

# SLEPc: Scalable Library for Eigenvalue Problem Computations

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## Outline

- 1 Introduction
- 2 Overview of SLEPc
- 3 Basic Usage
  - Eigenvalue Solvers
  - Spectral Transformation
  - SVD Solvers
- 4 Advanced Features

## Eigenvalue Problems

Consider the following eigenvalue problems

Standard Eigenproblem

$$Ax = \lambda x$$

Generalized Eigenproblem

$$Ax = \lambda Bx$$

where

- ▶  $\lambda$  is a (complex) scalar: *eigenvalue*
- ▶  $x$  is a (complex) vector: *eigenvector*
- ▶ Matrices  $A$  and  $B$  can be real or complex
- ▶ Matrices  $A$  and  $B$  can be symmetric (Hermitian) or not
- ▶ Typically,  $B$  is symmetric positive (semi-) definite

## Solution of the Eigenvalue Problem

There are  $n$  eigenvalues (counted with their multiplicities)

Partial eigensolution:  $nev$  solutions

$$\lambda_0, \lambda_1, \dots, \lambda_{nev-1} \in \mathbb{C}$$
$$x_0, x_1, \dots, x_{nev-1} \in \mathbb{C}^n$$

$nev$  = number of  
eigenvalues /  
eigenvectors  
(eigenpairs)

Different requirements:

- ▶ Compute a few of the dominant eigenvalues (largest magnitude)
- ▶ Compute a few  $\lambda_i$ 's with smallest or largest real parts
- ▶ Compute all  $\lambda_i$ 's in a certain region of the complex plane

## Spectral Transformation

A general technique that can be used in many methods

$$Ax = \lambda x \implies Tx = \theta x$$

In the transformed problem

- ▶ The eigenvectors are not altered
- ▶ The eigenvalues are modified by a simple relation
- ▶ Convergence is usually improved (better separation)

Shift of Origin

$$T_S = A + \sigma I$$

Shift-and-invert

$$T_{SI} = (A - \sigma I)^{-1}$$

Cayley

$$T_C = (A - \sigma I)^{-1}(A + \tau I)$$

Drawback:  $T$  not computed explicitly, linear solves instead

## Singular Value Problems

Consider the SVD decomposition of a rectangular matrix

$$A \in \mathbb{R}^{m \times n}$$

Singular Value Decomposition

$$A = U \Sigma V^T = \sum_{i=1}^n u_i \sigma_i v_i^T$$

where

- ▶  $\sigma_1, \sigma_2, \dots, \sigma_n$ : *singular values*
- ▶  $u_1, u_2, \dots, u_n$ : *left singular vectors*
- ▶  $v_1, v_2, \dots, v_n$ : *right singular vectors*

## Solution of the Singular Value Problem

There are  $n$  singular values (counted with their multiplicities)

Partial solution:  $nsv$  solutions

$$\begin{aligned}\sigma_0, \sigma_1, \dots, \sigma_{nsv-1} &\in \mathbb{R} \\ u_0, u_1, \dots, u_{nsv-1} &\in \mathbb{R}^m \\ v_0, v_1, \dots, v_{nsv-1} &\in \mathbb{R}^n\end{aligned}$$

$nsv$  = number of  
singular values /  
vectors (singular  
triplets)

- ▶ Compute a few smallest or largest  $\sigma_i$ 's

Alternatives:

- ▶ Solve eigenproblem  $A^T A$
- ▶ Solve eigenproblem  $H(A) = \begin{bmatrix} 0^{m \times m} & A \\ A^T & 0^{n \times n} \end{bmatrix}$
- ▶ Bidiagonalization

## Design Considerations

- ▶ Various problem characteristics: Problems can be real/complex, Hermitian/non-Hermitian
- ▶ Many ways of specifying which solutions must be sought
- ▶ Many formulations: not all eigenproblems are formulated as simply  $Ax = \lambda x$  or  $Ax = \lambda Bx$

Goal: provide a uniform, coherent way of addressing these problems

- ▶ Internally, solvers can be quite complex (deflation, restart, ...)
- ▶ Spectral transformations can be used irrespective of the solver
- ▶ Repeated linear solves may be required
- ▶ SVD can be solved via associated eigenproblem or bidiagonalization

Goal: hide eigensolver complexity and separate spectral transform

## What Users Need

### *Provided by PETSc*

- ▶ Abstraction of mathematical objects: vectors and matrices
- ▶ Efficient linear solvers (direct or iterative)
- ▶ Easy programming interface
- ▶ Run-time flexibility, full control over the solution process
- ▶ Parallel computing, mostly transparent to the user

### *Provided by SLEPc*

- ▶ State-of-the-art eigensolvers
- ▶ Spectral transformations
- ▶ SVD solvers

## Summary

### **PETSc:** Portable, Extensible Toolkit for Scientific Computation

Software for the scalable (parallel) solution of algebraic systems arising from partial differential equation (PDE) simulations

- ▶ Developed at Argonne National Lab since 1991
- ▶ Usable from C, C++, Fortran77/90
- ▶ Focus on abstraction, portability, interoperability
- ▶ Extensive documentation and examples
- ▶ Freely available and supported through email

<http://www.mcs.anl.gov/petsc>

Current version: **3.0.0** (released Dec 2008)

## Summary

**SLEPc**: Scalable Library for Eigenvalue Problem Computations

A *general* library for solving large-scale sparse eigenproblems on parallel computers

- ▶ For standard and generalized eigenproblems
- ▶ For real and complex arithmetic
- ▶ For Hermitian or non-Hermitian problems

Also support for the partial SVD decomposition

<http://www.grycap.upv.es/slepc>

Current version: **3.0.0** (released Feb 2009)

## Structure of SLEPc (1)

SLEPc extends PETSc with three new objects: **EPS**, **ST**, **SVD**

### EPS: Eigenvalue Problem Solver

- ▶ The user specifies an eigenproblem via this object
- ▶ Provides a collection of eigensolvers
- ▶ Allows the user to specify a number of parameters (e.g. which portion of the spectrum)



## Structure of SLEPc (2)

### ST: Spectral Transformation

- ▶ Used to transform the original problem into  $Tx = \theta x$
- ▶ Always associated to an EPS object, not used directly

### SVD: Singular Value Decomposition

- ▶ The user specifies the SVD problem via this object
- ▶ Transparently provides the associated eigenproblems or a specialized solver



## PETSc/SLEPc Numerical Components

### PETSc

<b>Nonlinear Systems</b>			<b>Time Steppers</b>			
Line Search	Trust Region	Other	Euler	Backward Euler	Pseudo Time Step	Other
<b>Krylov Subspace Methods</b>						
GMRES	CG	CGS	Bi-CGStab	TFQMR	Richardson	Chebyshev Other
<b>Preconditioners</b>						
Additive Schwarz	Block Jacobi	Jacobi	ILU	ICC	LU	Other
<b>Matrices</b>						
Compressed Sparse Row	Block Compressed Sparse Row	Block Diagonal	Dense	Other		
<b>Vectors</b>	<b>Index Sets</b>					
	Indices	Block Indices	Stride	Other		

### SLEPc

<b>SVD Solvers</b>			
Cross Product	Cyclic Matrix	Lanczos	Thick Res. Lanczos
<b>Eigensolvers</b>			
Krylov-Schur	Arnoldi	Lanczos	Other
<b>Spectral Transform</b>			
Shift	Shift-and-invert	Cayley	Fold

## EPS: Basic Usage

Usual steps for solving an eigenvalue problem with SLEPc:

1. Create an EPS object
2. Define the eigenvalue problem
3. (Optionally) Specify options for the solution
4. Run the eigensolver
5. Retrieve the computed solution
6. Destroy the EPS object

All these operations are done via a generic interface, common to all the eigensolvers

## EPS: Simple Example

```
EPS          eps;          /* eigensolver context */
Mat          A, B;        /* matrices of Ax=kBx  */
Vec          xr, xi;      /* eigenvector, x      */
PetscScalar kr, ki;      /* eigenvalue, k       */

EPSCreate(PETSC_COMM_WORLD, &eps);
EPSSetOperators(eps, A, B);
EPSSetProblemType(eps, EPS_GNHEP);
EPSSetFromOptions(eps);

EPSSolve(eps);

EPSGetConverged(eps, &nconv);
for (i=0; i<nconv; i++) {
    EPSGetEigenpair(eps, i, &kr, &ki, xr, xi);
}

EPSTDestroy(eps);
```



## Details: Solving the Problem

### EPSSolve(EPS eps)

Launches the eigensolver

Currently available eigensolvers:

- ▶ Power Iteration and RQI
- ▶ Subspace Iteration with Rayleigh-Ritz projection and locking
- ▶ Arnoldi method with explicit restart and deflation
- ▶ Lanczos method with explicit restart and deflation
  - ▶ Reorthogonalization: Local, Partial, Periodic, Selective, Full
- ▶ Krylov-Schur (default)

Also interfaces to external software: ARPACK, PRIMME, ...



## Details: Problem Definition

### EPSSetOperators(EPS eps, Mat A, Mat B)

Used for passing the matrices that constitute the problem

- ▶ A generalized problem  $Ax = \lambda Bx$  is specified by A and B
- ▶ For a standard problem  $Ax = \lambda x$  set B=PETSC\_NULL

### EPSSetProblemType(EPS eps, EPSProblemType type)

Used to indicate the problem type

Problem Type	EPSProblemType	Command line key
Hermitian	EPS_HEP	-eps_hermitian
Generalized Hermitian	EPS_GHEP	-eps_gen_hermitian
Non-Hermitian	EPS_NHEP	-eps_non_hermitian
Generalized Non-Herm.	EPS_GNHEP	-eps_gen_non_hermitian

## Details: Specification of Options

### EPSSetFromOptions(EPS eps)

Looks in the command line for options related to EPS

For example, the following command line

```
% program -eps_hermitian
```

is equivalent to a call `EPSSetProblemType(eps, EPS_HEP)`

Other options have an associated function call

```
% program -eps_nev 6 -eps_tol 1e-8
```

### EPSView(EPS eps, PetscViewer viewer)

Prints information about the object (equivalent to `-eps_view`)

## Details: Viewing Current Options

### Sample output of `-eps_view`

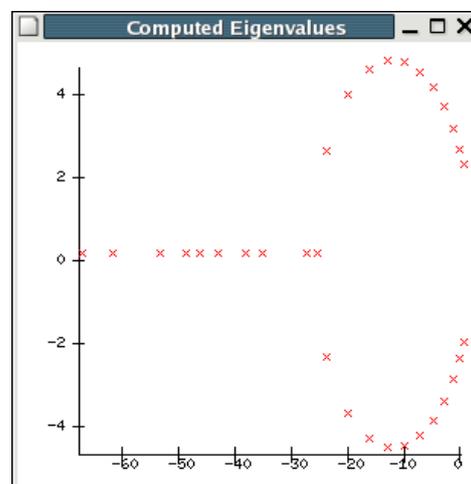
```
EPS Object:
  problem type: symmetric eigenvalue problem
  method: krylovschur
  selected portion of spectrum: largest eigenvalues in magnitude
  number of eigenvalues (nev): 1
  number of column vectors (ncv): 16
  maximum dimension of projected problem (mpd): 16
  maximum number of iterations: 100
  tolerance: 1e-07
  dimension of user-provided deflation space: 0
IP Object:
  orthogonalization method: classical Gram-Schmidt
  orthogonalization refinement: if needed (eta: 0.707100)
ST Object:
  type: shift
  shift: 0
```

## EPS: Run-Time Examples

```
% program -eps_view -eps_monitor  
  
% program -eps_type krylovschur -eps_nev 6 -eps_ncv 24  
  
% program -eps_type arnoldi -eps_tol 1e-8 -eps_max_it 2000  
  
% program -eps_type subspace -eps_hermitian -log_summary  
  
% program -eps_type lapack  
  
% program -eps_type arpack -eps_plot_eigs -draw_pause -1  
  
% program -eps_type primme -eps_smallest_real
```

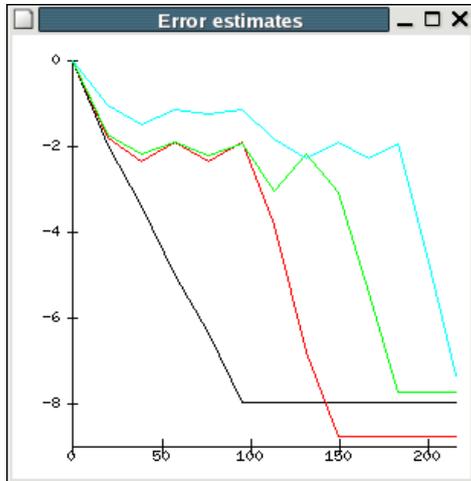
## Built-in Support Tools

- ▶ Plotting computed eigenvalues  
% program -eps\_plot\_eigs
- ▶ Printing profiling information  
% program -log\_summary
- ▶ Debugging  
% program -start\_in\_debugger  
% program -malloc\_dump





## Built-in Support Tools



- ▶ Monitoring convergence (textually)  
`% program -eps_monitor`
- ▶ Monitoring convergence (graphically)  
`% program -draw_pause 1`  
`-eps_monitor_draw`



## Spectral Transformation in SLEPc

An ST object is always associated to any EPS object

$$Ax = \lambda x$$

$\implies$

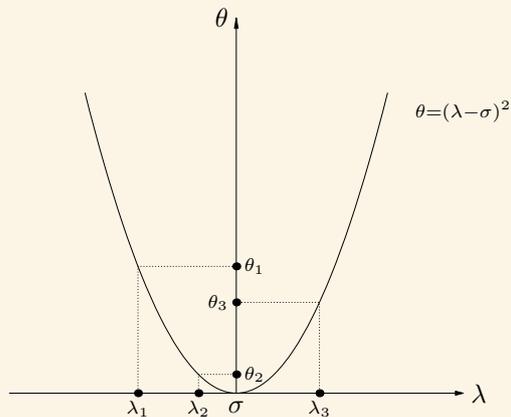
$$Tx = \theta x$$

- ▶ The user need not manage the ST object directly
- ▶ Internally, the eigensolver works with the operator  $T$
- ▶ At the end, eigenvalues are transformed back automatically

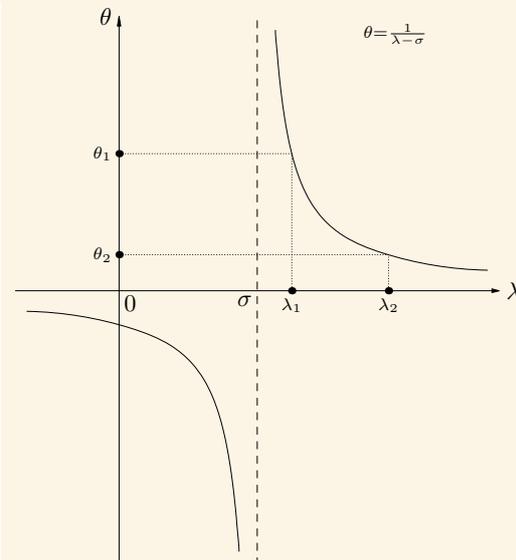
ST	Standard problem	Generalized problem
shift	$A + \sigma I$	$B^{-1}A + \sigma I$
fold	$(A + \sigma I)^2$	$(B^{-1}A + \sigma I)^2$
sinvert	$(A - \sigma I)^{-1}$	$(A - \sigma B)^{-1}B$
cayley	$(A - \sigma I)^{-1}(A + \tau I)$	$(A - \sigma B)^{-1}(A + \tau B)$

## Illustration of Spectral Transformation

### Spectrum folding



### Shift-and-invert



## Accessing the ST Object

The user does not create the ST object

```
EPSGetST(EPS eps, ST *st)
```

Gets the ST object associated to an EPS

Necessary for setting options in the source code

**Linear Solves.** Most operators contain an inverse

- ▶ Linear solves are handled internally via a KSP object

```
STGetKSP(ST st, KSP *ksp)
```

Gets the KSP object associated to an ST

All KSP options are available, by prepending the `-st_` prefix

## ST: Run-Time Examples

```
% program -eps_type power -st_type shift -st_shift 1.5

% program -eps_type power -st_type sinvert -st_shift 1.5

% program -eps_type power -st_type sinvert
          -eps_power_shift_type rayleigh

% program -eps_type arpack -eps_tol 1e-6
          -st_type sinvert -st_shift 1
          -st_ksp_type cgs -st_ksp_rtol 1e-8
          -st_pc_type sor -st_pc_sor_omega 1.3
```

## SVD: Basic Usage

Usual steps for solving an SVD problem with SLEPc:

1. Create an SVD object
2. Define the problem
3. (Optionally) Specify options for the solution
4. Run the solver
5. Retrieve the computed solution
6. Destroy the SVD object

All these operations are done via a generic interface, common to all the SVD solvers

## SVD: Simple Example

```
SVD          svd;          /* SVD solver context */
Mat          A;           /* matrix for A=USV^T */
Vec          u,v;        /* singular vectors */
PetscReal    s;          /* singular value */

SVDCreate(PETSC_COMM_WORLD, &svd);
SVDSsetOperator(svd, A);
SVDSsetFromOptions(svd);

SVDSsolve(svd);

SVDSgetConverged(svd, &nconv);
for (i=0; i<nconv; i++) {
    SVDSgetSingularTriplet(svd, i, &s, u, v);
}

SVDSdestroy(svd);
```

## Details: Solving the Problem

**SVDSolve(SVD svd)**

Launches the SVD solver

Currently available SVD solvers:

- ▶ Cross-product matrix with any EPS eigensolver
- ▶ Cyclic matrix with any EPS eigensolver
- ▶ Golub-Kahan-Lanczos bidiagonalization with explicit restart and deflation
- ▶ Golub-Kahan-Lanczos bidiagonalization with thick restart and deflation

## Details: Problem Definition and Specification of Options

`SVDSetOperators(SVD svd, Mat A)`

Used for passing the matrix that constitutes the problem

`SVDSetFromOptions(SVD svd)`

Looks in the command line for options related to SVD

For example, the following command line

```
% program -svd_tol 1e-8 -svd_max_it 100
```

is equivalent to a call `SVDSetTolerances(eps, 1e-8, 100)`

`SVDView(SVD svd, PetscViewer viewer)`

Prints information about the object (equivalent to `-svd_view`)

## Details: Viewing Current Options

Sample output of `-svd_view`

SVD Object:

method: trlanczos

transpose mode: explicit

selected portion of the spectrum: largest

number of singular values (nsv): 1

number of column vectors (ncv): 10

maximum dimension of projected problem (mpd): 10

maximum number of iterations: 100

tolerance: 1e-07

Lanczos reorthogonalization: two-side

IP Object:

orthogonalization method: classical Gram-Schmidt

orthogonalization refinement: if needed (eta: 0.707100)



## SVD: Run-Time Examples

```
% program -svd_view -svd_monitor  
  
% program -svd_type lanczos -svd_nsv 6 -svd_ncv 24  
  
% program -svd_type trlanczos -svd_tol 1e-8 -svd_max_it 2000  
  
% program -svd_type cross -svd_eps_type krylovschur  
  
% program -svd_type lapack  
  
% program -svd_type lanczos -svd_monitor_draw  
  
% program -svd_type trlanczos -svd_smallest
```



## Options for Subspace Generation

### Initial Subspace

- ▶ Provide an initial trial subspace, e.g. from a previous computation
- ▶ Current support only for a single vector ([EPSSetInitialVector](#))

### Deflation Subspace

- ▶ Provide a deflation space with [EPSAttachDeflationSpace](#)
- ▶ The eigensolver operates in the restriction to the orthogonal complement
- ▶ Useful for constrained eigenproblems or problems with a known nullspace

## Subspace Extraction

In some cases, convergence of the eigensolver may be very slow

→ Enhanced subspace **extraction**: try to extract better approximations from the available subspace

- ▶ Harmonic extraction
  - ▶ Compute harmonic Ritz values instead of Ritz values
  - ▶ Useful for computing interior eigenvalues (alternative to the spectral transformation)
  - ▶ Currently implemented in Krylov-Schur solver
- ▶ Other: refined extraction

## Computation of Many Eigenpairs

By default, a subspace of dimension  $2 \cdot nev$  is used...

For large  $nev$ , this is not appropriate

- ▶ Excessive storage and inefficient computation

$$\begin{array}{c} \boxed{A} \end{array} \begin{array}{c} \boxed{V_m} \end{array} = \begin{array}{c} \boxed{V_m} \end{array} \begin{array}{c} \boxed{S_m} \\ \boxed{b_{m+1}^*} \end{array}$$

**Strategy:** compute eigenvalues in chunks - restrict the dimension of the projected problem

```
% program -eps_nev 2000 -eps_mpd 300
```



## SLEPc Highlights

- ▶ Growing number of eigensolvers
- ▶ Seamlessly integrated spectral transformation
- ▶ Support for SVD
- ▶ Easy programming with PETSc's object-oriented style
- ▶ Data-structure neutral implementation
- ▶ Run-time flexibility, giving full control over the solution process
- ▶ Portability to a wide range of parallel platforms
- ▶ Usable from code written in C, C++ and Fortran
- ▶ Extensive documentation



## Future Directions

### Under Development

- ▶ Generalized Davidson and Jacobi-Davidson solvers
- ▶ Enable computational intervals for symmetric problems

### Mid Term

- ▶ Conjugate Gradient-type eigensolvers
- ▶ Non-symmetric Lanczos eigensolver
- ▶ Support for other types of eigenproblems: quadratic, structured, non-linear



## More Information



Homepage:

<http://www.grycap.upv.es/slepc>

Hands-on Exercises:

<http://www.grycap.upv.es/slepc/handson>

Contact email:

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