Outline:

- MPI Master–Worker paradigm
- Linear algebra
- LAPACK and the BLAS

References:

- $UWHPSC/codes mpi$
- class notes: MPI section
- class notes: Linear algebra
Another Send/Receive example

Computing the 1-norm of a matrix,

\[ \|A\|_1 = \max_j \sum_i |a_{ij}| = \max \text{ of 1-norm of column vectors} \]

\[ \implies \|Ax\|_1 \leq \|A\|_1 \|x\|_1 \text{ for all } x. \]

Sample codes are now in...

$UWHPSC/codes/mpi/matrix1norm1.f90$: 
   Same number of processes as columns,

$UWHPSC/codes/mpi/matrix1norm2.f90$: 
   Possibly more (or fewer) columns than processes.

The latter case shows the more typical situation where master process must send out new work as processes finish.

Can also view in class notes: MPI section
Another Send/Receive example

Master (Processor 0) sends \( j \)th column to Worker Processor \( j \),
gets back 1-norm to store in \( \text{anorm}(j) \), \( j = 1, \ldots, \text{ncols} \)

! code for Master (Processor 0):
if (proc_num == 0) then

    do j=1,ncols
        call MPI_SEND(a(1,j), nrows, MPI_DOUBLE_PRECISION,&
                       j, j, MPI_COMM_WORLD, ierr)
    enddo

    do j=1,ncols
        call MPI_RECV(colnorm, 1, MPI_DOUBLE_PRECISION, &
                      MPI_ANY_SOURCE, MPI_ANY_TAG, &
                      MPI_COMM_WORLD, status, ierr)
        jj = status(MPI_TAG)
        anorm(jj) = colnorm
    enddo
endif

Note: Master may receive back in any order!

MPI\_ANY\_SOURCE will match first to arrive.

The tag is used to tell which column’s norm has arrived (\( jj \)).
Send and Receive example — worker code

Master (Processor 0) sends $j$th column to Worker Processor $j$, gets back 1-norm to store in $\text{anorm}(j)$, $j = 1, \ldots, \text{ncols}$

! code for Workers (Processors 1, 2, ...):

if (proc_num /= 0) then

    call MPI_RECV(colvect, nrows, MPI_DOUBLE_PRECISION, &
                  0, MPI_ANY_TAG, &
                  MPI_COMM_WORLD, status, ierr)

    j = status(MPI_TAG) ! this is the column number
                        ! (should agree with proc_num)

    colnorm = 0.d0
    do i=1,nrows
        colnorm = colnorm + abs(colvect(i))
    enddo

    call MPI_SEND(colnorm, 1, MPI_DOUBLE_PRECISION, &
                  0, j, MPI_COMM_WORLD, ierr)

endif

Note: Sends back to Process 0 with tag $j$. 

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It is best to *use high-quality software* as much as possible, for several reasons:

- It will take *less time* to figure out how to use the software than to write your own version. (Assuming it’s well documented!)

- Good general software has been *extensively tested* on a wide variety of problems.

- Often general software is much *more sophisticated* than what you might write yourself, for example it may provide error estimates automatically, or it may be *optimized* to run fast.
Software sources

- Netlib: http://www.netlib.org
- Trilinos: http://trilinos.sandia.gov/
- DOE ACTS: http://acts.nersc.gov/
- PETSc nonlinear solvers: http://www.mcs.anl.gov/petsc/petsc-as/
- Many others!
The code in $UWHPSC/codes/fortran/zeroin illustrate how to use the function zero\text{in} obtained from the Golden Oldies (go) directory of Netlib.

See: http://www.netlib.org/go/index.html

Estimates a zero of the function $f(x)$ between $ax$ and $bx$ within some tolerance.

Note: Fortran 77 style!
Many routines for linear algebra.

Typical name: XYYZZZ

- **X** is precision
- **YY** is type of matrix, e.g. GE (general), BD (bidiagonal),
- **ZZZ** is type of operation, e.g. SV (solve system),
  EV (eigenvalues, vectors), SVD (singular values, vectors)
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Examples:

**DGESV** can be used to solve a general $n \times n$ linear system in double precision.

**DGTSV** can be used to solve a general $n \times n$ tridiagonal linear system in double precision.
Installing LAPACK

On Virtual Machine or other Debian or Ubuntu Linux:

    $ sudo apt-get install liblapack-dev

This will include BLAS (but not optimized for your system).
Alternatively can download tar files and compile.

See complete documentation at

http://www.netlib.org/lapack/
Basic Linear Algebra Subroutines

Core routines used by LAPACK (Linear Algebra Package) and elsewhere.

Generally optimized for particular machine architectures, cache hierarchy.

Can create optimized BLAS using ATLAS (Automatically Tuned Linear Algebra Software)

See notes and http://www.netlib.org/blas/faq.html

- Level 1: Scalar and vector operations
- Level 2: Matrix-vector operations
- Level 3: Matrix-matrix operations
Subroutine names start with:

- S: single precision
- D: double precision
- C: single precision complex
- Z: double precision complex

Examples:

- SAXPY: single precision replacement of $y$ by $\alpha x + y$.
- DDOT: dot product of two vectors
- DGEMV: matrix-vector multiply, general matrices
- DGEMM: matrix-matrix multiply, general matrices
- DSYMM: matrix-matrix multiply, symmetric matrices
If `program.f90` uses BLAS routines...

```
$ gfortran -c program.f90
$ gfortran program.o -lblas
```

or can combine as

```
$ gfortran program.f90 -lblas
```

When linking together `.o` files, will look for a file called `libblas.a` (probably in `/usr/lib`).

This is a archived static library.
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When linking together `.o` files, will look for a file called `libblas.a` *(probably in `/usr/lib`).*

This is a archived static library.

Can specify different library location using `-L/path/to/library`.
Making blas library

Download http://www.netlib.org/blas/blas.tgz.

Put this in desired location, e.g.  $HOME/lapack/blas.tgz

$ cd $HOME/lapack
$ tar -zxf blas.tgz  # creates BLAS subdirectory
$ cd BLAS
$ gfortran -O3 -c *.f
$ ar cr libblas.a *.o  # creates libblas.a

To use this library:

$ gfortran program.f90 -lblas \
   -L$HOME/lapack/BLAS

Note: Non-optimized Fortran 77 versions.

Better approach would be to use ATLAS.
Creating LAPACK library

Can be done from source at

http://www.netlib.org/lapack/

but somewhat more difficult.

Individual routines and dependencies can be obtained from netlib, e.g. the double precision versions from:

http://www.netlib.org/lapack/double

Download .tgz file and untar into directory where you want to use them, or make a library of just these files.
Often a program needs to be written to handle arrays whose size is not known until the program is running.

Fortran 77 approaches:

- Allocate arrays large enough for any application,
- Use “work arrays” that are partitioned into pieces.

We will look at some examples from LAPACK since you will probably see this in other software!
Often a program needs to be written to handle arrays whose size is not known until the program is running.

Fortran 77 approaches:
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We will look at some examples from LAPACK since you will probably see this in other software!

The good news:

Fortran 90 allows dynamic memory allocation.
DGESV — Solves a general linear system

http://www.netlib.org/lapack/double/dgesv.f

```
SUBROUTINE DGESV( N, NRHS, A, LDA, IPIV, 
    &    B, LDB, INFO )
```

\( N \) = size of system (square \( N \times N \))

\( A \) = matrix on input, L,U factors on output,

dimension(LDA,K) with LDA, K \( \geq N \)

\( LDA \) = **leading dimension of \( A \)**

(number of rows in declaration of \( A \))

**Example:**

```
real(kind=8) dimension(100,500) :: a
! fill a(1:20, 1:20) with 20x20 matrix
n = 20
lda = 100
```
DGESV — Solves a general linear system

Example:

```fortran
real(kind=8), dimension(100,500) :: a
real(kind=8), dimension(200,400) :: b
integer, dimension(600) :: ipiv
!

! fill a(1:20, 1:20) with 20x20 matrix
! b(1:20, 1:3) with 3 right hand sides
!

n = 20;  nrhs = 3;  lda = 100;  ldb = 200

call dgesv(n, nrhs, a, lda, ipiv, b, ldb, info)
```

What is passed to `dgesv` is **start_address**, the address of first element of `a`. (Matrix is stored by columns)

Whenever `a(i,j)` appears in code, address is:

```fortran
address = start_address + (j-1)*lda + (i-1)
```
DGESV — Solves a general linear system

SUBROUTINE DGESV( N, NRHS, A, LDA, IPIV, & B, LDB, INFO )

NRHS = number of right hand sides

B = matrix whose columns are right hand side(s) on input solution vector(s) on output.

LDB = leading dimension of B.

INFO = integer returning 0 if successful.

A = matrix on input, L,U factors on output,

IPIV = Returns pivot vector (permutation of rows) integer, dimension(N)
Row I was interchanged with row IPIV(I).
Gaussian elimination as factorization

If $A$ is nonsingular it can be factored as

$$PA = LU$$

where

$P$ is a permutation matrix (rows of identity permuted),

$L$ is lower triangular with 1’s on diagonal,

$U$ is upper triangular.

After returning from `dgesv`:
- $A$ contains $L$ and $U$ (without the diagonal of $L$),
- `IPIV` gives ordering of rows in $P$. 

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Gaussian elimination as factorization

Example:

\[
A = \begin{bmatrix}
2 & 1 & 3 \\
4 & 3 & 6 \\
2 & 3 & 4
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{bmatrix}\begin{bmatrix}
2 & 1 & 3 \\
4 & 3 & 6 \\
2 & 3 & 4
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 0 \\
1/2 & 1 & 0 \\
1/2 & -1/3 & 1
\end{bmatrix}\begin{bmatrix}
4 & 3 & 6 \\
0 & 1.5 & 1 \\
0 & 0 & 1/3
\end{bmatrix}
\]

\text{IPIV} = (2,3,1)

and \(A\) ends up as

\[
\begin{bmatrix}
4 & 3 & 6 \\
1/2 & 1.5 & 1 \\
1/2 & -1/3 & 1/3
\end{bmatrix}
\]
See $UWHPSC/codes/lapack/random.

Sample codes that solve the linear system $Ax = b$ with a random $n \times n$ matrix $A$, where the value $n$ is run-time input.

*randomsys1.f90* is with static array allocation.

*randomsys2.f90* is with dynamic array allocation.
dgesv examples

See $UWHPSC/codes/lapack/random$.

Sample codes that solve the linear system $Ax = b$ with a random $n \times n$ matrix $A$, where the value $n$ is run-time input.

`randomsys1.f90` is with static array allocation.

`randomsys2.f90` is with dynamic array allocation.

`randomsys3.f90` also estimates condition number of $A$.

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

Can bound relative error in solution in terms of relative error in data using this:

\[ Ax^* = b^* \quad \text{and} \quad A\tilde{x} = \tilde{b} \quad \implies \quad \frac{\|\tilde{x} - x^*\|}{\|x^*\|} \leq \kappa(A) \frac{\|\tilde{b} - b^*\|}{\|b^*\|} \]