Introduction to PETSc

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Outline

- Introduction
- Getting started
- PETSc objects
- `SNES`: Nonlinear solvers
- `TS`: Time stepping
- Profiling, debugging

Introduction

To set the stage

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 dffculties and reduce the development time, but it is not black-box PDE solver, nor a silver bullet

Barry Smith

More specifically...

Portable Extendable Toolkit for Scientific Computations

- Scientific Computations: parallel linear algebra, in particular linear and nonlinear solvers
- Toolkit: Contains high level solvers, but also the low level tools to roll your own.
- Portable: Available on many platforms, basically anything that has MPI

Why use it? It's big, powerful, well supported.

What does PETSc target?

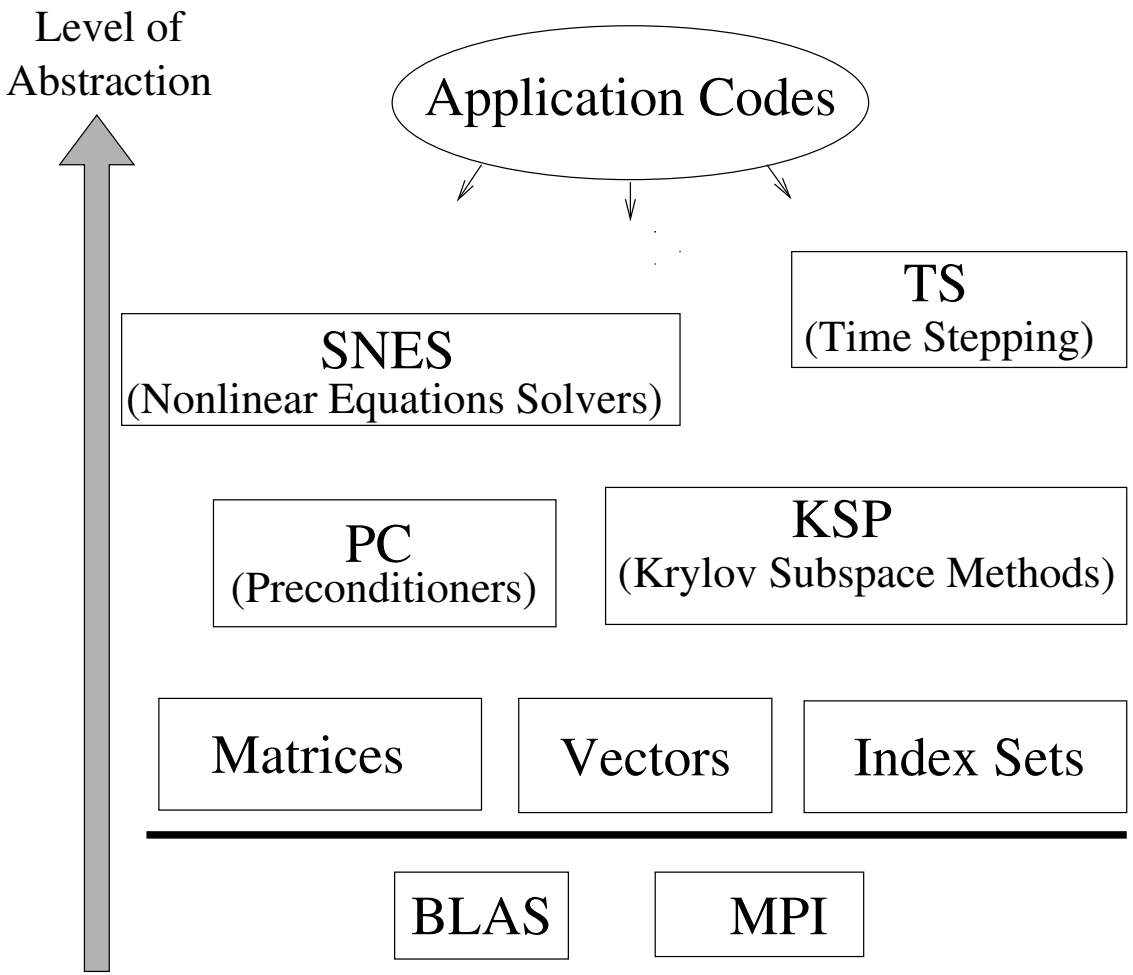
- Serial and Parallel
- Linear and nonlinear
- Finite difference and finite element
- Structured and unstructured

What is in PETSc?

- Linear system solvers (sparse/dense, iterative/direct)
- Nonlinear system solvers
- Tools for distributed matrices
- Support for profiling, debugging, graphical output

Documentation and help

- Web page: `http://tinyurl.com/PETSc-man-page`
- PDF manual: `http://tinyurl.com/PETSc-pdf-manual`
- PETSc on TACC clusters: consulting through TACC/XSEDE user portal
- General questions about PETSc: petsc-maint@mcs.anl.gov
- Follow-up to this tutorial: eijkhout@tacc.utexas.edu


Level of
Abstraction
Application Codes
TS
(Time Stepping)
SNES
(Nonlinear Equations Solvers)
PC
(Preconditioners)
KSP
(Krylov Subspace Methods)
Matrices
Vectors
Index Sets
BLAS
MPI

Parallel Numerical Components of PETSc

Nonlinear Solvers		
Newton−based Methods		Other
Line Search	Trust Region	

Time Steppers			
Euler	Backward Euler	Pseudo−Time Stepping	Other

Krylov Subspace Methods							
GMRES	CG	CGS	Bi−CG−Stab	TFQMR	Richardson	Chebychev	Other

Preconditioners						
Additive Schwarz	Block Jacobi	Jacobi	ILU	ICC	LU (sequential only)	Other

Matrices				
Compressed Sparse Row (AIJ)	Block Compressed Sparse Row (BAIJ)	Block Diagonal (BDiag)	Dense	Other

Vectors

Index Sets			
Indices	Block Indices	Stride	Other

External packages

PETSc does not do everything, but it interfaces to other software:

- Dense linear algebra: `Scalapack`, `Plapack`
- Grid partitioning software: `ParMetis`, `Jostle`, `Chaco`, `Party`
- ODE solvers: `PVODE`
- Eigenvalue solvers (including SVD): `SLEPc`
- Optimization: `TAO`

PETSc and parallelism

PETSc is layered on top of MPI

MPI has basic tools: send elementary datatypes between processors

PETSc has intermediate tools:
insert matrix element in arbitrary location,
do parallel matrix-vector product

$\Rightarrow$ you do not need to know much MPI when you use PETSc

PETSc and parallelism

All objects in Petsc are defined on a communicator;
can only interact if on the same communicator

Parallelism through MPI

No OpenMP used;
user can use shared memory programming

Transparent: same code works sequential and parallel

Object oriented design

Petsc uses objects: vector, matrix, linear solver, nonlinear solver

Overloading:

```
MATMult(A,x,y); // y <- A x
```

same for sequential, parallel, dense, sparse

Data hiding

To support this uniform interface, the implementation is hidden:

```
MatSetValue(A,i,j,v,INSERT_VALUES); // A[i,j] <- v
```

There are some direct access routines, but most of the time you don't need them.

Getting started

Program header, C

```
#include "petsc.h"

#undef __FUNCT__
#define __FUNCT__ "main"
int main(int argc,char **argv)
```

- Petsc include file: one at the top of the file
- Declare the name of each routine: helps with traceback
- Can also include `petscmat.h` if no higher functionality needed.

Program header, F

```
      program init

        implicit none
#include "finclude/petsc.h"
```

Include file once per subprogram

```
#include "finclude/petscsys.h"
#include "finclude/petscvec.h"
#include "finclude/petscmat.h"
```

Variable declarations, C

```
KSP             solver;
Mat             A;
Vec             x,y;
PetscInt        n = 20;
PetscScalar     v;
PetscReal       nrm;
```

Note Scalar vs Real

Variable declarations, F

```
KSP             :: solver
Mat             :: A
Vec             :: x,y
PetscInt        :: j(3)
PetscScalar     :: mv
PetscReal       :: nrm
```

Much like in C; uses cpp

Routine start/end, C

```
PetscFunctionBegin;
// all statements
PetscFunctionReturn(0);
```

only in C, not in Fortran

Library setup, C

```
  ierr = PetscInitialize(&argc,&argv,0,0); CHKERRQ(ierr);
// all the petsc work
  ierr = PetscFinalize();CHKERRQ(ierr);
```

Can replace `MPI_Init`

General: Every routine has an error return. Catch that value!

Library setup, F

```
        call PetscInitialize(PETSC_NULL_CHARACTER,ierr)
        CHKERRQ(ierr)
// all the petsc work
        call PetscFinalize(ierr)
        CHKERRQ(ierr)
```

Error code is now final parameter. This holds for every PETSc routine

Note to self

```
PetscInitialize
  (&argc,&args,0,"Usage: prog -o1 v1 -o2 v2\n");
```

run as

```
./program -help
```

This displays the usage note, plus all available petsc options.

Not available in Fortran

Let's do something useful, C

```
ierr = PetscOptionsGetInt
    (PETSC_NULL,"-n",&n,PETSC_NULL); CHKERRQ(ierr);
ierr = PetscPrintf
    (comm,"Input parameter: %d\n",n); CHKERRQ(ierr);
```

Read commandline argument, print out from processor zero

Let's do something useful, F

```
      character*80      msg
      call PetscOptionsGetInt(PETSC_NULL_CHARACTER,
     >     "-n",n,PETSC_NULL_CHARACTER,ierr)
      CHKERRQ(ierr)
      write(msg,10) n
 10   format("Input parameter:",i5)
      call PetscPrintf(PETSC_COMM_WORLD,msg,ierr)
      CHKERRQ(ierr)
```

Note the `PETSC_NULL_CHARACTER`, note that `PetscPrintf` has only one string argument

Lab 1

`init.c/init.F`

`Vec` datatype: vectors

Create calls

Everything in PETSc is an object, with create and destroy calls:

```
VecCreate(MPI_Comm comm,Vec *v);
VecDestroy(Vec v);

/* C */
Vec V;
ierr = VecCreate(MPI_COMM_SELF,&V); CHKERRQ(ierr);
ierr = VecDestroy(&V); CHKERRQ(ierr);

! Fortran
Vec V
call VecCreate(MPI_COMM_SELF,V,e)
CHKERRQ(ierr)
call VecDestroy(V,e)
CHKERRQ(ierr);
```

Note: in Fortran there are no "star" arguments

More about vectors

A vector is a vector of `PetscScalars`: there are no vectors of integers (see the `IS` datatype later)

The vector object is not completely created in one call:

```
VecSetSizes(Vec v, int m, int M);
```

Other ways of creating: make more vectors like this one:

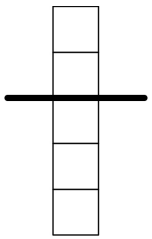
```
VecDuplicate(Vec v,Vec *w);
```

Parallel layout

Local or global size in

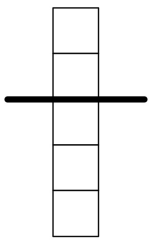
```
VecSetSizes(Vec v, int m, int M);
```

Global size can be specified as `PETSC_DECIDE`.



VecSetSizes(V,2,5)

VecSetSizes(V,3,5)



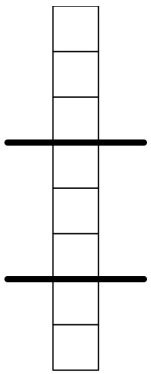
VecSetSizes(V,2,PETSC_DECIDE)

VecSetSizes(V,3,PETSC_DECIDE)

Parallel layout up to PETSc

```
VecSetSizes(Vec v, int m, int M);
```

Local size can be specified as `PETSC_DECIDE`.



VecSetSizes(V,PETSC_DECIDE,8)

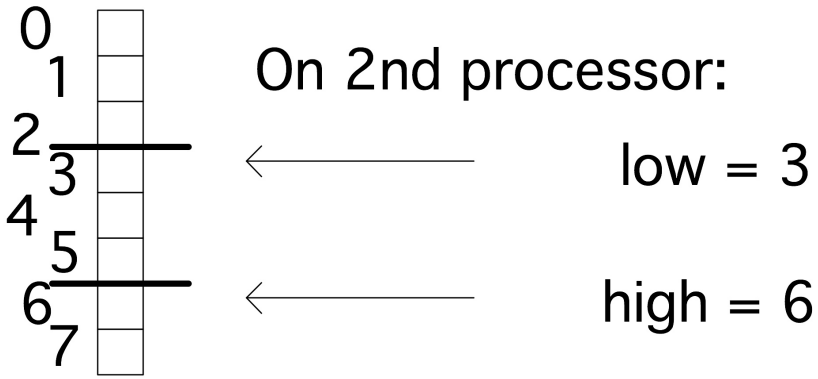
VecSetSizes(V,PETSC_DECIDE,8)

VecSetSizes(V,PETSC_DECIDE,8)

Query parallel layout

Query vector layout:

```
VecGetOwnershipRange(Vec x,PetscInt *low,PetscInt *high)
VecGetOwnershipRange(x,low,high,ierr) ! F
```



Query general layout:

```
PetscSplitOwnership(MPI_Comm comm,PetscInt *n,PetscInt *N)
PetscSplitOwnership(comm,n,N,ierr) ! F
```

(get local/global given the other)

Setting values

Set vector to constant value:

```
VecSet(Vec x,PetscScalar value);
```

Set individual elements (global indexing!):

```
VecSetValues(Vec x,int n,int *indices,PetscScalar *values,
    INSERT_VALUES); /* or ADD_VALUES */

i = 1; v = 3.14;
VecSetValues(x,1,&i,&v,INSERT_VALUES);
ii[0] = 1; ii[1] = 2; vv[0] = 2.7; vv[1] = 3.1;
VecSetValues(x,2,ii,vv,INSERT_VALUES);

call VecSetValues(x,1,i,v,INSERT_VALUES,ierr,e)
ii(1) = 1; ii(2) = 2; vv(1) = 2.7; vv(2) = 3.1
call VecSetValues(x,2,ii,vv,INSERT_VALUES,ierr,e)
```

Setting values

No restrictions on parallelism;
after setting, move values to appropriate processor:

```
VecAssemblyBegin(Vec x);
VecAssemblyEnd(Vec x);
```

Getting values (C)

Setting values is done without user access to the stored data
Getting values is often not necessary: many operations provided.
what if you do want access to the data?

- Create vector from user provided array:

```
VecCreateSeqWithArray(MPI_Comm comm,
  PetscInt n,const PetscScalar array[],Vec *V)
VecCreateMPIWithArray(MPI_Comm comm,
  PetscInt n,PetscInt N,const PetscScalar array[],Vec *vv)
```

- Get the internal array (local only; see `VecScatter` for more general mechanism):

```
VecGetArray(Vec x,PetscScalar *a[])
/* do something with the array */
VecRestoreArray(Vec x,PetscScalar *a[])
```

Getting values example

```
int localsize,first,i;
PetscScalar *a;
VecGetLocalSize(x,&localsize);
VecGetOwnershipRange(x,&first,PETSC_NULL);
VecGetArray(x,&a);
for (i=0; i<localsize; i++)
  printf("Vector element %d : %e\n",first+i,a[i]);
VecRestoreArray(x,&a);
```

Array handling in F90

```
PetscScalar, pointer :: xx_v(:)
....
call VecGetArrayF90(x,xx_v,ierr)
a = xx_v(3)
call VecRestoreArrayF90(x,xx_v,ierr)
```

More seperate F90 versions for 'Get' routines
(there are some ugly hacks for F77)

Basic operations

```
VecAXPY(Vec y,PetscScalar a,Vec x);   /* y <- y + a x */
VecAYPX(Vec y,PetscScalar a,Vec x);   /* y <- a y + x */
VecScale(Vec x, PetscScalar a);
VecDot(Vec x, Vec y, PetscScalar *r); /* several variants */
VecMDot(Vec x,int n,Vec y[],PetscScalar *r);
VecNorm(Vec x,NormType type, double *r);
VecSum(Vec x, PetscScalar *r);
VecCopy(Vec x, Vec y);
VecSwap(Vec x, Vec y);
VecPointwiseMult(Vec w,Vec x,Vec y);
VecPointwiseDivide(Vec w,Vec x,Vec y);
VecMAXPY(Vec y,int n, PetscScalar *a, Vec x[]);
VecMax(Vec x, int *idx, double *r);
VecMin(Vec x, int *idx, double *r);
VecAbs(Vec x);
VecReciprocal(Vec x);
VecShift(Vec x,PetscScalar s);
```

`Mat` Datatype: matrix

Matrix creation

The usual create/destroy calls:

```
MatCreate(MPI_Comm comm,Mat *A)
MatDestroy(Mat A)
```

Several more aspects to creation:

```
MatSetType(A,MATSEQAIJ) /* or MATMPIAIJ or MATAIJ */
MatSetSizes(Mat A,int m,int n,int M,int N)
MatSeqAIJSetPreallocation /* more about this later*/
  (Mat B,PetscInt nz,const PetscInt nnz[])
```

Local or global size can be `PETSC_DECIDE` (as in the vector case)

Matrix creation all in one

```
MatCreateSeqAIJ(MPI_Comm comm,PetscInt m,PetscInt n,
  PetscInt nz,const PetscInt nnz[],Mat *A)
MatCreateMPIAIJ(MPI_Comm comm,
  PetscInt m,PetscInt n,PetscInt M,PetscInt N,
  PetscInt d_nz,const PetscInt d_nnz[],
  PetscInt o_nz,const PetscInt o_nnz[],
  Mat *A)
```

If you already have a CRS matrix

```
PetscErrorCode  MatCreateSeqAIJWithArrays
  (MPI_Comm comm,PetscInt m,PetscInt n,
   PetscInt* i,PetscInt*j,PetscScalar *a,Mat *mat)
```

(also from triplets)

Do not use this unless you interface to a legacy code. And even then...

Matrix Preallocation

- PETSc matrix creation is very flexible:
- No preset sparsity pattern
- any processor can set any element
  $\Rightarrow$ potential for lots of malloc calls
- malloc is very expensive: (run your code with `-memory_info`, `-malloc_log`)
- tell PETSc the matrix' sparsity structure
  (do construction loop twice: once counting, once making)

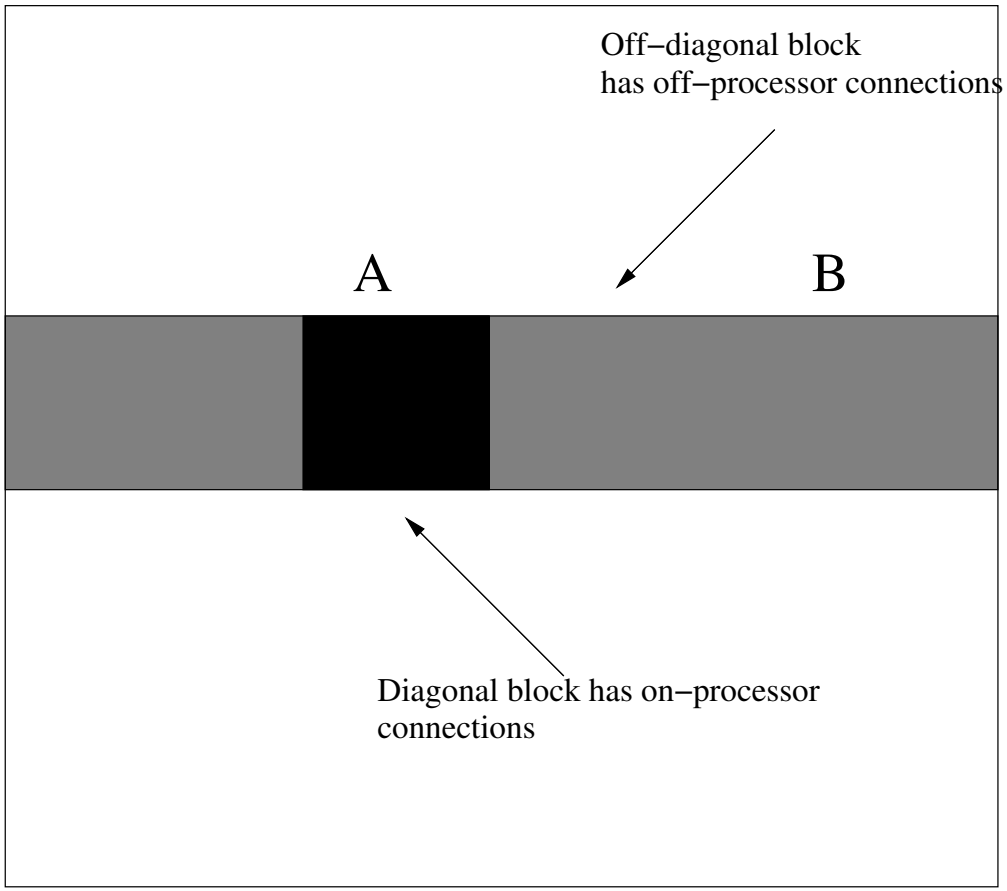
Sequential matrix structure

```
MatSeqAIJSetPreallocation
    (Mat B,PetscInt nz,const PetscInt nnz[])
/* or */
MatCreateSeqAIJ(comm,int m,int n,
    int nz,int *nnz,Mat *A);
```

- `nz` number of nonzeros per row
  (or slight overestimate)
- `nnz` array of row lengths (or overestimate)
- considerable savings over dynamic allocation!

In Fortran use `PETSC_NULL_INTEGER` if not specifying `nnz` array

Parallel matrix structure



(why does it do this?)

- $y \leftarrow Ax_A + Bx_b$
- x_B needs to be communicated; Ax_A can be computed in the meantime
- Algorithm
  - Initiate asynchronous sends/receives for x_b
  - compute Ax_A
  - make sure x_b is in
  - compute Bx_B
- so by splitting matrix storage into A, B part, code for the sequential case can be reused.
- This is one of the few places where PETSc's design is visible to the user.

Parallel matrix structure description

- `d_nz`: number of nonzeros per row in diagonal part
- `o_nz`: number of nonzeros per row in off-diagonal part
- `d_nnz`: array of numbers of nonzeros per row in diagonal part
- `o_nnz`: array of numbers of nonzeros per row in off-diagonal part

```
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);
```

In Fortran use `PETSC_NULL_INTEGER` if not specifying arrays

Querying parallel structure

Matrix partitioned by block rows:

```
MatGetSize(Mat mat,PetscInt *M,PetscInt* N);
MatGetLocalSize(Mat mat,PetscInt *m,PetscInt* n);
MatGetOwnershipRange(Mat A,int *first row,int *last row);
```

If the matrix is square, m, n will probably be equal, even though distribution by block rows

Setting values

Set one value:

```
MatSetValue(Mat v,
  PetscInt i,PetscInt j,PetscScalar va,InsertMode mode)
```

where insert mode is `INSERT_VALUES, ADD_VALUES`

Set block of values:

```
MatSetValues(Mat A,int m,const int idxm[],
    int n,const int idxn[],const PetscScalar values[],
    InsertMode mode)
```

(`v` is row-oriented)

Special case of the general case:

```
MatSetValues(A,1,&i,1,&j,&v,INSERT_VALUES); // C
MatSetValues(A,1,i,1,j,v,INSERT_VALUES,e); ! F
```

Assembling the matrix

Setting is independent of parallelism

```
MatAssemblyBegin(Mat A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(Mat A,MAT_FINAL_ASSEMBLY);
```

Cannot mix inserting/adding values: need to do assembly in between

Getting values (C)

- Values are often not needed: many matrix operations supported
- Matrix elements can only be obtained locally.

```
PetscErrorCode  MatGetRow(Mat mat,
 PetscInt row,PetscInt *ncols,const PetscInt *cols[],
 const PetscScalar *vals[])
PetscErrorCode MatRestoreRow(/* same parameters */
```

Note: for inspection only; possibly expensive.

Getting values (F)

```
MatGetRow(A,row,ncols,cols,vals,ierr)
```

where `cols(maxcols)`, `vals(maxcols)` are long enough arrays (allocated by the user)

Other matrix types

`MATBAIJ` : blocked matrices (dof per node)

(see `PETSC_DIR/include/petscmat.h`)

Dense:

```
MatCreateSeqDense(PETSC_COMM_SELF,int m,int n,
  PetscScalar *data,Mat *A);
MatCreateMPIDense(MPI Comm comm,int m,int n,int M,int N,
  PetscScalar *data,Mat *A)
```

Data argument optional

Matrix operations

Main operations are matrix-vector:

```
MatMult(Mat A,Vec in,Vec out);
MatMultAdd
MatMultTranspose
MatMultTransposeAdd
```

Simple operations on matrices:

```
MatNorm

MatScale
MatDiagonalScale
```

Matrix viewers

```
MatView(A,0);

row 0: (0, 1)  (2, 0.333333)  (3, 0.25)  (4, 0.2)
row 1: (0, 0.5)  (1, 0.333333)  (2, 0.25)  (3, 0.2)
....
```

- Shorthand for `MatView(A,PETSC_VIEWER_STDOUT_WORLD);` or even `MatView(A,0)` (Fortran: `PETSC_NULL_INTEGER`)
- also invoked by `-mat_view`
- Sparse: only allocated positions listed
- other viewers: for instance `-mat_view_draw` (X terminal)

General viewers

Any PETSc object can be viewed
binary dump is a view:

```
PetscViewer fd;
PetscViewerBinaryOpen
  (PETSC_COMM_WORLD,"matdata",FILE_MODE_WRITE,&fd);
MatView(A,fd);
PetscViewerDestroy(fd);
```

Shell matrices

What if the matrix is a user-supplied operator, and not stored?

```
MatSetType(A,MATSHELL); /* or */
MatCreateShell(MPI Comm comm,
    int m,int n,int M,int N,void *ctx,Mat *mat);

PetscErrorCode UserMult(Mat mat,Vec x,Vec y);

MatShellSetOperation(Mat mat,MatOperation MATOP_MULT,
  (void(*)(void)) PetscErrorCode (*UserMult)(Mat,Vec,Vec));
```

Inside iterative solvers, PETSc calls `MatMult(A,x,y)`:
no difference between stored matrices and shell matrices

Shell matrix context

Shell matrices need custom data

```
MatShellSetContext(Mat mat,void *ctx);
MatShellGetContext(Mat mat,void **ctx);
```

(This does not work in Fortran: use Common or Module)

User program sets context, matmult routine accesses it

Shell matrix example

```
...
MatSetType(A,MATSHELL);
MatShellSetOperation(A,MATOP_MULT,(void*)&mymatmult);
MatShellSetContext(A,(void*)&mystruct);
...

PetscErrorCode mymatmult(Mat mat,Vec in,Vec out)
{
  PetscFunctionBegin;
  MatShellGetContext(mat,(void**)&mystruct);
  /* compute out from in, using mystruct */
  PetscFunctionReturn(0);
}
```

Submatrices

Extract one parallel submatrix:

```
MatGetSubMatrix(Mat mat,
  IS isrow,IS iscol,PetscInt csize,MatReuse cll,
  Mat *newmat)
```

Extract multiple single-processor matrices:

```
MatGetSubMatrices(Mat mat,
  PetscInt n,const IS irow[],const IS icol[],MatReuse scall,
  Mat *submat[])
```

Collective call, but different index sets per processor

Load balancing

```
MatPartitioningCreate
    (MPI Comm comm,MatPartitioning *part);
```

Various packages for creating better partitioning: Chaco, Parmetis

KSP & PC: **Iterative solvers**

What are iterative solvers?

Solving a linear system $Ax = b$ with Gaussian elimination can take lots of time/memory.

Alternative: iterative solvers use successive approximations of the solution:

- Convergence not always guaranteed
- Possibly much faster / less memory
- Basic operation: $y \leftarrow Ax$ executed once per iteration
- Also needed: preconditioner $B \approx A^{-1}$

Basic concepts

- All linear solvers in PETSc are iterative (see below)
- Object oriented: solvers only need matrix action, so can handle shell matrices
- Preconditioners
- Fargoing control through commandline options
- Tolerances, convergence and divergence reason
- Custom monitors and convergence tests

Iterative solver basics

```
KSPCreate(comm,&solver); KSPDestroy(solver);

// general:
KSPSetOperators(solver,A,B,DIFFERENT_NONZERO_PATTERN);
// common:
KSPSetOperators(solver,A,A,DIFFERENT_NONZERO_PATTERN);
// also SAME_NONZERO_PATTERNS and SAME_PRECONDITIONER

KSPSolve(solver,rhs,sol);
/* optional */ KSPSetup(solver);
```

Solver type

```
KSPSetType(solver,KSPGMRES);
```

KSP can be controlled from the commandline:

```
KSPSetFromOptions(solver);
/* right before KSPSolve or KSPSetUp */
```

then options `-ksp....` are parsed.

- type: `-ksp_type gmres -ksp_gmres_restart 20`
- `-ksp_view`

Convergence

Iterative solvers can fail

- Solve call itself gives no feedback: solution may be completely wrong
- `KSPGetConvergedReason(solver,&reason)` :
  positive is convergence, negative divergence
  (`${PETSC_DIR}/include/petscksp.h` for list)
- `KSPGetIterationNumber(solver,&nits)` : after how many iterations did the method stop?

```
KSPSolve(solver,B,X);
KSPGetConvergedReason(solver,&reason);
if (reason<0) {
   printf("Divergence.\n");
} else {
   KSPGetIterationNumber(solver,&its);
   printf("Convergence in %d iterations.\n",(int)its);
}
```

Monitors and convergence tests

```
KSPSetTolerances(solver,rtol,atol,dtol,maxit);
```

Monitors can also be set in code, but easier:

- `-ksp_monitor`
- `-ksp_monitor_true_residual`

Monitors and convergence tests (adv)

```
KSPMonitorSet(KSP ksp,
 PetscErrorCode (*monitor)
      (KSP,PetscInt,PetscReal,void*),
 void *mctx,
 PetscErrorCode (*monitordestroy)(void*));
KSPSetConvergenceTest(KSP ksp,
 PetscErrorCode (*converge)
      (KSP,PetscInt,PetscReal,KSPConvergedReason*,void*),
 void *cctx,
 PetscErrorCode (*destroy)(void*))
```

Example of convergence tests

```
PetscErrorCode resconverge
(KSP solver,PetscInt it,PetscReal res,
 KSPConvergedReason *reason,void *ctx)
{
  MPI_Comm comm; Mat A; Vec X,R; PetscErrorCode ierr;
  PetscFunctionBegin;
  KSPGetOperators(solver,&A,PETSC_NULL,PETSC_NULL);
  PetscObjectGetComm((PetscObject)A,&comm);
  KSPBuildResidual(solver,PETSC_NULL,PETSC_NULL,&R);
  KSPBuildSolution(solver,PETSC_NULL,&X);
  /* stuff */
  if (sometest) *reason = 15;
  else *reason = KSP_CONVERGED_ITERATING;
  PetscFunctionReturn(0);
```

Advanced options

Many options fpr the (mathematically) sophisticated user
some specific to one method

`KSPSetInitialGuessNonzero`
`KSPGMRESSetRestart`
`KSPSetPreconditionerSide`
`KSPSetNormType`

Null spaces

```
MatNullSpace sp;
MatNullSpaceCreate /* constant vector */
    (PETSC_COMM_WORLD,PETSC_TRUE,0,PETSC_NULL,&sp);
MatNullSpaceCreate /* general vectors */
    (PETSC_COMM_WORLD,PETSC_FALSE,5,vecs,&sp);
KSPSetNullSpace(ksp,sp);
```

The solver will now properly remove the null space at each iteration.

PC basics

- PC usually created as part of KSP: separate create and destroy calls exist, but are (almost) never needed

```
KSP solver; PC precon;
KSPCreate(comm,&solver);
KSPGetPC(solver,&precon);
PCSetType(precon,PCJACOBI);
```

- `PCJACOBI`, `PCILU` (only sequential), `PCASM`, `PCBJACOBI`, `PCMG`, et cetera
- Controllable through commandline options:
  `-pc_type ilu -pc_factor_levels 3`

Preconditioner reuse

In context of nonlinear solvers, the preconditioner can sometimes be reused:

- If the jacobian doesn't change much, reuse the preconditioner completely
- If the preconditioner is recomputed, the sparsity pattern probably stays the same

`KSPSetOperators(solver,A,B,structureflag)`

- `B` is basis for preconditioner, need not be `A`
- `structureflag` can be `SAME_PRECONDITIONER`, `SAME_NONZERO_PATTERN`, `DIFFERENT_NONZERO_PATTERN`: avoid recomputation of preconditioner (sparsity pattern) if possible

Factorization preconditioners

Exact factorization: $A = LU$

Inexact factorization: $A \approx M = LU$ where L, U obtained by throwing away 'fill-in' during the factorization process.
Exact:

$$\forall_{i,j} : a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$

Inexact:

$$\forall_{i,j} : \text{if } a_{ij} \neq 0 \; a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$

Application of the preconditioner (that is, solve $Mx = y$) approx same cost as matrix-vector product $y \leftarrow Ax$

Factorization preconditioners are sequential

ILU

PCICC: symmetric, PCILU: nonsymmetric

```
PCFactorSetLevels(PC pc,int levels);
-pc_factor_levels <levels>
```

et cetera

Prevent indefinite preconditioners:

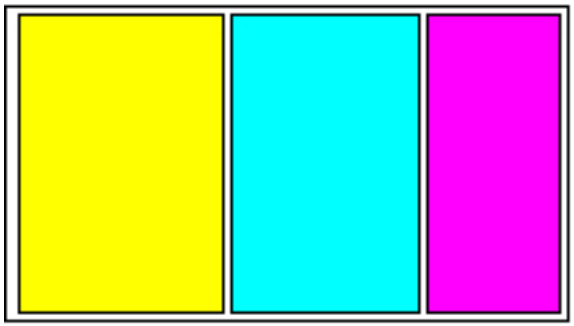
```
PCFactorSetShiftPd(PC pc,MatFactorShiftType type);
```

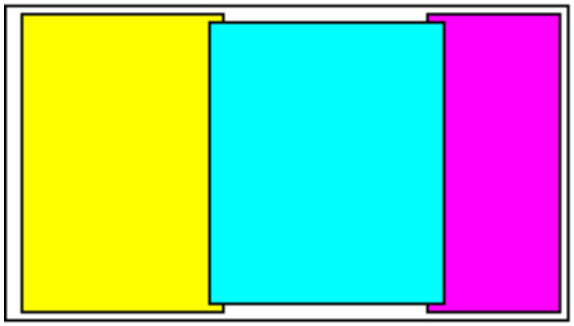
value MAT_SHIFT_POSITIVE_DEFINITE et cetera

Block Jacobi and Additive Schwarz

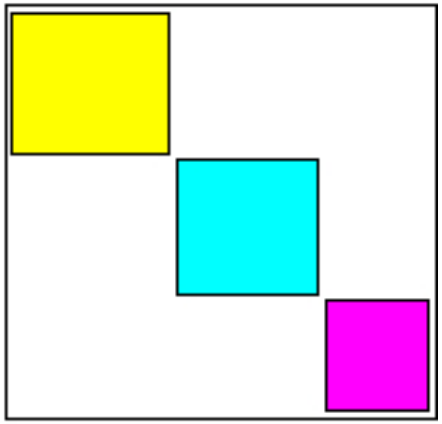
- Factorization preconditioners are sequential;
- can be made parallel by use in Block Jacobi or Additive Schwarz methods
- each processor has its own block(s) to work with

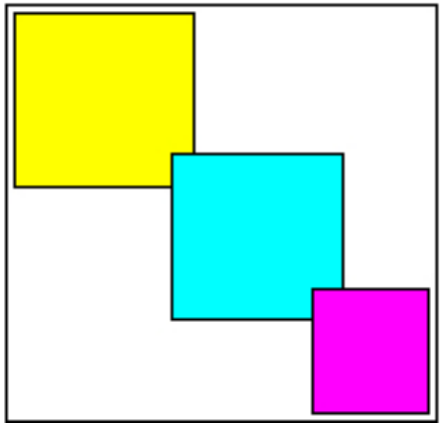
Domain partitioning





Matrix blocks





Block Jacobi and Additive Schwarz, theory

- Both methods parallel
- Jacobi fully parallel
  Schwarz local communication between neighbours
- Both require sequential local solver
- Jacobi limited reduction in iterations
  Schwarz can be optimal

Block Jacobi and Additive Schwarz, coding

```
KSP *ksps; int nlocal,firstlocal; PC pc;
PCBJacobiGetSubKSP(pc,&nlocal,&firstlocal,&ksps);
for (i=0; i<nlocal; i++) {
  KSPSetType( ksps[i], KSPGMRES );
  KSPGetPC( ksps[i], &pc );
  PCSetType( pc, PCILU );
}
```

Much shorter: commandline options `-sub_ksp_type` and `-sub_pc_type` (subksp is PREONLY by default)

```
PCASMSetOverlap(PC pc,int overlap);
```

Matrix-free solvers

Shell matrix requires shell preconditioner (or use different operators in `KSPSetOperators`):

```
PCSetType(pc,PCSHELL);
PCShellSetContext(PC pc,void *ctx);
PCShellGetContext(PC pc,void **ctx);
PCShellSetApply(PC pc,
    PetscErrorCode (*apply)(void*,Vec,Vec));
PCShellSetSetUp(PC pc,
    PetscErrorCode (*setup)(void*))
```

similar idea to shell matrices

Direct methods

- Iterative method with direct solver as preconditioner would converge in one step
- Direct methods in PETSc implemented as special iterative method: `KSPPREONLY` only apply preconditioner
- All direct methods are preconditioner type `PCLU`:

```
myprog -pc_type lu -ksp_type preonly \
    -pc_factor_mat_solver_package mumps
```

Other external PCs

If installed, other parallel preconditioner are available:

- From Hypre: `PCHYPRE` with subtypes `boomeramg`, `parasails`, `euclid`, `pilut`: `PCHYPRESetType(pc,parasails)` or `-pc_hypre_type parasails`
- `PCSPAI` for Sparse Approximate Inverse
- `PCPROMETHEUS`
- External packages' existence can be tested:

```
%% grep hypre $PETSC_DIR/$PETSC_ARCH/include/petscconf.
#ifndef PETSC_HAVE_HYPRE
#define PETSC_HAVE_HYPRE 1
#ifndef PETSC_HAVE_LIBHYPRE
#define PETSC_HAVE_LIBHYPRE 1
```

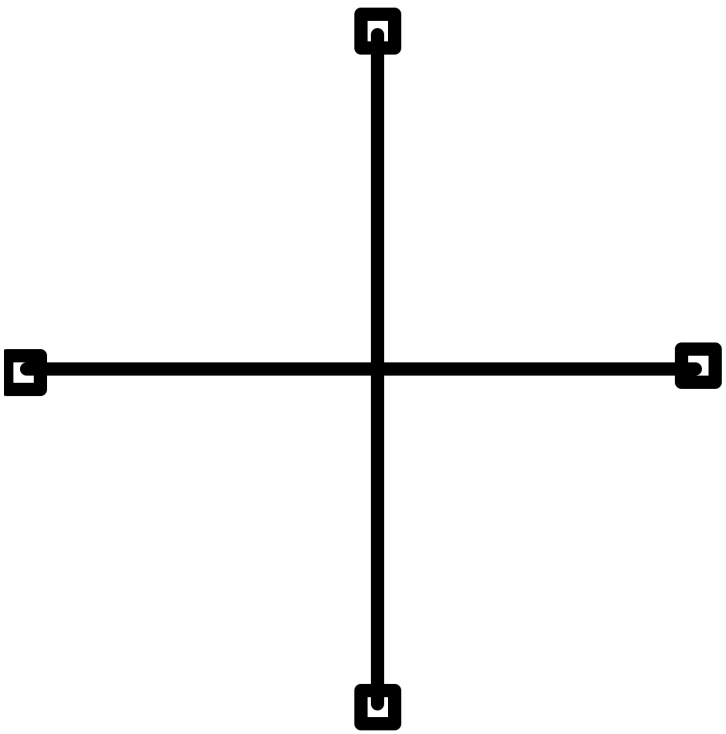
Grid manipulation

Regular grid: DMDA

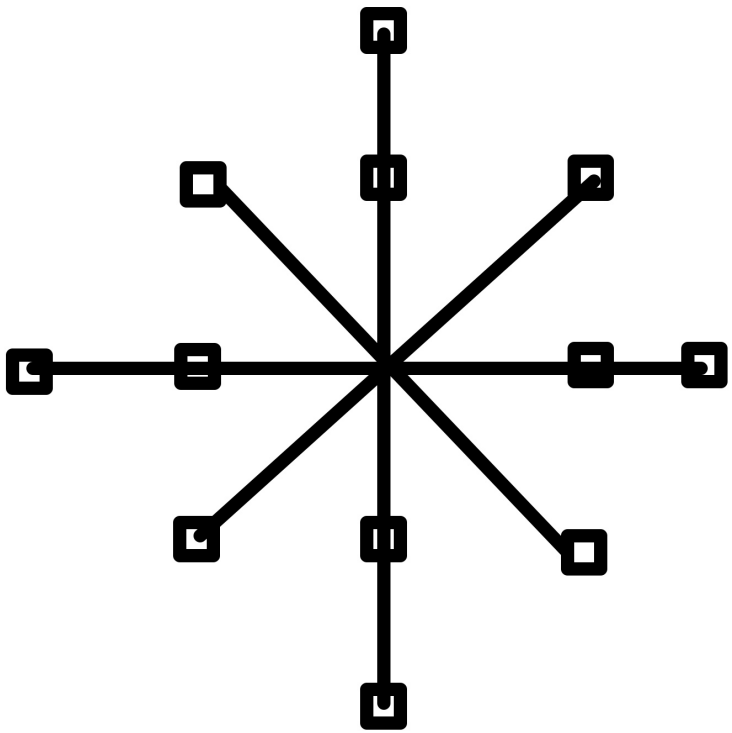
DMDAs are for storing vector field, not matrix.

Support for different stencil types:

Star stencil

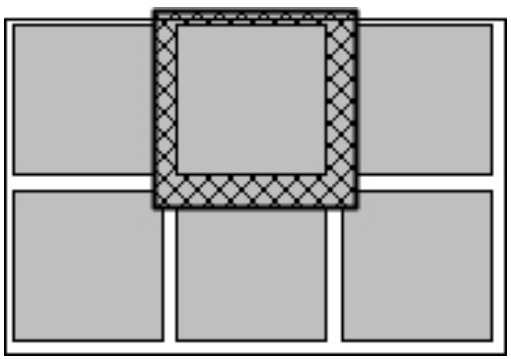


Box stencil



Ghost regions around processors

A DMDA defines a global vector, which contains the elements of the grid, and a local vector for each processor which has space for "ghost points".



DMDA construction

```
DMDACreate2d(comm, bndx,bndy, type, M, N, m, n,
  dof, s, lm[], ln[], DMDA *da)
```

`bndx,bndy` boundary behaviour: none/ghost/periodic

type: Specifies stencil
`DMDA_STENCIL_BOX` or `DMDA_STENCIL_STAR`

M/N: Number of grid points in x/y-direction
m/n: Number of processes in x/y-direction
dof: Degrees of freedom per node
s: The stencil width (for instance, 1 for 2D five-point stencil)

lm/n: array of local sizes (optional; Use `PETSC_NULL` for the default)

Associated vectors

```
DMCreateGlobalVector(DMDA da,Vec *g);
DMCreateLocalVector(DMDA da,Vec *l);

global -> local
DMGlobalToLocalBegin/End
    (DMDA da,Vec g,InsertMode iora,Vec l);

local -> global
DMLocalToGlobalBegin/End
    (DMDA da,Vec l,InsertMode mode,Vec g);

local -> global -> local :
DMLocalToLocalBegin/End
    (DMDA da,Vec l1,InsertMode iora,Vec l2);
```

Irregular grid: IS & VecScatter

Index Set is a set of indices (more later about their uses)

```
ISCreateGeneral(comm,n,indices,&is);
    /* indices can now be freed */
ISCreateGeneralWithArray(comm,n,indices,&is);
    /* indices are stored */
ISCreateStride (comm,n,first,step,&is);
ISCreateBlock  (comm,bs,n,indices,&is);

ISDestroy(is);
```

Various manipulations: `ISSum`, `ISDifference`, `ISInvertPermutations` et cetera.

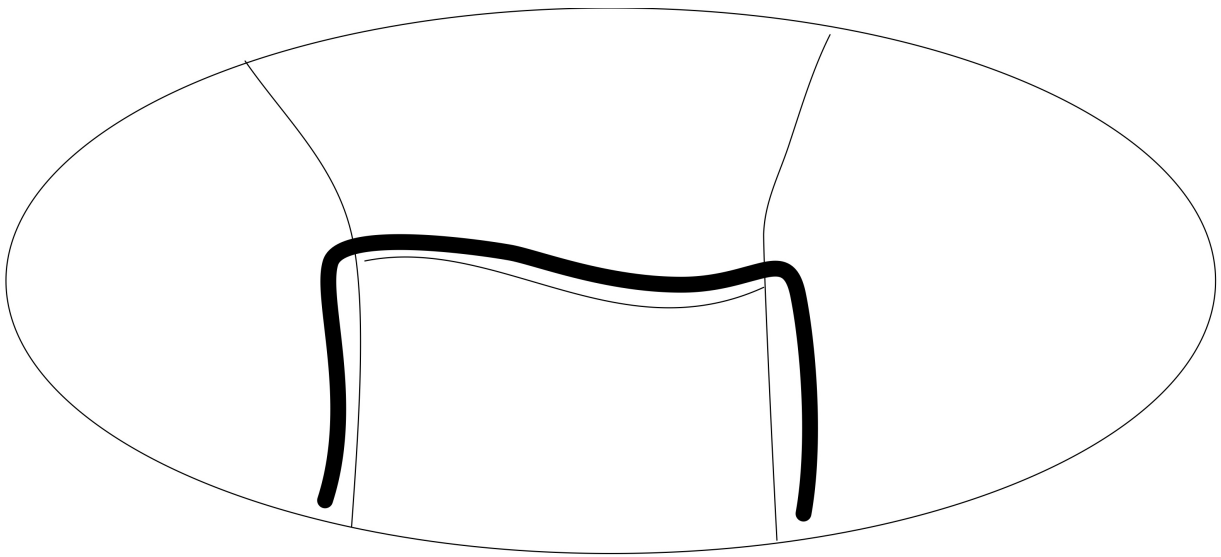
Retrieving information

ISGetIndices / ISRestoreIndices ISGetSize

VecScatter

```
VecScatterCreate(Vec,IS,Vec,IS,VecScatter*) \& Destroy
VecScatterBegin
  (VecScatter,Vec,Vec, InsertMode mode, ScatterMode direction)
VecScatterEnd
  (VecScatter,Vec,Vec, InsertMode mode, ScatterMode direction)
```

Example: collect distributed boundary onto a single processor:



SNES: Nonlinear solvers

Nonlinear problems

Basic equation

$$f(u) = 0$$

where u can be big, for instance nonlinear PDE.

Typical solution method:

$$u_{n+1} = u_n - J(u_n)^{-1} f(u_n)$$

Newton iteration.

Needed: function and Jacobian.

Basic SNES usage

User supplies function and Jacobian:

```
SNES            snes;

SNESCreate(PETSC_COMM_WORLD,&snes)
SNESSetType(snes,type);
SNESSetFromOptions(snes);
SNESDestroy(SNES snes);
```

where `type`:

- `SNESLS` Newton with line search
- `SNESTR` Newton with trust region
- several specialized ones

SNES specification

```
VecCreate(PETSC_COMM_WORLD,&r)
SNESSetFunction(snes,r,FormFunction,*ctx)

MatCreate(PETSC_COMM_WORLD,&J)
SNESSetJacobian(snes,J,J,FormJacobian,*ctx)

SNESSolve(snes,PETSC_NULL,x)
SNESGetIterationNumber(snes,&its)
```

Target function

```
PetscErrorCode FormFunction
    (SNES snes,Vec x,Vec f,void *dummy)
{
VecGetArray(x,&xx); VecGetArray(f,&ff);

ff[0] = PetscSinScalar(3.0*xx[0]) + xx[0];
ff[1] = xx[1];

VecRestoreArray(x,&xx); VecRestoreArray(f,&ff);
return 0;
}
```

Jacobian

```
PetscErrorCode FormJacobian
 (SNES snes,Vec x,Mat *jac,Mat *prec,MatStructure *flag,vo
{
PetscScalar    A[];
VecGetArray(x,&xx)
A[0] = ... ; /* et cetera */
MatSetValues(*jac,...,INSERT_VALUES)
MatSetValues(*prec,..,INSERT_VALUES)
*flag = SAME_NONZERO_PATTERN;
VecRestoreArray(x,&xx)
MatAssemblyBegin(*prec,MAT_FINAL_ASSEMBLY)
MatAssemblyEnd(*prec,MAT_FINAL_ASSEMBLY)
MatAssemblyBegin(*jac,MAT_FINAL_ASSEMBLY)
MatAssemblyEnd(*jac,MAT_FINAL_ASSEMBLY)
return 0;
}
```

Further possibilities

`SNESSetTolerances(SNES snes,double atol,double rtol,double stol, int its,int fcts);`

convergence test and monitoring, specific options for line search and trust region

adaptive converngence: `-snes_ksp_ew_conv` (Eisenstat Walker)

Solve customization

```
SNESSetType(snes,SNESTR); /* newton with trust region */
SNESGetKSP(snes,&ksp)
KSPGetPC(ksp,&pc)
PCSetType(pc,PCNONE)
KSPSetTolerances(ksp,1.e-4,PETSC_DEFAULT,PETSC_DEFAULT,20)
```

sophisticated stuff

- Jacobian through finite difference: `SNESDefaultComputeJacobian` or `-snes_fd`
- Matrix-free operation

TS: Time stepping

Profiling, debugging

Basic profiling

- `-log_summary` flop counts and timings of all PETSc events
- `-info` all sorts of information, in particular

```
%% mpiexec yourprogram -info | grep malloc
[0] MatAssemblyEnd_SeqAIJ():
    Number of mallocs during MatSetValues() is 0
```

- `-log_trace` start and end of all events: good for hanging code

Log summary: overall

	Max	Max/Min	Avg	Total
Time (sec):	5.493e-01	1.00006	5.493e-01	
Objects:	2.900e+01	1.00000	2.900e+01	
Flops:	1.373e+07	1.00000	1.373e+07	2.746e+07
Flops/sec:	2.499e+07	1.00006	2.499e+07	4.998e+07
Memory:	1.936e+06	1.00000		3.871e+06
MPI Messages:	1.040e+02	1.00000	1.040e+02	2.080e+02
MPI Msg Lengths:	4.772e+05	1.00000	4.588e+03	9.544e+05
MPI Reductions:	1.450e+02	1.00000		

Log summary: details

	Max	Ratio	Max	Ratio	Max	Ratio	Avg len	%T	%F	%M	%L	%R	%T	%F	%M	%L	%R	Mflop/s
MatMult	100	1.0	3.4934e-02	1.0	1.28e+08	1.0	8.0e+02	6	32	96	17	0	6	32	96	17	0	255
MatSolve	101	1.0	2.9381e-02	1.0	1.53e+08	1.0	0.0e+00	5	33	0	0	0	5	33	0	0	0	305
MatLUFactorNum	1	1.0	2.0621e-03	1.0	2.18e+07	1.0	0.0e+00	0	0	0	0	0	0	0	0	0	0	43
MatAssemblyBegin	1	1.0	2.8350e-03	1.1	0.00e+00	0.0	1.3e+05	0	0	3	83	1	0	0	3	83	1	0
MatAssemblyEnd	1	1.0	8.8258e-03	1.0	0.00e+00	0.0	4.0e+02	2	0	1	0	3	2	0	1	0	3	0
VecDot	101	1.0	8.3244e-03	1.2	1.43e+08	1.2	0.0e+00	1	7	0	0	35	1	7	0	0	35	243
KSPSetup	2	1.0	1.9123e-02	1.0	0.00e+00	0.0	0.0e+00	3	0	0	0	2	3	0	0	0	2	0
KSPSolve	1	1.0	1.4158e-01	1.0	9.70e+07	1.0	8.0e+02	26	100	96	17	92	26	100	96	17	92	194

User events

```
#include "petsclog.h"
int USER EVENT;
PetscLogEventRegister(&USER EVENT,"User event name",0);
PetscLogEventBegin(USER EVENT,0,0,0,0);
/* application code segment to monitor */
PetscLogFlops(number of flops for this code segment);
PetscLogEventEnd(USER EVENT,0,0,0,0);
```

Program stages

```
PetscLogStagePush(int stage); /* 0 <= stage <= 9 */
PetscLogStagePop();
PetscLogStageRegister(int stage,char *name)
```

Debugging

- Use of `CHKERRQ` and `SETERRQ` for catching and generating error
- Use of `PetscMalloc` and `PetscFree` to catch memory problems;
  `CHKMEMQ` for instantaneous memory test (debug mode only)