SLEPc:
Scalable Library for Eigenvalue Problem Computations

The DOE Advanced CompuTational Software Collection (ACTS)

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ACTS COLLECTION

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OUTLINE

- What is **SLEPc**?
- Computational Problems target by SLEPc
- **SLEPc**: Eigenvalue Solvers
- **SLEPc**: Spectral Transformation
- **SLEPc**: SVD Solvers
- **SLEPc**: Quadratic Eigenvalue Solvers
- Additional Features of **SLEPc**
- short DEMO

Scalable Library for Eigenvalue Problem computation

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Scalable Library for Eigenvalue Problem computation

SLEPc

- home page

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

- Additional Material:

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

  > module load slepc/3.1_g (there are more choices)

  > cp -r $SLEPC_DIR/src/eps/examples/ .

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Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Linear Least Squares Problems	Least Squares	$min_x \|\| b - Ax \|\|_2$	ScaLAPACK
	Minimum Norm Solution	$min_x \|\| x \|\|_2$	ScaLAPACK
	Minimum Norm Least Squares	$min_x \|\| b - Ax \|\|_2$ $min_x \|\| x \|\|_2$	ScaLAPACK
Standard Eigenvalue Problem	Symmetric Eigenvalue Problem	$Az = \lambda z$ *For* $A=A^H$ or $A=A^T$	ScaLAPACK (dense) SLEPc (sparse)
Singular Value Problem	Singular Value Decomposition	$A = U\Sigma V^T$ $A = U\Sigma V^H$	ScaLAPACK (dense) SLEPc (sparse)
Generalized Symmetric Definite Eigenproblem	Eigenproblem	$Az = \lambda Bz$ $ABz = \lambda z$ $BAz = \lambda z$	ScaLAPACK (dense) SLEPc (sparse)

Computational Problems

Computational Problem	Methodology	Algorithms	Library
• Eigenvalue Solvers • Spectral Transformations • SVD Solvers • Quadratic Eigenvalue Solvers	Availa in ACT	in ACTS	es that

[background]:Solving Eigenvalue Problems

Computational Problem

- Eigenvalue Solvers
- Spectral Transformations
- SVD Solvers
- Quadratic Eigenvalue Solvers

Standard Eigenproblem

$$Ax = \lambda x$$

Generalized Eigenproblem

$$Ax = \lambda Bx$$

Where,

- λ 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 (un)symmetric (Hermitian)
- Typically B is symmetric positive (semi-) definite

[background]: Solving Eigenvalue Problems

Computational Problem

- Eigenvalue Solvers
- Spectral Transformations
- SVD Solvers
- Quadratic Eigenvalue Solvers

Solutions

$$\lambda_0, \lambda_1, \ldots \lambda_{nev-1} \in \mathbb{C}$$

$$x_0, x_1, \ldots x_{nev-1} \in \mathbb{C}^n$$

Where,

- there are nev eigenvalues (counted with their multiplicities)

Computational requirements:

- Compute a few dominant eigenvalues
- Compute a few λ_i's with smallest or largest real parts
- Compute all λ_i's in a given region of the complex plane

[background]: Spectral Transformation

Computational Problem

- Eigenvalue Solvers
- Spectral Transformations
- SVD Solvers
- Quadratic Eigenvalue Solvers

A general techniques that can be used in many methods to improve convergence (better separation)

Original System ⇒ **Transformed System**

$$Ax = \lambda x \qquad \Rightarrow \qquad Tx = \theta x$$

In the transformed systems;

- λ_i's are modified by simple relation
- x_i's are not altered

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

[background] Singular Value Decomposition (SVD) Problems

Computational Problem	
• Eigenvalue Solvers • Spectral Transformations • **SVD Solvers** • Quadratic Eigenvalue Solvers	Compute the SVD of a rectangular matrix $A \in \mathbb{R}^{mxn}$

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

where

- Singular Values: $\sigma_1, \sigma_2, \ldots \sigma_n$
- Left singular vectors: $u_1, u_2, \ldots u_m$
- Right singular vectors : $v_1, v_2, \ldots v_n$

[background] Solving a SVD Problems

Computational Problem

- Eigenvalue Solvers
- Spectral Transformations
- **SVD Solvers**
- Quadratic Eigenvalue Solvers

Partial solution: nsv solutions:

- Singular values: $\sigma_0, \sigma_1, \ldots \sigma_{nsv-1} \in \mathbb{R}$
- Left singular vectors: $u_0, u_1, \ldots u_{nsv-1} \in \mathbb{R}^m$
- Right singular vectors : $v_0, v_1, \ldots v_{nsv-1} \in \mathbb{R}^n$

There are nsv singular values (counted with their multiplicities)

Computational requirements:

- Compute a few smallest or largest σ_i's
- Solve the eigenproblem A^TA
- Solve the eigenproblem $H(A) = \begin{bmatrix} 0^{mxm} & A \\ A^T & 0^{nxn} \end{bmatrix}$
- Bidiagonalization

[background] Quadratic Eigenvalue Problems

Computational Problem
• Eigenvalue Solvers
• Spectral Transformations
• SVD Solvers
• **Quadratic Eigenvalue Solvers**

Quadratic Eigenvalue Problem

$$(\lambda^2 M + \lambda C + K)x = 0$$

Where,

- λ is a (complex) scalar, eigenvalue
- x is a (complex) vector: eigenvector
- Matrices M, C and K can be real or complex
- Matrices M, C and K can be (un)symmetric (Hermitian)
- Typically some matrices are also symmetric positive (semi-) definite

[background] Solving Quadratic Eigenvalue Problems

Computational Problem

- Eigenvalue Solvers
- Spectral Transformations
- SVD Solvers
- **Quadratic Eigenvalue Solvers**

$$\lambda_0, \lambda_1, \ldots \lambda_{nev-1} \in \mathbb{C}$$

$$x_0, x_1, \ldots x_{nev-1} \in \mathbb{C}^n$$

Where,

- there are 2 X nev eigenvalues

Alternatives:

- Linearization $Az = \lambda Bz$

$$z = \begin{bmatrix} x \\ \lambda x \end{bmatrix} \qquad A = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \qquad B = \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix}$$

- Specific method (Q-Arnoldi)

SLEPc Design Considerations

- Various problem characteristics:
  - real/complex
  - Hermitian/non-hermitian
- Multiple ways to specify the solutions that are sought
- Many formulations (beyond $Ax = \lambda x$ or $Ax = \lambda Bx$)

Characteristics of the SLEPc Library

- Uniform abstract User Interfaces to address all the aforementioned problems
  - Through a simple and intuitive interphase, SLEPc provides internally solver implementations with a high-level of algorithmic complexity (deflation, restart, etc. .)
- Spectral transformations can be used irrespectively of the solver
- Recurrent linear solves may be necessary
- SVD and QEP can be solved via associated eigenproblem or specific methods (bidiagonalization/Q-Arnoldi)

Characteristics of the SLEPc Library

- General Purpose library for the solution of large-scale sparse eigenproblems on parallel computers
  - For standard, generalized and quadratic eigenproblems
  - For real and complex arithmetic
  - For Hermitian or non-Hermitian problems
  - For the partial SVD decomposition

  - Relies on PETSc Functionality
  - Current version 3.3 (released on August 2012). The major changes in this version are:
    - New EPS solvers: RQCG, GD2 and indefinite Krylov-Schur.
    - A major reorganization of code (now everything related to projected eigenproblems is encapsulated in a new auxiliary object DS).

Four Abstract Objects SLEPc

- Extends PETSc functionality with four objects
  - **EPS**: Eigenvalue Problem Solver

EPS is the abstract User Interface to:

- Describe an eigenvalue problem
- Access a collection of sparse eigensolver implementations and algorithmic parameters (e.g., eigenvalues of interest)

Four Abstract Objects SLEPc

- Extends PETSc functionality with four objects
  - **EPS**: Eigenvalue Problem Solver
  - **ST:** Spectral Transformation

- ST is abstract interface to transform the original system into $Tx = \theta x$
- ST is always associated to an EPS object and cannot be directly accessed

Four Abstract Objects SLEPc

- Extends PETSc functionality with four objects
  - **EPS**: Eigenvalue Problem Solver
  - **ST:** Spectral Transformation
  - **SVD:** Singular Value Decomposition

SVD is the abstract User Interface to:

- Describe a SVD problem
- Provides, transparently, access to eigensolvers for the associated eigenproblems or the specialized solver based on bidiagonalization

Four Abstract Objects SLEPc

- Extends PETSc functionality with four objects
  - **EPS**: Eigenvalue Problem Solver
  - **ST:** Spectral Transformation
  - **SVD:** Singular Value Decomposition
  - **QEP:** Quadratic Eigenvalue Problem

QEP is the abstract User Interface to:

- Describe a Quadratic Eigenproblem
- Provides, transparently, the linearlization to a generalized eigenproblem or the specialized solver (Q-Arnoldi)

Characteristics of the SLEPc Library

PETSc

SNES — Nonlinear Systems

Line Search	Trust Region	Other

TS — Time Steppers

Euler	Backward Euler	Time Stepping	Other

KSP — Krylov Subspace Methods

GMRES	CG	CGS	Bi-CGStab	TFQMR	Richardson	Chebychev	Other

PC — Preconditioners

Additive Schwarz	Block Jacobi	Jacobi	ILU	ICC	LU	Other

Mat — Matrices

Compressed Sparse Row	Block Compressed Sparse Row	Block Diagonal	Dense	Other

Vec — Vectors

IS — Index Sets

Indices	Block Indices	Stride	Other

SLEPc

SVD — SVD Solvers

Cross Product	Cyclic Matrix	Lanczos	Thick R. Lanczos

QEP — Quadratic

Linear-ization	Q-Arnoldi

EPS — Eigensolvers

Krylov-Schur	Arnoldi	Lanczos	GD	JD	Other

ST — Spectral Transformation

Shift	Shift-and-invert	Cayley	Fold	Preconditioner

Solving an Eigenvalue Problem with SLEPc

- Usual steps:
  - Declare a SLEPc EPS object and create the EPS object
  - Define the eigenvalue problem
  - Optionally specify algorithmic parameters for the solution
  - Invoke the eigensolver
  - Retrieve the computed solution
  - Don't forget to **Destroy** the EPS object

Solving an Eigenvalue Problem with SLEPc

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);
}

EPSDestroy(eps);
```

Functionality available in the EPSSolve

Currently available eigensolvers:

- Power Iteration and Rayleigh-Quatient Iteration (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**)
- Preconditioned solvers: Generalized Davison and Jacobi-Davidson (non-hermitian)
- ***new:*** Rayleigh-Quatient CG (RQCG)
- ***new:*** GD2
- ***new:*** Indefinite Krylov-Schur

Defining the Eigenproblem in SLEPc

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

Standard Eigenproblem

$$Ax = \lambda x$$

Specified through `Mat A`, while `Mat B` is set to `PETSC_NULL`

Generalized Eigenproblem

$$Ax = \lambda Bx$$

Specified through `Mat A` and `Mat B`

```
EPSSetProblemType( EPS eps, EPSProblemType type)
```

Problem Type	EPSProblemType	Command line option
Hermitian	EPS_HEP	-eps_hermitian
Generalized Hermitian	EPS_GHEP	-eps_gen_hermitian
non-Hermitian	EPS_NHEP	-eps_non_hermitian
Generalized non-Hermitian	EPS_GNHEP	-eps_gen_non_hermitian
GNHEP with B > 0	EPS_PGNHEP	-eps_pos_gen_non_hermitian

Defining the Eigenproblem in SLEPc

`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`)

Profiling in SLEPc (EPS)

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
```

Built-In Profiling/Debugging Support SLEPc

- Plotting computed eigenvalues

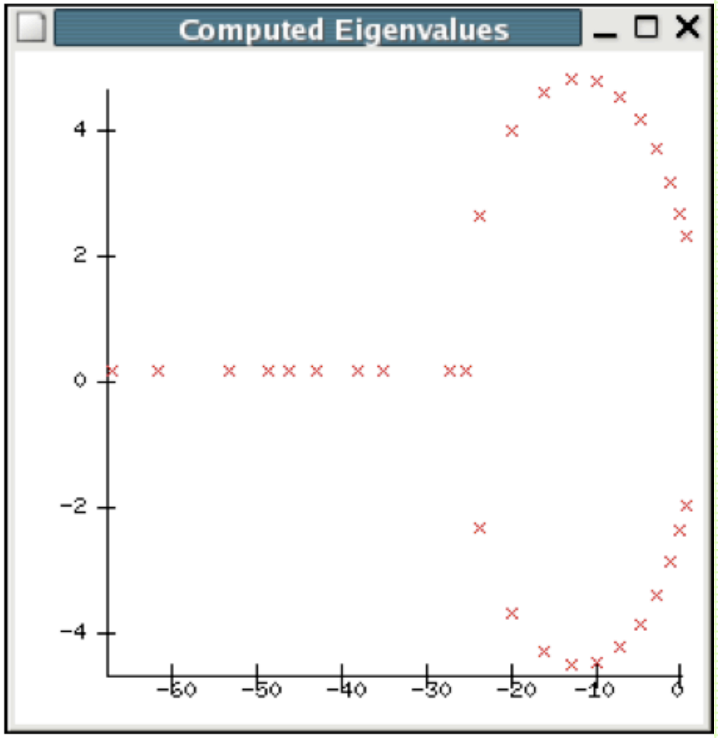
```
% program -eps_plot_eigs
```

- Printing profiling information

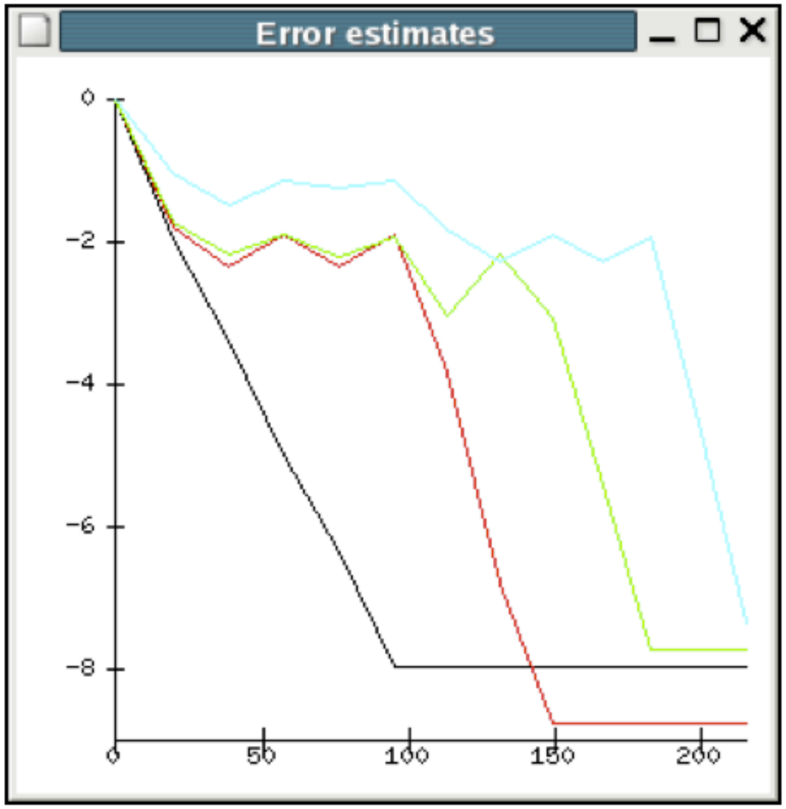
```
% program -log_summary
```

- Debugging

```
% program -start_in_debugger
% program -malloc_dump
```



Built-In Profiling/Debugging Support SLEPc



- Monitoring convergence (textually)

  ```
  % program -eps_monitor
  ```

- Monitoring convergence (graphically)

  ```
  % program -draw_pause 1
          -eps_monitor_draw_all
  ```

Spectral Transformation in SLEPc

Original System	$\Rightarrow$	Transformed System
$Ax = \lambda x$		$Tx = \theta x$

- A **ST** object is always associated to a **EPS** object
- Internally, the eigensolver works with the operator T
- At the end, eigenvalues are transformed back automatically

ST Type	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	$(A - \sigma I)^{-1}(A + \tau I)$	$(A - \sigma B)^{-1}(A + \tau B)$
precond	$K^{-1} \approx (A - \sigma I)^{-1}$	$K^{-1} \approx (A - \sigma B)^{-1}$

Accessing SLEPc's ST Object

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

- **ST** objects are not created by the user instead it is obtained
- Users only need *st to set options inside the code
- Linear solve are handled internally through PETSc's **KSP**

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

Gets the KSP object associated to an ST

All KSP options are available to the user, in the command line by prepending the **-st_** prefix

ST Run-Time Examples

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

% program -eps_type power -st_type sinvert -eps_target 1.5

% program -eps_type power -st_type sinvert
          -eps_power_shift_type rayleigh

% program -eps_type krylovschur -eps_tol 1e-6
          -st_type sinvert -eps_target 1
          -st_ksp_type cgs -st_ksp_rtol 1e-8
          -st_pc_type sor  -st_pc_sor_omega 1.3

% program -eps_type jd -eps_target 2
```

Solving a SVD Problem with SLEPc

- Usual steps:
  - Declare a SLEPc SVD object and create the SVD object
  - Define the problem
  - Optionally specify algorithmic parameters for the solution
  - Invoke the solver
  - Retrieve the computed solution
  - Don’t forget to **Destroy** the SVD object

Example of Solving a SVD Problem with SLEPc

```
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);
SVDSetOperator(svd, A);
SVDSetFromOptions(svd);

SVDSolve(svd);

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

SVDDestroy(svd);
```

Functionality available in the SVDSolve

Currently available SVD solver:

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

Additional Parameters for the SVD in SLEPc

```
SVDSetOperators( SVD svd, Mat A)
```

Specified through `Mat A` as the operator

```
SVDSetFromOptions( SVD svd)
```

Overwrite options from command-line arguments

```
SVDView( SVD svd, PetscViewer viewer)
```

Equivalent to -svd_view

Solving a QEP with SLEPc

- Usual steps:
  - Declare a SLEPc QEP object and create the QEP object
  - Define the eigenvalue problem
  - Optionally specify algorithmic parameters for the solution
  - Invoke the solver
  - Retrieve the computed solution
  - Don't forget to **Destroy** the QPD object

Example of Solving a QEP with SLEPc

```
QEP         qep;        /*  eigensolver context   */
Mat         M, C, K;    /*  matrices of the QEP   */
Vec         xr, xi;     /*  eigenvector, x        */
PetscScalar kr, ki;     /*  eigenvalue, k         */

QEPCreate(PETSC_COMM_WORLD, &qep);
QEPSetOperators(qep, M, C, K);
QEPSetProblemType(qep, QEP_GENERAL);
QEPSetFromOptions(qep);

QEPSolve(qep);

QEPGetConverged(qep, &nconv );
for (i=0; i<nconv; i++) {
  QEPGetEigenpair(qep, i, &kr, &ki, xr, xi );
}

QEPDestroy(qep);
```

Functionality available in the QEPSolve

Currently available eigensolvers:

- Linearization with any EPS solver
  - Non-symmetric $\begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} - \lambda \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix}$
  - Symmetric $\begin{bmatrix} 0 & -K \\ -K & -C \end{bmatrix} - \lambda \begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix}$
  - Hamiltonian $\begin{bmatrix} K & 0 \\ C & K \end{bmatrix} - \lambda \begin{bmatrix} 0 & K \\ -M & 0 \end{bmatrix}$
- Q-Arnoldi

Defining the QEP in SLEPc

```
QEPSetOperators( QEP qep, Mat M, Mat C, Mat K)
```

Define the QEP through matrices M,C, and K

```
QEPSetProblemType( QEP qep, QEPProblemType type)
```

Problem Type	EPSProblemType	Command line option
General	QEP_GENERAL	-qep_general
hermitian	QEP_HERMITIAN	-qep_hermitian
Gyroscopic	QEP_GYROSCOPIC	-qep_gyroscopic

Additional Parameters for the QEP in SLEPc

`QEPSetFromOptions(QEP qep)`

Overwrite options from command-line arguments

`QEPView(QEP qep, PetscViewer viewer)`

Equivalent to -qep_view

`QEPLinearSetCompanionForm(QEP qep, PetscInt cform)`

Selects among the different available expressions for linearization

Options for Subspace Generation in SLEPc

Initial Subspace

- Provide an initial trial subspace with **`EPSSetInitialSpace`** (e.g., from previous computations)
- Krylov solvers only support a single vector

Deflation Subspace

- Provide an initial trial subspace with **`EPSSetDeflationSpace`**
- The eigensolver operates in the restriction to the orthogonal compliment
- Useful for constraint eigenproblems or problems with a known nullspace

SLEPc Highlights

- Growing number of eigensolvers
- Seamlessly integrated spectral transformation
- Support for SVD and QEP
- PETSc style user interfaces and extensibility
- Supported run-time options to drive the solver and parameter selection
- Portability to a wide range of platforms
- Supports C, C++ and different flavors of fortran
- Extensive documentation
- ***Got PETSc?*** then, very easy to install

Acknowledgements

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