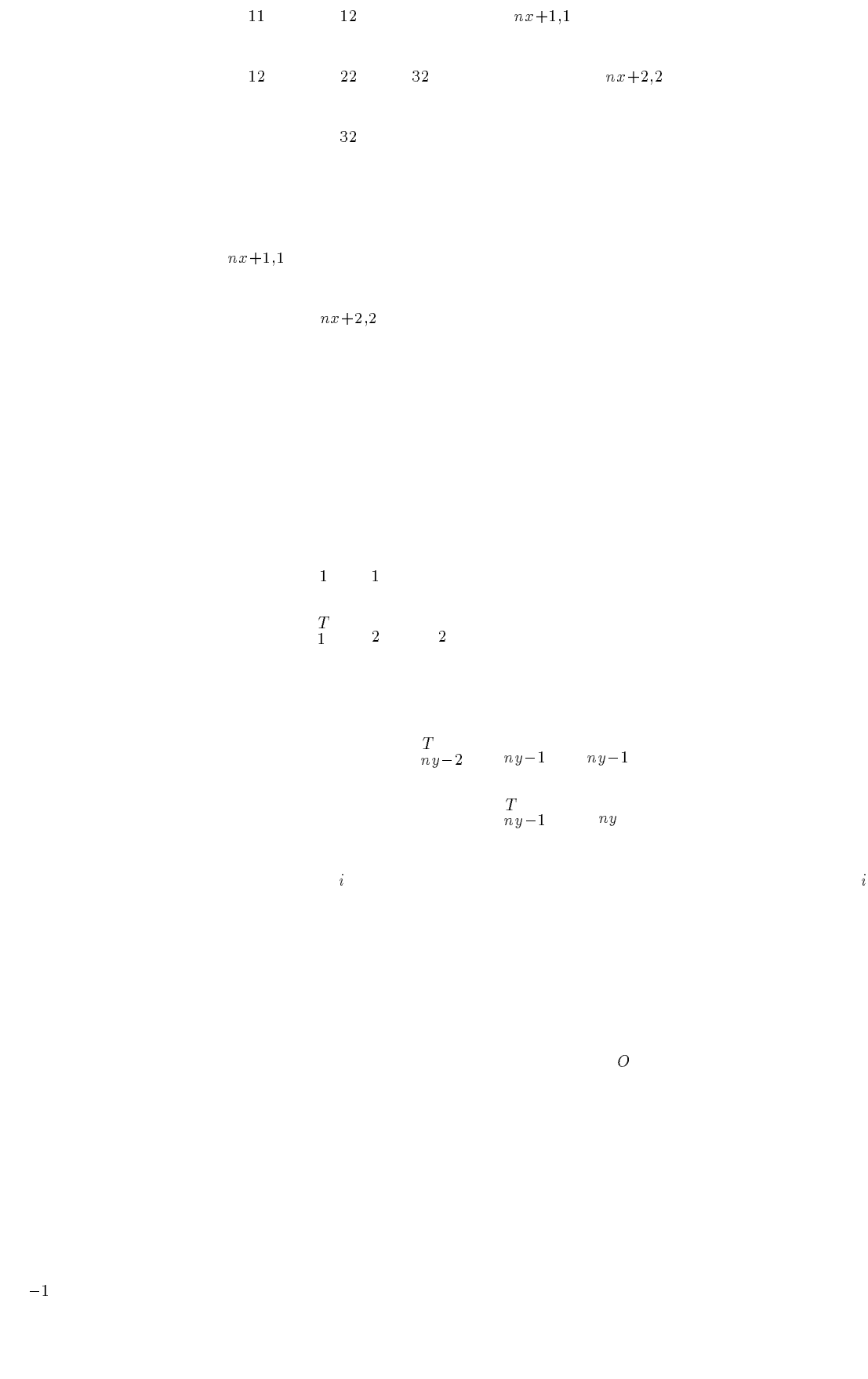
is zero, since both the δ_I and δ_P are zero there. At the production well, $\delta_P = 1$, and so $f = q$ there. At the injection well f is not constant, since it involves the pressure p, and thus

$$f = -\gamma(p_{BH} - p)$$

The p term is taken over to the differential side of the equation, and hence at the injection well, the problem turns into a Helmholtz equation. Following the notation of equation (2.16), λ_O is converted into $\lambda_O + \gamma$ and the right hand side term of equation (2.16) becomes $-\Delta x \Delta y\, \gamma\, p_{BH}$.

$$i+\tfrac{1}{2},j \qquad \overline{\qquad}_{ij} \qquad \overline{\qquad}_{i+1,j}^{-1}$$

$$- \qquad -$$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2.4 Sample Problems

For the purposes of this dissertation, it is assumed that the viscosity of the fluid is unity, i.e. $\mu = 1$, and so the mobility λ is the same as the permeability k. The forcing function (2.5) has values of its parameters set as

$$\begin{aligned} \gamma &= 1.0 \\ p_{BH} &= 2.5 \\ q &= -1.0 \end{aligned}$$

The region Ω is the unit square $[0,1] \times [0,1]$. The injection and production wells are at point $(0,0)$ and $(1,1)$ respectively. Two choices are given for the permeability function k.

2.4.1 Problem 1

The permeability is chosen so that it is constant everywhere

$$k(x,y) \equiv 1,\ (x,y) \in [0,1] \times [0,1]$$

On a 20 by 20 grid, scaling the output pressure so that it is in the range zero to one (the pressure at $(0,0)$ is 3.50973, and that at $(1,1)$ is 3.50000), the pressure distribution over Ω, as seen in Figure 2.2, is obtained.

The corresponding fluid flow field, obtained by calculating the gradient direction for each point in the pressure distribution, is shown in Figure 2.3, where the flow direction is shown by the arrow direction, and the magnitude of the flow shown by the arrow body lengths.

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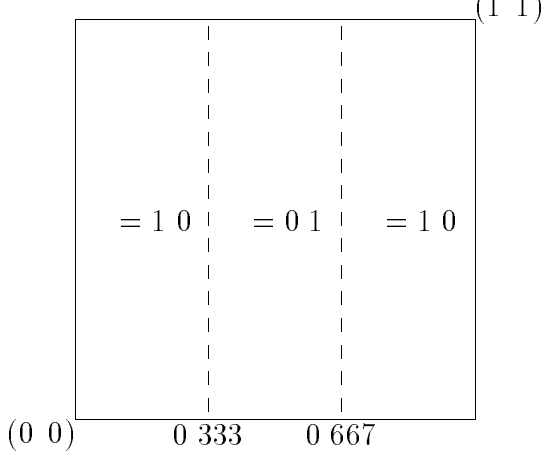

Figure 2.4: Diagram of ( ) for problem 2

The permeability is chosen to be a non-uniform function, such that

$$(\quad) = \begin{cases} 0\,1 & 0\,333 \quad 0\,667 \\ 1\,0 & \text{otherwise} \end{cases}$$

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IW

First, this chapter briefly describes the standard iterative methods for the solution of the matrix equation

$$\_ = \_ \qquad (3\ 1)$$

assuming is symmetric and positive definite, conditions satisfied by the discretisation of the partial differential equation in Chapter 2. Next, the Conjugate Gradient Method is developed and some of its properties are given. Lastly, the idea of preconditioning is presented, and a number of preconditioning strategies are described.

The standard iterative methods given in [7] are based on rearranging equation (3.1) by splitting the matrix into = , and forming the iteration

$$\_^{k+1} = \_^{k} + \_$$

$$\_^{k+1} \quad -1 \quad \_^{k} \quad -1 \_$$

where is the iteration number. The emphasis is on a choice of M so that an equation such as _ = _ is easy to solve at each iteration.

ration.

21

31 32

$n1$ $n2$ $n,n-1$

11 nn

12 $1n$

$n-2,n$

$n-1,n$

-1

-1

-1

to be performed in order to find an optimum , although there do exist adaptive methods that will converge to the optimum as the iterations proceed.

Another way to accelerate the convergence of an iterative method is to combine

The global convergence of the steepest descent method [7] is obtained from the inequality

$$\phi(\underline{x}^{k+1}) + \frac{1}{2}\underline{b}^T A^{-1}\underline{b} \leq \left(1 - \frac{1}{\kappa_2(A)}\right)\left(\phi(\underline{x}^k) + \frac{1}{2}\underline{b}^T A^{-1}\underline{b}\right)$$

As can be seen from this inequality, if $\kappa_2(A)$ is large, then the rate of convergence is slow. To overcome this problem, instead of minimising along the set of residual vectors $\{\underline{r}^0, \underline{r}^1, \ldots\}$, we minimise along a set of 'search directions' $\{\underline{p}^0, \underline{p}^1, \ldots\}$. Defining the new iterate this time as

$$\underline{x}^{k+1} = \underline{x}^k + \alpha \underline{p}^k \tag{3.7}$$

and, again, minimising ϕ^{k+1} by setting

$$\frac{\partial \phi^{k+1}}{\partial \alpha} = 0$$

gives

$$\alpha = \frac{(\underline{p}^k)^T \underline{r}^k}{(\underline{p}^k)^T A \underline{p}^k} \tag{3.8}$$

In order to ensure a reduction in the size of ϕ, $\underline{p}^k$ must not be orthogonal to $\underline{r}^k$, i.e. $(\underline{p}^k)^T \underline{r}^k \neq 0$, and the search directions $\underline{p}^k$ are taken as A-conjugate to all the previous search vectors [7], i.e. $P_{k-1}^T A \underline{p}^k = 0$ where $P_{k-1} = \{\underline{p}^0, \ldots, \underline{p}^{k-1}\} \in \mathbb{R}^{n \times k}$. This is the basis of the Conjugate Gradient (CG) method. From [7], the required search directions are given by

$$\underline{p}^k = \underline{r}^k + \beta \underline{p}^{k-1} \tag{3.9}$$

where

$$\beta = \frac{(\underline{r}^k)^T \underline{r}^k}{(\underline{r}^{k-1})^T A \underline{r}^{k-1}} \tag{3.10}$$

3.2.2 CG Method

Using equation

$$(\underline{p}^k)^T \underline{r}^k = (\underline{r}^k)^T \underline{r}^k$$

from [20] and equation

$$\underline{r}^{k+1} = \underline{b} - A\underline{x}^{k+1} = \underline{r}^k - \alpha A\underline{p}^k$$

from [5] we can rearrange the equations (3.6), (3.7), (3.8), (3.9), and (3.10) into the standard CG algorithm, as devised by Hestenes and Stiefel (1952):- Choose an initial guess $\underline{x}^0$, set $\underline{r}^0 = \underline{b} - A\underline{x}^0$ and $\underline{p}^0 = \underline{r}^0$ then do for $k = 0, 1, 2, \ldots, n$

$$\begin{aligned} \alpha^k &= \frac{(\underline{r}^k)^T \underline{r}^k}{(\underline{p}^k)^T A\underline{p}^k} \\ \underline{x}^{k+1} &= \underline{x}^k + \alpha^k \underline{p}^k \\ \underline{r}^{k+1} &= \underline{r}^k - \alpha^k A\underline{p}^k \\ \beta^k &= \frac{(\underline{r}^{k+1})^T \underline{r}^{k+1}}{(\underline{r}^k)^T \underline{r}^k} \\ \underline{p}^{k+1} &= \underline{r}^{k+1} + \beta^k \underline{p}^k \end{aligned} \tag{3.11}$$

3.2.3 Convergence of CG

If algorithm (3.11) is performed in exact arithmetic, the (exact) solution is obtained in at most n steps (and the method would be a direct one). However, when finite precision arithmetic is used, rounding errors lead to a gradual loss of orthogonality among the residuals, and the finite termination property is lost. This is not serious, since in 1971, Reid [20] showed that when CG is treated purely as an iterative method for large, sparse systems, convergence to a required accuracy usually occurs in many less than n steps. If the matrix A has m distinct eigenvalues, then CG will converge in at most m iterations. Thus, if A has a series of

clustered eigenvalues, then the convergence will be more rapid. The termination criterion is based on a maximum number of iterations, $_{max}$, and some measure of the size of $_^{k}$.

From [7] an error bound on the CG method can be obtained in terms of the -norm, $_{A}$, and after iterations

$$_ \quad _^{k} \ _{A} \quad 2 \ _ \quad _^{0} \ _{A} \quad \frac{\sqrt{\ _{2}(\ )} \quad 1}{\sqrt{\ _{2}(\ )} + 1}^{k} \tag{3 12}$$

This bound is usually far too pessimistic, and the accuracy of the $_^{k}$ is often better than inequality (3.12) predicts. One useful consequence of inequality (3.12) is that the CG method converges very quickly in the -norm if $_{2}(\ ) \quad 1$.

As noted above, if $_{2}(\ ) \quad 1$, then CG converges quickly. The idea of precondi-

$$_ \quad _$$

^{2}

$$^{n \times n}$$

$$^{-1} \quad _ \quad ^{-1} \ _$$

$$^{-1} \quad _ \quad _ \quad _ \quad ^{-1} \ _$$

In order to get $\tilde{}$ close to the identity it is required that is a good approximation for , so that $^{-1}$.

Note that the basic CG algorithm is the preconditioned CG algorithm with the identity matrix as the preconditioner.

$\underline{\ }^{0}$ $\underline{\ }^{0}$ $\underline{\ }$ $\underline{\ }^{0}$

$\underline{\ }^{0}$ $^{-1}\underline{\ }^{0}$

$$_k \quad \frac{\underline{\ }^{k\ T}\ ^{-1}\underline{\ }^{k}}{\underline{\ }^{k\ T}\ \underline{\ }^{k}}$$

$$\underline{\ }^{k+1} \quad \underline{\ }^{k} \quad ^{k}\underline{\ }^{k}$$

$$\underline{\ }^{k+1} \quad \underline{\ }^{k} \quad ^{k} \quad \underline{\ }^{k}$$

$$_k \quad \frac{\underline{\ }^{k+1\ T}\ ^{-1}\underline{\ }^{k+1}}{\underline{\ }^{k\ T}\ ^{-1}\underline{\ }^{k}}$$

$$\underline{\ }^{k+1} \quad ^{-1}\underline{\ }^{k+1} \quad ^{k}\underline{\ }^{k}$$

$^{-1}$

This section details various types of preconditioner . There are five main types considered:-

1. based on splittings of , i.e. =

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$11 \quad 22 \qquad nn$

-1

2

Tridiagonal Preconditioning

Due to the structure of the matrix equations arising from the discretisation in Chapter 2, that is 5-diagonal matrices, another choice for M is the tridiagonal part of A, i.e.

$$T = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 \\ a_{21} & a_{22} & a_{23} & & \vdots \\ 0 & a_{32} & \ddots & \ddots & \\ \vdots & & \ddots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & \cdots & 0 & a_{n,n-1} & a_{nn} \end{bmatrix}$$

This choice of T is relatively simple to invert, being just a forward and backward substitution. As mentioned in Section 2.3, the A obtained from the problem discretisation is actually block tridiagonal, and thus T consists of ny tridiagonal blocks each of size nx by nx.

Another tridiagonal preconditioner would be the tridiagonal part of A^{-1}, which should be more a accurate approximation than the inverse of the tridiagonal part of A, but, unfortunately, a way to compute this inexpensively could not be found.

Block Diagonal Preconditioning

Instead of taking just the diagonal elements of the matrix A, diagonal blocks of A can be used, e.g. s such blocks A_i, possibly of differing sizes

$$M = \begin{bmatrix} A_1 & 0 & \cdots & \cdots & 0 \\ 0 & A_2 & 0 & & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & A_{s-1} & 0 \\ 0 & 0 & \cdots & 0 & A_s \end{bmatrix}$$

and thus, the solution of $M\underline{z} = \underline{r}$ in the PCG algorithm reduces to the solutions to a series of smaller independent problems.

In the discretisation in Chapter 2, a natural block size is nx, and in this case all the A_i's are tridiagonal. Another natural size is any integer multiple of nx, and here all the A_i's are 5-diagonal.

Blocked Tridiagonal Preconditioning

As above, tridiagonal preconditioning can be 'blocked' to introduce independent smaller subsystems. With a block size of nx, this reduces to the Block Diagonal Preconditioning with block size of nx, and incidentally, it is the same as Tridiagonal Preconditioning.

3.4.2 Factorisations of A

Standard techniques for the direct solution of equation (3.1), involve factorising A into the product of two matrices A_1 and A_2 such that systems $A_i\underline{x} = \underline{b},\ i = 1, 2$ are trivial to solve.

If is symmetric and positive definite, then can be written as

$$= \quad ^{T} \tag{3 15}$$

where is lower triangular [7]. quation (3.15) then uniquely defines , and since is lower triangular $^{-1}\_$ and $^{-T}\_$ are easily calculated for any vector _, and the solution to (3.1) is given as

$$\_ = (\ ^{-T})(\ ^{-1}\_)$$

 quation (3.15) can be solved column by column recursively to obtain [7] as follows

$$\begin{aligned} &\text{do} \quad = 1 \ \ 2 \ \ldots \\ &\qquad _{ii} = \sqrt{\ _{ii} \quad \sum_{k=1}^{i-1} \ ^{2}_{jk}} \\ &\qquad \text{do} \quad = \ +1 \quad +2 \ \ldots \\ &\qquad\qquad _{ji} = \frac{A_{ji} - \sum_{k=1}^{i-1} L_{jk} L_{ik}}{L_{ii}} \end{aligned} \tag{3.16}$$

The square root operation is expensive to calculate and often inaccurate, so there exists an alternative statement of Cholesky which avoids it, where is written as

$$= \quad ^{T}$$

where the diagonal of consists of all ones.

preconditioning (calculation of the complete decomposition would solve the problem immediately!), the Incomplete Cholesky Decomposition of A can be defined. First, a sparsity pattern is defined to impose on L, i.e. a set of matrix entries, P, are chosen which are forced to be zero in L. Algorithm (3.16) is still used, but whenever an L_{ij} arises with $(i,j) \in P$, it is set to zero and the algorithm continues. Thus, these elements of L are neither calculated or stored. The simplest choice for P is

$$P = \{\, (i,j) \,|\, A_{ij} = 0;\ i,j = 1,2,\ldots,n \,\}$$

that is, the sparsity pattern of A is enforced on L. In [15], this choice of P is referred to ICCG(0), one of a family of methods. This choice of P is used throughout this dissertation, and is referred to as ICCG. Thus

$$A = LL^T + E$$

where E is a small error matrix whose non-zero entries all lie in P, and the preconditioning matrix M can be taken as LL^T, which only requires a forward and backward substitution to invert.

In algorithm (3.16) it is crucial that all the L_{ii} are greater than zero. If $L_{ii} = 0$ then the algorithm breaks down, and if $L_{ii} < 0$, then LL^T is not positive definite [12] and the CG method cannot be used. It is shown in [15] that if A is an M-matrix[1] then the ICCG algorithm always gives $L_{ii} > 0$, but, unfortunately, ICCG on an arbitrary positive definite matrix is not guaranteed to work. A

[1] $A = (a_{ij})$ is an M-matrix if $a_{ij} \leq 0$ for $i \neq j$, A is non-singular, and $A^{-1} \geq 0$.

simple counter-example is given in [12],

$$\begin{bmatrix} 3 & -2 & 0 & 2 \\ -2 & 3 & -2 & 0 \\ 0 & -2 & 3 & -2 \\ 2 & 0 & -2 & 3 \end{bmatrix}$$

Complete Cholesky decomposition gives $L_{44} = \frac{1}{2}$, while ICCG gives $L_{44} = -5$. All is not lost though, since an exact decomposition of A is not required, and [12] suggests that if an L_{ii} arises such that $L_{ii} < 0$, it is simply set to some positive value[2] and the algorithm is continued. This only causes the ith diagonal element of E to be non-zero, all other non-zeros are still in P. If $L_{ii} < 0$ rarely occurs, i.e. if the decomposition is mostly stable, this adaptation should work quite well, and the experiences in [12] confirm this.

A small modification can be made to the ICCG algorithm, and that is to enforce the equality of the row-sums of A and LL^T by altering the diagonal elements. This leads to a slightly better approximation of A [10].

Blocked Incomplete Cholesky

In Section 3.4.1, the idea of Block Diagonal Preconditioning was introduced to introduce smaller subproblems which were more easily solved. The idea here is to solve each subproblem obtained with the Block Diagonal Preconditioner with the ICCG algorithm, instead of calculating the exact solution, for the same reasons that the ICCG algorithm was developed above.

[2] In [12] $L_{ii} = \sum_{j=1}^{i-1} |L_{ij}| + \sum_{j=i+1}^{n} |L_{ij}|$.

3.4.3 Polynomial Approximation

If $\rho(J) < 1$, then from [22], the inverse of $I - J$ can be expressed as a power series in J, i.e.

$$(I - J)^{-1} = \sum_{k=0}^{\infty} J^k = I + J + J^2 + J^3 + \ldots \tag{3.17}$$

If A is written as $A = \quad + L + U$, as in equation (3.3), then $J = - \quad ^{-1}(L+U)$ is the Jacobi iteration matrix (see Section (3.1.2)), and [7] shows that $\rho(J) < 1$. Thus, if A is written as $A = \quad (I - J)$, and $(I - J)^{-1}$ expanded as in equation (3.17), the inverse of A can be expressed as

$$\begin{aligned} A^{-1} &= (\quad (I - J))^{-1} \\ &= (I - J)^{-1} \quad ^{-1} \\ &= \{\sum_{k=0}^{\infty} J^k\} \quad ^{-1} \\ &= \sum_{k=0}^{\infty} (-1)^k (\quad ^{-1}(L + U))^k \quad ^{-1} \end{aligned} \tag{3.18}$$

The idea of polynomial preconditioning is to truncate the power series (3.18) after m terms and obtain an approximation M_m^{-1} for A^{-1}. If the series is truncated after the $k = 1$ term, then

$$M_1^{-1} = \quad ^{-1} - \quad ^{-1}(L + U) \quad ^{-1} \tag{3.19}$$

has the same sparsity pattern as A, hence no fill-in has occurred. The idea in [11] is instead of having a truncated power series of the form (3.18), a parameter is introduced for each term in the approximation, thus

$$M_m^{-1} \approx \sum_{k=0}^{m} \gamma_k (-1)^k (\quad ^{-1}(L + U))^k \quad ^{-1} \tag{3.20}$$

and then to choose the γ_i's such that the spectral radius, $\rho(M_m^{-1}A)$, is minimised, i.e. the convergence of the PCG method maximised. The observation for equa-

tion (3.19) still holds, i.e. M_1^{-1} still has the same sparsity as A. This method is also used in [4], although there it is for approximating the inverse of a tridiagonal matrix, and three sets of values are given for γ_0 and γ_1 with $m = 1$; approximately 0.9412 and -0.4706, 1 and -1, and 1.1429 and -1.1429. The values given in [11] for γ_0 and γ_1 are 1.0 and -1.0, and $\frac{7}{6}$ and $-\frac{5}{6}$. See [11] for details of how these values were obtained.

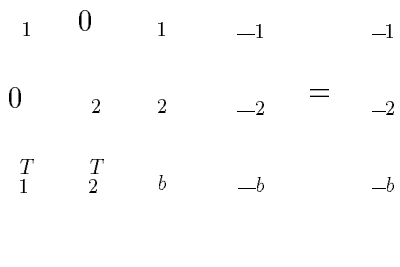
3.4.4 Iterative Methods

Since each iteration of the PCG algorithm involves the solution of a system of the form $M\underline{z} = \underline{r}$, an idea is to perform a number of iterations of one of the standard iterative methods as described in Section 3.1, where M is the required part of A. Hence, any iterative method based on the splitting of $A = M - N$ may be accelerated by the use of the CG method, as long as M is symmetric and positive definite. The case where one iteration of the Jacobi (Section 3.1.2) iteration is performed corresponds to the diagonal scaling method in Section 3.3.

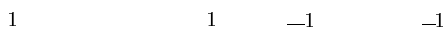
3.4.5 Domain Decomposition

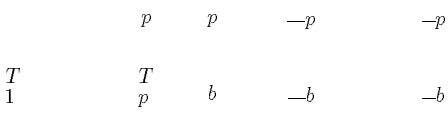
The idea of domain decomposition can be illustrated by dividing the region the problem is being solved on, Ω, into two non-overlapping subregions Ω_1 and Ω_2 ($\Omega = \Omega_1 \cup \Omega_2$). The mesh points are ordered so that those in Ω_1 come first, those in Ω_2 come next, and all those not in Ω_1 or Ω_2 (the mesh points on the interface $\partial\Omega_1 \cup \partial\Omega_2$ and those on the global boundary $\partial\Omega$) come last. The three groups of mesh points are called $\underline{x}_1$, $\underline{x}_2$ and $\underline{x}_b$ respectively, and the resulting matrix system

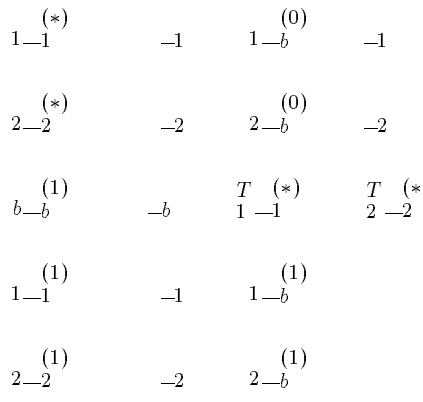
is of the form



(3 21)







Ch pter

Seri l Implement tion

This chapter outlines the serial implementation of the PCG algorithm (3.14) with some of the preconditioners in Section 3, complete with any implementation peculiarities. The metrics used for the comparison of various preconditioners are then introduced, and finally, results for all of the serial preconditioners are presented.

4.1 Serial P G Algorithm

Algorithm (3.14) is not the most efficient algorithm in terms of work and storage space; only one matrix-vector product $A\underline{p}^k$ and only one M^{-1} calculation (solution of $M\underline{z} = \underline{r}$) need be done per iteration. Values can be saved from previous iterations, and the indices of the vectors $\underline{x}$, $\underline{r}$, $\underline{p}$, etc. can be dropped, just by using them to represent the latest vectors. The following algorithm uses, apart from the storage of the problem (3.1) and the preconditioner matrix M, three

vectors and five scalars of storage,

$$
\begin{aligned}
&\underline{z} = A\underline{x} \\
&\underline{r} = \underline{b} \quad \underline{z} \\
&\underline{p} = M^{-1}\underline{r} \\
&\text{lip} = \underline{r}^T\underline{p} \\
&\text{do } i = 0, 1, \ldots, \\
&\qquad \underline{z} = A\underline{p} \\
&\qquad \text{nip} = \underline{p}^T\underline{z} \\
&\qquad \alpha = \frac{\text{nip}}{\text{lip}} \\
&\qquad \underline{x} = \underline{x} + \alpha\underline{p} \\
&\qquad \underline{r} = \underline{r} \quad \alpha\underline{z} \\
&\qquad \underline{z} = M^{-1}\underline{z} \\
&\qquad \text{nip} = \underline{r}^T\underline{z} \\
&\qquad \beta = \frac{\text{nip}}{\text{lip}} \\
&\qquad \underline{p} = \underline{z} + \beta\underline{p} \\
&\qquad \text{lip} = \text{nip}
\end{aligned}
\tag{4.1}
$$

An extra vector of storage may be needed in the parts of algorithm (4.1) where the inverse of the preconditioner M^{-1} is involved. The iterating is stopped after a predetermined maximum number of iterations, or when a measure of the residual size is small enough, e.g.

$$\|\underline{r}\|_2^2 = \underline{r}^T\underline{r} < \text{tol}^2$$

The nature of the problem being solved, and the types of preconditioner chosen to be implemented, allow several storage and time saving optimisations to be done. The preconditioners chosen to be implemented in serial were :-

CG - Standard Conjugate Gradients (Algorithm 3.11)

DCG - Diagonal Scaled CG (Section 3.4.1)

DBCG - Diagonal Block Preconditioned CG (Section 3.4.1)

ICCG - Incomplete Cholesky Preconditioned CG (Section 3.4.2)

DBICCG - Diagonal Block Incomplete Cholesky Preconditioned CG (Section 3.4.2)

DBTCG - Tridiagonal Diagonal Block Preconditioned CG (Section 3.4.1)

POLCG - Polynomial Preconditioned CG (Section 3.4.3)

The tridiagonal preconditioner (Section 3.4.1) has not been included, because, as noted in Section 3.4.1, it is equivalent, for the problem discretisation in Chapter 2, to the DBCG method with block size , and also the DBTCG method. The Iterative accelerated methods (Section 3.4.4) were not considered due to lack of time. The Domain Decomposition methods (Section 3.4.4) were not considered due to lack of time.

$\_^{(d)}$ $\_^{(1)}$

$\_^{(2)}$, so

$$\begin{array}{ccccccc}
_{}_{11} & _{}_{12} & 0 & & _{}_{1,s+1} & 0 & \\
_{}_{21} & _{}_{22} & _{}_{23} & \ddots & 0 & _{}_{2,s+2} & \\
0 & _{}_{32} & _{}_{33} & \ddots & & & \ddots \\
\vdots & \ddots & \ddots & \ddots & & & \\
_{}_{s+1,1} & 0 & & & \ddots & \ddots & 0 \\
0 & _{}_{2,s+2} & & & \ddots & _{}_{n-1,n-1} & _{}_{n-1,n} \\
\vdots & & \ddots & & 0 & _{}_{n,n-1} & _{}_{nn}
\end{array}$$

maps to

$$\begin{array}{ccccccc}
_{}_{1}^{(d)} & _{}_{1}^{(1)} & 0 & & _{}_{1}^{(2)} & 0 & \\
_{}_{1}^{(1)} & _{}_{2}^{(d)} & _{}_{2}^{(1)} & \ddots & 0 & _{}_{2}^{(2)} & \\
0 & _{}_{2}^{(1)} & _{}_{3}^{(d)} & \ddots & & & \ddots \\
\vdots & \ddots & \ddots & \ddots & & & \\
_{}_{1}^{(2)} & 0 & & & \ddots & \ddots & 0 \\
0 & _{}_{2}^{(2)} & & & \ddots & _{}_{n-1}^{(d)} & _{}_{n-1}^{(1)} \\
\vdots & & \ddots & & 0 & _{}_{n-1}^{(1)} & _{}_{n}^{(d)}
\end{array}$$

Similar types of storage mechanism can be used for most of the preconditioners,

CG

Since CG is PCG with the identity matrix, $M = I$, and thus M, or its inverse, M^{-1}, never need to be calculated, and the algorithm (4.1) simplifies slightly.

DCG

In DCG, the preconditioner is the diagonal of A, and hence to multiply by M^{-1}, division by the diagonal elements of A is performed.

DBCG

In this case M consists of diagonal blocks M_i of A, and each of these diagonal blocks is either tridiagonal or 5-diagonal. In the tridiagonal case, the solution of $M_i \underline{z} = \underline{r}$ is obtained by a simple forward and backward substitution to obtain the two factors of M_i, but in the 5-diagonal case a full[1] Cholesky decomposition has to be done to obtain the factors. This requires a problem dependent amount of extra storage for the factors, and, unfortunately, Fortran 77 cannot allocate dynamic storage, thus the arrays are just made very large at the start, hoping there is enough space for the factors given the required problem size.

In the preconditioning phase, the problem is split up into p subproblems (the size of each problem is automatically determined to make sure each one is an integer multiple of nx), and M is factored so that $M = LL^T$, i.e. each M_i is factored so that $M_i = L_i L_i^T$. During the iteration, each subproblem $M_i \underline{z} = \underline{r}$ is solved using the factor L_i by forward and backward substitution. As mentioned in Section 4.1, an extra vector of storage is required for this substitution phase.

[1]Actually, since A is banded, a banded Cholesky decomposition can be done, re uiring less storage space and time.

The splitting of the problem such as above is unnatural, in that the code required to do the splitting is rather complex, but it has been done here more for the comparison with a parallel version of the method than to give an efficient serial implementation.

The matrix is factorised using the Cholesky decomposition (3.16) with the modifications in Section 3.4.2 for the incomplete decomposition, but by using

– –

The polynomial approximation (3.20) $^{-1}$ to $^{-1}$ given in Section 3.4.3, with $= 1$, has the same sparsity as , thus only three vectors are needed to store it (Section 4.2.1). It is precalculated before the iteration starts, and the equation $\_ = \_$ is solved by a matrix multiplication $\_ = \ ^{-1}\_$.

In order to compare preconditioning strategies, some metrics for determining efficiency, rate of convergence, etc. , are required.

The easiest thing to do is to time how long each part of the PCG algorithms take for a certain problem size, and count the number of iterations required to reach a certain accuracy. The four chosen here are

4.3.2 Iteration Matrix Metrics

The idea of preconditioning is to make the condition number of $\tilde{A} = M^{-1}A$ close to one, so that $\tilde{A} \approx I$. This also means that all of the eigenvalues of $\tilde{A}$ are required to be bunched around one, and hence the spectral radius of $\tilde{A}$ needs to be small.

Using the ISPACK [21] library of eigenvalue and eigenvector routines, a complete eigenvalue spectrum, $\lambda(\tilde{A})$, can be obtained from the $\tilde{A}$'s from each preconditioner. From $\lambda(\tilde{A})$ it is possible to obtain the condition number, $\kappa_2(\tilde{A})$, and the spectral radius, $\rho(\tilde{A})$.

4.4 Serial Implementation Results

The preconditioners in Section (4.2.2) were implemented in Fortran 77. All the timings were obtained by running the programs on a single transputer (See Chapter 5). All of the graphs were obtained using the UNIRAS graphics library, and the eigenvalue spectra were obtained using the ISPACK subroutines, both on Sun Sparc computers.

Since the DBCG and DBICCG methods require a block size, or alternatively, the number of subproblems to split the problem into, and the fact that the transputer system available (See Chapter 5) has five processors, it was decided, for both of these methods, to have the number of subproblems as one, two, three, four, or five (to allow direct comparisons with the parallel versions (See Section 5.7)). The number of subproblems is indicated by following DBCG or DBICCG by the number, e.g. DBCG2 for two subproblems. DBCG1 is equivalent to directly solv-

Method	γ_0	γ_1
POLCG1	1.0	-1.0
POLCG2	1.1429	-1.1429
POLCG3	0.9412	-0.4706
POLCG4	1.16666	-0.83333

Table 4.1: Parameters for the POLCG method

ing the problem by Cholesky Decomposition (3.16), ignoring the time spent in performing one iteration of the PCG method, and DBICCG1 is equivalent to ICCG. Four versions of the POLCG were used, with their γ_0 and γ_1 defined as in Table 4.1. Occasionally, the results show a TRICG method. This is just a full tridiagonal preconditioner, and in terms of performance is just about equivalent to DBTCG (the solution stage takes slightly longer, but the end result is the same).

4.4.1 Timings

Tables 4.2, 4.3, 4.4, and 4.5 show, in order of increasing total iteration time, the number of iterations required to reach convergence (in this case for the 2-norm of the residual to fall below 10^{-8}), the preconditioning time, the time per iteration, and the total time for each of the investigated methods on two problem sizes (10 by 10 and 20 by 20) and for both of the sample problems (Section 2.4). The times involved are measured in ticks of $\frac{1}{16525}$ths of a second.

The Figures 4.1 and 4.2 show the number of iterations and total time required as the problem size increases (from 5 by 5, i.e. 25 unknowns, to 30 by 30, i.e. 900

Method	Iterations	Preconditioning Time	Iteration Time	Total Time
DBCG1	1	1511	376	1886
ICCG	17	156	137	2493
POLCG4	27	120	135	3764
DBICCG2	25	166	147	3848
POLCG3	28	120	135	3899
CG	44	55	91	4090
DCG	42	58	100	4282
DBICCG3	27	170	154	4351
DBICCG4	29	178	164	4952
POLCG2	37	120	135	5119
DBTCG	43	96	120	5281
TRICG	43	103	128	5647
DBICCG5	32	186	176	5827
POLCG1	37	120	135	5827
DBCG2	15	1409	347	6625
DBCG3	23	1306	327	8841
DBCG4	27	1205	307	9514
DBCG5	30	1109	287	9740

Table 4.2: Iterations and timings for Problem 1 (10 by 10)

Method	Iterations	Preconditioning Time	Iteration Time	Total Time
ICCG	30	634	554	17279
DBCG1	1	17904	2510	20414
DBICCG2	43	673	596	26338
POLCG4	52	484	546	28785
DBICCG3	46	700	634	29885
POLCG3	58	484	546	32080
DBICCG4	48	740	680	33427
CG	93	223	368	34476
DBICCG5	50	775	722	36899
DCG	91	234	405	36962
DBTCG	88	386	484	43033
TRICG	88	417	517	45998
POLCG1	86	484	546	47454
POLCG2	86	484	546	47454
DBCG2	18	17249	2398	60428
DBCG3	31	16581	2318	88469
DBCG4	38	15955	2239	101066
DBCG5	43	15333	2160	108230

Table 4.3: Iterations and timings for Problem 1 (20 by 20)

Method	Iterations	Preconditioning Time	Iteration Time	Total Time
DBCG1	1	1510	376	1886
ICCG	21	157	137	3042
DBICCG2	25	166	147	3848
DBICCG3	28	170	154	4505
DBICCG4	30	178	164	5116
DBTCG	44	96	120	5402
DBICCG5	31	186	176	5651
DCG	56	58	100	5706
TRICG	44	104	128	5776
POLCG3	42	120	135	5798
DBCG2	15	1408	347	6624
POLCG4	57	120	135	7830
CG	87	55	92	8063
DBCG3	23	1306	327	8841
DBCG4	27	1206	307	9515
DBCG5	31	1110	287	10029
POLCG2	85	120	135	11627
POLCG1	86	120	135	11763

Table 4.4: Iterations and timings for Problem 2 (10 by 10)

Method	Iterations	Preconditioning Time	Iteration Time	Total Time
DBCG1	1	17904	2510	20414
ICCG	38	635	554	21709
DBICCG2	43	672	596	26338
DBICCG3	46	700	634	29886
DBICCG4	48	740	680	33427
DBICCG5	51	774	722	37621
DBTCG	88	385	484	43032
POLCG3	83	484	547	45807
TRICG	88	417	517	45998
DCG	120	234	405	48846
DBCG2	19	17249	2398	62825
CG	188	223	370	69837
POLCG4	128	484	547	70517
DBCG3	31	16582	2319	88471
DBCG4	38	15955	2239	101067
DBCG5	43	15335	2160	108233
POLCG1	218	484	547	119937
POLCG2	218	484	547	119937

Table 4.5: Iterations and timings for Problem 2 (20 by 20)

unknowns).

A number of observations can be made from these tables and figures,

In terms of iteration count the ICCG method is only beaten by the DBCG methods with a small number of subproblems.

In terms of total time the ICCG method is only ever beaten by the DBCG1 method (the direct solution), and as the problem size increases the difference between them decreases, and for large problem sizeseum2nBffsizktheOI fr3eI

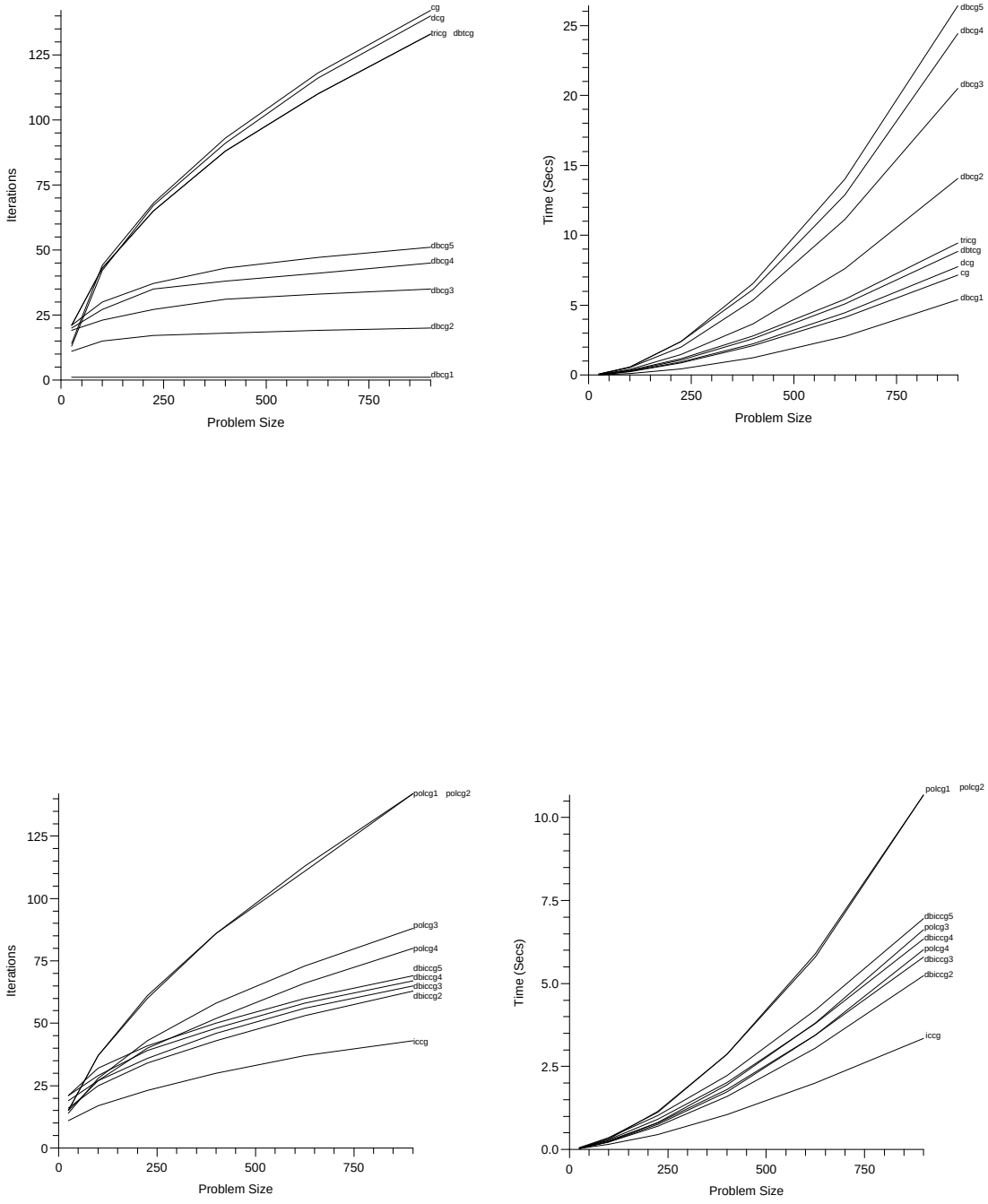
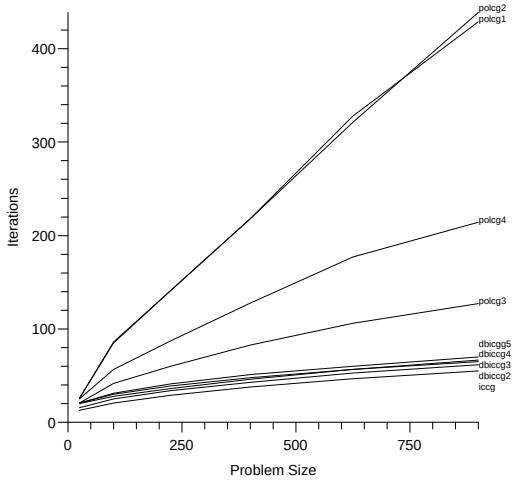
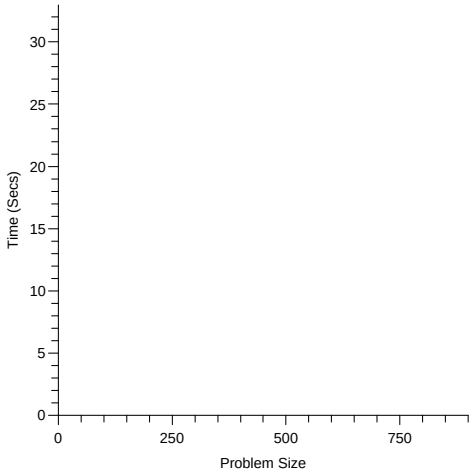
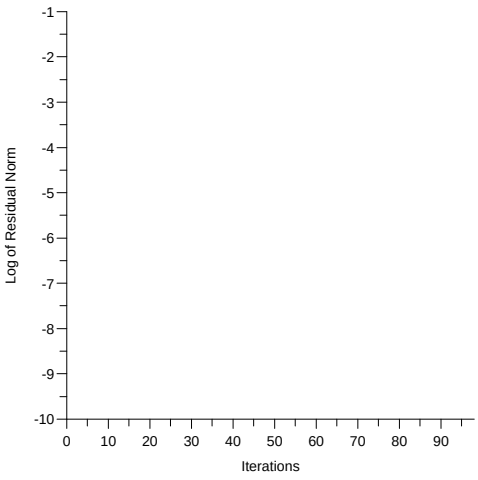


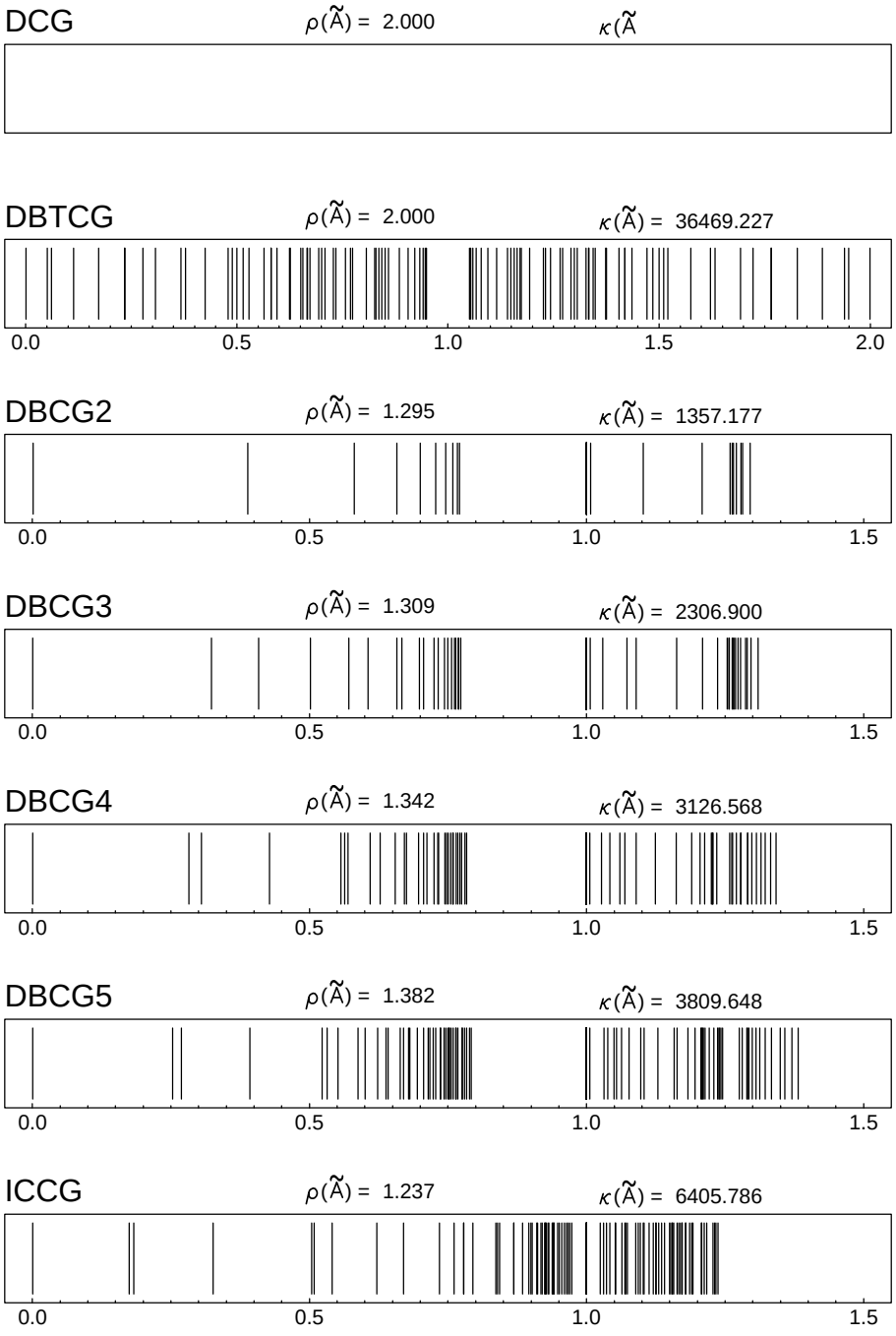
Figure 4.1: Work involved in problem 1 as problem size increases

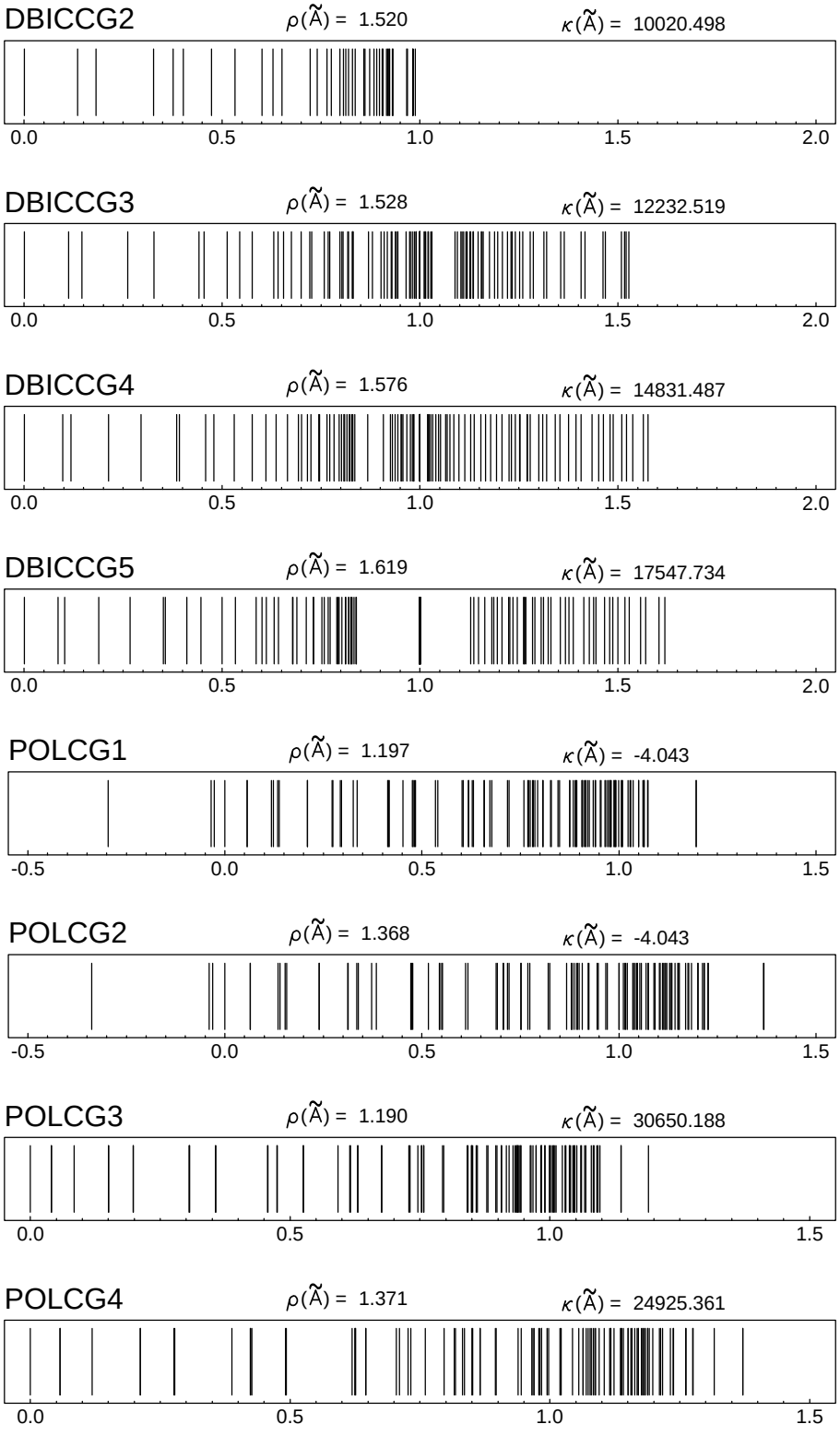

polcg2
polcg1
polcg4
polcg3
dbicgg5
dbiccg4
dbiccg3
dbiccg2
iccg
Iterations
Problem Size
0
100
200
300
400
0
250
500
750


Time (Secs)
Problem Size
0
5
10
15
20
25
30
0
250
500
750


-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
Log of Residual Norm
0
10
20
30
40
50
60
70
80
90
Iterations

Section 3.2, the Figures 4.1 and 4.2, the Tables 4.2, 4.3, 4.4, and 4.5, and the above eigenvalue spectrum figures, a number of observations can be made;


DCG
$\rho(\tilde{A}) = 2.000$
$\kappa(\tilde{A}$
DBTCG
$\rho(\tilde{A}) = 2.000$
$\kappa(\tilde{A}) = 36469.227$
0.0
0.5
1.0
1.5
2.0
DBCG2
$\rho(\tilde{A}) = 1.295$
$\kappa(\tilde{A}) = 1357.177$
0.0
0.5
1.0
1.5
DBCG3
$\rho(\tilde{A}) = 1.309$
$\kappa(\tilde{A}) = 2306.900$
0.0
0.5
1.0
1.5
DBCG4
$\rho(\tilde{A}) = 1.342$
$\kappa(\tilde{A}) = 3126.568$
0.0
0.5
1.0
1.5
DBCG5
$\rho(\tilde{A}) = 1.382$
$\kappa(\tilde{A}) = 3809.648$
0.0
0.5
1.0
1.5
ICCG
$\rho(\tilde{A}) = 1.237$
$\kappa(\tilde{A}) = 6405.786$
0.0
0.5
1.0
1.5


DBICCG2
$\rho(\tilde{A})$ = 1.520
$\kappa(\tilde{A})$ = 10020.498
0.0 0.5 1.0 1.5 2.0
DBICCG3
$\rho(\tilde{A})$ = 1.528
$\kappa(\tilde{A})$ = 12232.519
0.0 0.5 1.0 1.5 2.0
DBICCG4
$\rho(\tilde{A})$ = 1.576
$\kappa(\tilde{A})$ = 14831.487
0.0 0.5 1.0 1.5 2.0
DBICCG5
$\rho(\tilde{A})$ = 1.619
$\kappa(\tilde{A})$ = 17547.734
0.0 0.5 1.0 1.5 2.0
POLCG1
$\rho(\tilde{A})$ = 1.197
$\kappa(\tilde{A})$ = -4.043
-0.5 0.0 0.5 1.0 1.5
POLCG2
$\rho(\tilde{A})$ = 1.368
$\kappa(\tilde{A})$ = -4.043
-0.5 0.0 0.5 1.0 1.5
POLCG3
$\rho(\tilde{A})$ = 1.190
$\kappa(\tilde{A})$ = 30650.188
0.0 0.5 1.0 1.5
POLCG4
$\rho(\tilde{A})$ = 1.371
$\kappa(\tilde{A})$ = 24925.361
0.0 0.5 1.0 1.5

POLCG3

POLCG4 $\rho(\tilde{A}) = 2.070$ $\kappa(\tilde{A}) = -4.799$

DBTCG has a better bunching of its eigenvalues around one, and, as predicted by theory, better convergence than DCG (in terms of iterations).

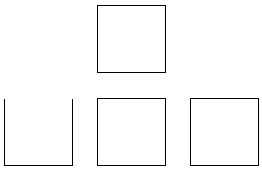
The DBCG methods all have similar spectra, and although not shown, DBCG1 has all its eigenvalues equal to one, and converges in one iteration! DBCG2 has a lot of repeated eigenvalues, and DBCG3-5 just have these repeated eigenvalues spreading out. All of them are pretty well bunched, and their convergence (in iterations) echoes this.

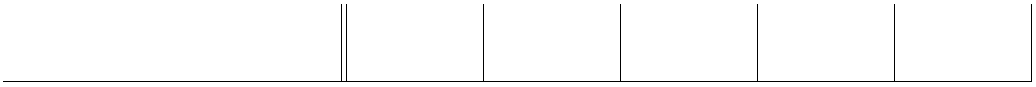
[1]The system is currently on loan from the Rutherford Appleton Laboratory as part of the

memory, a RISC[2] processor, a hardware process queue to allow concurrent running of multiple processes on a single transputer, and four bi-directional serial communication links to connect to other transputers, all on a single VLSI[3] chip.

[2]Reduced Instruction Set Computer, the idea being it is easier to make a very fast simple processor than a complex slower one.

[3]Very Large Scale Integration.





instructions to the data it is processing. Since a transputer system is built up from a number of independent processors, each with their own memory, a transputer system is a member of the MIMD (Multiple Instruction stream, Multiple Data stream) class of parallel computers. If, however, each transputer executes the same program, but on its own data, then it can be considered to be a SIMD (Single Instruction stream, Multiple Data stream) system. This is how it has been chosen to use the Reading System, due to the nature of the problem to be solved, i.e. give each processor part of the matrix system.

5.1.4 Software Model

The transputer is designed to efficiently implement the OCCAM language. However since the standard numerical analysts' language is FORTRAN 77, parallel FORTRAN 77 is available, e.g. Reading has the 3L parallel FORTRAN 77 package [1].

There are two main types of software parallelisation available in 3L FORTRAN, tasks and threads.

Tasks

A task is a FORTRAN program. The structure of tasks within a system is static, i.e. tasks are not created and destroyed dynamically during execution, and no hierarchy exists, e.g. tasks cannot have subtasks. The structure of tasks is controlled in the 3L system by a configuration file that indicates the distribution of tasks among the various available processors and describes the links between them [1, 16]. ach task is a separate entity, no data is shared between them, even

if they are on the same transputer. They can only communicate via channels which are fixed one way communication paths. A complete transputer application consists of a collection of one or more tasks. A task may contain several concurrent threads.

A thread is a FORTRAN subroutine. They can be created and destroyed dynamically and a thread my be created within another thread. Starting a thread is like making a subroutine call, except that the calling program regains control immediately, and the thread runs concurrently with the calling program. Threads can share FORTRAN common blocks, and thus can communicate directly.

The 3L FORTRAN runtime library provides a simple interface to allow tasks to communicate. Basically, it consists of send message and receive message function calls which send and receive a packet of data to or from a channel. The possible channels are determined indirectly by the configuration file [16].

The most obvious approach to parallelise an algorithm is to examine it and convert it into a procedure that operates on composite mathematical objects, such as

inherent parallelism, and be more adaptable.

When a problem is split into a number of subproblems, it is desired that each of the subproblems are independent from the others. This would allow each problem to be solved on a separate processor. Unfortunately, very few algorithms split up into totally independent subproblems, and some global communication needs to be done, e.g. calculation of an inner product where both vectors are distributed over the network. During such a global communication, all processors have to wait to receive their information from the others before they can continue processing[5]. This global synchronisation limits the amount of work that can be done in parallel, and thus affects the performance of the algorithm, thus, each transputer should do a large amount of computation with respect to communication.

5.2.1 Alternative parallel PCG algorithm

The serial PCG algorithm (4.1) given in Section 4 has two vector inner products (three depending on the termination condition) requiring global communication between the processors, and they do not appear in the same position in the algorithm. An alternative algorithm, proposed by Meurant, described in [13], has an extra inner product and two extra vectors of storage, but all the inner products appear at the same point, and thus they can all be calculated at the

[5]In SIMD or shared memory MIMD systems each processor can have access to all of the memory, so the problems are not as serious.

same time.

$$\underline{w} = A\underline{x}$$

$$\underline{r} = \underline{b} - \underline{w}$$

$$\underline{z} = M^{-1}\underline{r}$$

$$\underline{p} = \underline{z}$$

do $i = 0, 1, \ldots, \{$

$$\begin{aligned}
\underline{w} &= A\underline{p} \\
\underline{v} &= M^{-1}\underline{w} \\
\text{ip1} &= \underline{v}^T\underline{w} \\
\text{ip2} &= \underline{w}^T\underline{p} \\
\text{ip3} &= \underline{r}^T\underline{z} \\
\alpha &= \frac{(\text{ip3})}{(\text{ip2})} \\
s &= \alpha^2\,(\text{ip1}) - (\text{ip3}) \\
\beta &= \frac{s}{(\text{ip3})} \\
\underline{x} &= \underline{x} + \alpha\underline{p} \\
\underline{r} &= \underline{r} - \alpha\underline{w} \\
\underline{z} &= \underline{z} - \alpha\underline{v} \\
\underline{p} &= \underline{z} + \beta\underline{p}
\end{aligned} \tag{5.1}$$

}

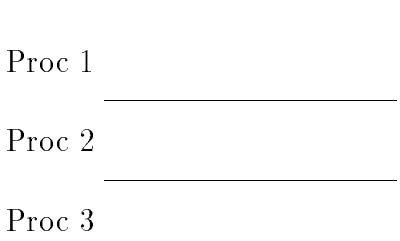


Figure 5.3: Sample split of over three processors

The by matrix problem, where = ,

$$\_ = \_$$

now has to be split up so that it can be solved on processors. It is sensible to allocate similar size parts of the problem to each processor, to make sure that each processor does a similar amount of work. Noting from Section 3.4.1 that the block preconditioners require the block size, $_i$ to be an integer multiple of , for the ease of programming, we enforce these restrictions for all the preconditioners. The matrix is split up into parts of $_i$ contiguous rows of , where = 1 2 ... . The same happens for all vectors on each processor. ach processor stores its part of in the same way as Section 4.2.1 for the serial case, e.g. for a 18 by 18

$$\begin{matrix} \_^{d}_{7} & \_^{d}_{12} & \_^{1}_{6} & \_^{1}_{12} & & \_^{2}_{4} & \_^{2}_{12} \\ & & & & & \_^{d}_{i} & \_^{d}_{i+s-1} \end{matrix}$$

$$\_^{1}_{i-1} \quad \_^{1}_{i+s-1} \quad \_^{2}_{i-nx} \quad \_^{2}_{i+s-1}$$

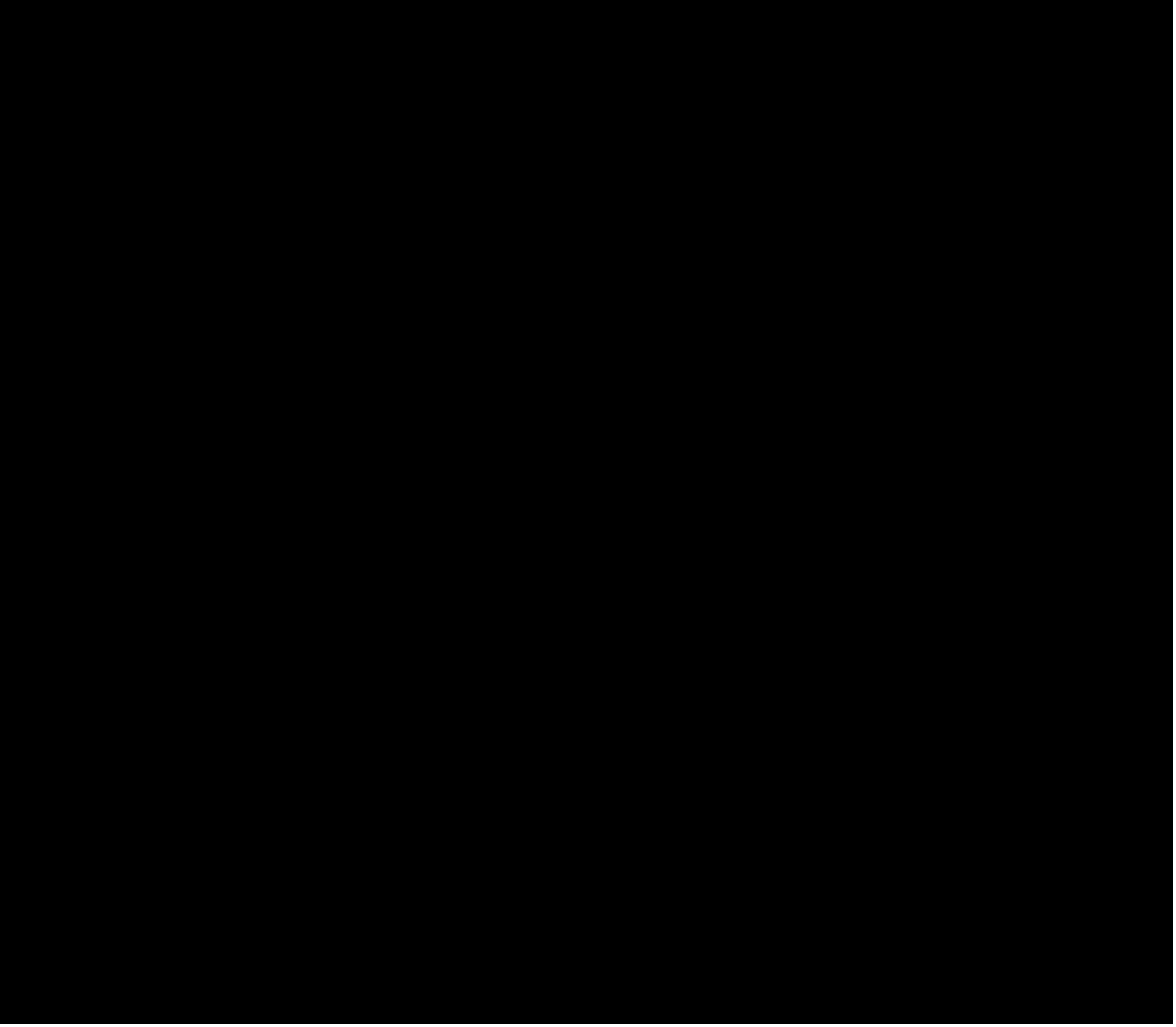
$$\_$$

$$\_ \qquad\qquad \_^{i-nx}_{} \quad \_^{i-1}_{} \qquad\qquad \_$$

from the 'below' processor $\_{i+s}$ to $\_{i+s+nx-1}$.

In order to effectively implement an algorithm on an arbitrary number of processors connected in an arbitrary communications network, it is necessary to have an effective communications harness [3] that takes out the need for the user to know the details of the network. This harness provides a transparent message routing system that allows any processor to send a message to any other, irrespective of the network topology. The harness runs in parallel with the processes on each transputer. The harness is implemented as a library of function calls, which the user links in when compiling their program. The main process on each transputer calls an initialise function which sets up all the required information about the network, and then all communication is done via the harness library calls. The main advantage of harnesses is that if, say, an algorithm was developed on a pipeline transputer system, to move it to a two dimensional array network would only require the writing of an array harness, the actual algorithm would remain unchanged.

In a similar vein, it is a good idea to write a library of subroutines for doing various useful things, such as matrix-vector multiplication or vector inner products, where the matrices or vectors are distributed over the network (See [14] for the implementation of a complete matrix and vector package on a Hypercube).



as opposed to $O(p)$ for the pipeline [14].

5.4.3 Matrix-vector Multiplication

This subroutine is called before the transputer does its local matrix-vector multiplication to obtain the parts of the vector that are stored in the 'above' and 'below' transputers (See Section 5.3).

5.4.4 Solution Collection

This subroutine collects all of the partial solutions $\underline{x}_i$ and assembles them into the solution, $\underline{x}$, on the master transputer.

5.5 Parallel Preconditioner Implementation

The preconditioners investigated in parallel are the same ones that were looked at in Section 4. All of those, except the ICCG algorithm and the POLCG algorithm, are inherently parallel, that is the work involved in putting the problem on a set of processors and the implementation of the harness suffices to allow the parallel implementation to be done.

5.5.1 POLCG Preconditioner

The POLCG algorithm, can be easily implemented in parallel if the storage of A on each processor (Section 5.3) is modified slightly. The diagonal of A, $\underline{a}^d$, has to extend nx positions above the first equation in the block, i.e. as in Section 5.3 we need $\underline{a}^d_{i-nx}$ to $\underline{a}^d_{i+s-1}$, $\underline{a}^1_{i-1}$ to $\underline{a}^1_{i+s-1}$, and $\underline{a}^2_{i-nx}$ to $\underline{a}^2_{i+s-1}$. This modification

allows the storage of the equivalent part of the $^{-1}$ approximation as that of in each processor, thus the $\_$ and the approximate $^{-1}\_$ multiplications have the same form.

$^{T}\_\quad\_$

$$T_{\_\quad\_}$$

$$\_\quad\_$$

$$T_{\_\quad\_}$$

Although this preconditioner was not considered in serial due to the structure of the matrix from the problem discretisation, an efficient tridiagonal solver for a pipeline network was discovered in [19]. It used the technique of cyclic reduction

p

p

exists,

$$\frac{*}{p} = \frac{\text{execution time on one processor with best serial algorithm}}{\text{execution time on processors with parallel algorithm}}$$

The best serial algorithm in this case is the ICCG algorithm. There are other

ICCG algorithm, the S_p^* speedup is not calculated. The number of iterations is obviously the same as for the serial case. The times given when one processor is being used are not the same as those obtained when using the serial algorithm, they are slightly larger. This is due to the fact that the modified PCG algorithm is being used, not the basic PCG algorithm.

- All the results show a decrease in iteration time for increasing the processors from one to five. As the results for the 5x5 systems show, this decrease may not last for much longer after five processors.

- The rate of decline of the parallel efficiency drops as the problem size gets larger.

- The smaller the problem size and the larger the number of processors, the less efficient the method will be, due to the increase in communication traffic compared to computation.

- Parallel efficiencies of over 90% are obtained when the problem size is greater than or equal to 20 by 20.

- Some of the entries in the E_p column are greater than 100% due to the unequal splitting of the problem over the transputers. As shown in Table 5.1, not all the transputers are the same speed, and, for example, a 20 by 20 problem on 3 processors will put 120 equations on the first, and 140 each on the second and third, and since transputers 2 and 3 are faster than the first, the equations get solved in the time that it should take for 360.

Problem Size	Processors	Time	$_p$	$_p$
5x5	1	553	1.00	100
	2	298	1.85	92.8
	3	240	2.30	76.8
	4	237	2.33	58.3
	5	206	2.68	53.7
10x10	1	6128	1.00	100
	2	3257	1.88	94.1
	3	2092	2.93	97.6
	4	1628	3.76	94.1
	5	1542	3.97	79.5
20x20	1	50172	1.00	100
	2	25487	1.97	98.4
	3	15658	3.20	107
	4	13237	3.79	94.8
	5	10816	4.63	92.8
30x30	1	175373	1.00	100
	2	88135	1.99	99.5
	3	59045	2.97	99.0
	4	41870	4.18	104
	5	36191	4.84	97.0

Problem Size	Processors	Time	$_p$	$_p$
	1	999	1.00	100
	2	514	1.94	97.2

Problem Size	Processors	Time	S_p	E_p
5x5	1	534	1.00	100
	2	283	1.89	94.3
	3	229	2.33	77.7
	4	224	2.38	59.6
	5	196	2.72	54.5
10x10	1	6119	1.00	100
	2	3309	1.85	92.5
	3	2114	2.89	96.5
	4	1631	3.75	93.8
	5	1552	3.94	78.9
20x20	1	51429	1.00	100
	2	26129	1.97	98.4
	3	16031	3.21	107
	4	13537	3.80	95.0
	5	11041	4.66	93.2
30x30	1	177309	1.00	100
	2	89224	1.98	99.4
	3	59843	2.96	98.8
	4	42423	4.17	104
	5	36661	4.84	96.7

Table 5.4: DCG for problem 1 with increasing number of processors

Problem Size	Processors	Time	$_p$	$_p$
5x5	1	874	1.00	100
	2	465	1.88	94.0
	3	374	2.34	77.9
	4	369	2.37	59.2
	5	318	2.75	55.0
10x10	1	8118	1.00	100
	2	4290	1.89	94.6
	3	2742	2.96	98.7

Of all the serial preconditioning strategies investigated in Chapter 4, the ICCG method was found to outperform all the rest, and on the larger problem sizes, outperformed a direct Cholesky Decomposition of the matrix . For problem 1, a surprising number of the preconditioning strategies were outperformed by the standard CG method, although for problem 2, most did outperform CG. The only other methods, apart from ICCG, that performed well over both the sample problems were the DBICCG methods, although some success was had with the POLCG methods used on problem 1. The overall performance of the POLCG methods was not as good as expected, especially on problem 2. The same applied to the DBTCG method, although this was better on problem 2. Since most physical problems would be far closer to problem 2 than problem 1, we would want to investigate further the methods which work well on problem 2.

No concrete evidence was obtained for direct links between condition number of the iteration matrix and the CG convergence, or spectral radius and CG

lation. The clustering of eigenvalues appears to have a greater effect, although no quantitative measure of eigenvalue clustering could be found in order to examine the effect in detail.

A transputer library for the Reading transputer system was successfully implemented for the pipeline of processors, but, unfortunately, only the CG and DCG methods could be implemented in parallel, and further work is required to debug the remaining preconditioners. This has not stopped the investigation of the parallelisation of the CG and DCG methods, and Chapter 5 has shown that where problem size was far greater than number of processors, parallel efficiencies of over 90% can be achieved. Since most of the remaining preconditioners are all of a similar structure to CG and DCG (they are all inherently 'blocked' into independent subproblems), the high efficiencies should also be obtainable. The ease of obtaining these high parallel efficiencies was surprising considering that the communication network was a pipeline, but the possible overheads involved with a pipeline probably would not appear until a far larger number of processors were used. Further work is required on the parallelisation of the ICCG method, although, as shown in the serial case, the DBICCG methods can perform well over both sample problems (and, in theory

Appendix A

Basic Matrix Theory

This appendix describes some of the basic matrix theory associated with this dissertation. Unless otherwise stated, the theory applies to n by n real, square matrices. The elements of the matrix A are denoted a_{ij}, where i and j range from 1 to n.

Symmetry

The matrix A is symmetric if

$$A = A^T$$

Positive Definite

The matrix A is positive definite if

$$\forall \underline{x} \neq 0, \quad \underline{x}^T A \underline{x} > 0$$

Diagonal Dominance

The matrix A is diagonally dominant if

$$\forall i, \quad |a_{ii}| \geq \sum_{j=1}^{i-1} |a_{ij}| + \sum_{j=i+1}^{n} |a_{ij}|$$

It is strictly diagonally dominant if the inequality $\geq$ is a strict inequality $>$.

Irreducible

The matrix A is irreducible if

$$\nexists P \text{ such that } P^T A P = \begin{bmatrix} A_1 & A_2 \\ 0 & A_3 \end{bmatrix}$$

i.e. the matrix A cannot be partitioned so that there are two or more independent groups of equations.

Irreducible Diagonal Dominance

The matrix A is irreducibly diagonally dominant if it is diagonally dominant, with a strict inequality for at least one i, and it is irreducible.

Existence of A^{-1}

If A is irreducibly diagonally dominant, $a_{ii} > 0$, and $a_{ij} \leq 0$ for $i \neq j$, then A is positive definite and A^{-1} exists.

Eigenvalues

The n eigenvalues, λ_i, of the matrix A are the solutions of

$$\det(A - \lambda I) = 0$$

They are all real if A is symmetric, and all positive if A is positive definite.

Spectrum

The spectrum of the matrix A, $\lambda(A)$, is the set of all the eigenvalues of A

$$\lambda(A) = \{ \lambda_i \,|\, i = 1, 2, \ldots, n \}$$

Spectral Radius

The spectral radius, $\rho(A)$, of the matrix A is defined by

$$\rho(A) = \max_{1 \le i \le n} (|\lambda_i|)$$

Vector Norms

A vector norm on $\mathbb{R}^n$ is a function $f : \mathbb{R}^n \mapsto \mathbb{R}$, denoted $f(\underline{x}) = ||\underline{x}||$, such that

$$\begin{aligned} f(\underline{x}) &\ge 0 && \underline{x} \in \mathbb{R}^n,\ f(\underline{x}) = 0 \text{ iff } \underline{x} = 0 \\ f(\underline{x} + \underline{y}) &\le f(\underline{x}) + f(\underline{y}) && \underline{x},\ \underline{y} \in \mathbb{R}^n \\ f(\alpha \underline{x}) &= |\alpha| f(\underline{x}) && \alpha \in \mathbb{R},\ \underline{x} \in \mathbb{R}^n \end{aligned}$$

Some useful norms are the p-norms, where

$$||\underline{x}||_p = \sqrt[p]{\sum_{i=1}^{n} |\underline{x}_i|^p}, \qquad p \ge 1$$

of which the 1, 2, and ∞ norms are the most important

$$\begin{aligned} ||\underline{x}||_1 &= \sum_{i=1}^{n} |\underline{x}_i| \\ ||\underline{x}||_2 &= \sqrt{\sum_{i=1}^{n} |\underline{x}_i|^2} = \sqrt{\underline{x}^T \underline{x}} \\ ||\underline{x}||_\infty &= \max_{1 \le i \le n} |\underline{x}_i| \end{aligned}$$

Another useful norm is the A-norm

$$||\underline{x}||_A = \sqrt{\underline{x}^T A \underline{x}}$$

Matrix Norms

Similar to the vector norms, matrix norms are a function $f : \mathbb{R}^{m\times n} \mapsto \mathbb{R}$, denoted $f(A) = ||A||$, such that

$$\begin{aligned} f(A) &\geq 0 && A \in \mathbb{R}^{m\times n},\ f(A) = 0 \text{ iff } A = 0 \\ f(A+B) &\leq f(A) + f(B) && A,\ B \in \mathbb{R}^{m\times n} \\ f(\alpha A) &= |\alpha| f(A) && \alpha \in \mathbb{R},\ A \in \mathbb{R}^{m\times n} \end{aligned}$$

The frequently used norms are the Frobenius norm

$$||A||_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} |a_{ij}|^2}$$

and the p-norms

$$||A||_p = \sup_{\underline{x}\neq 0} \frac{||A\underline{x}||_p}{||\underline{x}||_p}$$

The 1, 2, and ∞ matrix norms have alternative expressions

$$\begin{aligned} ||A||_1 &= \max_{1\leq j\leq n} \sum_{i=1}^{m} |a_{ij}| \\ ||A||_2 &= \sqrt{\rho(A^T A)} \\ ||A||_\infty &= \max_{1\leq i\leq m} \sum_{j=1}^{n} |a_{ij}| \end{aligned}$$

Condition Number

The condition number of a matrix A, $\kappa(A)$, is defined as

$$\kappa(A) = ||A||\ ||A^{-1}||$$

with the convention that $\kappa(A) = \infty$ if A is singular. It is a measure of how sensitive the $A\underline{x} = \underline{b}$ problem is to numerical solution, the larger the condition number the more sensitive the problem is to rounding errors. Note that $\kappa(A)$

depends on the underlying matrix norm, and when this norm is to be stressed, subscripts are used, e.g.

$$_2(\ ) = \quad _2 \quad ^{-1} \ _2$$

The $_2(\ )$ norm can also be expressed as

$$_2(\ ) = \frac{max}{min}$$

where $_{max}$ and $_{min}$ are the maximum and minimum eigenvalues of .

The matrix is weakly cyclic index (1) if there exists a permutation matrix such that ^{T} is of the form

$$^T = \begin{bmatrix} 0 & 0 & & & 0 & _{1,k} \\ _{21} & 0 & & & 0 & 0 \\ 0 & _{32} & \ddots & & & \vdots \\ \vdots & 0 & \ddots & \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & & 0 & _{k,k-1} & 0 \end{bmatrix}$$

If the Jacobi matrix, $= \ ^{-1}(+)$, where is the diagonal of , is the lower triangular part of , and is the upper triangular part of , is weakly cyclic index (2), then is a -cyclic matrix. It can be shown that a block tridiagonal matrix is a 2-cyclic matrix [22].

[1] 3L Ltd. , December 1990. Software version 2.1.3.

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