PETSc and SLEPc

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[1] **PETSc Users Manual 3.6**.
[2] **SLEPc Users Manual** .

Outline

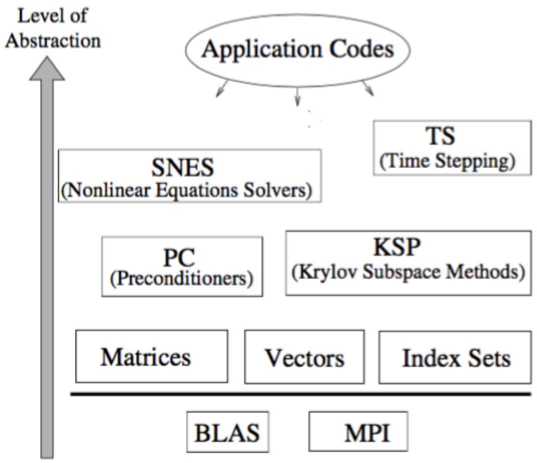
Version

- PETSc
  - The current version is 3.6; released June 9, 2015.
  - Users Manual Revision 3.6.
- SLEPc
  - The current version is 3.6; released June, 2015.
  - Users Manual June, 2015.

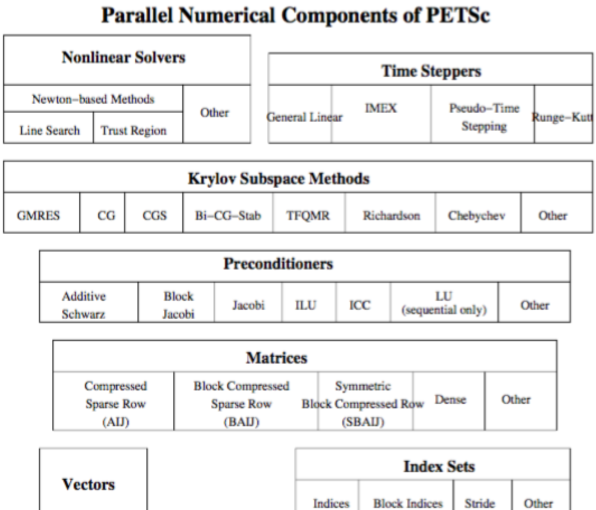
PETSc and SLEPc

- PETSc: Portable, Extensible Toolkit for Scientific Computation
- SLEPc: Scalable Library for Eigenvalue Problem Computations
- SLEPc is an extension of PETSc

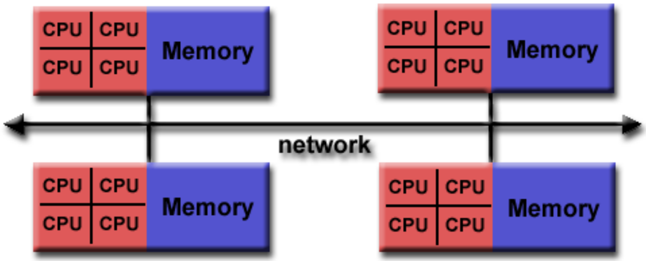
Organization of the PETSc Libraries



Numerical Libraries of PETSc



Message Passing Interface (MPI)



[3]

[3] **https://computing.llnl.gov/tutorials/mpi/**.

Threads

- PETSc: pure MPI, no OpenMP.
- Active OpenMP with ./configure only when one has many small systems (or sets of ODEs).

GPU

https://www.mcs.anl.gov/petsc/features/gpus.html

- CUDA (NVIDIA)
- OpenCL (NVIDIA, AMD, Intel MIC)

Supported languages

- PETSc: written in C
- C++
- Fortran
- Python
- MATLAB (limited)

Objects

- IS: index sets;
- Vec: vectors;
- Mat: matrices;
- DM: managing interactions between mesh data structures and vectors and matrices;
- KSP: Krylov subspace mthdos;
- PC: preconditioners;
- SNES: onlinear solvers;
- TS: timesteppers for solving time-dependent PDEs.

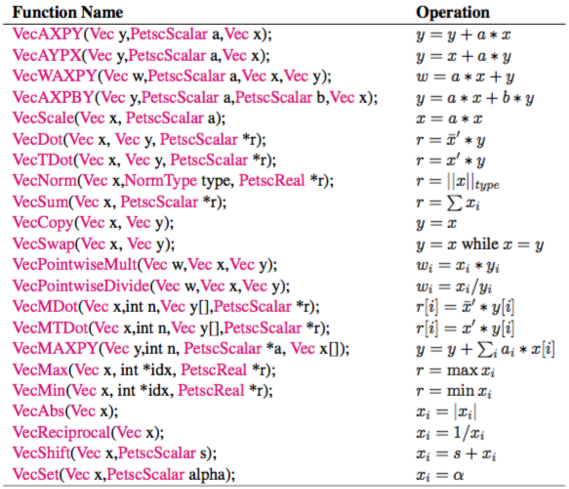
Vectors

- Sequential:
  VecCreateSeq(PETSC_COMM_SELF,int m,Vec *x);
- Parallel:
  VecCreateMPI(MPI_Comm comm,int m,int M,Vec *x);
- Or,
  VecCreate(MPI_Comm comm,Vec *v);
  VecSetSizes(Vec v, int m, int M);
  VecSetFromOptions(Vec v);

Vectors

- Assigning a single value to all components:
  VecSet(Vec x,PetscScalar value);
- Assigning a set of components:
  call
  VecSetValues(Vec x,int n,int *indices,PetscScalar *values,
  INSERT VALUES);
  any number of times, then call
  VecAssemblyBegin(Vec x);
  VecAssemblyEnd(Vec x);

Basic vector operations



Function Name	Operation
VecAXPY(Vec y,PetscScalar a,Vec x);	$y = y + a * x$
VecAYPX(Vec y,PetscScalar a,Vec x);	$y = x + a * y$
VecWAXPY(Vec w,PetscScalar a,Vec x,Vec y);	$w = a * x + y$
VecAXPBY(Vec y,PetscScalar a,PetscScalar b,Vec x);	$y = a * x + b * y$
VecScale(Vec x, PetscScalar a);	$x = a * x$
VecDot(Vec x, Vec y, PetscScalar *r);	$r = \bar{x}' * y$
VecTDot(Vec x, Vec y, PetscScalar *r);	$r = x' * y$
VecNorm(Vec x,NormType type, PetscReal *r);	$r = \|\|x\|\|_{type}$
VecSum(Vec x, PetscScalar *r);	$r = \sum x_i$
VecCopy(Vec x, Vec y);	$y = x$
VecSwap(Vec x, Vec y);	$y = x$ while $x = y$
VecPointwiseMult(Vec w,Vec x,Vec y);	$w_i = x_i * y_i$
VecPointwiseDivide(Vec w,Vec x,Vec y);	$w_i = x_i / y_i$
VecMDot(Vec x,int n,Vec y[],PetscScalar *r);	$r[i] = \bar{x}' * y[i]$
VecMTDot(Vec x,int n,Vec y[],PetscScalar *r);	$r[i] = x' * y[i]$
VecMAXPY(Vec y,int n, PetscScalar *a, Vec x[]);	$y = y + \sum_i a_i * x[i]$
VecMax(Vec x, int *idx, PetscReal *r);	$r = \max x_i$
VecMin(Vec x, int *idx, PetscReal *r);	$r = \min x_i$
VecAbs(Vec x);	$x_i = \|x_i\|$
VecReciprocal(Vec x);	$x_i = 1/x_i$
VecShift(Vec x,PetscScalar s);	$x_i = s + x_i$
VecSet(Vec x,PetscScalar alpha);	$x_i = \alpha$

Matrices: Supported matrix formats

- Dense matrices
- Sparse matrices
- Block matrices
- Matrix-Free matrices (function handle in MATLAB)

Creating and assembling matrices

```
MatCreate(MPI_Comm comm,Mat *A)
MatSetSizes(Mat A,int m,int n,int M,int N)
MatSetValues(Mat A,int m,const int idxm[],int n,const int idxn[],
        const PetscScalar values[], INSERT VALUES);
MatAssemblyBegin(Mat A,MAT FINAL ASSEMBLY);
MatAssemblyEnd(Mat A,MAT FINAL ASSEMBLY);
```

Dense matrices

- Column major order, different from C/C++
- Sequential:
  ```
  MatCreateSeqDense(PETSC_COMM_SELF,int m,int n,
          PetscScalar *data,Mat *A);
  ```
- Parallel:
  ```
  MatCreateDense(MPI_Comm comm,int m,int n,int M,int N,
          PetscScalar *data,Mat *A);
  ```

Sparse matrices

The general sparse AIJ format (CSR: compressed sparse row)

$$\boldsymbol{A} = \begin{pmatrix} 10 & 20 & 0 & 0 \\ 0 & 30 & 0 & 0 \\ 0 & 0 & 40 & 50 \\ 70 & 0 & 0 & 80 \end{pmatrix}$$

$$VA = [10, 20, 30, 40, 50, 70, 80]$$
$$JA = [0, 1, 1, 2, 3, 0, 3]$$
$$IA = [0, 2, 3, 5]$$

Sequential AIJ sparse matrices

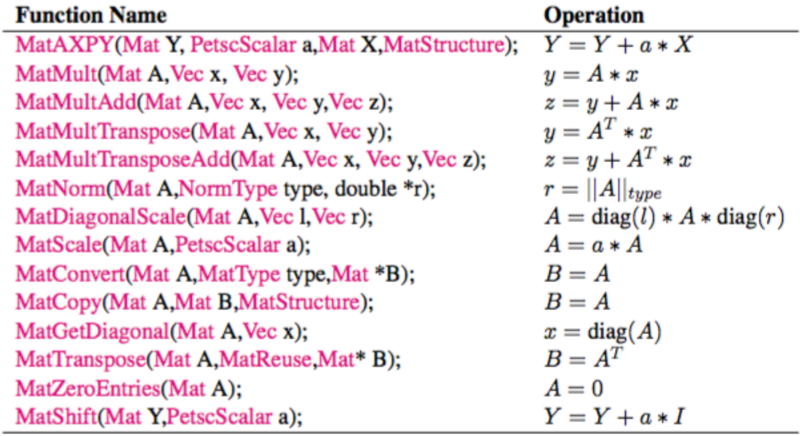
MatCreateSeqAIJ(PETSC_COMM_SELF,int m,int n,
        int nz, int *nnz,Mat *A);
nz: the expected number of nonzeros in a given row.
Eg: the tridiagonal matrix
nnz: the array of length m, which indicate the exact number of elements for each row.
int nnz[m];
nnz[0]= nonzeros in row 0;
nnz[1]=nonzeros in row 1;
...
nnz[m-1]=nonzeros in row m-1;

Parallel AIJ sparse matrices

```
MatCreateMPIAIJ(MPI_Comm comm,int m,int n,int M,int N,int d_nz,
        int *d_nnz, int o_nz,int *o_nnz,Mat *A);
```

$$\left(\begin{array}{ccc|ccc|cc}
1 & 2 & 0 & 0 & 3 & 0 & 0 & 4 \\
0 & 5 & 6 & 7 & 0 & 0 & 8 & 0 \\
9 & 0 & 10 & 11 & 0 & 0 & 12 & 0 \\
\hline
13 & 0 & 14 & 15 & 16 & 17 & 0 & 0 \\
0 & 18 & 0 & 19 & 20 & 21 & 0 & 0 \\
0 & 0 & 0 & 22 & 23 & 0 & 24 & 0 \\
\hline
25 & 26 & 27 & 0 & 0 & 28 & 29 & 0 \\
30 & 0 & 0 & 31 & 32 & 33 & 0 & 34
\end{array}\right)$$

Basic matrix operations



Function Name	Operation
MatAXPY(Mat Y, PetscScalar a,Mat X,MatStructure);	$Y = Y + a * X$
MatMult(Mat A,Vec x, Vec y);	$y = A * x$
MatMultAdd(Mat A,Vec x, Vec y,Vec z);	$z = y + A * x$
MatMultTranspose(Mat A,Vec x, Vec y);	$y = A^T * x$
MatMultTransposeAdd(Mat A,Vec x, Vec y,Vec z);	$z = y + A^T * x$
MatNorm(Mat A,NormType type, double *r);	$r = \|\|A\|\|_{type}$
MatDiagonalScale(Mat A,Vec l,Vec r);	$A = \text{diag}(l) * A * \text{diag}(r)$
MatScale(Mat A,PetscScalar a);	$A = a * A$
MatConvert(Mat A,MatType type,Mat *B);	$B = A$
MatCopy(Mat A,Mat B,MatStructure);	$B = A$
MatGetDiagonal(Mat A,Vec x);	$x = \text{diag}(A)$
MatTranspose(Mat A,MatReuse,Mat* B);	$B = A^T$
MatZeroEntries(Mat A);	$A = 0$
MatShift(Mat Y,PetscScalar a);	$Y = Y + a * I$

KSP: Linear equation solvers

Solve

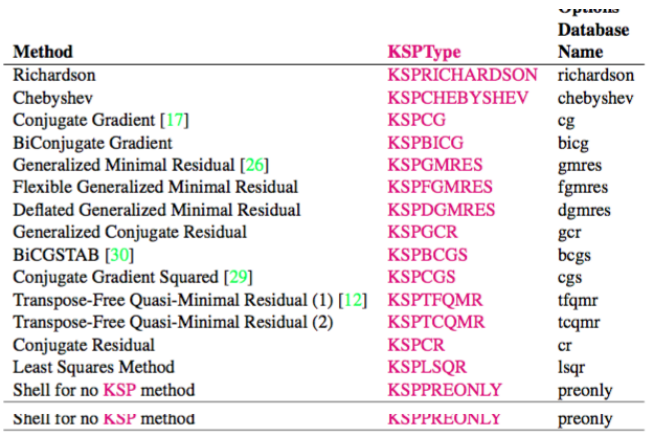
$$\boldsymbol{A}\mathbf{x} = \mathbf{b}$$

where $\boldsymbol{A}$ is nonsingular.

Using KSP

```
KSPCreate(MPI_Comm comm,KSP *ksp);
KSPSetOperators(KSP ksp,Mat Amat,Mat Pmat);
KSPSetFromOptions(KSP ksp);
KSPSolve(KSP ksp,Vec b,Vec x);
KSPDestroy(KSP *ksp);
```

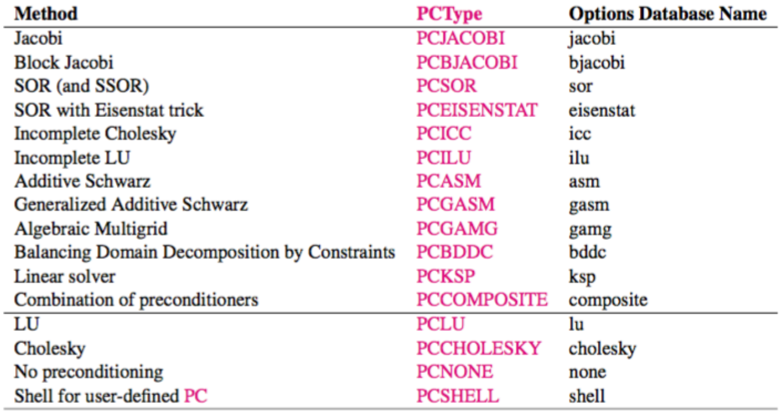
KSP objects



Method	KSPType	Options Database Name
Richardson	KSPRICHARDSON	richardson
Chebyshev	KSPCHEBYSHEV	chebyshev
Conjugate Gradient [17]	KSPCG	cg
BiConjugate Gradient	KSPBICG	bicg
Generalized Minimal Residual [26]	KSPGMRES	gmres
Flexible Generalized Minimal Residual	KSPFGMRES	fgmres
Deflated Generalized Minimal Residual	KSPDGMRES	dgmres
Generalized Conjugate Residual	KSPGCR	gcr
BiCGSTAB [30]	KSPBCGS	bcgs
Conjugate Gradient Squared [29]	KSPCGS	cgs
Transpose-Free Quasi-Minimal Residual (1) [12]	KSPTFQMR	tfqmr
Transpose-Free Quasi-Minimal Residual (2)	KSPTCQMR	tcqmr
Conjugate Residual	KSPCR	cr
Least Squares Method	KSPLSQR	lsqr
Shell for no KSP method	KSPPREONLY	preonly

Shell for no KSP method KSPPREONLY preonly

KSP preconditioners



Method	PCType	Options Database Name
Jacobi	PCJACOBI	jacobi
Block Jacobi	PCBJACOBI	bjacobi
SOR (and SSOR)	PCSOR	sor
SOR with Eisenstat trick	PCEISENSTAT	eisenstat
Incomplete Cholesky	PCICC	icc
Incomplete LU	PCILU	ilu
Additive Schwarz	PCASM	asm
Generalized Additive Schwarz	PCGASM	gasm
Algebraic Multigrid	PCGAMG	gamg
Balancing Domain Decomposition by Constraints	PCBDDC	bddc
Linear solver	PCKSP	ksp
Combination of preconditioners	PCCOMPOSITE	composite
LU	PCLU	lu
Cholesky	PCCHOLESKY	cholesky
No preconditioning	PCNONE	none
Shell for user-defined PC	PCSHELL	shell

Installation

- Linux with default installation options
  - ./configure –with-cc=gcc –with-cxx=g++ –with-fc=gfortran –download-fblaslapack –download-mpich
  - make all test
- Different architecture, external packages
  http://www.mcs.anl.gov/petsc/documentation/installation.html

Compiling: Makefile

```
include ${PETSC_DIR}/lib/petsc/conf/variables
include ${PETSC_DIR}/lib/petsc/conf/rules

ex1: ex1.o  chkopts
       -${CLINKER} -o ex1 ex1.o  ${PETSC_KSP_LIB}
       ${RM} ex1.o

ex2: ex2.o  chkopts
       -${CLINKER} -o ex2 ex2.o  ${PETSC_KSP_LIB}
       ${RM} ex2.o
```

Execution

mpiexec -np 8 ./petsc-program-name petsc-options

petsc-options:

- -log_summary
- -malloc_dump
- -info
- -ksp_type
- -pc_type

Example

/u/u24/zhang701/cse/day2/PETSc/ex2.c

- Solve $\boldsymbol{A}\mathbf{x} = \mathbf{b}$ using krylov subspace method with different preconditioners
  make ex2.c
  make run2

Eigenvalue problems

- the standard eigenvalue problem:

$$\boldsymbol{A}\mathbf{x} = \lambda\mathbf{x}$$

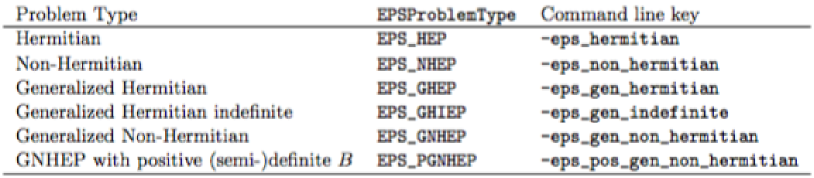
- the generalized eigenvalue problem:

$$\boldsymbol{A}\mathbf{x} = \lambda\boldsymbol{B}\mathbf{x}$$

Basic usage

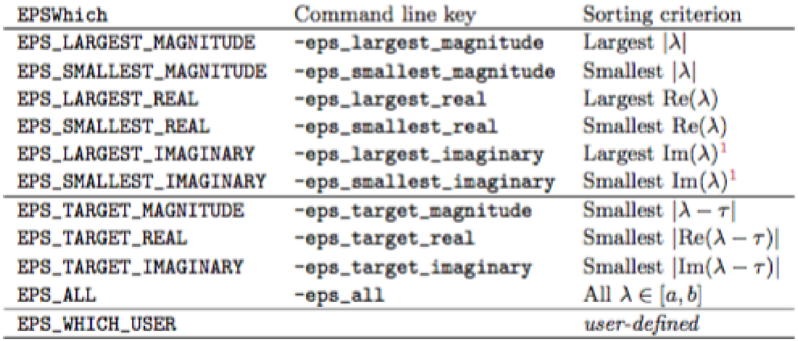
```
EPS         eps;       /*  eigensolver context  */
Mat         A;         /*  matrix of Ax=kx      */
Vec         xr, xi;    /*  eigenvector, x       */
PetscScalar kr, ki;    /*  eigenvalue, k        */
PetscInt    j, nconv;
PetscReal   error;

EPSCreate( PETSC_COMM_WORLD, &eps );
EPSSetOperators( eps, A, NULL );
EPSSetProblemType( eps, EPS_NHEP );
EPSSetFromOptions( eps );
EPSSolve( eps );
EPSGetConverged( eps, &nconv );
for (j=0; j<nconv; j++) {
  EPSGetEigenpair( eps, j, &kr, &ki, xr, xi );
  EPSComputeError( eps, j, EPS_ERROR_RELATIVE, &error );
}
EPSDestroy( &eps );
```

Problem type in eps



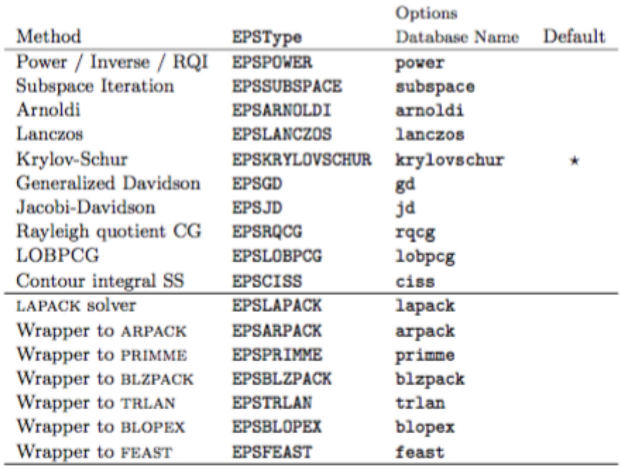
Problem Type	EPSProblemType	Command line key
Hermitian	`EPS_HEP`	`-eps_hermitian`
Non-Hermitian	`EPS_NHEP`	`-eps_non_hermitian`
Generalized Hermitian	`EPS_GHEP`	`-eps_gen_hermitian`
Generalized Hermitian indefinite	`EPS_GHIEP`	`-eps_gen_indefinite`
Generalized Non-Hermitian	`EPS_GNHEP`	`-eps_gen_non_hermitian`
GNHEP with positive (semi-)definite B	`EPS_PGNHEP`	`-eps_pos_gen_non_hermitian`

Available selections in eps



EPSWhich	Command line key	Sorting criterion
EPS_LARGEST_MAGNITUDE	-eps_largest_magnitude	Largest $\lvert\lambda\rvert$
EPS_SMALLEST_MAGNITUDE	-eps_smallest_magnitude	Smallest $\lvert\lambda\rvert$
EPS_LARGEST_REAL	-eps_largest_real	Largest $\mathrm{Re}(\lambda)$
EPS_SMALLEST_REAL	-eps_smallest_real	Smallest $\mathrm{Re}(\lambda)$
EPS_LARGEST_IMAGINARY	-eps_largest_imaginary	Largest $\mathrm{Im}(\lambda)$[1]
EPS_SMALLEST_IMAGINARY	-eps_smallest_imaginary	Smallest $\mathrm{Im}(\lambda)$[1]
EPS_TARGET_MAGNITUDE	-eps_target_magnitude	Smallest $\lvert\lambda-\tau\rvert$
EPS_TARGET_REAL	-eps_target_real	Smallest $\lvert\mathrm{Re}(\lambda-\tau)\rvert$
EPS_TARGET_IMAGINARY	-eps_target_imaginary	Smallest $\lvert\mathrm{Im}(\lambda-\tau)\rvert$
EPS_ALL	-eps_all	All $\lambda\in[a,b]$
EPS_WHICH_USER		*user-defined*

Eigensolvers in eps



Method	EPSType	Options Database Name	Default
Power / Inverse / RQI	EPSPOWER	power	
Subspace Iteration	EPSSUBSPACE	subspace	
Arnoldi	EPSARNOLDI	arnoldi	
Lanczos	EPSLANCZOS	lanczos	
Krylov-Schur	EPSKRYLOVSCHUR	krylovschur	⋆
Generalized Davidson	EPSGD	gd	
Jacobi-Davidson	EPSJD	jd	
Rayleigh quotient CG	EPSRQCG	rqcg	
LOBPCG	EPSLOBPCG	lobpcg	
Contour integral SS	EPSCISS	ciss	
LAPACK solver	EPSLAPACK	lapack	
Wrapper to ARPACK	EPSARPACK	arpack	
Wrapper to PRIMME	EPSPRIMME	primme	
Wrapper to BLZPACK	EPSBLZPACK	blzpack	
Wrapper to TRLAN	EPSTRLAN	trlan	
Wrapper to BLOPEX	EPSBLOPEX	blopex	
Wrapper to FEAST	EPSFEAST	feast	

Supported problem types for all eigensolvers in eps

Method	Portion of spectrum	Problem type	Real/Complex
`power`	Largest $\|\lambda\|$	any	both
`subspace`	Largest $\|\lambda\|$	any	both
`arnoldi`	any	any	both
`lanczos`	any	EPS_HEP, EPS_GHEP	both
`krylovschur`	any	any	both
`gd`	any	any	both
`jd`	any	any	both
`rqcg`	Smallest $\mathrm{Re}(\lambda)$	EPS_HEP, EPS_GHEP	both
`lobpcg`	Smallest $\mathrm{Re}(\lambda)$	EPS_HEP, EPS_GHEP	both
`ciss`	All λ in region	any	both
`lapack`	any	any	both
`arpack`	any	any	both
`primme`	Largest and smallest $\mathrm{Re}(\lambda)$	EPS_HEP	both
`blzpack`	Smallest $\mathrm{Re}(\lambda)$	EPS_HEP, EPS_GHEP	real
`trlan`	Largest and smallest $\mathrm{Re}(\lambda)$	EPS_HEP	real
`blopex`	Smallest $\mathrm{Re}(\lambda)$	EPS_HEP, EPS_GHEP	both
`feast`	All λ in an interval	EPS_HEP, EPS_GHEP	complex

Installation

- export PETSC_DIR = PETSC directory name
- export PETSC_ARCH = arch name
- export SLEPC_DIR = SLEPc directory name
- ./configure
- make
- make test

Note that the compiler used to compile SLEPc must be the same compiler used to compiler PETSc.

Compiling: Makefile

```
include ${SLEPC_DIR}/lib/slepc/conf/slepc_common

ex1: ex1.o chkopts
        -${CLINKER} -o ex1 ex1.o ${SLEPC_EPS_LIB}
        ${RM} ex1.o
```

Execution

mpiexec -np 8 ./slepc-program-name slepc-options

slepc-options:

- -n
- -eps_nev
- -eps_type
- -eps_monitor

Example

make ex1.c
make runex1_1
make runex1_all
make runex1_all_plot
make ex9.c
make runex9
make runex9_mo
make runex9_mo_lg

When to use PETSc+SLEPc

PETSc+SLEPc is not intended for the classes of problems for which effective MATLAB code can be written

How to learn PETSc+SLEPc

- PETSc+SLEPc manual
- References on the web page (with examples for each functions)
- Examples in the src/.

How to write a new application program using PETSc+SLEPc

1. Install and test PETSc+SLEPc according to the instructions at the PETSc+SLEPc web site.
2. Copy one of the many PETSc+SLEPc examples in the directory that corresponds to the class of problem of interest.
3. Copy the corresponding makefile within the example directory; compile and run the example program.
4. Use the example program as a starting point for developing a custom code.

Questions?