Lecture 09 – Krylov Methods and Third Party Libraries

Prof. Brendan Kochunas

NERS/ENGR 570 - Methods and Practice of Scientific Computing (F20)

COLLEGE OF ENGINEERING
NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

Outline

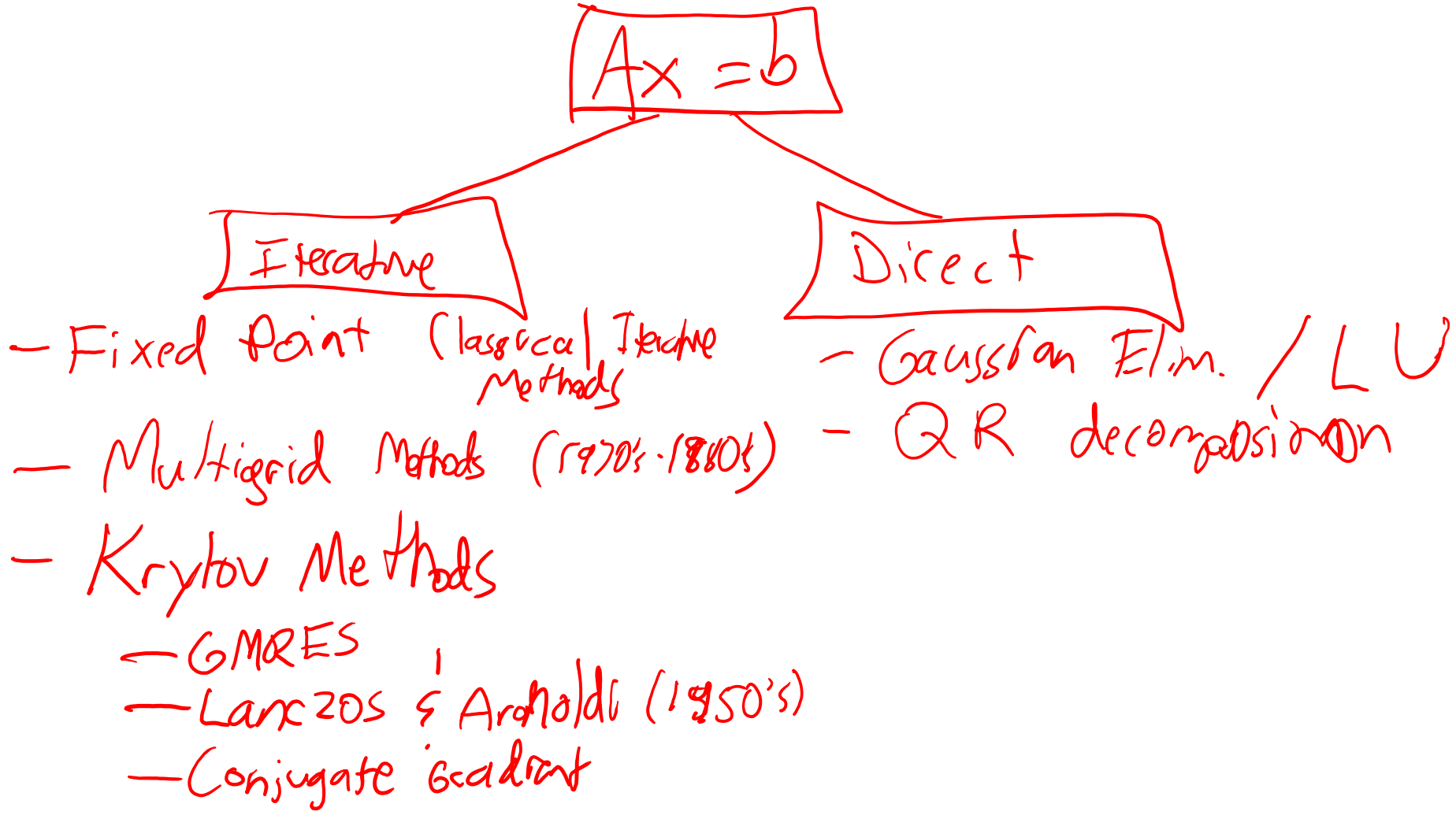
- Krylov Methods
- Convergence and Preconditioning
- Third Party Libraries
  - BLAS/LAPACK
  - PETSc
  - Trilinos

Learning Objectives: By the end of Today's Lecture you should be able to

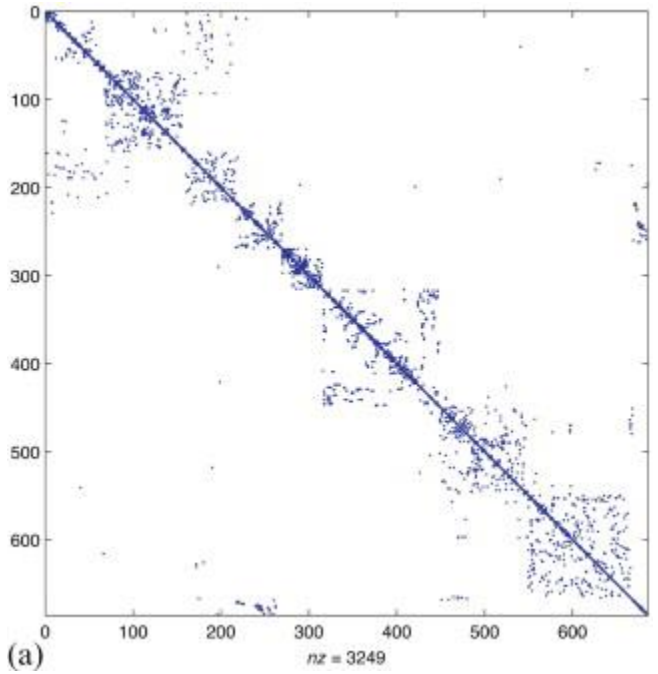
- (Knowledge) explain what defines a Krylov method
- (Knowledge) explain the underlying algorithmic features of GMRES
- (Knowledge) have an intuition about how well a Krylov method will converge
- (Knowledge) describe how preconditioners work
- (Knowledge) quickly navigate documentation for BLAS, LAPACK, PETSc, and Trilinos to find more information about a particular capability of the library

Review/Recap

Overview of Solution Methods



Krylov Methods



Reference: Yousef Saad, *Iterative Methods for Sparse Linear Systems*, SIAM

Krylov (subspace) Methods

- Use Krylov subspaces

$$K_p(\mathbf{A},\mathbf{b}) = \text{span}\left\{\mathbf{b}, \mathbf{Ab}, \mathbf{A^2b}, \ldots, \mathbf{A^pb}\right\}$$

- Krylov subspaces are easy and efficient to construct
  - Use only matrix-vector operations (this is good for large sparse systems!)

- Krylov methods also rely on projection
  - Specifically projection to the Krylov subspace

General Idea: Projection Methods

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$$

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}(\mathbf{x}_0 + \delta) \perp L$$

$$\mathbf{r}_0 - \mathbf{A}\delta \perp L$$

$$\mathbf{r}_{new} = \mathbf{r}_0 - \mathbf{A}\delta$$

- Two types: orthogonal and oblique
- For a linear system: $\mathbf{A}\mathbf{x} = \mathbf{b}$
  - $\mathbf{A}$ exists in $\boldsymbol{R}^n$ and $\boldsymbol{K}$ and $\boldsymbol{L}$ are two subspaces within $\boldsymbol{R}^n$ where $\boldsymbol{K} \perp \boldsymbol{L}$
  - An approximation of the solution is: $\tilde{\mathbf{x}} = \mathbf{x}_0 + \delta$
  - which has the residual: $\mathbf{r} = \mathbf{A}\tilde{\mathbf{x}} - \mathbf{b}$
- Solution by orthogonal projection means

Find $\tilde{\mathbf{x}} \in \mathbf{x}_0 + K$ such that $\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}^{(\ell)} \perp L$

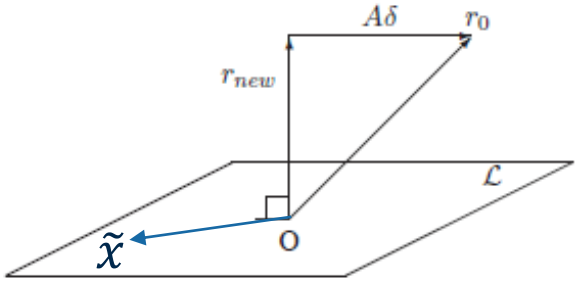


Figure 5.1: Interpretation of the orthogonality condition.

Orthogonalization Schemes: Arnoldi and GMRES

Arnoldi

- Uses Gram-Schmidt procedure to build an orthonormal basis

GMRES

- Generalized Minimum Residual

ALGORITHM 6.4 *Full Orthogonalization Method (FOM)*

1. Compute $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, and $v_1 := r_0/\beta$
2. Define the $m \times m$ matrix $H_m = \{h_{ij}\}_{i,j=1,\ldots,m}$; Set $H_m = 0$
3. For $j = 1, 2, \ldots, m$ Do:
4. Compute $w_j := Av_j$
5. For $i = 1, \ldots, j$ Do:
6. $h_{ij} = (w_j, v_i)$
7. $w_j := w_j - h_{ij}v_i$
8. EndDo
9. Compute $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ set $m := j$ and Goto 12
10. Compute $v_{j+1} = w_j/h_{j+1,j}$.
11. EndDo
12. Compute $y_m = H_m^{-1}(\beta e_1)$ and $x_m = x_0 + V_m y_m$

ALGORITHM 6.9 *GMRES*

1. Compute $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, and $v_1 := r_0/\beta$
2. For $j = 1, 2, \ldots, m$ Do:
3. Compute $w_j := Av_j$
4. For $i = 1, \ldots, j$ Do:
5. $h_{ij} := (w_j, v_i)$
6. $w_j := w_j - h_{ij}v_i$
7. EndDo
8. $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ set $m := j$ and go to 11
9. $v_{j+1} = w_j/h_{j+1,j}$
10. EndDo
11. Define the $(m+1) \times m$ Hessenberg matrix $\bar{H}_m = \{h_{ij}\}_{1 \le i \le m+1, 1 \le j \le m}$.
12. Compute y_m the minimizer of $\|\beta e_1 - \bar{H}_m y\|_2$ and $x_m = x_0 + V_m y_m$.

Arnoldi Factorization

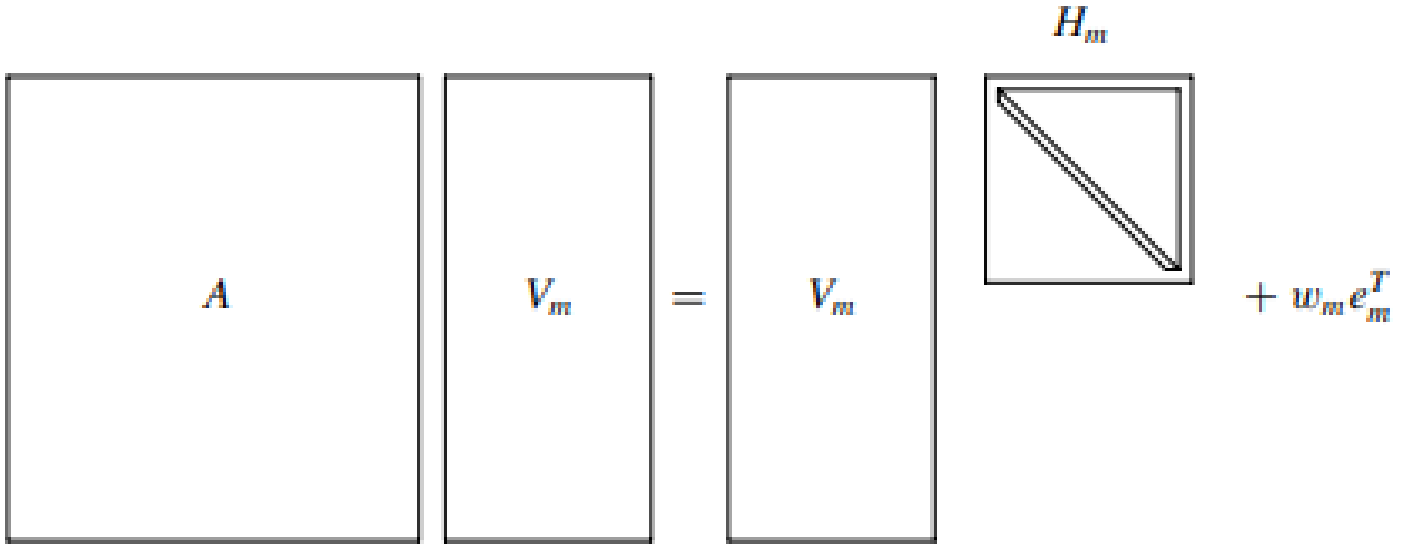


Figure 6.1. *The action of A on V_m gives $V_m H_m$ plus a rank-one matrix.*

Special cases: Symmetric Matrices

Lanczos algorithm for symmetric matrices

- This is a simplification of Arnoldi's method, where the Hessenberg matrix is tridiagonal

ALGORITHM **6.15** *The Lanczos Algorithm*

1. *Choose an initial vector* v_1 *of 2-norm unity. Set* $\beta_1 \equiv 0, v_0 \equiv 0$
2. *For* $j = 1, 2, \ldots, m$ *Do:*
3. $w_j := Av_j - \beta_j v_{j-1}$
4. $\alpha_j := (w_j, v_j)$
5. $w_j := w_j - \alpha_j v_j$
6. $\beta_{j+1} := \|w_j\|_2$. *If* $\beta_{j+1} = 0$ *then Stop*
7. $v_{j+1} := w_j / \beta_{j+1}$
8. *EndDo*

Conjugate Gradient (CG)

- Only for symmetric systems

ALGORITHM **6.16** *Lanczos Method for Linear Systems*

1. *Compute* $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, *and* $v_1 := r_0/\beta$
2. *For* $j = 1, 2, \ldots, m$ *Do:*
3. $w_j = Av_j - \beta_j v_{j-1}$ *(If* $j = 1$ *set* $\beta_1 v_0 \equiv 0$*)*
4. $\alpha_j = (w_j, v_j)$
5. $w_j := w_j - \alpha_j v_j$
6. $\beta_{j+1} = \|w_j\|_2$. *If* $\beta_{j+1} = 0$ *set* $m := j$ *and go to 9*
7. $v_{j+1} = w_j / \beta_{j+1}$
8. *EndDo*
9. *Set* $T_m = \text{tridiag}\ (\beta_i, \alpha_i, \beta_{i+1})$, *and* $V_m = [v_1, \ldots, v_m]$.
10. *Compute* $y_m = T_m^{-1}(\beta e_1)$ *and* $x_m = x_0 + V_m y_m$

Bi-Orthognalization Schemes: Lanczos and BiCGSTAB

Lanczos (Generalize for non-symmetric)

- Build 2 subspaces

$$\mathcal{K}_m(A, v_1) = \text{span}\{v_1, Av_1, \ldots, A^{m-1}v_1\}$$
$$\mathcal{K}_m(A^T, w_1) = \text{span}\{w_1, A^T w_1, \ldots, (A^T)^{m-1}w_1\}$$

ALGORITHM 7.1 *The Lanczos Biorthogonalization Procedure*

1. *Choose two vectors* v_1, w_1 *such that* $(v_1, w_1) = 1$.
2. *Set* $\beta_1 = \delta_1 \equiv 0$, $w_0 = v_0 \equiv 0$
3. *For* $j = 1, 2, \ldots, m$ *Do:*
4. $\quad \alpha_j = (Av_j, w_j)$
5. $\quad \hat{v}_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$
6. $\quad \hat{w}_{j+1} = A^T w_j - \alpha_j w_j - \delta_j w_{j-1}$
7. $\quad \delta_{j+1} = |(\hat{v}_{j+1}, \hat{w}_{j+1})|^{1/2}$. *If* $\delta_{j+1} = 0$ *Stop*
8. $\quad \beta_{j+1} = (\hat{v}_{j+1}, \hat{w}_{j+1})/\delta_{j+1}$
9. $\quad w_{j+1} = \hat{w}_{j+1}/\beta_{j+1}$
10. $\quad v_{j+1} = \hat{v}_{j+1}/\delta_{j+1}$
11. *EndDo*

BiCGSTAB

- Variation of Conjugate Gradient Squared (Transpose free Bi-Conjugate Gradient)

ALGORITHM 7.7 *BICGSTAB*

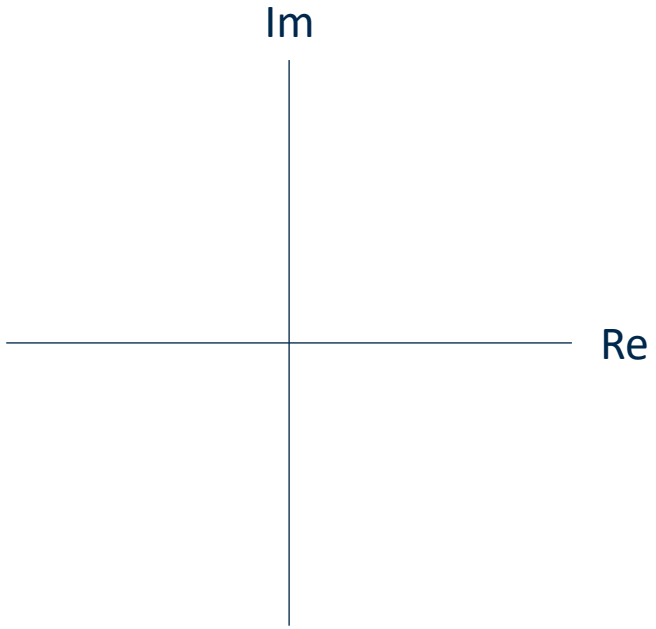
1. *Compute* $r_0 := b - Ax_0$; r_0^* *arbitrary;*
2. $p_0 := r_0$.
3. *For* $j = 0, 1, \ldots,$ *until convergence Do:*
4. $\quad \alpha_j := (r_j, r_0^*)/(Ap_j, r_0^*)$
5. $\quad s_j := r_j - \alpha_j Ap_j$
6. $\quad \omega_j := (As_j, s_j)/(As_j, As_j)$
7. $\quad x_{j+1} := x_j + \alpha_j p_j + \omega_j s_j$
8. $\quad r_{j+1} := s_j - \omega_j As_j$
9. $\quad \beta_j := \frac{(r_{j+1}, r_0^*)}{(r_j, r_0^*)} \times \frac{\alpha_j}{\omega_j}$
10. $\quad p_{j+1} := r_{j+1} + \beta_j(p_j - \omega_j Ap_j)$
11. *EndDo*

Convergence of Krylov Methods

- Convergence is related to properties of the eigenspectrum of the coefficient matrix, $\mathbf{A}$.
  - But more specifically the condition number:

$$\left\|\mathbf{r}^{(\ell)}\right\| \propto \kappa(\mathbf{A})$$

- Convergence is often not monotonic
- GMRES does well if eigenvalues of $\mathbf{A}$ are clustered.
- BiCGSTAB does well if eigenvalues are spread out
  - It isolates extremal eigenvalues



More about condition numbers

- Generally it tells us how much an output value can change relate to a small change in the input
  - Bounds accuracy of approximate solution to a linear system
- Generally given by:

$$\kappa(\mathbf{A}) = \frac{\sigma_{\max}(\mathbf{A})}{\sigma_{\min}(\mathbf{A})}$$

- Recall that under certain conditions the SVD may be equivalent to the eigendecomposition so sometimes:

$$\kappa(\mathbf{A}) = \frac{|\lambda_{\max}(\mathbf{A})|}{|\lambda_{\min}(\mathbf{A})|}$$

- Note that this differs from the classical iterative techniques where generally convergence is given by:

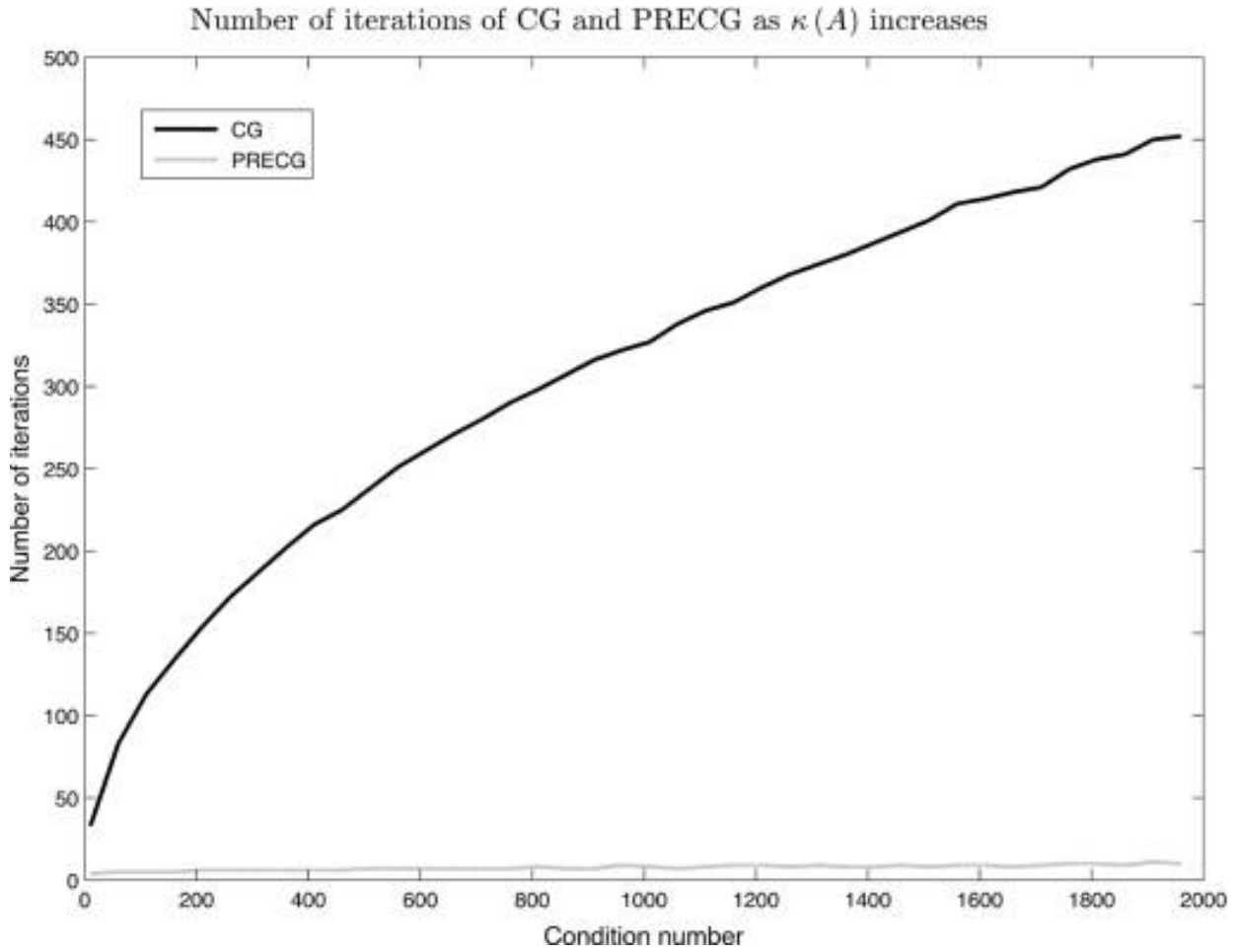
$$\rho(\mathbf{A}) = \max_i |\lambda_i(\mathbf{A})| = |\lambda_{\max}(\mathbf{A})|$$

- The discretization of most PDE's give condition numbers that are ***unbounded***, and *increase as the problem size increases*.

Preconditioning

- Objective: Lower the condition number of $\mathbf{A}$ to achieve faster convergence
  - Left Preconditioner: $\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}$
  - Right Preconditioner: $\mathbf{A}\mathbf{M}^{-1}\mathbf{M}\mathbf{x} = \mathbf{b}$ solve $\mathbf{A}\mathbf{M}^{-1}\mathbf{u} = \mathbf{b},$ then $\mathbf{u} = \mathbf{M}\mathbf{x}$
- Properties of a good preconditioner
  - Large decrease in condition number for a wide range of A
  - Efficient to construct and apply
- Krylov methods generally only as good as their preconditioner.
  - This is conservation of misery.
  - Research into preconditioners still an active topic
  - Consequently, for some problems classical iteration schemes are still the best choice

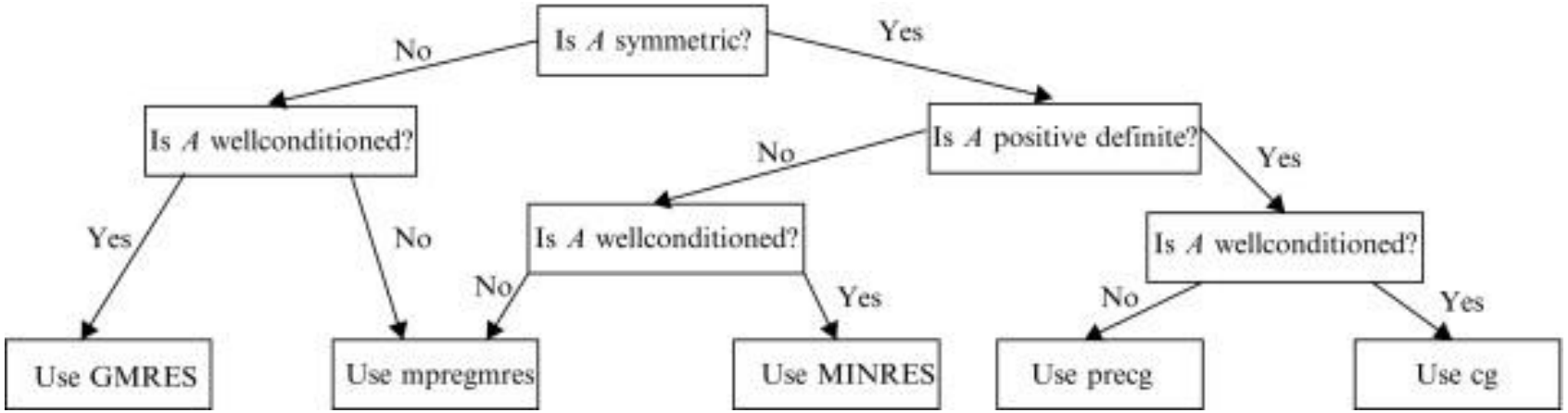
Importance of a Preconditioner



Lots of Types of Preconditioners

- Classical methods; Jacobi, SOR, SSOR
- Decomposition:
  - Incomplete LU (ILU): do an LU factorization but don't change sparsity
    - Very difficult to parallelize
  - Cholesky
- Polynomials: Chebyshev, Least-Squares
- Multigrid
- "Physics-based"

Choosing a Krylov Method



Summary of Krylov Methods

Orthogonalization

- Usually requires more storage
  - e.g. Hessenberg matrix and GMRES vectors
  - Restarted forms attempt to mitigate this
- Guaranteed to converge
  - May require full orthogonalization

Bi-Orthogonalization

- Avoid storage by doing twice the work (bi-orthogonalization)
  - Uses 3-term recurrence for orthogonalizing
- Not guaranteed to converge, but it usually does

Probably need a preconditioner

Scientific Computing Libraries

BLAS, LAPACK, PETSc, Trilinos, and Others

BLAS (Basic Linear Algebra Subprograms)

- BLAS is a (Fortran) programming interface to low-level linear algebra routines.
- Examples of basic linear algebra operations:
  - Dot products, addition of vectors, scalar multiplication of vectors.
  - Matrix-vector multiplications.
  - Matrix-matrix multiplications.
- Why BLAS?
  - Handwritten simple linear algebra routines can run at widely varying speeds.
  - Loop unrolling and finding correct compiler flags is key and sometimes becomes difficult
  - when using a new compiler or computer.
  - Basic linear algebra routines form the backbone of many sophisticated solvers and BLAS package tries to provide most optimized version of basic linear algebra routines.
  - Linking to BLAS, we get code that runs much faster than hand-written version of code.

BLAS (Basic Linear Algebra Subprograms)

- BLAS-1 operations:
  - Routines which involve only vector operations: dot-products, vector norms.
  - S – Single Precision, D - Double Precision, C – Complex, Z – Double precision complex

_SWAP	x <---> y	S, D
_SCAL	x <-- alpha * x	S, D, C, Z, CS, ZD
_COPY	x <-- y	S, D, C, Z
_AXPY	y <-- alpha * x + y	S, D, C, Z
_DOT	dot <--	S, D, DS
_DOTU	dot <-- x^T*y	C, Z
_DOTC	dot <-- x^H*y	C, Z
_NRM2	nrm2 <-- || x ||_2	S, D, SC, DZ
_ASUM	nrm1 <-- || x ||_1	S, D, SC, DZ

BLAS (Basic Linear Algebra Subprograms)

- BLAS-2 operations:
  - This level contains matrix-vector operations including, among other things, a generalized matrix-vector multiplication (gemv):

```
_GEMV      y <-- alpha*A*x + beta*y, y <-- alpha*A^T*x + beta*y  (General Real Matrix)
_GBMV      y <-- alpha*A*x + beta*y, y <-- alpha*A^T*x + beta*y  (General Banded)
_HEMV      y <-- alpha*A*x + beta*y                              (Hermitian (complex))
_HBMV      y <-- alpha*A*x + beta*y                              (Hermitian (banded))
_SYMV      y <-- alpha*A*x + beta*y                              (Symmetric)
_SBMV      y <-- alpha*A*x + beta*y                              (Symmetric banded)
_TRMV      y <-- A*x , x <-- A^T*x                               (Triangular)
_TBMV      y <-- A*x , x <-- A^T*x                               (Triangular banded)
_TRSV      y <-- inv(A)*x , x <-- inv(A^T) * x
```

BLAS (Basic Linear Algebra Subprograms)

- BLAS-3 Matrix-matrix operations:
  - This level operations are matrix-matrix multiplications.

```
_GEMM  C <-- alpha op(A) op(B) + beta C
_SYMM  C <-- alpha AB + beta C
_HEMM  C <-- alpha AB + beta C
_SYRK  C <-- alpha A A^T + beta C
_HERK  C <-- alpha A A^H + beta C
_SYRK2 C <-- alpha A B^T + alpha B A^T + beta C
_TRMM  B <-- alpha op(A) B
_TRSM  B <-- alpha op(inv(A)) B
```

BLAS-Example Code

http://www.netlib.org/lapack/explore-html/

```
*  =====================================================================
      DOUBLE PRECISION FUNCTION ddot(N,DX,INCX,DY,INCY)
*
*  -- Reference BLAS level1 routine (version 3.4.0) --
*  -- Reference BLAS is a software package provided by Univ. of Tennessee,    --
*  -- Univ. of California Berkeley, Univ. of Colorado Denver and NAG Ltd..--
*     November 2011
*
*     .. Scalar Arguments ..
      INTEGER INCX,INCY,N
*     ..
*     .. Array Arguments ..
      DOUBLE PRECISION DX(*),DY(*)
*     ..
*
*  =====================================================================
*
*     .. Local Scalars ..
      DOUBLE PRECISION DTEMP
      INTEGER I,IX,IY,M,MP1
*     ..
*     .. Intrinsic Functions ..
      INTRINSIC mod
*     ..
      ddot = 0.0d0
      dtemp = 0.0d0
      IF (n.LE.0) RETURN
      IF (incx.EQ.1 .AND. incy.EQ.1) THEN
*
*        code for both increments equal to 1
*
*
*        clean-up loop
*
         m = mod(n,5)
         IF (m.NE.0) THEN
            DO i = 1,m
               dtemp = dtemp + dx(i)*dy(i)
            END DO
            IF (n.LT.5) THEN
               ddot=dtemp
            RETURN
            END IF
         END IF
         mp1 = m + 1
         DO i = mp1,n,5
          dtemp = dtemp + dx(i)*dy(i) + dx(i+1)*dy(i+1) +
     $            dx(i+2)*dy(i+2) + dx(i+3)*dy(i+3) + dx(i+4)*dy(i+4)
         END DO
      ELSE
*
```

LAPACK

- LA Pack is a collection of Fortran functions that can help you solve Linear Algebra related problems based on BLAS routines.
- LAPACK provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems.
- The associated matrix factorizations (LU, Cholesky, QR, SVD, Schur, generalized Schur) are also provided,
- Dense and banded matrices are handled, but not general sparse matrices. In all areas, similar functionality is provided for real and complex matrices, in both single and double precision.
- Online Reference: http://www.netlib.org/lapack

LAPACK Routines

- Simple driver routines: Simple driver routines solve a linear algebra problem
- Eg: Finding eigenvalues of a matrix, solving a set of linear equations etc.,
- Expert driver routines: Expert driver routines do the same things as simple driver routines, but will provide more options or information to the user.
- Eg: SGESV is used to solve linear systems whereas the expert driver SGESVX not only solves the linear system but will also provide the estimate of the condition number of input matrix.
- Computational routines: Routines are mainly for internal use by LA Pack itself and called by driver routines.
- Eg: LU, QR and other factorizations or reduction of symmetric matrix to tridiagonal form.

LAPACK Naming conventions

- Lapack functions are usually named in the form XYYZZZ

X = type of problem that the routine solves
S Single precision real
D Double precision real
C Single complex
Z Double precision complex

YY = matrix types
GE General
BD Bidiagonal
HE Hermitian
HB Hermitian Band
SB Symmetric Band

ZZZ = indicate the computation performed
Eg: SV = Solve, SVX = Solve Expert

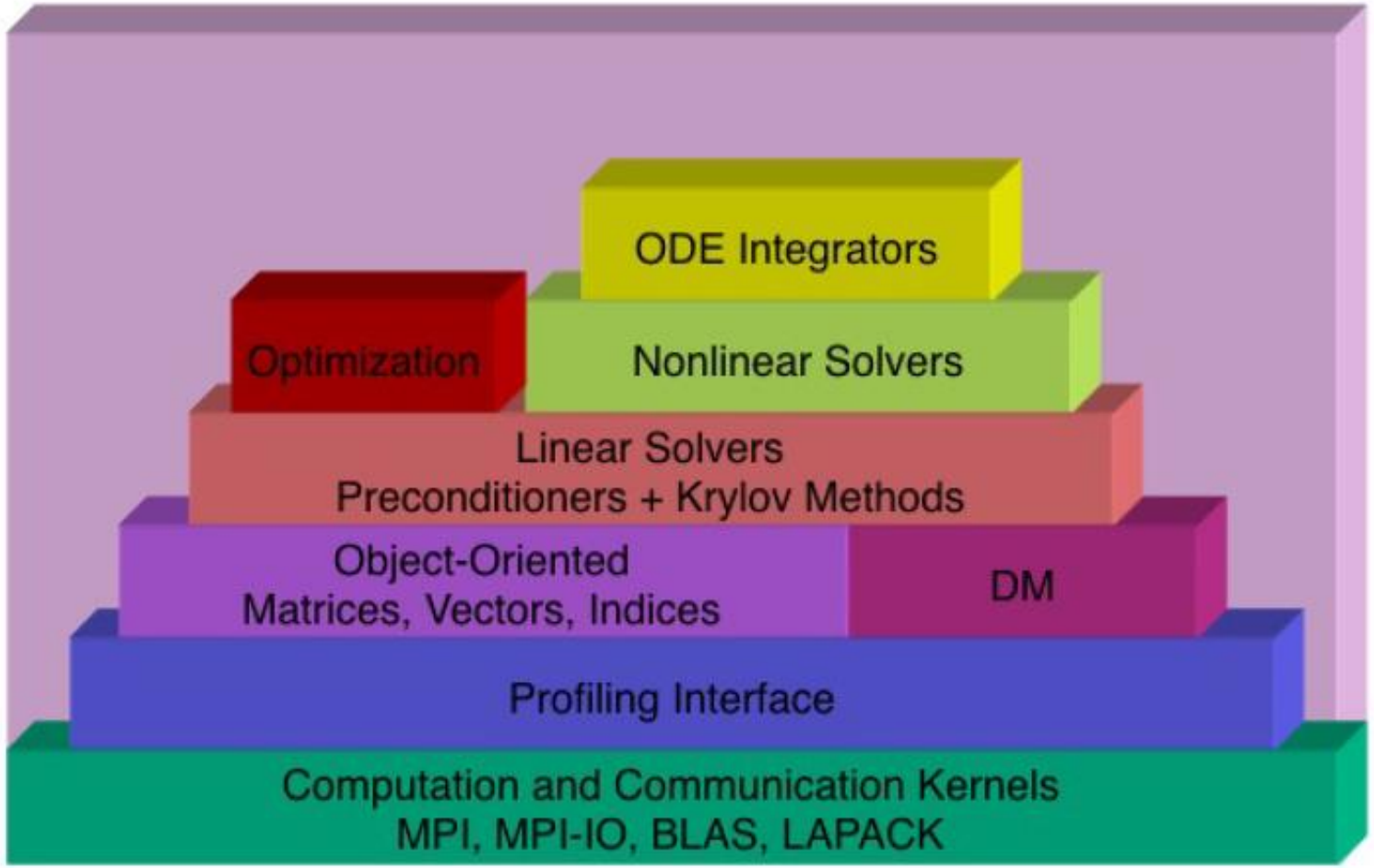
PETSc

- **P**ortable **E**xtensible **T**oolkit for **S**cientific computing:

  Developing parallel, nontrivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort. PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver, nor a silver bullet. — Barry Smith

- Philosophy: Everything has a plugin architecture
  - Vectors, Matrices, Partitioning algorithms
  - Preconditioners, Krylov accelerators
  - Nonlinear solvers, Time integrators
  - Spatial discretizations
  - Application user loads plugin at run, no source code in sight. PETSc tries to keep solvers independent of physics and discretization.

PETSc Structure



Basic PETSc object usage

Every object in PETSc supports a basic interface

Function	Operation
`Create()`	create the object
`Get/SetName()`	name the object
`Get/SetType()`	set the implementation type
`Get/SetOptionsPrefix()`	set the prefix for all options
`SetFromOptions()`	customize object from the command line
`SetUp()`	preform other initialization
`View()`	view the object
`Destroy()`	cleanup object allocation

Also, all objects support the `-help` option.

PETSc Vectors

- PETSc vectors are fundamental datatypes of PETSc which is used represent field solutions, right-hand sides etc. Each process locally owns a subvector of contiguous global data.
- Creating PETSc vectors:
  - `VecCreate(MPI_Comm, Vec *)`
  - `VecSetSizes(Vec, int n, int N)`
  - `VecSetTypes(Vec, VecType typename)`
  - `VecSetFromOptions(Vec)`
- Supports all vector space operations `VecDot()`, `VecNorm()`, `VecScale()`

PETSc Vectors

- Inserting entries into PETSc vectors:
  - Each process sets or add values and begins communications to send values to correct process and complete the communication.

  - `VecSetValues(Vec v, int n, int rows[], PetscScalar values[], mode)`
  - `VecAssemblyBegin(Vec v)`
  - `VecAssemblyEnd(Vec v)`

- PETSc allows you to access the local storage with `VecGetArray()` functions.

PETSc Matrices

- PETSc handles both sparse and dense matrix formats in parallel.

```
MatCreate(MPI_Comm, Mat *)
MatSetSizes(Mat, int m, int n, int M, int N)
MatSetType(Mat, MatType typeName)
MatSetFromOptions(Mat)
```
Can set the type at runtime

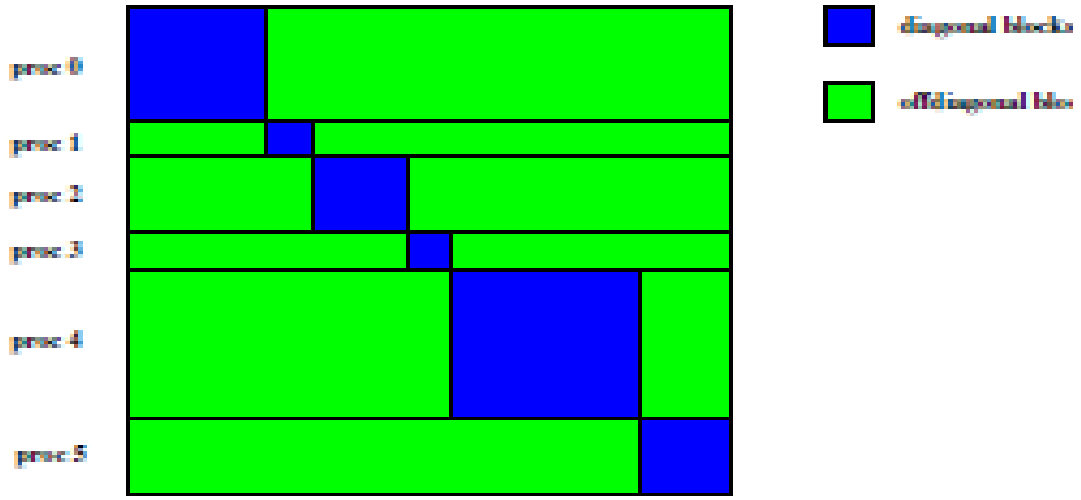
```
MatMPIBAIJSetPreallocation(Mat,...)
```
important for assembly performance

```
MatSetBlockSize(Mat, int bs)
```
for vector problems

```
MatSetValues(Mat,...)
```
MUST be used, but does automatic communication
MatSetValuesLocal, MatSetValuesStencil,
MatSetValuesBlocked

Parallel sparse matrix in PETSc

Each process locally owns a submatrix of contiguous global rows
Each submatrix consists of diagonal and off-diagonal parts




```
MatGetOwnershipRange(Mat A,int *start,int *end)
```

start: first locally owned row of global matrix
end-1: last locally owned row of global matrix

Other useful features of PETSc

- Iterative solvers:
  - Linear solvers in PETSc KSP: Conjugate Gradient, Bi Conjugate Gradient, GMRES, etc.
  - Lots of sophisticated Preconditioners like block Jacobi, SOR, Multigrid, field-split, etc.
  - Nonlinear solvers (SNES):
    - Newton type with line search and trust-region
    - Quasi Newton methods
    - Nonlinear conjugate gradients
    - User-defined methods.
- Time Integration strategies

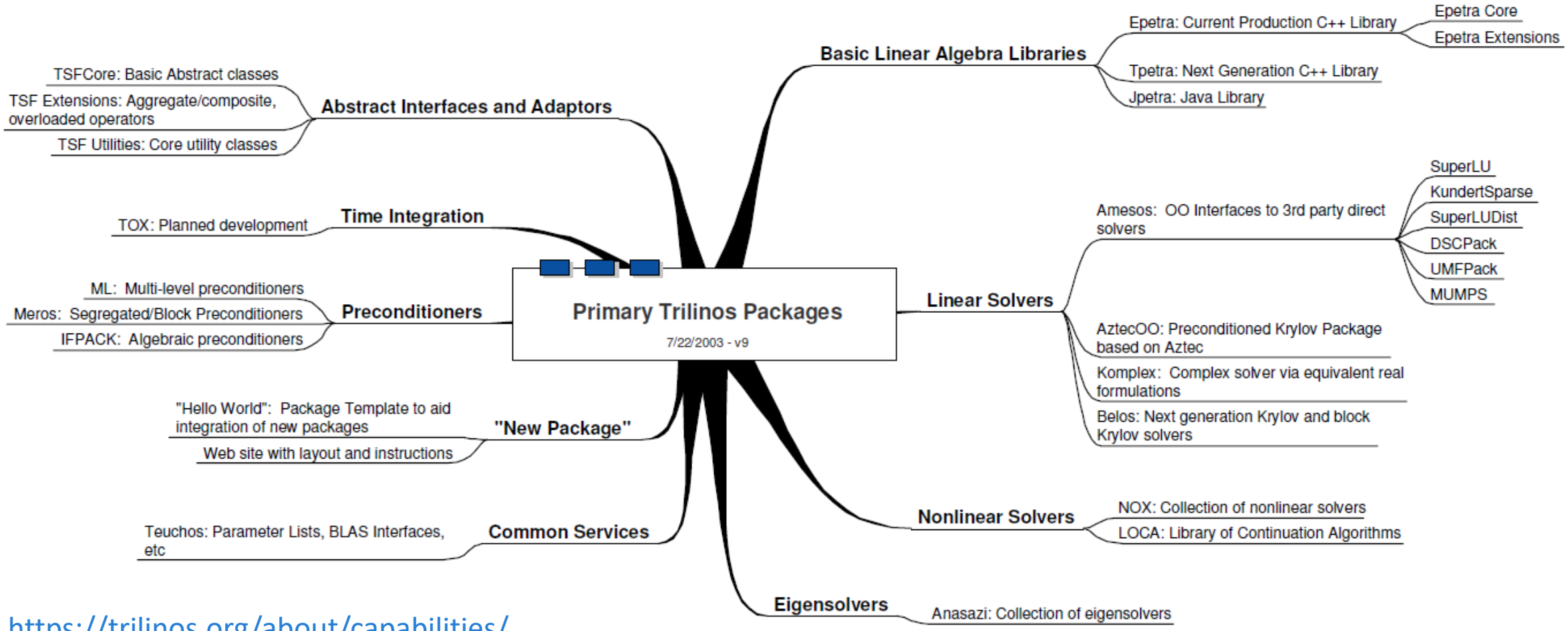
TRILINOS

- The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages.
- More extensive than PETSc and more complex to use.
- Trilinos tries to provide an environment for solving FEM problems and PETSc provides an environment for solving sparse linear algebra problems.

Capabilities

- Trilinos – Greek for “String of Pearls”
  - Most package names are Greek
  - Duplication of capability
  - Some are deprecated

User Experience	Parallel Programming Environments	I/O Support
Mesh & Geometry	Framework & Tools	Discretization
Linear Algebra Services	Linear & Eigen Solvers	Embedded Nonlinear Analysis
Software Engineering		



https://trilinos.org/about/capabilities/

- Contains Tools for:
  - Problem Discretization
  - Solution of Algebraic Systems
  - Uncertainty Quantification
  - Numerical Optimization

https://fastmath-scidac.llnl.gov/software-catalog.html

Integrating Libraries with your Code
eXstreme-scale Software Development Kit