CEE 618 Scientific Parallel Computing (Lecture 3)

Linear Algebra Basics using LAPACK

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Convection-Diffusion-Reaction Equation

- General form

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - \nabla \cdot (\boldsymbol{v} C) - kC \quad (1)$$

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- In 2D with a **constant** diffusion coefficient

$$0 = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \quad (3)$$

Laplacian eq.
$\nabla^2 C = 0$

Convection-Diffusion-Reaction Equation

- General form

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - \nabla \cdot (\boldsymbol{v} C) - kC \tag{1}$$

- In a steady state without convection and reaction

$$0 = \nabla \cdot (D \nabla C) \tag{2}$$

- In 2D with a **constant** diffusion coefficient

$$0 = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \tag{3}$$

- Mathematically identical to heat diffusion ($C \to T$)

$$0 = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \tag{4}$$

- Examples? Let's watach some videos in http://albertsk.org/videos/physical/

Example problem

Solve the following equation using the method of separation of variables:

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = 0 \tag{5}$$

- Boundary conditions $(0 < x, y < L)$
  1. $C\left(x = 0, y\right) = 0$
  2. $C\left(x, y = 0\right) = 0$
  3. $C\left(x, y = L\right) = 0$
  4. $C\left(x = L, y\right) = 10 \sin\left(\frac{\pi y}{L}\right)$

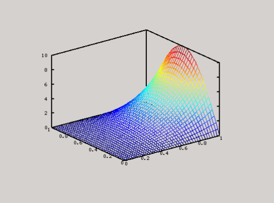


Figure: How does your solution look like?

Solution

1. By the method of the separation of variables

$$C(x, y) = X(x)\, Y(y) \tag{6}$$

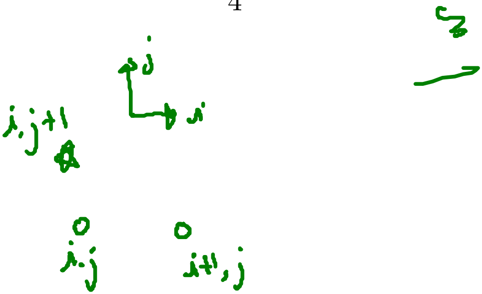
$$C = \frac{10}{\sinh \pi} \sinh \frac{\pi x}{L} \sin \frac{\pi y}{L} \tag{7}$$

Prove.

Solution

2. By MS Excel: *I am nothing but an average of my neighbors.*

$$C_{ij} = \frac{C_{i+1,j} + C_{i-1,j} + C_{i,j+1} + C_{i,j-1}}{4} \tag{8}$$



Outline

Example

Tony is two years odlder than Sam and the sum of their current ages is twenty. How old are Tony and Sam? Use a two by two matrix to solve this problem.

Cramer's rule

$$T - S = 2 \quad (9)$$

$$T + S = 20 \quad (10)$$

$2T + 0\cdot S = 22$

$T = 11, \; S = 9$

$\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} T \\ S \end{bmatrix} = \begin{bmatrix} 2 \\ 20 \end{bmatrix}$

$\text{Det} = \begin{vmatrix} 1 & -1 \\ 1 & 1 \end{vmatrix} = 1 - (-1) = 2$

$T = \dfrac{\begin{vmatrix} 2 & -1 \\ 20 & 1 \end{vmatrix}}{\text{Det}} = \dfrac{2-(-20)}{2} = \dfrac{22}{2} = 11$

$S = \dfrac{\begin{vmatrix} 1 & 2 \\ 1 & 20 \end{vmatrix}}{\text{Det}} = \dfrac{20-2}{2} = 9$

A Linear System

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b} \tag{11}$$

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}_{n\times n}, \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{n\times 1} \text{ and } \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}_{n\times 1}$$

where $\mathbf{A}$ is a $n \times n$ **square matrix**, and $\mathbf{b}$ is a $n \times 1$ **column vector**, of which all elements are known.

Then, how can we calculate $\mathbf{x}$?

LU decomposition

The square matrix $\mathbf{A}$ can be decomposed into

$$\mathbf{A} = \mathbf{L} \cdot \mathbf{U} \tag{12}$$

where $\mathbf{L}$ and $\mathbf{U}$ are **lower** and **upper** triangular matrixes, respectively, and calculated as

$$L = \begin{pmatrix} \alpha_{11} & 0 & \cdots & 0 \\ \alpha_{21} & \alpha_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n1} & \alpha_{n2} & \cdots & \alpha_{nn} \end{pmatrix}, U = \begin{pmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1n} \\ 0 & \beta_{22} & \cdots & \beta_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \beta_{nn} \end{pmatrix}$$

Then,

$$\mathbf{A} \cdot \mathbf{x} = (\mathbf{L} \cdot \mathbf{U}) \cdot \mathbf{x} = \mathbf{L} \cdot (\mathbf{U} \cdot \mathbf{x}) = \mathbf{b} \tag{13}$$

Let's set $\mathbf{U} \cdot \mathbf{x} = \mathbf{y}$, then

$$\mathbf{L} \mathbf{y} = \mathbf{b} \tag{14}$$

Forward substitution with known $\mathbf{L}$ and $\mathbf{b}$ to solve for $\mathbf{y}$

$\alpha_{11} y_1 + 0 \cdots = b_1$

$$\mathbf{L} \cdot \mathbf{y} = \mathbf{b}$$

$$\begin{pmatrix} \alpha_{11} & 0 & \cdots & 0 \\ \alpha_{21} & \alpha_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n1} & \alpha_{n2} & \cdots & \alpha_{nn} \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Then,

$$y_1 =$$

Forward substitution with known $\mathbf{L}$ and $\mathbf{b}$ to solve for $\mathbf{y}$

$y = U \cdot x$

$$\mathbf{L} \cdot \mathbf{y} = \mathbf{b}$$

$$\begin{pmatrix} \alpha_{11} & 0 & \cdots & 0 \\ \alpha_{21} & \alpha_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n1} & \alpha_{n2} & \cdots & \alpha_{nn} \end{pmatrix} \cdot \begin{pmatrix} \mathrm{y}_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \mathrm{b}_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Then,

$$y_1 = \frac{b_1}{\alpha_{11}}, \quad y_2 = \frac{b_2 - \alpha_{11} y_1}{\alpha_{22}}, \quad \dots \tag{15}$$

Using back substitution,

$$y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=1}^{i-1} \alpha_{ij} y_j \right] \tag{16}$$

where $i = 2, 3, ..., n$.

Backward substitution with $\mathbf{U}$ and $\mathbf{y}$ to solve for $\mathbf{x}$

$$\mathbf{U} \cdot \mathbf{x} = \mathbf{y} \tag{17}$$

$$\begin{pmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1n} \\ 0 & \ddots & \cdots & \vdots \\ \vdots & \vdots & \beta_{n-1,n-1} & \beta_{n-1,n} \\ 0 & \cdots & 0 & \beta_{nn} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_{n-1} \\ \mathrm{x_n} \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_{n-1} \\ \mathrm{y_n} \end{pmatrix}$$

Then,

$$x_n =$$

Backward substitution with $\mathbf{U}$ and $\mathbf{y}$ to solve for $\mathbf{x}$

$$\mathbf{U} \cdot \mathbf{x} = \mathbf{y} \tag{17}$$

$$\begin{pmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1n} \\ 0 & \ddots & \cdots & \vdots \\ \vdots & \vdots & \beta_{n-1,n-1} & \beta_{n-1,n} \\ 0 & \cdots & 0 & \beta_{\mathrm{nn}} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_{n-1} \\ \mathrm{x_n} \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_{n-1} \\ \mathrm{y_n} \end{pmatrix}$$

Then,

$$x_n = \frac{y_n}{\beta_{nn}}, \quad x_{n-1} = \frac{y_{n-1} - \beta_{n-1,n} x_n}{\beta_{n-1,n-1}}, \quad \ldots \tag{18}$$

Using back substitution,

$$x_i = \frac{1}{\beta_{ii}} \left[y_i - \sum_{j=i+1}^{n} \beta_{ij} x_j \right] \tag{19}$$

where $i = n-1, n-2, ..., 1$.

Combined matrix of α's and β's with less memory

Using $\alpha_{ii} = 1$ where $i = 1, 2, ..., n$

$$\mathbf{L} \oplus \mathbf{U} \to \mathbf{C} = \begin{pmatrix} \beta_{11} & \beta_{12} & \beta_{13} & \cdots & \beta_{1,n-1} & \beta_{1n} \\ \alpha_{21} & \beta_{22} & \beta_{23} & \cdots & \beta_{2,n-1} & \beta_{2n} \\ \alpha_{31} & \alpha_{32} & \beta_{33} & \cdots & \beta_{3,n-1} & \beta_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \alpha_{n-1,1} & \alpha_{n-1,2} & \alpha_{n-1,3} & \cdots & \beta_{n-1,n-1} & \beta_{n-1,n} \\ \alpha_{n1} & \alpha_{n2} & \alpha_{n3} & \cdots & \alpha_{n,n-1} & \beta_{nn} \end{pmatrix}$$

Example:

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b} \tag{20}$$

$$A = \begin{pmatrix} 1 & 3 & 1 \\ 1 & 1 & 2 \\ 2 & 3 & 4 \end{pmatrix}, b = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} =? \tag{21}$$

$$C = \begin{pmatrix} 2.000000 & 3.000000 & 4.000000 \\ 0.500000 & 1.500000 & -1.000000 \\ 0.500000 & -0.333333 & -0.333333 \end{pmatrix}, x = \begin{pmatrix} 2 \\ 0 \\ -1 \end{pmatrix} \tag{22}$$

However, C does not directrly represent L and U of matrix A because pivoting exchanges row index during the LU decomposition.

Makefile

1. Use files in "/opt/cee618s13/class03/" to solve this problem using **ludcmp** and **lubksb** subroutines from NRF77[1]
2. Use LAPACK routines[2] of **DGETRF** and **DGETRS**.
3. Check how to link LAPACK in Makefile.

[1] Section 2.3 of "Numerical Recipes in FORTRAN 77", available at http://www.nrbook.com/a/bookfpdf.php

[2] LAPACK user's guide at http://www.netlib.org/lapack/lug/index.html

Using subroutines in NRF: ludcmp & lubksb

```
program LU
implicit none
integer :: i,j, indx(3)
real    :: a(3,3)=(/1.,1.,2.,3.,1.,3.,1.,2.,4./)
real    :: d,b(3)=(/1.,0.,0./)

open(11, file='lu.dat')
!  Display the given matrix, A and b
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6))") (a(i,j),j=1,3), b(i)
enddo
!  Decomposition of the given matrix A
call ludcmp(a,3,3,indx,d)
!  Display the decomposed matrix, A and b
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6))") (a(i,j),j=1,3)
enddo
!  Solving for x with the decomposed matrix using backsubsitution
call lubksb(a,3,3,indx,b)
!  Display the decomposed matrix, A and the solution x
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6))") (a(i,j),j=1,3), b(i)
enddo
stop
end
```

unit

to write a blank line to '11'

$$A = \begin{pmatrix} 1 & 3 & 1 \\ 1 & 1 & 2 \\ 2 & 3 & 4 \end{pmatrix}$$

$a_{11}\ a_{12}\ a_{13}\ b_1$

$a_{11}\ a_{12}\ a_{13}$
$a_{21}\ a_{22}\ a_{23}$
$a_{31}\ a_{32}\ a_{33}$

$\Rightarrow a_{11}\ a_{21}\ a_{31}\ a_{12}\ a_{22}$

./codes/LU/LU3.f90

Results using ludcmp & lubksb

$$\begin{pmatrix} 1 & 3 & 1 \\ 1 & 1 & 2 \\ 2 & 3 & 4 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{23}$$

```
   1.000000     3.000000     1.000000     1.000000
   1.000000     1.000000     2.000000     0.000000
   2.000000     3.000000     4.000000     0.000000

   2.000000     3.000000     4.000000
   0.500000     1.500000    -1.000000
   0.500000    -0.333333    -0.333333

   2.000000     3.000000     4.000000     2.000000
   0.500000     1.500000    -1.000000     0.000000
   0.500000    -0.333333    -0.333333    -1.000000
```

./codes/LU/lu.dat

```
      SUBROUTINE ludcmp(a,n,np,indx,d)
      INTEGER n,np,indx(n),NMAX
      REAL d,a(np,np),TINY
      PARAMETER (NMAX=500,TINY=1.0e-20)
      INTEGER i,imax,j,k
      REAL aamax,dum,sum,vv(NMAX)
      d=1.
      do 12 i=1,n
        aamax=0.
        do 11 j=1,n
          if (abs(a(i,j)).gt.aamax) aamax=abs(a(i,j))
11      continue
        if (aamax.eq.0.) pause 'singular matrix in ludcmp'
        vv(i)=1./aamax
12    continue
      do 19 j=1,n
        do 14 i=1,j-1
          sum=a(i,j)
          do 13 k=1,i-1
            sum=sum-a(i,k)*a(k,j)
13        continue
          a(i,j)=sum
14      continue
```

```
      SUBROUTINE lubksb(a,n,np,indx,b)
      INTEGER n,np,indx(n)
      REAL a(np,np),b(n)
      INTEGER i,ii,j,ll
      REAL sum
      ii=0
      do 12 i=1,n
        ll=indx(i)
        sum=b(ll)
        b(ll)=b(i)
        if (ii.ne.0)then
          do 11 j=ii,i-1
            sum=sum-a(i,j)*b(j)
11        continue
        else if (sum.ne.0.) then
          ii=i
        endif
        b(i)=sum
12    continue
      do 14 i=n,1,-1
        sum=b(i)
        do 13 j=i+1,n
          sum=sum-a(i,j)*b(j)
```

Using subroutines in LAPACK: dgetrf & dgetrs

```
program LUlapack
implicit none
integer              :: i,j, ipiv(3), info
double precision     :: a(3,3)=(/1.,1.,2.,3.,1.,3.,1.,2.,4./)
double precision     :: b(3)=(/1.,0.,0./)

open(11,file='lulapack.dat')
!                 Display the given matrix, A and b
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6)) ") (a(i,j),j=1,3), b(i)
end do
!                 Decomposition of the given matrix A
call dgetrf(3,3,a,3,ipiv,info)
!                 Display the decomposed matrix, A and b
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6)) ") (a(i,j),j=1,3), b(i)
end do
!                 Solving for x with the decomposed matrix using backsubsitution
call dgetrs('N',3,1,a,3,ipiv,b,3,info)
!                 Display the decomposed matrix, A and the solution x
write(11,*)
do i=1,3
   write(11,"(4(2x,F12.6)) ") (a(i,j),j=1,3), b(i)
end do
stop
end
```

./codes/LUlapack/LU3dlapack.f90

Archives

- **Linear Equations** at `http://www.netlib.org/lapack/lug/node38.html`
- **Individual** at `http://www.netlib.org/lapack/individualroutines.html`
- **Single, REAL** at `http://www.netlib.org/lapack/single/`
- **Double, REAL** at `http://www.netlib.org/lapack/double/`
- **dgetrf** at `http://www.netlib.org/lapack/double/dgetrf.f`
- **dgetrs** at `http://www.netlib.org/lapack/double/dgetrs.f`
- **dgetri** at `http://www.netlib.org/lapack/double/dgetri.f`

Specifically

- call dgetrf (3 , 3 , a , 3 , ipiv , info)

- call dgetrs(’N’ , 3 , 1 , a , 3 , ipiv , b , 3 , info)

Outline

Eigen Value & Eigen Vector

Example: Rotate to principal axes the quadratic surface

$$x^2 + 6xy - 2y^2 - 2yz + z^2 = 24 \tag{24}$$

In matrix form this equation is

$$\begin{pmatrix} x & y & z \end{pmatrix} \begin{pmatrix} 1 & 3 & 0 \\ 3 & -2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 24 \tag{25}$$

or

$$X^T M X = 24 \tag{26}$$

The characteristic equation of this matrix is

$$\begin{vmatrix} 1-\mu & 3 & 0 \\ 3 & -2-\mu & -1 \\ 0 & -1 & 1-\mu \end{vmatrix} = -\mu^3 + 13\mu - 12 = -(\mu - 1)(\mu + 4)(\mu - 3) = 0 \tag{27}$$

The characteristic values are $\underline{\mu = 1, \ -4, \ 3}$.

From

$$\begin{pmatrix} x & y & z \end{pmatrix} \begin{pmatrix} 1 & 3 & 0 \\ 3 & -2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 24 \tag{28}$$

relative to the principal axes (x', y', z'), the quadratic sufrace equation becomes

$$\begin{pmatrix} x' & y' & z' \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = 24 \tag{29}$$

or

$$1 \cdot {x'}^2 + (-4) \cdot {y'}^2 + 3 \cdot {z'}^2 = 24 \tag{30}$$

or

$${X'}^T M' X' = 24 \tag{31}$$

where

$$M' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \tag{32}$$

Eigen vectors are

$$\left(\frac{1}{\sqrt{10}}, \frac{0}{\sqrt{10}}, \frac{3}{\sqrt{10}}\right) \quad \text{for} \quad \mu = 1 \tag{33}$$

$$\left(\frac{-3}{\sqrt{35}}, \frac{5}{\sqrt{35}}, \frac{1}{\sqrt{35}}\right) \quad \text{for} \quad \mu = -4 \tag{34}$$

$$\left(\frac{-3}{\sqrt{14}}, \frac{-2}{\sqrt{14}}, \frac{1}{\sqrt{14}}\right) \quad \text{for} \quad \mu = 3 \tag{35}$$

$$\begin{pmatrix} \frac{1}{\sqrt{10}} & \frac{-3}{\sqrt{35}} & \frac{-3}{\sqrt{14}} \\ 0 & \frac{5}{\sqrt{35}} & \frac{-2}{\sqrt{14}} \\ \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{35}} & \frac{1}{\sqrt{14}} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \tag{36}$$

or

$$C \cdot X = X'$$

$$X^T \cdot C^T = X'^T$$

In other words,

$$\begin{pmatrix} \frac{1}{\sqrt{10}} & 0 & \frac{3}{\sqrt{10}} \\ \frac{-3}{\sqrt{35}} & \frac{5}{\sqrt{35}} & \frac{1}{\sqrt{35}} \\ \frac{-3}{\sqrt{14}} & \frac{-2}{\sqrt{14}} & \frac{1}{\sqrt{14}} \end{pmatrix} \begin{pmatrix} 1 & 3 & 0 \\ 3 & -2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{10}} & \frac{-3}{\sqrt{35}} & \frac{-3}{\sqrt{14}} \\ 0 & \frac{5}{\sqrt{35}} & \frac{-2}{\sqrt{14}} \\ \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{35}} & \frac{1}{\sqrt{14}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \tag{37}$$

- In the eigen vector matrix, the columns can be exchanged and **signs** can be reverted. It is a matter of using right-handed or left-haded coordinates.
- Using transformed coordinates makes the problem mathematically so convenient.
- In quantum mechanics, eigen values are energy and eigen vectors are quantum states.

```fortran
PROGRAM EIGENVV
 IMPLICIT NONE
INTEGER             :: I, INFO, J,  N,   LWORK
DOUBLE PRECISION :: DUMMY(1,1)
DOUBLE PRECISION, ALLOCATABLE, DIMENSION (:,:) :: A, B , VR
DOUBLE PRECISION, ALLOCATABLE, DIMENSION (:)   :: ALPHAR, ALPHAI, BETA, WORK
   open (11,file='mat.in',status='old')
   read (11,*) N
   LWORK = 8*N
   allocate(A(N,N),B(N,N),ALPHAR(N),ALPHAI(N),BETA(N),VR(N,N),WORK(LWORK))
   B = 0.0; do i = 1, N; B(i,i) = 1.0; end do
   READ (11,*) ((A(I,J),J=1,N),I=1,N)
   CALL DGGEV('N','V',N,A,N,B,N, ALPHAR,ALPHAI,BETA,DUMMY,1,VR,N,WORK,LWORK,INFO)
   write(*,*) 'Eigen values are (diagonal) :'
   write(*,"(3(2X,F12.8))") ((A(i,j),J=1,N),I=1,N)
   write(*,*)
   call eigvec_norm (N,VR)
   write(*,*) 'Eigen vectors are :'
   write(*,"(3(2X,F12.8))") ((VR(i,j),J=1,N),I=1,N)
   write(*,*)
   deallocate(A,B,ALPHAR,ALPHAI,BETA,VR,WORK)

contains

    subroutine eigvec_norm (N,VR)
    DOUBLE PRECISION :: VR(N,N)
    integer          :: N, i, j
    double precision :: norm
    do i = 1, 3
       norm = DOT_PRODUCT (VR(:,i)   , VR(:,i)   )
       VR(:,i) = VR(:,i) / sqrt(norm)
    enddo
    end subroutine eigvec_norm
end program
```

(:,:,:) → for 3D

./codes/eigen/eigvv.f90

Makefile

```
srcroot=eigvv
srcfile=$(srcroot).f90
exefile=$(srcroot).x

all:
	ifort $(srcfile) -o $(exefile) -llapack

run:
	./$(exefile)


edit:
	vim $(srcfile)

clean:
	rm -f *.x *.o
```

./codes/eigen/Makefile

Output

```
./eigvv.x
 Eigen values are (diagonal) :
   -4.00000000    -0.00000000     0.00000000
    0.00000000     3.00000000     0.00000000
    0.00000000     0.00000000     1.00000000

 Eigen vectors are :
   -0.50709255    -0.80178373     0.31622777
    0.84515425    -0.53452248    -0.00000000
    0.16903085     0.26726124     0.94868330
```

./codes/eigen/output.dat

Outline

sample0.pbs & sample1.pbs

```
#PBS -S /bin/bash
#PBS -V
uname -n
echo $PBS_O_JOBID
```

./codes/PBS/sample0.pbs

```
#!/bin/bash
#PBS -l walltime=12:00:00
#PBS -N MyJob
#PBS -V
uname -n
echo $PBS_O_JOBID
cd $PBS_O_WORKDIR
pwd
```

./codes/PBS/sample1.pbs

sample2.pbs

```
#!/bin/bash
#PBS -l host=fractal
#PBS -l walltime=12:00:00
#PBS -l select=1:mpiprocs=4:ncpus=4
#PBS -N Sample
#PBS -V
#PBS -j oe
cd $PBS_O_WORKDIR
### put your specific job here after 'time' command ###
time ls -laF
#####################################################
qstat -f $PBS_JOBID
```

./codes/PBS/sample2.pbs

Commands

1. $␣qsub␣<␣sample0.pbs
2. $␣qstat

- The first comman is to submit a job described in "sample0.pbs" to a queueing system, i.e. "torque".
- The second comman is to monitor a status of the job, of which job number was assigned automatically by the first command.
- Observe the directory since each command of "qsub" will generate two files with the job number.
- Look at contents of newly generated files.