PETSc Developers Manual

by

The PETSc Team
http://www.mcs.anl.gov/petsc

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Abstract:

PETSc is a set of extensible software libraries for scientific computation. PETSc is designed using a object-oriented architecture. This means that libraries consist of objects that have certain, defined functionality. This document defines how these objects are implemented.

This manual discusses the PETSc library design and describes how to develop new library codes that are compatible with other PETSc components including PETSc 3.0. The idea is not to develop one massive library that everyone shoves code into; rather, to develop an architecture that allows many people to (as painlessly as possible) contribute (and maintain) their own libraries, in a distributed fashion.

The text assumes that you are familiar with PETSc and have access to PETSc source code and documentation (available via http://www.mcs.anl.gov/petsc.)

Before contributing code to PETSc please read Chapter 1, which contains the source code style guide. http://www.mcs.anl.gov/petsc/developers/index.html contains information on how to submit patches to PETSc.

Please direct all comments and questions regarding PETSc design and development to petsc-dev@mcs.anl.gov. Note that all bug reports and questions regarding the use of PETSc should continue to be directed to petsc-maint@mcs.anl.gov.
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Chapter 1

Answering petsc-maint@mcs.anl.gov and petsc-users@mcs.anl.gov

• Try to be polite (this is not always easy)
• Address the person by name (when it is possible to determine their name)
• Apologize for the problem when it is appropriate (but not otherwise)
• Thank the person for their patience if it is more than six hours since the report came in.
• If the person drops the petsc-maint or petsc-users from the mailing list add it back in.

Often it pays to not ask too many questions or give too many suggestions in the same email. The user often only responds to the first of them anyways.
Chapter 2

Style Guide

The PETSc team uses certain conventions to make our source code consistent. Groups
developing classes compatible with PETSc are, of course, free to organize their own source
code anyway they like.

2.1 Names

Consistency of names for variables, functions, etc. is extremely important in making the
package both usable and maintainable. We use several conventions:

- All function names and enum types consist of words, each of which is capitalized, for
  example KSPSolve() and MatGetOrdering().

- All enum elements and macro variables are capitalized. When they consist of several
  complete words, there is an underscore between each word.

- Functions that are private to PETSc (not callable by the application code) either
  – have an appended _Private (for example, StashValues_Private) or
  – have an appended _Subtype (for example, MatMult_SeqAIJ).
  – have an appended _Default (for example, KSPBuildSolutionDefault) if used
    by several classes.

In addition, functions that are not intended for use outside of a particular file are
declared static.

- Function names in structures are the same as the base application function name with-
  out the object prefix, and all are in small letters. For example, MatMultTranspose()
  has a structure name of multtranspose().

- Each application usable function begins with the name of the class object, followed by
  any subclass name, for example, ISInvertPermutation(), MatMult() or KSPGMRES-
  SetRestart().

- Functions that PETSc provides as defaults for user provideable functions end with
  Default (for example, KSPMonitorDefault() or PetscSignalHandlerDefault())
• Options database keys are lower case, have an underscore between words and match the function name associated with the option without the word set. For example, 
\[-ksp_gmres_restart\].

### 2.2 Coding Conventions and Style Guide

Within the PETSc source code, we adhere to the following guidelines so that the code is uniform and easily maintainable:

• Public PETSc includes, `petsc*.h`, cannot include private PETSc `petsc/private/*impl.h` includes.

• Public and private PETSc includes, cannot include include files in the PETSc source tree.

• All PETSc function bodies are indented two characters.

• Each additional level of loops, if statements, etc. is indented two more characters.

• Wrapping lines should be avoided whenever possible.

• Source code lines do not have a hard length limit, generally we like them less than 150 characters wide.

• The local variable declarations should be aligned. For example, use the style

  ```
  Scalar a;
  int    i,j;
  ```

  instead of

  ```
  int i,j;
  Scalar a;
  ```

• Array and pointer arguments to functions where the array values are not changed should be labeled as `const` arguments.

• Scalar values passed to functions should **never** be labeled as `const`.

• The prototypes for functions should not include the names of the variables; for example write

  ```
  PetscErrorCode MyFunction(PetscInt);
  ```

  not

  ```
  PetscErrorCode MyFunction(PetscInt myvalue);
  ```
• All local variables of a particular type (e.g., int) should be listed on the same line if possible; otherwise, they should be listed on adjacent lines.

• Equal signs should be aligned in regions where possible.

• There must be a single blank line between the local variable declarations and the body of the function.

• The first line of the executable statements must be PetscFunctionBegin;

• The following text should be before each function

  #undef __FUNCT__
  #define __FUNCT__ "FunctionName"

  this is used by various macros (for example the error handlers) to always know what function the process is in.

• Use PetscFunctionReturn(returnvalue); not return(returnvalue);

• Never put a function call in a return statement; do not do

  PetscFunctionReturn( somefunction(...) );

• Do not put a blank line immediately after PetscFunctionBegin; or a blank line immediately before PetscFunctionReturn(0);

• Indentation for if statements must be done as as

  if ( ) {
      ....
  } else {
      ....
  }

• Never have

  if( )
      a single indented line

or

  for ( )
      a single indented line

instead use either

  if ( ) a single line
or

    if( ) {
        a single indented line
    }

• No tabs are allowed in *any* of the source code.

• Do not use sqrt(), pow(), sin() etc directly in PETSc source code or examples, rather use PetscSqrtScalar(), PetscSqrtReal() etc depending on the context. See petscmath.h for expressions to use.

• The open bracket { should be on the same line as the if () test, for (), etc. never on its own line unless followed by an else or else if, for example

    } else {

        never

    }

else {

    The closing bracket } should **always** be on its own line.

• Do not leave chunks of commented out code in the source files.

• In function declaration the open bracket { should be on the **next** line, not on the same line as the function name and arguments. This is an exception to the rule above.

• assert.h should not be included in PETSc source and assert() should not be used. It doesn’t play well in the parallel MPI world.

• The macros SETERRQ() and CHKERRQ() should be on the same line as the routine to be checked unless this violates the 150 character width rule. Try to make error messages short, but informative.

• *No* space after a ( or before a ). No space before the CHKXXX(). That is, do not write

    ierr = PetscMalloc1( 10,&a ); CHKERRQ(ierr);

instead write

    ierr = PetscMalloc1(10,&a); CHKERRQ(ierr);

• Except in code that may be called before PETSc is fully initialized, always use PetscMalloc(), PetscNew(), and PetscFree(), not *malloc()* and *free()*.
• *No* space after the ) in a cast, no space between the type and the * in a caste.

• *No* space before or after a , in lists That is, do not write

\[
\text{int a, b,c;}
\text{ierr = func(a, 22.0);CHKERRQ(ierr);}
\]

instead write

\[
\text{int a,b,c;}
\text{ierr = func(a,22.0);CHKERRQ(ierr);}
\]

• Subroutines that would normally have void ** argument to return a pointer to some data, should actually be protyped as as void*. This prevents the caller from having to put a (void**) caste in each function call. See, for example, DMDAVecGetArray().

• Do not use the register directive.

• Never use a local variable counter like PetscInt flops = 0; to accumulate flops and then call PetscLogFlops() always just call PetscLogFlops() directly when needed.

• Do not use if (rank == 0) or if (v == NULL) or if (flg == PETSC_TRUE) or if (flg == PETSC_FALSE) instead use if (!rank) or if (!v) or if (flg) or if (!flg).

• Do not use #ifdef or #ifndef rather use #if defined(… or #if !defined(…

• MPI routines and macros that are not part of the 1.0 or 1.1 standard should not be used in PETSc without appropriate .configure checks and #if defined() checks the code. Code should also be provided that works if the MPI feature is not available. For example,

\[
\begin{align*}
\text{#ifdef(PETSC_HAVE_MPI_IN_PLACE)} \\
\text{ierr = MPIAllgatherv(MPI_IN_PLACE,0,MPI_DATATYPE_NULL,lens,recvcounts,displs,MPIU_INT,comm);CHKERRQ(ierr);} \\
\text{#else} \\
\text{ierr = MPIAllgatherv(lens,sendcount,MPIU_INT,lens,recvcounts,displs,MPIU_INT,comm);CHKERRQ(ierr);} \\
\text{#endif}
\end{align*}
\]

• There shall be no PETSc routines introduced that provide essentially the same functionality as an available MPI routine. For example, one should not write a routine PetscGlobalSum() that takes a scalar value and performs an MPI_Allreduce() on it. One should use MPI_Allreduce() directly in the code.

• XXXTypes (for example KSPType) do not have an underscore in them, unless they refer to another package that uses an underscore, for example MATSOLVER SUPERLU DIST.
2.3 Formatted Comments for Documentation and Fortran Interfaces

PETSc uses formatted comments and the Sowing packages to generate documentation (manual pages) and the fortran interfaces. Documentation for Sowing and the formatting may be found at http://www.cs.uiuc.edu/homes/wgropp/projects/software/sowing/doctext.pdf.

 *@ indicates a formatted comment of a function that will be used for both documentation and a Fortran interface.
 *@C a formatted comment of a function that will be used only for documentation
 /*E a formatted comment of an enum used for documentation only
 /*M a formatted comment of a CPP macro used for both documentation and a Fortran interface
 /*MC a formatted comment of a CPP macro for documentation

 Functions that take char* or function pointer arguments must have the C symbol since the Fortran interface generator cannot handle them so the Fortran interface for them must be created manually.

 The Fortran interface files go into the three directories depending on how they are created: ftn-auto, ftn-custom, ftn-f90.
Chapter 3

The PETSc Kernel

PETSc provides a variety of basic services for writing scalable, component based libraries; these are referred to as the PETSc kernel. The source code for the kernel is in src/sys. It contains systematic support for

- PETSc types
- error handling
- memory management
- profiling
- object management
- file IO
- options database
- basic objects for viewing and drawing.

Each of these is discussed in a section below.

3.1 PETSc Types

For maximum flexibility, the basic data types int, double etc are generally not used in source code, rather it has:

- PetscScalar
- PetscInt
- PetscMPIInt
- PetscBLASInt
- PetscBool
- PetscBT - bit storage of logical true and false
PetscInt can be set using ./configure (option --with-64-bit-indices) to be either int (32 bit) or long long (64 bit) to allow indexing into very large arrays. PetscMPIInt are for integers passed to MPI as counts etc, these are always int since that is what the MPI standard uses. Similarly PetscBLASInt are for counts etc passed to BLAS and LAPACK routines. These are almost always int unless one is using a special “64 bit integer” BLAS/LAPACK (this is available, for example on Solaris systems).

In addition there a special types

- PetscClassId
- PetscErrorCode
- PetscLogEvent

in fact, these are currently always int but their use clarifies the code.

### 3.2 Implementation of Error Handling

PETSc uses a “call error handler; then (depending on result) return error code” model when problems are detected in the running code.

The public include file for error handling is include/petscerror.h, the source code for the PETSc error handling is in src/sys/error/.

#### 3.2.1 Simplified Interface

The simplified C/C++ macro-based interface consists of the following two calls

- SETERRQ(comm,error code,"Error message");
- CHKERRQ(ierr);

The macro SETERRQ() is given by

```
return PetscError(comm,_,LINE_,_,FUNCT_,_,FILE_,error code,error type,
"Error message");
```

It calls the error handler with the current function name and location: line number, file and directory, plus an error code and an error message. Normally comm is PETSC_COMM_SELF, it can only be another communicator if one is absolutely sure the same error will be generated on all processes in the communicator. This is to prevent the same error message from being printed by many processes. The error type is PETSC_ERROR_INITIAL on detection of the initial error and PETSC_ERROR_REPEAT for any additional calls. This is so that the detailed error information is only printed once instead of for all levels of returned errors.

The macro CHKERRQ() is defined by

```
if (ierr) PetscError(PETSC_COMM_SELF,_,LINE_,_,PETSC_FUNC_,_,FILE_,
ierr,PETSC_ERROR_REPEAT," ");
```
In addition to `SETERRQ()` are the macros `SETERRQ1()`, `SETERRQ2()`, `SETERRQ3()` and `SETERRQ4()` that allow one to include additional arguments that the message string is formated. For example,

```
SETERRQ2(comm,PETSC_ERR,"Iteration overflow: its %d norm %g",its,norm);
```

The reason for the numbered format is because CPP macros cannot handle a variable number of arguments.

### 3.2.2 Error Handlers

The error handling function `PetscError()` calls the “current” error handler with the code

```
PetscErrorCode PetscError(MPI_Comm,int line,const char *func,const char *file,
const char *dir,error code, error type,const char *mess)
{
    PetscErrorCode ierr;
    PetscFunctionBegin;
    if (!eh) ierr = PetscTraceBackErrorHandler(line,func,file,dir,error code,error type,mess,0);
    else ierr = (*eh->handler)(line,func,file,dir,error code,error type,mess,eh->ctx);
    PetscFunctionReturn(ierr);
}
```

The variable `eh` is the current error handler context and is defined in `src/sys/error/err.c` as

```c
typedef struct _EH*EH;
struct _EH {
    PetscErrorCode handler(MPI_Comm,int,const char*,const char*,const char *,
    PetscErrorCode,PetscErrorType,const char*,void *);
    void *ctx;
    EH previous;
};
```

One can set a new error handler with the command

```
PetscErrorCode PetscPushErrorHandler(PetscErrorCode (*handler)(int,const char *,const char*,
    const char*,PetscErrorCode,PetscErrorType,const char*,void *),
    void *ctx)
{
    PetscErrorCode ierr;
    EH neweh;
    PetscFunctionBegin;
    ierr = PetscNew(&neweh);CHKERRQ(ierr);
    if (eh) neweh->previous = eh;
    else neweh->previous = 0;
    neweh->handler = handler;
    neweh->ctx = ctx;
    ```
eh = neweh;
PetscFunctionReturn(0);
}

which maintains a linked list of error handlers. The most recent error handler is removed via

PetscErrorCode PetscPopErrorHandler(void)
{
    EH tmp;
    PetscErrorCode ierr;
    PetscFunctionBegin;
    if (!eh) PetscFunctionReturn(0);
    tmp = eh;
    eh = eh->previous;
    ierr = PetscFree(tmp);CHKERRQ(ierr);
    PetscFunctionReturn(0);
}

PETSc provides several default error handlers

- PetscTraceBackErrorHandler(),
- PetscAbortErrorHandler(), -on_error_abort,
- PetscReturnErrorHandler(),
- PetscEmacsClientErrorHandler(),
- PetscMPIAbortErrorHandler(), and
- PetscAttachDebuggerErrorHandler(). -on_error_attach_debugger.

### 3.2.3 Error Codes

The PETSc error handler takes a generic error code. The generic error codes are defined in include/petscerror.h, the same generic error code would be used many times in the libraries. For example the generic error code PETSC_ERR_MEM is used whenever requested memory allocation is not available.

### 3.2.4 Detailed Error Messages

In a modern parallel component oriented application code it does not make sense to simply print error messages to the screen (more than likely there is no “screen”, for example with Windows applications). PETSc provides the replaceable function pointer

(*PetscErrorPrintf)(“Format”,...);

that, by default prints to standard out. Thus error messages should not be printed with printf() or fprintf() rather it should be printed with (*PetscErrorPrintf)(). One can direct all error messages to stderr with the command line options -error_output_stderr.
3.3 Implementation of Profiling

This section provides details about the implementation of event logging and profiling within the PETSc kernel. The interface for profiling in PETSc is contained in the file `include/petsclog.h`. The source code for the profile logging is in `src/sys/plog/`.

3.3.1 Profiling Object Create and Destruction

The creation of objects is profiled with the command

```c
PetscLogObjectCreate(PetscObject h);
```

which logs the creation of any PETSc object. Just before an object is destroyed, it should be logged with

```c
PetscLogObjectDestroy(PetscObject h);
```

These are called automatically by `PetscHeaderCreate()` and `PetscHeaderDestroy()` which are used in creating all objects inherited off the basic object. Thus these logging routines should never be called directly.

If an object has a clearly defined parent object (for instance, when a work vector is generated for use in a Krylov solver), this information is logged with the command,

```c
PetscLogObjectParent(PetscObject parent,PetscObject child);
```

It is also useful to log information about the state of an object, as can be done with the command

```c
PetscLogObjectState(PetscObject h,const char *format,...);
```

For example, for sparse matrices we usually log the matrix dimensions and number of nonzeros.

3.3.2 Profiling Events

Events are logged using the pair

```c
PetscLogEventBegin(PetscLogEvent event,PetscObject o1,...,PetscObject o4);
PetscLogEventEnd(PetscLogEvent event,PetscObject o1,...,PetscObject o4);
```

This logging is usually done in the abstract interface file for the operations, for example, `src/mat/interface/matrix.c`.

3.3.3 Controlling Profiling

Several routines that control the default profiling available in PETSc are are

```c
PetscLogDefaultBegin();
PetscLogAllBegin();
PetscLogDump(const char *filename);
PetscLogView(PetscViewer);
```

These routines are normally called by the `PetscInitialize()` and `PetscFinalize()` routines when the option `-log_summary` is given.

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Chapter 4

Basic Object Design

PETSc is designed using strong data encapsulation. Hence, any collection of data (for instance, a sparse matrix) is stored in a way that is completely private from the application code. The application code can manipulate the data only through a well-defined interface, as it does not “know” how the data is stored internally.

4.1 Introduction

PETSc is designed around several classes (e.g. Vec (vectors), Mat (matrices, both dense and sparse)). These classes are each implemented using C structs, that contain the data and function pointers for operations on the data (much like virtual functions in classes in C++). Each class consists of three parts:

- a (small) common part shared by all PETSc compatible libraries.
- another common part shared by all PETSc implementations of the class and
- a private part used by only one particular implementation written in PETSc.

For example, all matrix (Mat) classes share a function table of operations that may be performed on the matrix; all PETSc matrix implementations share some additional data fields, including matrix size; while a particular matrix implementation in PETSc (say compressed sparse row) has its own data fields for storing the actual matrix values and sparsity pattern. This will be explained in more detail in the following sections. People providing new class implementations must use the PETSc common part.

We will use `<class>_<implementation>` to denote the actual source code and data structures used for a particular implementation of an object that has the `<class>` interface.

4.2 Organization of the Source Code

Each class has

- Its own, application public, include file `include/petsc<class>.h`
- Its own directory, `src/<class>`
• A data structure defined in the file include/petsc/private/<class>impl.h. This data structure is shared by all the different PETSc implementations of the class. For example, for matrices it is shared by dense, sparse, parallel, and sequential formats.

• An abstract interface that defines the application callable functions for the class. These are defined in the directory src/<class>/interface. This is how polymorphism is supported with code that implements the abstract interface to the operations on the object. Essentially, these routines do some error checking of arguments and logging of profiling information and then call the function appropriate for the particular implementation of the object. The name of the abstract function is <class>Operation, for instance, MatMult() or PCCreate(), while the name of a particular implementation is <class>Operation_<implementation>, for instance, MatMult_SeqAIJ() or PCCreate_ILU(). These naming conventions are used to simplify code maintenance.

• One or more actual implementations of the class (for example, sparse uniprocessor and parallel matrices implemented with the AIJ storage format). These are each in a subdirectory of src/<class>/impls. Except in rare circumstances data structures defined here should not be referenced from outside this directory.

Each type of object, for instance a vector, is defined in its own public include file, by
typedef _p_<class>* <class>; (for example, typedef _p_Vec* Vec;).

This organization allows the compiler to perform type checking on all subroutine calls while at the same time completely removing the details of the implementation of _p_<class> from the application code. This capability is extremely important because it allows the library internals to be changed without altering or recompiling the application code.

4.3 Common Object Header

All PETSc/PETSc objects have the following common header structures defined in include/petsc/private/petscimpl.h

/* Function table common to all PETSc compatible classs */

typedef struct {
    int (*getcomm)(PetscObject, MPI_Comm *);
    int (*view)(PetscObject, Viewer);
    int (*destroy)(PetscObject);
    int (*query)(PetscObject, const char *, PetscObject *);
    int (*compose)(PetscObject, const char*, PetscObject);
    int (*composefunction)(PetscObject, const char*, void(*)(void));
    int (*queryfunction)(PetscObject, const char *, void (*)(void));
} PetscOps;

/* Data structure header common to all PETSc compatible classs */
Here `<class>ops` is a function table (like the `PetscOps` above) that contains the function pointers for the operations specific to that class. For example, the PETSc vector class object looks like

```c
/* Function table common to all PETSc compatible vector objects */

typedef struct _VecOps* VecOps;
struct _VecOps {
    PetscErrorCode (*duplicate)(Vec,Vec*), /* get single vector */
    (*duplicatevecs)(Vec,int,Vec**), /* get array of vectors */
    (*destroyvecs)(Vec*,int), /* free array of vectors */
    (*dot)(Vec,Vec,Scalar*), /* z = x'H * y */
    (*norm)(Vec,NormType,double*), /* z = sqrt(x'H * x) */
    (*tdot)(Vec,Vec,Scalar*), /* x'y */
    (*scale)(Scalar*,Vec), /* x = alpha * x */
    (*copy)(Vec,Vec), /* y = x */
    (*set)(Scalar*,Vec), /* y = alpha */
    (*swap)(Vec,Vec), /* exchange x and y */
    (*axpy)(Scalar*,Vec,Vec), /* y = y + alpha * x */
    (*axpby)(Scalar*,Scalar*,Vec,Vec), /* y = y + alpha * x + beta * y */
};
```
/* Data structure header common to all PETSc vector classes */

struct _p_Vec {
  PetscClassId classid;
  PetscOps *bops;
  VecOps *ops;
  MPI_Comm comm;
  PetscLogDouble flops,time,mem;
  int id;
  int refct;
  int tag;
  DLList qlist;
  OList olist;
  char *type_name;
  PetscObject parent;
  char *name;
  char *prefix;
  void **fortran_func_pointers;
  void *data; /* implementation-specific data */
  PetscLayout map; ISLocalToGlobalMapping mapping; /* mapping used in VecSetValuesLocal() */
  ISLocalToGlobalMapping bmapping; /* mapping used in VecSetValuesBlockedLocal() */
};

Each PETSc object begins with a PetscClassId which is used for error checking. Each different class of objects has its value for the classid; these are used to distinguish between classes. When a new class is created one needs to call
ierr = PetscClassIdRegister(const char *classname,PetscClassId *classid); CHKERRQ(ierr);

For example,

ierr = PetscClassIdRegister("index set", &IS_CLASSID); CHKERRQ(ierr);

**Question:** Why is a fundamental part of PETSc objects defined in PetscLog when PETSc Log is something that can be "turned off"? One can verify that an object is valid of a particular class with

PetscValidHeaderSpecific(x, VEC_CLASSID, 1);

The third argument to this macro indicates the position in the calling sequence of the function the object was passed in. This is generate more complete error messages.

To check for an object of any type use

PetscValidHeader(x, 1);

### 4.4 Common Object Functions

Several routines are provided for manipulating data within the header, these include the specific functions in the PETSc common function table.

- **getcomm(PetscObject, MPI_Comm **)** obtains the MPI communicator associated with this object.

- **view(PetscObject, Viewer)** allows one to store or visualize the data inside an object. If the Viewer is null then should cause the object to print information on the object to standard out. PETSc provides a variety of simple viewers.

- **destroy(PetscObject)** causes the reference count of the object to be decreased by one or the object to be destroyed and all memory used by the object to be freed when the reference count drops to zero. If the object has any other objects composed with it then they are each sent a destroy(), i.e. the destroy() function is called on them also.

- **compose(PetscObject, const char *name, PetscObject)** associates the second object with the first object and increases the reference count of the second object. If an object with the same name was previously composed that object is dereferenced and replaced with the new object. If the second object is null and object with the same name has already been composed that object is dereferenced (the destroy() function is called on it, and that object is removed from the first object); i.e. this is a way to remove, by name, an object that was previously composed.

- **query(PetscObject, const char *name, PetscObject **)** retrieves an object that was previously composed with the first object. Retreives a null if no object with that name was previously composed.
composefunction(PetscObject, const char *name, const char *fname, void *func)
associates a function pointer to an object. If the object already had a composed
function with the same name, the old one is replace. If the fname is null it is removed
from the object. The string fname is the character string name of the function; it
may include the path name or URL of the dynamic library where the function is
located. The argument name is a “short” name of the function to be used with the
queryfunction() call. On systems that support dynamic libraries the func argument
is ignored; otherwise func is the actual function pointer.

For example, fname may be libpetscksp:PCCreate_LU or http://www.mcs.anl.gov/
petsc/libpetscksp:PCreate_LU.

queryfunction(PetscObject, const char *name, void **func) retrieves a function
pointer that was associated with the object. If dynamic libraries are used the function
is loaded into memory at this time (if it has not been previously loaded), not when the
composefunction() routine was called.

Since the object composition allows one to only compose PETSc objects with PETSc
objects rather than any arbitrary pointer, PETSc provides the convenience object Petsc-
Container, created with the routine PetscContainerCreate(MPI_Comm, PetscContainer*) to
allow one to wrap any kind of data into a PETSc object that can then be composed with a
PETSc object.

4.5 PETSc Implementation of the Object Functions

This sections discusses how PETSc implements the compose(), query(), composefunction(),
and queryfunction() functions for its object implementations. Other PETSc compatible
class implementations are free to manage these functions in any manner; but generally they
would use the PETSc defaults so that the library writer does not have to “reinvent the
wheel.”

4.5.1 Compose and Query

In src/sys/objects/olist.c PETSc defines a C struct
typedef struct _PetscObjectList *PetscObjectList;
struct _PetscObjectList {
    char name[128];
    PetscObject obj;
    PetscObjectList next;
};

from which linked lists of composed objects may be constructed. The routines to manipulate
these elementary objects are

int PetscObjectListAdd(PetscObjectList *fl, const char *name, PetscObject obj);
int PetscObjectListDestroy(PetscObjectList fl);
int PetscObjectListFind(PetscObjectList fl, const char *name, PetscObject *obj)
int PetscObjectListDuplicate(PetscObjectList fl, PetscObjectList *nl);
The function PetscObjectListAdd() will create the initial PetscObjectList if the argument
fp1 points to a null.

The PETSc object compose() and query() functions are then simply (defined in src/sys/objects/inheri-

PetscErrorCode PetscObjectCompose_Petsc(PetscObject obj, const char *name, PetscObject ptr)
{
    PetscErrorCode ierr;

    PetscFunctionBegin;
    ierr = PetscObjectListAdd(&obj->olist, name, ptr); CHKERRQ(ierr);
    PetscFunctionReturn(0);
}

PetscErrorCode PetscObjectQuery_Petsc(PetscObject obj, const char *name, PetscObject *ptr)
{
    PetscErrorCode ierr;

    PetscFunctionBegin;
    ierr = PetscObjectListFind(obj->olist, name, ptr); CHKERRQ(ierr);
    PetscFunctionReturn(0);
}

4.5.2 Compose and Query Function

PETSc allows one to compose functions bying name and function pointer. In src/sys/dll/reg.c,
PETSc defines the linked list structure

typedef struct _PetscFunctionList *PetscFunctionList;
struct _PetscFunctionList {
    void (*routine)(void);
    char *name;
    PetscFunctionList *next;
};

Each PETSc object contains a PetscFunctionList object. The composefunction() and
queryfunction() are given by

PetscErrorCode PetscObjectComposeFunction_Petsc(PetscObject obj, const char *name,
        void *ptr)
{
    PetscErrorCode ierr;

    PetscFunctionBegin;
    ierr = PetscFunctionListAdd(&obj->qlist, name, fname, ptr); CHKERRQ(ierr);
    PetscFunctionReturn(0);
}
PetscErrorCode PetscObjectQueryFunction(PetscObject obj, const char *name, void (**ptr)(void))
{
    PetscErrorCode ierr;

    PetscFunctionBegin;
    ierr = PetscFunctionListFind(obj->qlist, name, ptr); CHKERRQ(ierr);
    PetscFunctionReturn(0);
}

In addition to using the PetscFunctionList mechanism to compose functions into PETSc objects, it is also used to allow registration of new class implementations; for example, new preconditioners, see Section 5.2.3.

4.5.3 Simple PETSc Objects

There are some simple PETSc objects that do not need PETSCHEADER - and the associated functionality. These objects are internally named as _n_<class> as opposed to _p_<class>. For eg: _n_PetscTable vs _p_Vec.
Chapter 5

PetscObjects

5.1 Elementary Objects: IS, Vec, Mat

5.2 Solver Objects: PC, KSP, SNES, TS

5.2.1 Preconditioners: PC

The base PETSc PC object is defined in the include/petsc/private/pcimpl.h include file. A carefully commented implementation of a PC object can be found in src/ksp/pc/impls/jacobi/jacobi.c.

5.2.2 Krylov Solvers: KSP

The base PETSc KSP object is defined in the include/petsc/private/kspimpl.h include file. A carefully commented implementation of a KSP object can be found in src/ksp/ksp/impls/cg/cg.c.

5.2.3 Registering New Methods

See src/ksp/examples/tutorials/ex12.c for an example of registering a new preconditioning (PC) method.
Chapter 6

The Various Matrix Classes

PETSc provides a variety of matrix implementations, since no single matrix format is appropriate for all problems. This section first discusses various matrix blocking strategies, and then describes the assortment of matrix types within PETSc.

6.1 Matrix Blocking Strategies

In today’s computers, the time to perform an arithmetic operation is dominated by the time to move the data into position, not the time to compute the arithmetic result. For example, the time to perform a multiplication operation may be one clock cycle, while the time to move the floating point number from memory to the arithmetic unit may take 10 or more cycles. To help manage this difference in time scales, most processors have at least three levels of memory: registers, cache, and random access memory, RAM. (In addition, some processors have external caches, and the complications of paging introduce another level to the hierarchy.)

Thus, to achieve high performance, a code should first move data into cache, and from there move it into registers and use it repeatedly while it remains in the cache or registers before returning it to main memory. If one reuses a floating point number 50 times while it is in registers, then the “hit” of 10 clock cycles to bring it into the register is not important. But if the floating point number is used only once, the “hit” of 10 clock cycles becomes very noticeable, resulting in disappointing flop rates.

Unfortunately, the compiler controls the use of the registers, and the hardware controls the use of the cache. Since the user has essentially no direct control, code must be written in such a way that the compiler and hardware cache system can perform well. Good quality code is then be said to respect the memory hierarchy.

The standard approach to improving the hardware utilization is to use blocking. That is, rather than working with individual elements in the matrices, one employs blocks of elements. Since the use of implicit methods in PDE-based simulations leads to matrices with a naturally blocked structure (with a block size equal to the number of degrees of freedom per cell), blocking is extremely advantageous. The PETSc sparse matrix representations use a variety of techniques for blocking, including

- storing the matrices using a generic sparse matrix format, but storing additional information about adjacent rows with identical nonzero structure (so called I-nodes); this
I-node information is used in the key computational routines to improve performance (the default for the MATSEQAIJ and MATMPIAIJ formats);

- storing the matrices using a fixed (problem dependent) block size (via the MATSEQBAIJ and MATMPIBAIJ formats); and

The advantage of the first approach is that it is a minimal change from a standard sparse matrix format and brings a large percent of the improvement one obtains via blocking. Using a fixed block size gives the best performance, since the code can be hardwired with that particular size (for example, in some problems the size may be 3, in others 5, etc.), so that the compiler will then optimize for that size, removing the overhead of small loops entirely.

The following table presents the floating point performance for a basic matrix-vector product using these three approaches: a basic compressed row storage format (using the PETSc runtime options -mat_seqaij -mat_no_unroll); the same compressed row format using I-nodes (with the option -mat_seqaij); and a fixed block size code, with a block size of three for these problems (using the option -mat_seqbaij). The rates were computed on one node of an older IBM SP, using two test matrices. The first matrix (ARCO1), courtesy of Rick Dean of Arco, arises in multiphase flow simulation; it has 1501 degrees of freedom, 26,131 matrix nonzeros and, a natural block size of 3, and a small number of well terms. The second matrix (CFD), arises in a three-dimensional Euler flow simulation and has 15,360 degrees of freedom, 496,000 nonzeros, and a natural block size of 5. In addition to displaying the flop rates for matrix-vector products, we also display them for triangular solve obtained from an ILU(0) factorization.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Block size</th>
<th>Basic</th>
<th>I-node version</th>
<th>Fixed block size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiphase</td>
<td>3</td>
<td>27</td>
<td>43</td>
<td>70</td>
</tr>
<tr>
<td>Euler</td>
<td>5</td>
<td>28</td>
<td>58</td>
<td>90</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Problem</th>
<th>Block size</th>
<th>Basic</th>
<th>I-node version</th>
<th>Fixed block size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiphase</td>
<td>3</td>
<td>22</td>
<td>31</td>
<td>49</td>
</tr>
<tr>
<td>Euler</td>
<td>5</td>
<td>22</td>
<td>39</td>
<td>65</td>
</tr>
</tbody>
</table>

These examples demonstrate that careful implementations of the basic sequential kernels in PETSc can dramatically improve overall floating point performance, and users can immediately benefit from such enhancements without altering a single line of their application codes. Note that the speeds of the I-node and fixed block operations are several times that of the basic sparse implementations. The disappointing rates for the variable block size code occur because even on a sequential computer, the code performs the matrix-vector products and triangular solves using the coloring introduced above and thus does not utilize the cache particularly efficiently. This is an example of improving the parallelization capability at the expense of using each processor less efficiently.

### 6.1.1 Sequential AIJ Sparse Matrices

The default matrix representation within PETSc is the general sparse AIJ format (also called the Yale sparse matrix format or compressed sparse row format, CSR).
6.1.2 Parallel AIJ Sparse Matrices

This matrix type, which is the default parallel matrix format; additional implementation details are given in [1].

6.1.3 Sequential Block AIJ Sparse Matrices

The sequential and parallel block AIJ formats, which are extensions of the AIJ formats described above, are intended especially for use with multiclass PDEs. The block variants store matrix elements by fixed-sized dense $\mathbf{n} \times \mathbf{n}$ blocks. The stored row and column indices begin at zero.

The routine for creating a sequential block AIJ matrix with $\mathbf{m}$ rows, $\mathbf{n}$ columns, and a block size of $\mathbf{nb}$ is

$$
ierr = \text{MatCreateSeqBAIJ}(\text{MPI Comm comm}, \text{int nb}, \text{int m}, \text{int n}, \text{int nz}, \text{int *nnz}, \text{Mat *A})$$

The arguments nz and nnz can be used to preallocate matrix memory by indicating the number of block nonzeros per row. For good performance during matrix assembly, preallocation is crucial; however, the user can set nz=$0$ and nnz=NULL for PETSc to dynamically allocate matrix memory as needed. The PETSc users manual discusses preallocation for the AIJ format; extension to the block AIJ format is straightforward.

Note that the routine MatSetValuesBlocked() can be used for more efficient matrix assembly when using the block AIJ format.

6.1.4 Parallel Block AIJ Sparse Matrices

Parallel block AIJ matrices with block size $\mathbf{nb}$ can be created with the command

$$
ierr = \text{MatCreateBAIJ}(\text{MPI Comm comm}, \text{int nb}, \text{int m}, \text{int n}, \text{int M}, \text{int N}, \text{int d_nz}, \text{int *d_nnz}, \text{int o_nz}, \text{int *o_nnz}, \text{Mat *A});$$

$\mathbf{A}$ is the newly created matrix, while the arguments $\mathbf{m}$, $\mathbf{n}$, $\mathbf{M}$, and $\mathbf{N}$, indicate the number of local rows and columns and the number of global rows and columns, respectively. Either the local or global parameters can be replaced with PETSC_DECIDE, so that PETSc will determine them. The matrix is stored with a fixed number of rows on each processor, given by $\mathbf{m}$, or determined by PETSc if $\mathbf{m}$ is PETSC_DECIDE.

If PETSC_DECIDE is not used for $\mathbf{m}$ and $\mathbf{n}$ then the user must ensure that they are chosen to be compatible with the vectors. To do this, one first considers the product $y = Ax$. The $\mathbf{m}$ that one uses in MatCreateBAIJ() must match the local size used in the VecCreateMPI() for $\mathbf{y}$. The $\mathbf{n}$ used must match that used as the local size in VecCreateMPI() for $\mathbf{x}$.

The user must set $\text{d_nz}=0$, $\text{o_nz}=0$, $\text{d_nnz}=\text{NULL}$, and $\text{o_nnz}=\text{NULL}$ for PETSc to control dynamic allocation of matrix memory space. Analogous to nz and nnz for the routine MatCreateSeqBAIJ(), these arguments optionally specify block nonzero information for the diagonal ($\text{d_nz}$ and $\text{d_nnz}$) and off-diagonal ($\text{o_nz}$ and $\text{o_nnz}$) parts of the matrix. For a square global matrix, we define each processor’s diagonal portion to be its local rows and the corresponding columns (a square submatrix); each processor’s off-diagonal portion encompasses the remainder of the local matrix (a rectangular submatrix). The PETSc users manual gives an example of preallocation for the parallel AIJ matrix format; extension to the block parallel AIJ case is straightforward.
6.1.5 Sequential Dense Matrices

PETSc provides both sequential and parallel dense matrix formats, where each processor stores its entries in a column-major array in the usual Fortran77 style.

6.1.6 Parallel Dense Matrices

The parallel dense matrices are partitioned by rows across the processors, so that each local rectangular submatrix is stored in the dense format described above.
Bibliography