Third day

Practice for numerical issues

RIKEN CCS HPC Summer School
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Numerical Library
What is it? For what?

Numerical Library

Computer simulations create the future

- **Numerical Library is one of building blocks for ENSURING your advanced programming.**
- **It supports an API for very complex mathematical features, algorithm, schemes, also data handling…**
  - FFT, Eigenvalue calculation, SVD, etc…
- **There are reference codes.**
  - They might be examples of good (bad) programming.
- **It provides us with better performance and finer accuracy.**
  - Commercial library: faster and more accurate but expensive
  - Open Source library: fast and free (sometimes faster than commercial library)
  - You must check them before you run your application codes.

Example of Numerical Libraries

Computer simulations create the future

- **When you SPEED UP your code, use (probably being linked in most utility programs) the BLAS (Basic Linear Algebra Subprograms) library!**

  - Standard API for linear algebra kernels.
    - GEMM : Matrix-matrix multiplication ($C := \alpha AB + \beta C$)
    - AXPY: linear combination of 2 Vectors ($y := \alpha x + y$)
    - NRM2: Norm of a vector, etc. ($a = \|x\|_2$)

    Reference codes are available from netlib@UTK.

    http://www.netlib.org/BLAS/

  - Commercial: Intel MKL, AMD ACML (free)
  - Open Source: ATLAS(@UTK), GotoBLAS(@TACC), OpenBLAS for general purposed microprocessors
  - nVIDIA CUBLAS, AMD clMATH, MAGMABLAS(@UTK), KBLAS(@KAUST), ASPEN.K2(@RIKEN) : for GPGPU

Example of Numerical Libraries

Computer simulations create the future

If you want solve more complex problems, use followings;

- LAPACK (http://www.netlib.org/lapack/)
- ScaLAPACK (http://www.netlib.org/scalapack/)
- Elemental (http://libelemental.org/)

Dense, General

- EigenExa (http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html)
- ELPA (http://elpa.rzg.mpg.de/)

Dense Eigenvalue

- PETSc (http://www.mcs.anl.gov/petsc/)
- Trillions (https://trilinos.org/)

Sparse, General

- ARPACK (http://www.caam.rice.edu/software/ARPACK/)

Sparse, Eigenvalue

- FFTW (http://www.fftw.org/)
- FFTE (http://www.ffte.jp/)
- 2decomp&FFT (http://www.2decomp.org/)

FFT

- MT, MTGP, dSFMT (http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/SFMT/index.html)
- GMP big number librart(https://gmplib.org/)

Random number

- QD pack, MPACK, and so on

Multi-precision number

Review back on the CFD code

Core computational part in the CFD code

Computer simulations create the future

- **Solving a Poisson equation**

$$\Delta\phi = d$$

- **Discretization:**

$$\frac{\phi^k_{i-1,j} - 2\phi^{k+1}_{i,j} + \phi^k_{i+1.j}}{\Delta x^2} + \frac{\phi^k_{i,j-1} - 2\phi^{k+1}_{i,j} + \phi^k_{i.j+1}}{\Delta y^2} - d^k_{i,j} = 0$$

$$A\phi = d$$

$$A = \frac{1}{\Delta_x^2}(I_{N_y-1} \otimes X_{N_x-1}) + \frac{1}{\Delta_y^2}(X_{N_y-1} \otimes I_{N_x-1})$$

$$X_m = \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & & & & \\ & & 1 & -2 & 1 & \\ & & & 1 & -2 & \end{bmatrix}_{m\times m}$$

- **Finally, we have the Core iteration**

```
for(j=1; j<col_m_1; j++)
    for(i=2; i<row_m_1 - 1; i++)
      *(at(phiT,i,j)) = const1 * ( (L(phi,i+1,j  ) + L(phi,i-1,j  )) * const2 +
                                   (L(phi,i  ,j+1) + L(phi,i  ,j-1)) * const3 - L(d,i,j));
```

Solving Poisson' eq

- **You can write a Jacobi iteration code easily. BUT,**
  - wasting your time (programming, execution time).
  - Poisson's eq has a mathematical difficulty of convergence (sometimes diverge).
- **Many algorithms are implemented as library codes.**

You can choose **Faster and reliable** library routine to Solve Poisson'eq.

Today we try to use PETSc libary

Krylov Subspace method GMRES, CG, GCR, etc.. with Preconditioners

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- **Jacobi iteration**

$$x^{n+1} = D^{-1}((A - D)x^n) - b)$$

Convergence condition is very strict and the Jacobi method sometimes (or often?) diverges or stagnates. (diagonal dominant property is well known condition).

Similar algorithms:
Gauss-Seidel, SOR, SSOR, etc.

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- **GMRES**

$$\mathrm{argmin}_y\{\|AVy - b\| | V \in \mathcal{K}_A^n(v_0)\}$$

Based on Krylov subspace iteration and Arnoldi procedure, it finds a local solution vector by using the Least square approximation within a spanned subspace.

Generally, GMRES is known as best method for a non-symmetric case.

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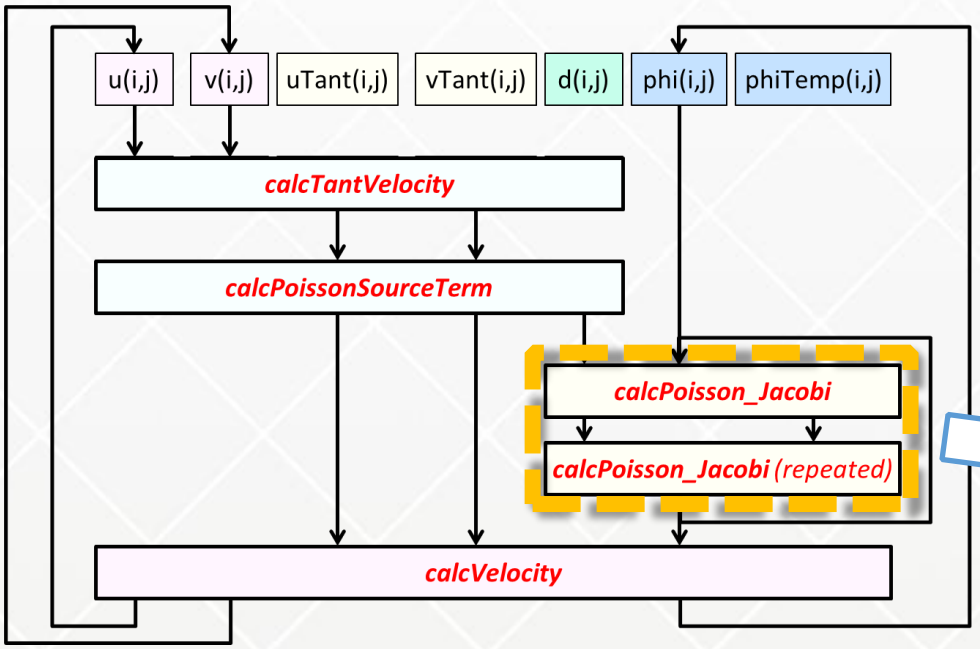

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GMRES, CG, GCR, etc..
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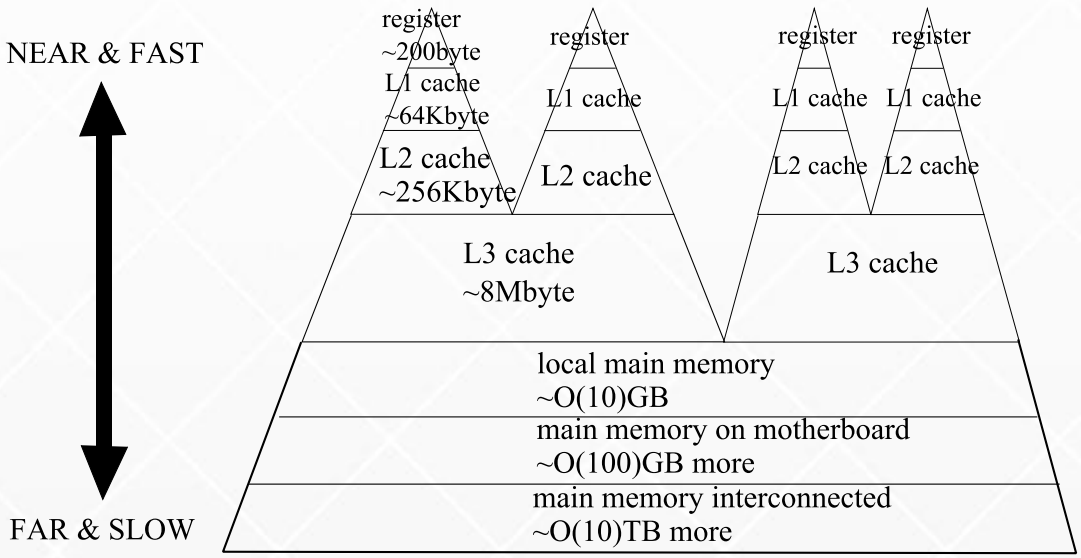
How does Numerical library achieve high Performance?

How can user utilize it with higher performance?

Difficulties in multicore computing

- **Difficulties in handling multicore.**
  - They are hiding in the deep and complex hierarchy of cache and memory structures.



  - To access the data with a tiny latency, the data must be prefetched on a cache memory, and dealt with carefully. In fact, we should have a view in a mind thoroughly to the cache conflict and memory traffic.
- **Memory bandwidth**
  - Improvement in the memory bandwidth is extremely gradual.
  - It is inevitable to change the software according to such an evolution and complication of hardware.

Balance of flops/memory access

- **BLAS has three categories with respect to the ratio of flops/memory access. Assumption: Data loaded from main memory is stored in a buffer memory on a processor chip and recycle until the procedure completes.**
  - Level 1: vector-vector operations
    - O(N) / O(N) ~O(1)

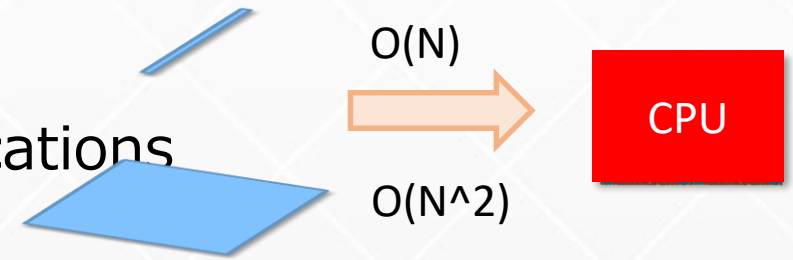
      $y := \alpha x + y$

  - Level 2: Matrix-vector multiplications
    - O(N^2)/O(N^2) ~O(1)

      $y := \alpha Ax + \beta y$

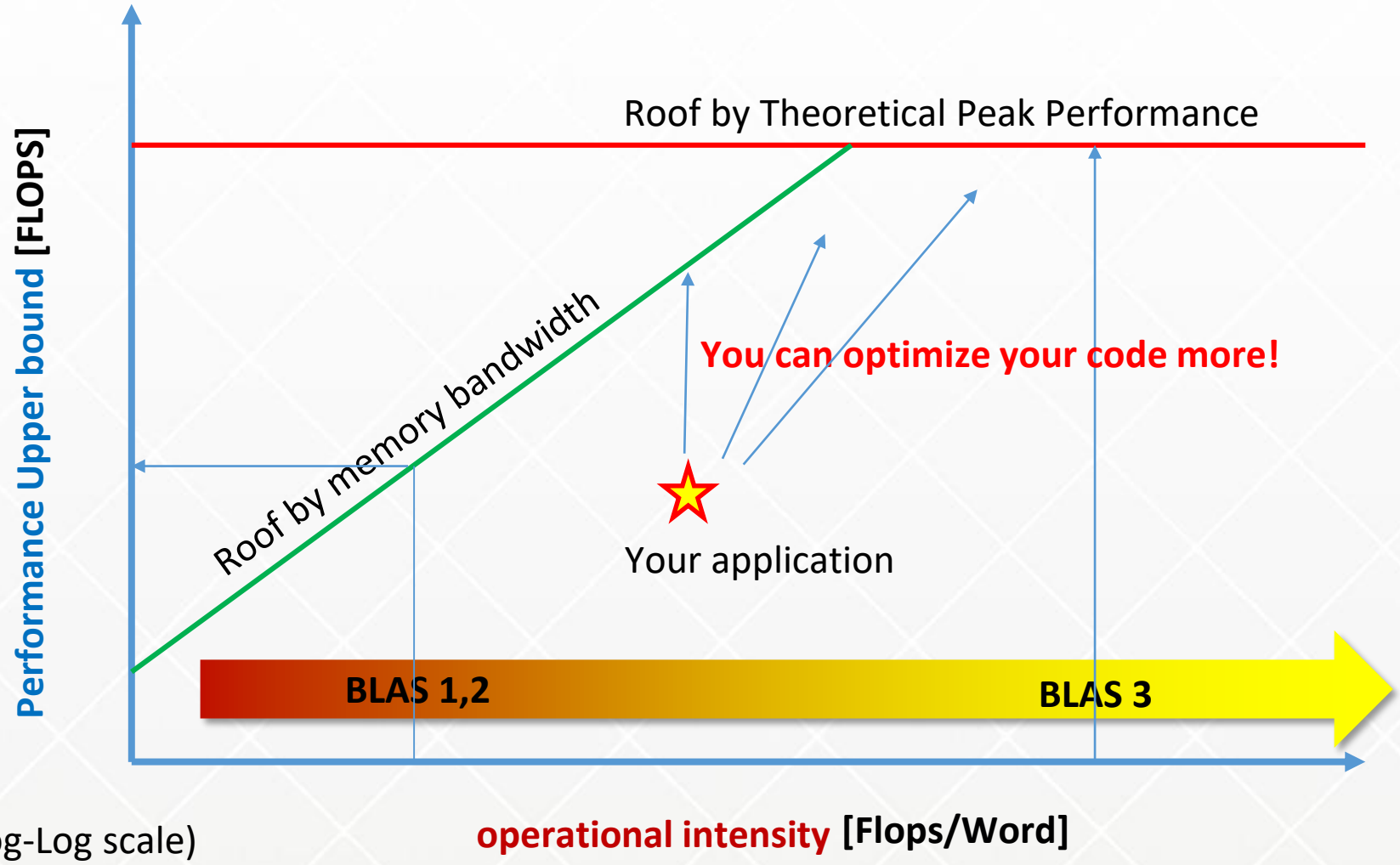
  - Level 3: Matrix-Matrix multiplication
    - O(N^3)/O(N^2) ~O(N) >> O(1)

      $C := \alpha AB + \beta C$



The metric defined by 'flops/Byte' or 'flops/words' is called **'operational intensity'.** It is strongly related to the Roofline model.

Roofline model



(Log-Log scale)

Recent trends of Optimization

Computer simulations create the future

- **Block algorithm**
  - Since block algorithm reduces memory traffic, it leads to larger operational intensity.
  - Re-write your code by using GEMM (or level3 BLAS) calls.
- **Tiling algorithm**
  - It is also one of the block algorithms, but the tiling algorithm reformats the data layout.
    - A(1:NX,1:NY) → A(1:BX,1:BY, 1:NX/BX, 1:NY/BY)

      Submatrix is contiguously stored in memory
  - Contiguous data/stream data can be store into L1/L2 cache.
  - Reduce and avoid TLB-miss trouble

How to use Numerical Libraries

ScaLAPACK, EigenExa, SLEPC

ScaLAPACK

For Dense linear algebra

From the developer site

- **http://www.netlib.org/scalapack/examples/**

Download "sample_pdsyev_call.f".

How to use ScaLAPACK on K

Computer simulations create the future

- **Link on the K computer or other Fujitsu environments**

```
% mpifrtpx -o exe sample_pdsyev_call.f -SCALAPACK -SSL2BLAMP
```

- **Job script**

```
#!/bin/bash
#PJM --rsc-list "rscgrp=small"
#PJM --rsc-list "node=2x2"
#PJM --rsc-list "elapse=00:10:00"
#PJM -S
#PJM --stg-transfiles all
#PJM --mpi "use-rankdir"
#PJM --mpi "proc=4"
#PJM --stgin "rank=* ./exe %r:./"
```

```
. /work/system/Env_base

export OMP_NUM_THREADS=8

date
mpiexec ./exe
date
```

Let's learn the sample code

- **Matrix generator: PDLAMODHILB**
- **Eigensolver: PDSYEV**
- **Output routine: PDLAPRNT**

Other routines are required, such as initializer (BLACS_XXX), finalizer (BLACS_EXIT), and definer of descriptors (DESCINIT), which represent matrix data structures.

BLACS: runtime system that organizes communication on ScaLAPACK.
PDSYEV: QR iteration algorithm
other algorithms are supported in PDSYEVX, PDSYEVD, PDSYEVR.

Matrix format: the 2D block-cyclic distribution and column major ordering

Read the source code

- **PDLAMODHILB**
  - Specialized parallelization or parallel calls are encapsulated in PDELSET routine. **The routine may be called in duplicate manner, however, the owner process only update its local memory** stored in 2D block-cyclic distribution.

```
SUBROUTINE PDLAMODHILB( N, A, IA, JA, DESCA, INFO )
DO 20 J = 1, N
DO 10 I = 1, N
IF( I.EQ.J ) THEN
        CALL PDELSET( A, I, J, DESCA,  ¥
        ( DBLE( N-I+1 ) ) / DBLE( N )+ONE /  ( DBLE( I+J )-ONE ) )
ELSE
        CALL PDELSET( A, I, J, DESCA, ONE / ( DBLE( I+J )-ONE ) )
ENDIF

END
```

EigenExa

One of the R-CCS software for solving a dense eigenvalue problem

How to use EigenExa on K

- **Link on the K computer or other Fujitsu environments**

```
% cp home/ra001016/a03572/SCHOOL/EigenExa/EigenExa-2.4p1-patched-all.tgz .
% tar -zxvf EigenExa-2.4p1-patched-all.tgz
% ./bootstrap; ./configure --host=K
% make
Then cd benchmark/
```

- **Job script**

```
#!/bin/bash
#PJM --rsc-list "rscgrp=small"
#PJM --rsc-list "node=2x2"
#PJM --rsc-list "elapse=00:10:00"
#PJM -S
#PJM --stg-transfiles all
#PJM --mpi "use-rankdir"
#PJM --mpi "proc=4"
#PJM --stgin
"rank=* ./eigenexa_benchmark %r:./“
#PJM --stgin "rank=* ./IN %r:./"

. /work/system/Env_base

export OMP_NUM_THREADS=8

date
mpiexec ./eigenexa_benchmark
date
```

Let's learn the sample code

Computer simulations create the future

- **Matrix generator: mat_set**
- **Eigensolver: eigen_sx**

- **As ScaLAPACK does, initializer (eigen_init) and finalizer (eigen_free) are obligately called in appropriate timing.**
- **EigenExa takes advantage of also 2D cyclic-cyclic distribution (in detail, fixed in NB as one both COL and ROW). Compatible to ScaLAPACK and other utility functions, reciprocally.**

- **Therefore, if descriptor defined with NB=1 and generated by PDLMODHILB can be passed to EigenExa and diagonalized.**

Benchmark code

- **On the benchmark directory,**
  - You can submit a job by `pjsub job-script.sh`.

```
Env_base: K-1.2.0-24
Mon Jul  2 11:07:14 JST 2018
 INPUT FILE='IN'
 ==========================================================
 ## EigenExa version (2.4a) / (May 25, 2017) / (Hanachirusato)
 Solver = eigen_sx / via penta-diagonal format
 Block width =  48 / 128
 NUM.OF.PROCESS= 4 ( 2 2 )
 NUM.OF.THREADS= 8
 Matrix dimension =  1000
 Matrix type =  2  (Random matrix)
 Internally required memory =  8472688  [Byte]
 The number of eigenvectors computed =  1000
 mode 'A' :: all the eigenpairs
 Elapsed time =  0.3770818118937314  [sec]
 FLOP        =  6826626901.333333
 Performance  =  18.10383499286145  [GFLOPS]
 ==========================================================
```

All eigenvalues and corresponding eigenvectors of a randomized matrix N=1000.

Edit an input file

- **Look at 'IN' file, you can edit N and nvec fields.**

```
!
! Input file format
!
! N bx by mode matrix solver
!
! N      : matrix dimension
! nvec   : the number of eigenvetors to be computed
! bx     : block width for the forward transformation
! by     : block width for the backward transformation
! mode   : solver mode { 0 : only eigenvalues }
!                      { 1 : eigenvalues and corresponding eigenv
ectors}
!                      { 2 : mode 1 + accuracy improvement for ei
genvalues}
! matrix : test matrix { 11 types, 0 ... 10 }
!        run with -L option shows the list of test matrices
!        typical ones are as follows
!        { 0 : Frank matrix}
!        { 1 : Toeplitz matrix}
!        { 2 : Random matrix}
! solver : { 0 : eigen_sx, new algorithm, faster on the K }
!        { 1 : eigen_s,  conventional algorithm }
! check_error : { 0 : off, 1 : on }
```

```
!
! if a line starts from '!', the line is treated as a commen
t
!   N  nvec bx  by m t s e
 1000  1000 48 128 1 2 0 0
 1000  1000 48 128 1 2 0 0
 1000  1000 48 128 1 2 0 0
 1000  1000 48 128 1 2 0 0
 1000  1000 48 128 1 2 0 0
-1
```

End mark

Accuracy Check

Random matrix

Mode: solving eigenvalues and vectors

Block factors

N. of eigenvectors to be computed

Matrix dimension

PETSc(SLEPC)

Official site on PETSc and SLEPC

Hands-on exercises

https://www.mcs.anl.gov/petsc/petsc-3.8/src/ksp/ksp/examples/tutorials/

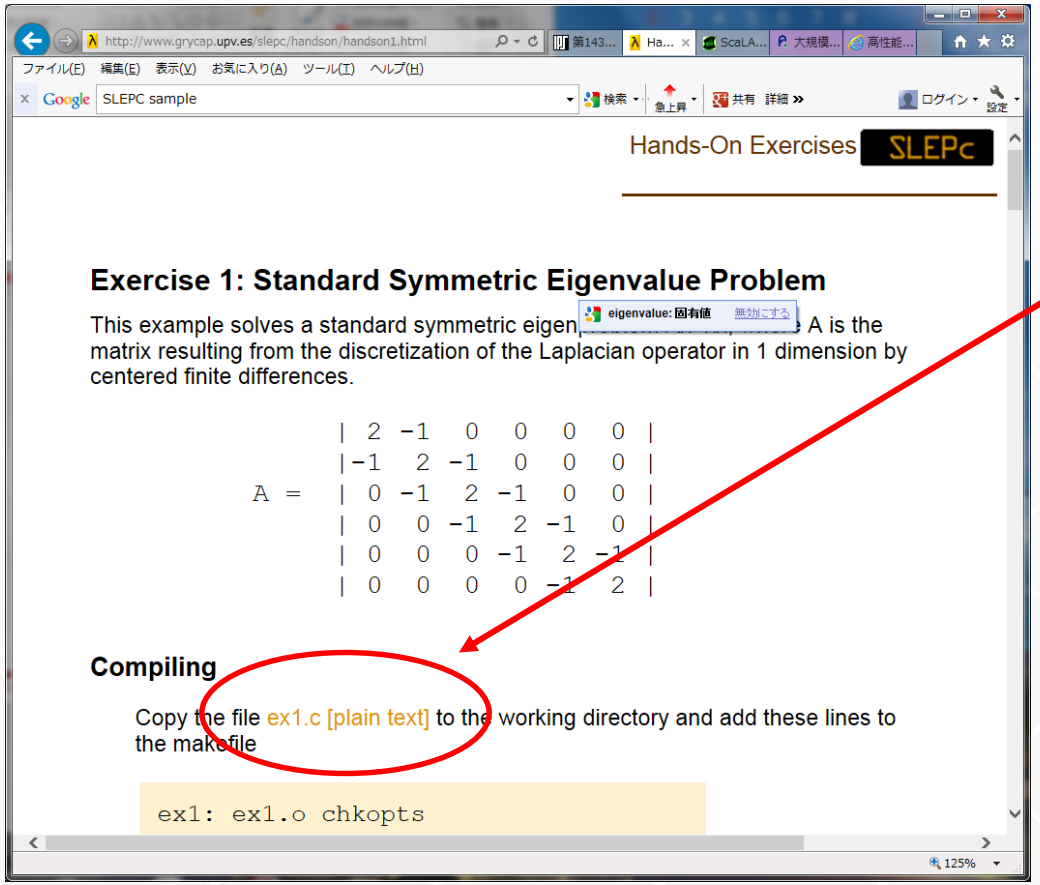
EigenExa | PROJE... | LINKS | 大規模並... | Krylov Meth... | RIKEN Internatio...

https://www.mcs.anl.gov/p

ex29.c: Solves 2D inhomogeneous Laplacian using multigrid
ex30.c: * Example code testing SeqDense matrices with an LDA (leading dimension of the user-allocated arrray) larger than M
ex31.c: Solves 2D compressible Euler
ex32.c: Solves 2D inhomogeneous Laplacian using multigrid
ex34.c: Solves 3D Laplacian using multigrid
ex41.c: Reads a PETSc matrix and vector from a socket connection, solves a linear system and sends the result back
ex42.c: Solves the incompressible, variable viscosity stokes equation in 3d using Q1Q1 elements, ¥n¥
ex43.c: Solves the incompressible, variable viscosity Stokes equation in 2d on the unit domain ¥n¥
ex45.c: Solves 3D Laplacian using multigrid
ex46.c: Solves a linear system in parallel with KSP and DM
ex49.c: Solves the compressible plane strain elasticity equations in 2d on the unit domain using Q1 finite elements
ex50.c: Solves 2D Poisson equation using multigrid
ex51.c: This example solves a linear system in parallel with KSP
ex52.c: Solves a linear system in parallel with KSP
ex53.c: Solves a tridiagonal linear system with KSP
ex54.c: Creates a matrix from quadrilateral finite elements in 2D, Laplacian ¥n¥
ex55.c: 2D, bi-linear quadrilateral (Q1), displacement finite element formulation¥n¥
ex56.c: 3D, tri-linear quadrilateral (Q1), displacement finite element formulation¥n¥
ex58.c: Solves a tridiagonal linear system with KSP
ex62.c: Illustrates use of PCGASM
ex63.cxx:
ex64.c: Illustrates use of the preconditioner GASM
ex65.c: Solves 1D constant coefficient Laplacian using DMSHELL and multigrid
ex66.c: Solves 2D Poisson equation using multigrid
ex67.c: Krylov methods to solve u'' = f in parallel with periodic boundary conditions
ex68.c:
ex69.c:
makefile

ex50.c

http://www.grycap.upv.es/slepc/handson/handson1.html



ex1.c

Compile and link

Makefile

```
ARCH=
PETSC_DIR=/home/ra001016/a03572/petsc-real
PETSC2_DIR=/home/ra001016/a03572/petsc-complex
SLEPC_DIR=/home/ra001016/a03572/slepc

CC=mpifccpx
FC=mpifrtpx
BLAS=-SSL2BLAMP -SCALAPACK

CCFLAGS_PETSC=-Xg -Kfast,openmp -I$(PETSC_DIR)/include
LDFLAGS_PETSC=-L$(PETSC_DIR)/lib -lpetsc $(BLAS)
CCFLAGS_SLEPC=-Xg -Kfast,openmp -I$(PETSC2_DIR)/include -I$(SLEPC_DIR)/include
LDFLAGS_SLEPC=-L$(SLEPC_DIR)/lib -lslepc -L$(PETSC2_DIR)/lib -lpetsc $(BLAS)

all: ksp_exec eps_exec
ksp_exec: ex50.o
	$(CC) $(CCFLAGS_PETSC) -o $@ $< $(LDFLAGS_PETSC)
ex50.o: ex50.c
	$(CC) $(CCFLAGS_PETSC) -c $<

eps_exec: ex1.o
	$(CC) $(CCFLAGS_SLEPC) -o $@ $< $(LDFLAGS_SLEPC)
ex1.o: ex1.c
	$(CC) $(CCFLAGS_SLEPC) -c $<
clean:
	¥rm *.o ksp_exec eps_exec
```

Use **make** command

→

ksp_exec (ex50) and eps_exec are (ex1) generated.

Job submission

```
#!/bin/bash
#PJM --rsc-list "rscgrp=small"
#PJM --rsc-list "node=4"
#PJM --rsc-list "elapse=00:10:00"
#PJM -S
#PJM --stg-transfiles all
#PJM --mpi "use-rankdir"
#PJM --mpi "proc=4"
#PJM --stgin "rank=* ./eps_exec %r:./“

. /work/system/Env_base
export OMP_NUM_THREADS=8

mpiexec ./eps_exec -n 540 -m 180 -eps_type gd -eps_nev 4 -eps_monitor -
eps_view
```

C version

1-D Laplacian Eigenproblem, n=100

Number of iterations of the method: 19
Solution method: krylovschur

Number of requested eigenvalues: 1
Stopping condition: tol=1e-08, maxit=100
Number of converged eigenpairs: 2

```
        k          ||Ax-kx||/||kx||
----------------- ------------------
    3.999033       4.02784e-09
    3.996131       4.31174e-09
```

C version

F90 version

1-D Laplacian Eigenproblem, n =100 (Fortran)

Number of iterations of the method: 19
Solution method: krylovschur
Number of requested eigenvalues: 1
Stopping condition: tol=1.0000E-08, maxit= 100
Number of converged eigenpairs: 2

```
        k          ||Ax-kx||/||kx||
----------------- ------------------
    3.9990E+00       4.0278E-09
    3.9961E+00       4.3117E-09
```

F90 version

Play with PETSc/SLEPC

- **From the tutorial page,**

```
$ ./eps_exec -n 400 -eps_nev 3 -eps_tol 1e-7
```

1-D Laplacian Eigenproblem, n=400

Number of iterations of the method: 100
Solution method: krylovschur

Number of requested eigenvalues: 3
Stopping condition: tol=1e-07, maxit=100
Number of converged eigenpairs: 1

k	||Ax-kx||/||kx||
3.999939	9.48781e-08

```
$ ./eps_exec -n 400 -eps_nev 3 -eps_ncv 24
```

1-D Laplacian Eigenproblem, n=400

Number of iterations of the method: 60
Solution method: krylovschur

Number of requested eigenvalues: 3
Stopping condition: tol=1e-08, maxit=100
Number of converged eigenpairs: 5

k	||Ax-kx||/||kx||
3.999939	9.48494e-09
3.999754	7.19493e-09
3.999448	1.18552e-09
3.999018	6.43926e-10
3.998466	1.04213e-09

```
$ ./eps_exec -n 100 -eps_nev 4 -eps_type lanczos
```

1-D Laplacian Eigenproblem, n=100

Number of iterations of the method: 62
Solution method: lanczos

Number of requested eigenvalues: 4
Stopping condition: tol=1e-08, maxit=100
Number of converged eigenpairs: 4

k	||Ax-kx||/||kx||
3.999033	9.95783e-09
3.996131	1.97435e-09
3.991299	9.15231e-09
3.984540	3.55339e-09

Learn the sample code (Pseudo code)

Computer simulations create the future

```
SlepcInitialize( PETSC_NULL_CHARACTER, ierr )

MatCreate( PETSC_COMM_WORLD, A, ierr )
MatSetSizes( A, …., n, n, ierr )
MatSetUp( A, ierr )


(…. Calculation of matrix elements and others …..)


ESPCreate( PETSC_COMM_WORLD, eps, ierr )
ESPSetOperators( eps, A, PETSC_NULL_OBJECT, ierr )
EPSSetProblemType( eps, EPS_HEP, ierr )

EPSSolve( eps, ierr )

EPSGetEigenPair( eps, …… )

EPSDestroy( eps, ierr )
SlepcFinalize( ierr )
```

How to setup a matrix? (in fortran90)

Computer simulations create the future

- **PETSc handles internal data format and interface data flexibly. Because of PETSc management mechanism, user does not to see actual state on memory . Matrix A is dealt with a handler variable, and matrix elements are accessed via a query API.**

```
! Simple matrix format
Mat         A
EPS         eps
EPSType     tname
PetscReal   tol, error, values(:)

MatCreate( PETSC_COMM_WORLD, A, ierr )
MatSetSizes( A, PETSC_DECIDE, PETSC_DECIDE, M, N, ierr )

MatGetOwnershipRange(A, Istart, Iend, ierr )
MatSetValues(  A, m, idxm, n, idxn, values, INSERT_VALUES|ADD_VALUES, ierr)

MatAssemblyBegin( A, MAT_FINAL_ASSEMBLY, ierr)
MatAssemblyEnd( A, MAT_FINAL_ASSEMBLY, ierr)
```

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MatAssemblyBegin( A, MAT_FINAL_ASSEMBLY, ierr)
MatAssemblyEnd( A, MAT_FINAL_ASSEMBLY, ierr)
```

Create a matrix handler

How to setup a matrix? (in fortran90)

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MatSetSizes( A, PETSC_DECIDE, PETSC_DECIDE, M, N, ierr )

MatGetOwnershipRange(A, Istart, Iend, ierr )
MatSetValues(  A, m, idxm, n, idxn, values, INSERT_VALUES|ADD_VALUES, ierr)

MatAssemblyBegin( A, MAT_FINAL_ASSEMBLY, ierr)
MatAssemblyEnd( A, MAT_FINAL_ASSEMBLY, ierr)
```

Matrix size MxN

How to setup a matrix? (in fortran90)

Computer simulations create the future

- **PETSc handles internal data format and interface data flexibly. Because of PETSc management mechanism, user does not to see actual state on memory . Matrix A is dealt with a handler variable, and matrix elements are accessed via a query API.**

```
! Simple matrix format
Mat         A
EPS         eps
EPSType     tname
PetscReal   tol, error, values(:)

MatCreate( PETSC_COMM_WORLD, A, ierr )
MatSetSizes( A, PETSC_DECIDE, PETSC_DECIDE, M, N, ierr )

MatGetOwnershipRange(A, Istart, Iend, ierr )
MatSetValues(  A, m, idxm, n, idxn, values, INSERT_VALUES|ADD_VALUES, ierr)

MatAssemblyBegin( A, MAT_FINAL_ASSEMBLY, ierr)
MatAssemblyEnd( A, MAT_FINAL_ASSEMBLY, ierr)
```

For a mxn block matrix, array values are set.

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MatAssemblyBegin( A, MAT_FINAL_ASSEMBLY, ierr)
MatAssemblyEnd( A, MAT_FINAL_ASSEMBLY, ierr)
```

Assemble the matrix data set on a distributed manner

Play back the CFD code and link it with PETSc

Core computational part in the CFD code

Computer simulations create the future

- **Solving a Poisson equation**

$$\Delta\phi = d$$

- **Discretization:**

$$\frac{\phi^k_{i-1,j} - 2\phi^{k+1}_{i,j} + \phi^k_{i+1.j}}{\Delta x^2} + \frac{\phi^k_{i,j-1} - 2\phi^{k+1}_{i,j} + \phi^k_{i.j+1}}{\Delta y^2} - d^k_{i,j} = 0$$

$$A\phi = d$$

$$A = \frac{1}{\Delta_x^2}(I_{N_y-1} \otimes X_{N_x-1}) + \frac{1}{\Delta_y^2}(X_{N_y-1} \otimes I_{N_x-1})$$

$$X_m = \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & & & & \\ & & 1 & -2 & 1 & \\ & & & 1 & -2 & \end{bmatrix}_{m\times m}$$

- **Finally, Core iteration: well-know iteration**

```
for(j=1; j<col_m_1; j++)
    for(i=2; i<row_m_1 - 1; i++)
      *(at(phiT,i,j)) = const1 * ( (L(phi,i+1,j  ) + L(phi,i-1,j  )) * const2 +
                                   (L(phi,i  ,j+1) + L(phi,i  ,j-1)) * const3 - L(d,i,j));
```

Use a PETSc KSP solver

Computer simulations create the future

- **What I did were,**
  - Download a sample source code
  - Modify main.cpp and cfd.cpp
  - Key points are i) initialization of PETSc environment and matrix generation, ii) calling a solver routine.

PETSc supports DMDA (distributed multi-dimentional array format) for vector data and a stencil mechanism for matrix representation.

- Prepare 3 call-back and 1 utility functions;
  - **ComputeRHS,**
  - **ComputeStencil,**
  - **SetInitialGuess,** and
  - **GetComputedResult.**

- Then, associate them with a DM handler.
- KSPSolve() organizes RHS and MatVec, etc.

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Use a PETSc KSP solver

Computer simulations create the future

1. **ComputeStencil**
   - Jacobi iteration is written in a 5-point Stencil fashion. Any stencil codes are

$$u_{i,j}^{new} := au_{i-1,j} + bu_{i,j-1} + cu_{i,j} + du_{i+1,j} + eu_{i,j+1} + f_{i,j}$$

   - Translate above relation into a Matrix-vector product.

2. **ComputeRHS**
   - Update the vector which appears in Right hand side

3. **SetInitialGuess**
   - Set up an initial guess for Krylov iterative solver

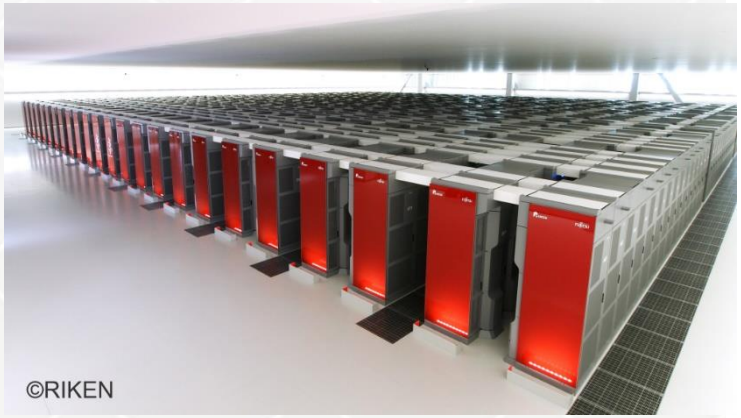
4. **GetComputedResult.**
   - Retrieve the result computed by using PETS.

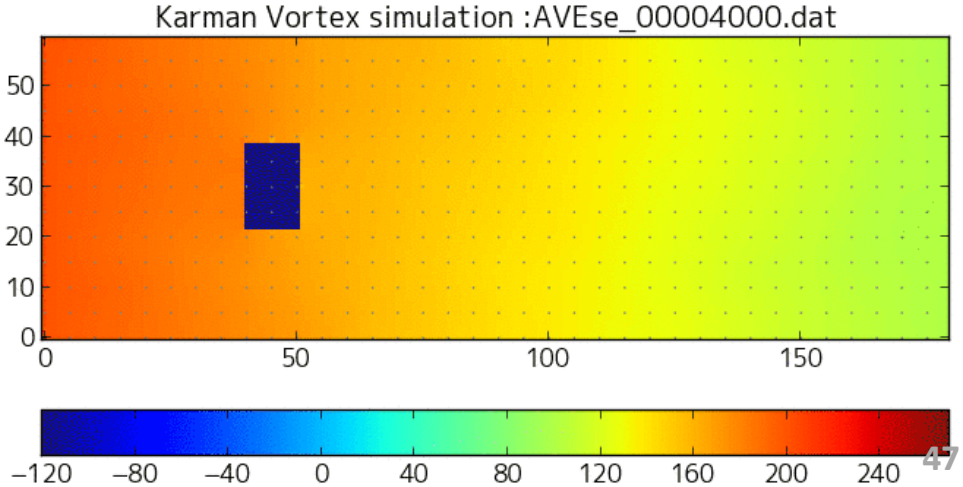
Let's Run the CFD code on K computer

Computer simulations create the future

```
% cp /home/ra001016/a03572/SCHOOL/CFD/mpi-petsc_merged_v4.tgz .
% tar zxvf mpi-petsc_merged_v4.tgz
% cd mpi-petsc_merged_v4
% make
```

Examples of job scripts are stored in scripts/.
If you want to run larger jobs, modify NX and NY larger (aspect must be 3:1), and smaller DT defined in cfd.h. Do, make clean, then again, make.
NOTE: We are sharing a CPU group account. So, please specify the CPU time limit less than 30min so as not to waste CPU time!





Example of Problem Settings (cfd.h)

Computer simulations create the future

- **For a large test**

```
#define NX (360)
#define NY (120)
#define DT  (5e-5)
#define NU  (0.01)
#define END_TIMESTEP        (10000)
#define SAVE_INTERVAL        (200)
```

- **For a huge case**

```
#define NX (540)
#define NY (180)
#define DT  (2.5e-5)
#define NU  (0.01)
#define END_TIMESTEP        (20000)
#define SAVE_INTERVAL        (400)
```

- **For a Challenging case**

```
#define NX (2700)
#define NY (900)
#define DT  (1e-6)
#define NU  (0.01)
#define END_TIMESTEP
(10000*3)
#define SAVE_INTERVAL
(10000)
```

Large test

1. **Edit cfd.h** *(make available LARGE and disable others)*

   #define TEST_CASE _LARGE_

2. **Compile by 'make'.**
3. **Prepare files required to a job** *(in case of 48 nodes)*

   - Make a work directory and change directory to it.
   - Copy **../script/run_batch_48mpi.sh** and the executable ../**solver_fractional** on the directory.

4. **Submit a job script**

   % pjsub run_batch_48mpi.sh

5. **Find and visualize a result on the directory.**

   - Data files are packed into a tar file.

   % tar -zxvf AVEse_data_48.tgz

   - You may also find **run_batch_48mpi.sh.oXXXXX**.

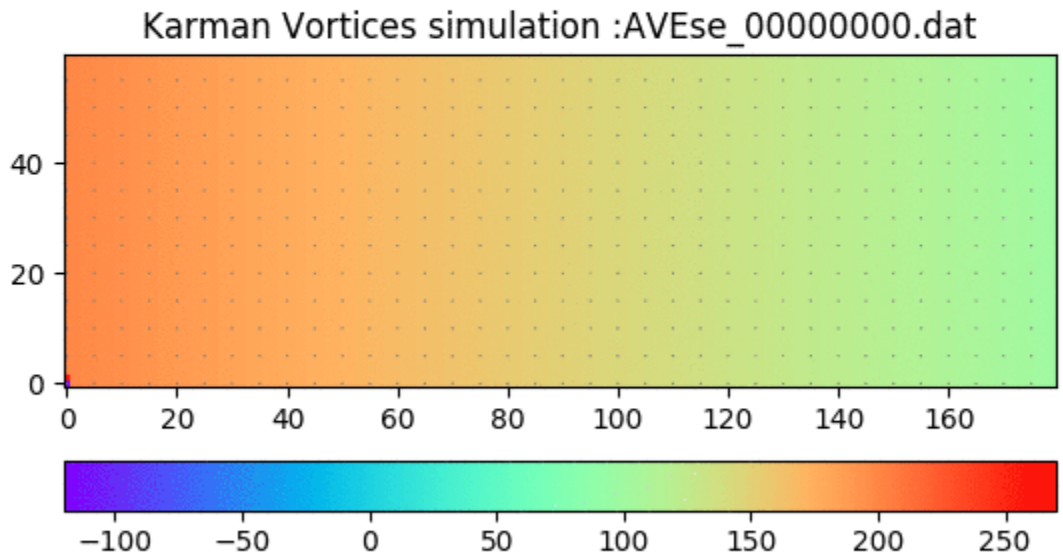
Visualize a result

- **Use a python script**

Now you are on the work directory.

```
% tar -zxvf AVEse_data_48.tgz
% python2.7 view.py
```

Huge case computed with 48 nodes



Hands-on time

Please access /home/ra001016/a03572/SCHOOL

ScaLAPACK/ → a sample code, a jobscript and Makefile
EigenExa/ → a sample code, a jobscript and Makefile
PETSc/ → PETSc sample codes, a jobscript and Makefile
CFD/ → Karman Vortex CFD codes

Basic hand-on works

Computer simulations create the future

BASE:

1. Run a sample code provided by the official developer site of ScaLAPACK.
2. Run a PETSc/SLEPc sample codes.
3. Confirm the CFD code with 'large' or 'huge' cases.

PRACTICAL:

For ScaLAPACK practices,

1. Modify **PDLAMODHILB**, then solve a real symmetric eigenvalue problem as you define or choose freely.
2. Also, vary the matrix dimension **N,** which is fixed in a source code, and the number of processes （**NPROW, NPCOL**）, then confirm parallel efficiency!
3. If you want to move advanced problem, try another routine pdsyevd!

Additional hands-on works

Computer simulations create the future

MORE ADVANCED:
For CFD practices,

1. **Try the challenging parameter case of the CFD code!** Please do not forget the CPU time limitation specified in the job script. Since to visualize Karman vortices takes a lot of iteration (delta T is too small), just stop the run at a couple of hundred iterations.
2. **Compare the two cases if PETSc uses or not.** You can switch them by activating the next macro in cfd.c (1: PETSC, 0: non-PETSC). Also, be aware of the CPU time, because the Jacobi iterative algorithm often fails in case of a challenging problem.

```
#defined USE_PETSC 1
```

MORE^2 ADVANCED:
(See next pages) Compute 9 eigenmodes of a Elastic plate analysis whose eigenvalues are from the largest by using SLEPSc/PETSc, and visualize the corresponding eigenvectors as a set of m x m images.

Advanced Lesson

- **Governing equation of vibration of an Elastic rectangular plate:**
  - Bi-harmonic equation

$$D\left(\frac{\partial^4 u}{\partial x^4}+2\frac{\partial^4 u}{\partial x^2\partial y^2}+\frac{\partial^4 u}{\partial y^4}\right)+\nu\frac{\partial^2 u}{\partial t^2}=0$$

$$D=\frac{Eh^3}{12(1-\mu^2)},\ \ \nu=\rho h$$

- **(E: Young ratio, h: width, ρ: density, μ: Poisson ratio)**
- **By using the variable separation method, we obtain**

$$\frac{\partial^4 u}{\partial x^4}+2\frac{\partial^4 u}{\partial x^2\partial y^2}+\frac{\partial^4 u}{\partial y^4}=\lambda u$$ **: eigenvalue problem**

Try then!

- **Boundary (Dirichlet)+Clamped Edge(Neumann) → Discretization**

$$u(\Gamma) = 0 \qquad \frac{\partial u}{\partial n}(\Gamma) = 0 \quad n : \text{normal} \quad \text{direction}$$

- **Using Kronecker tensor product notation, we present**

$$A = \frac{1}{h_x^4}(I_{N_y-1} \otimes X_{N_x-1}) + \frac{2}{h_x^2 h_y^2}(Y_{N_y-1} \otimes Y_{N_x-1}) + \frac{1}{h_y^4}(X_{N_y-1} \otimes I_{N_x-1})$$

$$X_m = \begin{bmatrix} 7 & -4 & 1 & & & \\ -4 & 6 & -4 & 1 & & \\ & & & & & \\ & & 1 & -4 & 6 & -4 \\ & & & 1 & -4 & 7 \end{bmatrix}_{m \times m} \qquad Y_m = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & & & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}_{m \times m}$$

Try then!

- **For the simplicity, the domain to be computed is fixed as a square shape and other parameters are supposed to be Nx=Ny=m, hx=hy=1.**

$$A = \begin{bmatrix} X_m & & & \\ & X_m & & \\ & & \ddots & \\ & & & X_m \end{bmatrix} + 2 \begin{bmatrix} -2Y_m & Y_m & & & \\ Y_m & -2Y_m & Y_m & & \\ & & & \ddots & \\ & & & Y_m & -2Y_m \end{bmatrix}$$

$$+ \begin{bmatrix} 7I & -4I & I & & \\ -4I & 6I & -4I & I & \\ & & & \ddots & \\ & & I & -4I & 7I \end{bmatrix}$$