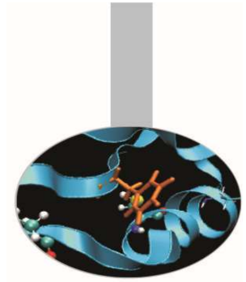

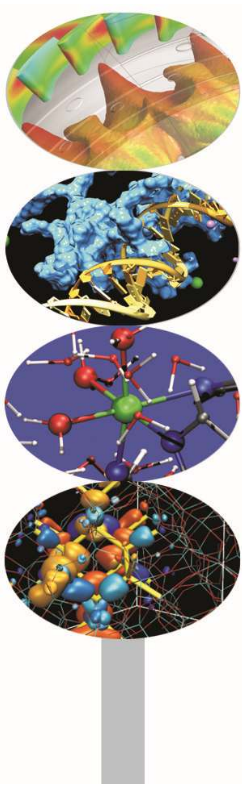

Numerical libraries

Exercises

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Library installation

As a beginning effort try download and install LAPACK from NETLIB:

- Download from http://www.netlib.org/lapack/lapack-3.5.0.tgz
- Configure *make.inc* (just copy make.inc.example for GNU compilers)
- cd *SRC*
- Run *make*
- cd ../*lapacke*
- Run *make*
- cd ../*BLAS/SRC*
- Run *make*

E1 – exercise – Matrix Multiply

It should be straightforward, although usually rather inefficient to implement a matrix multiplication routine. Try doing it and later add an alternative implementation that uses the BLAS routine:

```
FUNCTION DDOT(N,X,INCX,Y,INCY) RESULT(XtY)
   REAL(8) :: XtY  ! Y transpose
   INTEGER, INTENT(IN) :: N, INCX, INCY
   REAL(8), DIMENSION(:), INTENT(IN) :: X,Y
END FUNCTION DDOT
```

Source code: *MatrMult*

E2 – example - Rotation

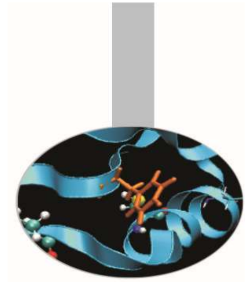
Wallace Givens was a researcher at Argonne National Laboratory when he introduced the so called *Givens rotation algorithm*, a rotation in the plane that is useful for transforming matrices in linear algebra computations.

The BLAS library contains routines to compute plane rotations and we could use them with the goal of rotating geometrical figures.

As an example, given a matrix PLANE(:,:) that represents a rectangle in a bi-dimensional plane and a set of points within the rectangle that defines a figure, at first we compute the angular parameters of the rotation, given by $c = \cos(\theta)$ and $s = \sin(\theta)$, then we calculate the result of the rotation applied to the figure.

The routine IntData2pgm() will help to visualize the rotated figure.

Source code: *Rotation*



Matrix norms

Consider $\mathcal{F}$ to be the space of *Real* or *Complex* numbers and $\mathcal{F}_{m,n}$ the space of matrices with MxN elements belonging to $\mathcal{F}$.

A matrix norm is a function $||.|| : \mathcal{F}_{m,n} \to \mathcal{F}$ with the following properties:

- $||A|| = 0$ iff $A = 0$
- $||A|| >= 0$
- $||x \cdot A|| = |x| \cdot ||A||$
- $||A+B|| <= ||A|| + ||B||$

With: $A, B \in \mathcal{F}_{m,n}$; $x \in \mathcal{F}$

Matrix norms

It follows that ($A, B \in \mathcal{F}_{m,n}$; $x, y \in \mathcal{F}$):

- $|x|.||A||' <= |x|.||A||'' <= |y|.||A||'$ [equivalence of matrix norm]
- $||.|| : \mathcal{F}_{m,n} \to \mathcal{F}$ is a continuous function

Relevant norms:

$||A||_1 = \mathrm{Max}_{1<=j<=N}\mathrm{Sum}_{1<=i<=M}|A_{i,j}|$ [max abs sum col elements]

$||A||_\infty = \mathrm{Max}_{1<=i<=M}\mathrm{Sum}_{1<=j<=N}|A_{i,j}|$ [max abs sum row elements]

$||A||_2 = \mathrm{SQRT}(\mathrm{Sum}_{1<=i<=M,1<=j<=N}|A^2_{i,j}|)$ [sqrt(sum squares)]

Condition number

A system of linear equations is solved when a vector $x \in \mathcal{F}_n$ is found such that $A \cdot x = b$ for given $A \in \mathcal{F}_{n,n}$ and $b \in \mathcal{F}_n$.

Suppose that $A \cdot y = b+e$ for a given e: $||e|| << ||b||$

It follows that $||y-x|| = ||A^{-1} \cdot e||$ and

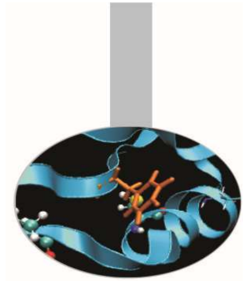
$$\frac{||y-x|| \,/\, ||x||}{||e|| \,/\, ||b||} = \frac{||A^{-1} \cdot e|| \,/\, ||A^{-1} \cdot b||}{||e|| \,/\, ||b||} = ||A^{-1}|| \cdot ||A|| = K(A)$$

Condition number

K(A) is the condition number with respect to the inversion of the matrix A or simply the *condition number* of A.

The value of the condition number depends on the used norm but, since matrix norms are equivalent, the order of magnitude of the condition numbers are similar.

The condition number gives a hint of how accurate is the solution of a linear system or how fast the solution varies as rhs values change.



E3 – exercise - Condition number

It can be demonstrated that $1 <= K(A) <= \infty$

The nearest K(A) is to 1 the more precise is the solution.

As an exercise a program could be written that calculates the condition number of a real NxN matrix A.

To do this the function DGECON of the LAPACK library can be used. Other useful functions are: DGETRF (LAPACK), DASUM (BLAS)

Example code: *CondNumber*

E3 – exercise - Condition number

```
FUNCTION DASUM( N, X, INCX ) RESULT(S)
        ! Sum of absolute values of a vector
          INTEGER, INTENT(IN) :: N, INCX
          REAL(8), DIMENSION(N), INTENT(IN) :: X
          REAL(8) :: S
END FUNCTION DASUM
```

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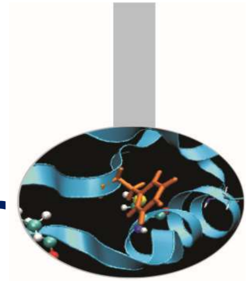
E3 – exercise - Condition number

```
SUBROUTINE  DGETRF ( M, N, A, LDA, IPIV, INFO)
!          Matrix factorization
           INTEGER, INTENT(IN) :: M, N, LDA
           REAL(8), dimension( LDA, N ), INTENT(IN OUT) ::      A
           INTEGER, dimension( * ), INTENT(OUT) ::IPIV
           INTEGER, INTENT(OUT) ::       INFO
 END SUBROUTINE DGETRF
```

E3 – exercise - Condition number



```
SUBROUTINE DGECON ( NORM, N, A, LDA, ANORM, RCOND, WORK,   &
      &                        IWORK,  INFO  )
!        Reciprocal of the condition number of a general real matrix A
      CHARACTER(1), INTENT(IN) :: NORM        !  May be "1" or "I"
      INTEGER, INTENT(IN) :: LDA, N
      REAL(8), DIMENSION( LDA, N ), INTENT(IN) :: A
      REAL(8), INTENT(IN) :: ANORM
      REAL(8), INTENT(OUT) :: RCOND
      REAL(8), DIMENSION( 4*N ), INTENT(IN OUT) :: WORK
      INTEGER, DIMENSION( N ), INTENT(IN OUT) :: IWORK
      INTEGER, INTENT(OUT) :: INFO
 END SUBROUTINE DGECON
```

E4 – example – Linear equation

Let us take into consideration the following equation in the [(1,1), (1,2), (2,2), (2,1)] 2D-square:

$$\partial^2 F(x,y)/ \partial x^2 + \partial^2 F(x,y)/ \partial y^2 = x + y$$

The exact solution is $F(x,y) = (x^3 + y^3) / 6$

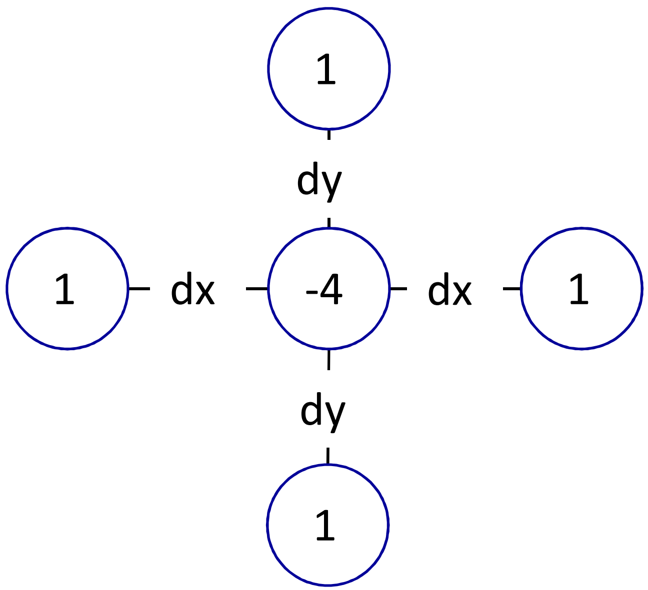
Let us pretend we do not know the exact solution but we know the values of the function on the perimeter of the square only and we are interested in computing the value of the function in a sufficient number of points within the square.

A finite difference approach could be easily implemented.

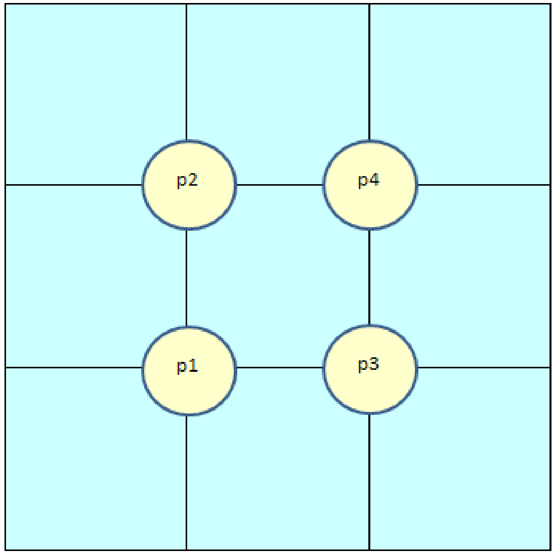
E4 – example – Linear equation

$\partial^2 F(x,y)/ \partial x^2$ approximated by $[F(x+dx,y) + F(x-dx,y) - 2 * F(x,y)] / dx^2$

$$\partial^2 F(x,y)/ \partial x^2 + \partial^2 F(x,y)/ \partial y^2 \Rightarrow [F(x+dx,y) + F(x-dx,y) + F(x,y+dy) + F(x,y-dy) - 4 * F(x,y)] / dx^2$$



E4 – example – Linear equation



- Divide the square in NxN grid cells
- Inner points represent the unknown values. LA = (N-1)*(N-1)
- A(LA,LA) matrix (finite difference coefficients) and B(LA) RHS vector (rhs x+y value and peripheral values) can be generated.

E4 – example – Linear equation

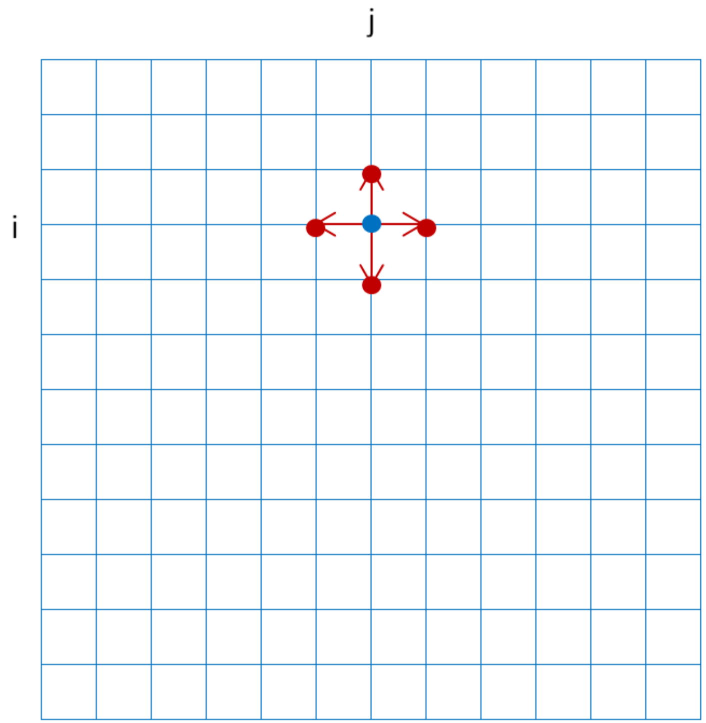
- The program could be designed as follow:
- Memorize inner point coords in Points(LA,2) vector
- Build A(LA,LA) matrix
- Build B(LA) = (x+y)/(dx*dy)-p; p = sum values peripheral points
- Factorize matrix: A => L·U
- Solve the system
- Compare computed solution to exact known solution

- Source code: LinearEquation

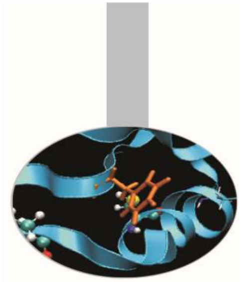
E5 – exercise – Band matrix

In the previous example a matrix has been generated to solve a PDE equation in a 2D-square. Grid points that are related each other may be a dimension length far each other

=> A is a band matrix



E5 – exercise – Band matrix

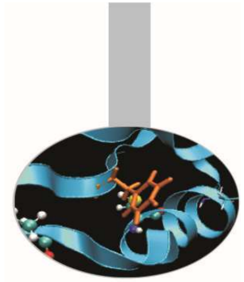


- Matrix A(LA,LA), LA=(N-1)*(N-1) of former example should have lower and upper bands with length N.

- Try modifying the source code in order to use Lapack routines DGBTRF and DGBTRS for band matrices.

- Source code: BandMatrix

E5 – exercise – Band matrix



```
SUBROUTINE  DGBTRF( M, N, KL, KU, AB, LDAB, IPIV, INFO )
!          Band matrix factorization
           INTEGER, INTENT(IN) :: M, N    ! Rows and columns
           INTEGER, INTENT(IN) :: KL, KU   ! Number of lower and
                                          !          upper bands
           REAL(8), DIMENSION( LDAB, N ), INTENT(IN OUT) :: AB
           INTEGER, INTENT(IN) :: LDAB      ! LDAB >= 2*KL+KU+1
           INTEGER, DIMENSION( * ), INTENT(OUT) ::IPIV
           INTEGER, INTENT(OUT) :: INFO
 END SUBROUTINE DGBTRF
```

E5 – exercise – Band matrix

```
lapack_int LAPACKE_dgbtrf    (int  matrix_order, // input
                lapack_int  m, //  input: Rows
                lapack_int  n, //  input: Columns
                lapack_int  kl, // input: Number of lower bands
                lapack_int  ku, // input: Number of upper bands
                double *  ab,  // input/output: Matrix ab[ldab,n]
                lapack_int  ldab, // input: LDAB >= 2*KL+KU+1
                lapack_int *  ipiv  // output
        )
```

E5 – exercise – Band matrix

```
SUBROUTINE  DGBTRS( TRANS, N, KL, KU, NRHS, AB, LDAB, IPIV,  &
  &        B, LDB, INFO )
   !       Solve a system of equation with band matrix
           CHARACTER(1) , INTENT(IN) :: TRANS    ! "N" = no transpose
           INTEGER, INTENT(IN) ::  N, KL, KU    ! Matrix order and bands
           INTEGER, INTENT(IN) :: NRHS      ! Right hand sides
           REAL(8), DIMENSION( LDAB, N ), INTENT(IN) :: AB
           INTEGER, INTENT(IN) :: LDAB      ! LDAB >= 2*KL+KU+1
           INTEGER, DIMENSION( * ), INTENT(IN) ::IPIV
           REAL(8), DIMENSION(LDB,NRHS), INTENT(IN OUT) :: B
           INTEGER, INTENT(IN) :: LDB
           INTEGER, INTENT(OUT) :: INFO
 END SUBROUTINE DGBTRS
```

E5 – exercise – Band matrix

```
lapack_int LAPACKE_dgbtrs (int  matrix_order, // input
        char  trans,  // input: “N” = no transpose
        lapack_int  n, // input:  Matrix order
        lapack_int  kl, // input:  Lower bands
        lapack_int  ku, // input:  Upper bands
        lapack_int  nrhs, // input: Right hand sides
        const double *  ab, // input: Matrix ab[ldab,n]
        lapack_int  ldab, // input: LDAB >= 2*KL+KU+1
        const lapack_int *  ipiv,  // input
        double *  b,  // input-output: matrix b[ldb,nrhs]
        lapack_int  ldb  // input
  )
```