PETSc: Platform for Scientific Computing

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ME 964: High Performance Computing for Engineering Applications
University of Wisconsin – Madison
April 21, 2011
Introduction

- Who uses and develops PETSc?
- Stuff for Windows
- How can I get PETSc?
- How do I Configure PETSc?
- How do I Build PETSc?
- How do I run an example?
- How do I get more help?

Version Control

Vector Algebra

Matrix Algebra
What I Need From You

- Tell me if you do not understand
- Tell me if an example does not work
- Suggest better wording or figures
- Followup problems at petsc-maint@mcs.anl.gov
Ask Questions!!!

- Helps **me** understand what you are missing
- Helps **you** clarify misunderstandings
- Helps **others** with the same question
How We Can Help at the Tutorial

- Point out relevant documentation
- Quickly answer questions
- Help install
- Guide design of large scale codes
- Answer email at petsc-maint@mcs.anl.gov
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PETSc was developed as a Platform for Experimentation

We want to experiment with different
- Models
- Discretizations
- Solvers
- Algorithms
  - which blur these boundaries
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
What is PETSc?

A freely available and supported research code
- Download from http://www.mcs.anl.gov/petsc
- Free for everyone, including industrial users
- Hyperlinked manual, examples, and manual pages for all routines
- Hundreds of tutorial-style examples
- Support via email: petsc-maint@mcs.anl.gov
- Usable from C, C++, Fortran 77/90, and Python
What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems
    - Cray XT5, BG/Q, NVIDIA Fermi, Earth Simulator
  - Loosely coupled systems, such as networks of workstations
    - IBM, Mac, iPad/iPhone, PCs running Linux or Windows

PETSc History
- Begun September 1991
- Over 60,000 downloads since 1995 (version 2)
- Currently 400 per month

PETSc Funding and Support
- Department of Energy
  - SciDAC, MICS Program, AMR Program, INL Reactor Program
- National Science Foundation
  - CIG, CISE, Multidisciplinary Challenge Program
Timeline

1991
PETSc-1
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed

1995
PETSc-2

2000
PETSc-3

2005

2010
What Can We Handle?

- PETSc has run implicit problems with over 500 billion unknowns
  - UNIC on BG/P and XT5
  - PFLOTRAN for flow in porous media

- PETSc has run on over 224,000 cores efficiently
  - UNIC on the IBM BG/P Intrepid at ANL
  - PFLOTRAN on the Cray XT5 Jaguar at ORNL

- PETSc applications have run at 22 Teraflops
  - Kaushik on XT5
  - LANL PFLOTRAN code
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New Model for Scientific Software

sympy
symbolics

Application

eqn. definition

data structures
integration/assembly

FFC/SyFi

solvers

petsc4py

numpy

PyCUDA

PETSc

CUDA
OpenCL

M. Knepley ( )

PETSc

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Who Uses PETSc?

Computational Scientists

Earth Science
- PyLith (CIG)
- Underworld (Monash)
- Magma Dynamics (LDEO, Columbia)

Subsurface Flow and Porous Media
- STOMP (DOE)
- PFLOTRAN (DOE)
Who Uses PETSc?

Computational Scientists

- CFD
  - OpenFOAM
  - freeCFD
  - OpenFVM

- MicroMagnetics (MagPar)

- Fusion (NIMROD)
Algorithm Developers

- **Iterative methods**
  - Deflated GMRES
  - LGMRES
  - QCG
  - SpecEst

- **Preconditioning researchers**
  - *Prometheus* (Adams)
  - *ParPre* (Eijkhout)
  - *FETI-DP* (Klawonn and Rheinbach)
Who Uses PETSc?

Algorithm Developers

- Finite Elements
  - PETSc-FEM
  - libMesh
  - Deal II
  - OOFEM

- Fast Multipole Method (PetFMM)

- Radial Basis Function Interpolation (PetRBF)

- Eigensolvers (SLEPc)

- Optimization (TAO)
The PETSc Team

Bill Gropp  Barry Smith  Satish Balay

Jed Brown  Matt Knepley  Lisandro Dalcin

Hong Zhang  Victor Eijkhout  Dmitry Karpeev
1. **Introduction**
   - Who uses and develops PETSc?
   - **Stuff for Windows**
     - How can I get PETSc?
     - How do I Configure PETSc?
     - How do I Build PETSc?
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Questions for Windows Users

Have you installed cygwin?
- Need python, make, and build-utils packages

Will you use the GNU compilers?
- If not, remove `link.exe`
- If MS, check compilers from `cmd window` and use `win32fe`

Which MPI will you use?
- You can use `-with-mpi=0`
- If MS, need to install MPICH2
- If GNU, can use `-download-mpich`
Introduction

Who uses and develops PETSc?
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How do I Configure PETSc?
How do I Build PETSc?
How do I run an example?
How do I get more help?
How can I get PETSc?

**Downloading PETSc**

- The latest tarball is on the PETSc site
  - We no longer distribute patches (everything is in the distribution)

- There is a Debian package
- There is a FreeBSD Port
- There is a Mercurial development repository
Cloning PETSc

- The full development repository is open to the public
  - http://petsc.cs.iit.edu/petsc/petsc-dev
  - http://petsc.cs.iit.edu/petsc/BuildSystem
- Why is this better?
  - You can clone to any release (or any specific ChangeSet)
  - You can easily rollback changes (or releases)
  - You can get fixes from us the same day
- We also make release repositories available
  - http://petsc.cs.iit.edu/petsc/releases/petsc-3.1
  - http://petsc.cs.iit.edu/petsc/releases/BuildSystem-3.1
Introduction

How can I get PETSc?

Unpacking PETSc

- Just clone development repository
  - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
  - `hg clone -rrelease-3.1 petsc-dev petsc-3.1`

- or

- Unpack the tarball
  - `tar xzf petsc.tar.gz`
Exercise 1

Download and Unpack PETSc!
Outline

1 Introduction

- Who uses and develops PETSc?
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- How can I get PETSc?
- **How do I Configure PETSc?**
- How do I Build PETSc?
- How do I run an example?
- How do I get more help?
Set `$PETSC_DIR` to the installation root directory

Run the configuration utility

- `$PETSC_DIR/configure`
- `$PETSC_DIR/configure -help`
- `$PETSC_DIR/configure -download-mpich`
- `$PETSC_DIR/configure -prefix=/usr`

There are many examples on the installation page

Configuration files are in `$PETSC_DIR/$PETSC_ARCH/conf`

- Configure header is in `$PETSC_DIR/$PETSC_ARCH/include`
- `$PETSC_ARCH` has a default if not specified
You can easily reconfigure with the same options

```bash
./${PETSC_ARCH}/conf/reconfigure-${PETSC_ARCH}.py
```

Can maintain several different configurations

```bash
./configure -PETSC_ARCH=linux-fast -with-debugging=0
```

All configuration information is in the logfile

```bash
./${PETSC_ARCH}/conf/configure.log
```

ALWAYS send this file with bug reports
Automatic Downloads

- Starting in 2.2.1, some packages are automatically
  - Downloaded
  - Configured and Built (in `$PETSC_DIR/externalpackages`)
  - Installed with PETSc

- Currently works for
  - petsc4py
  - PETSc documentation utilities (Sowing, lgrind, c2html)
  - BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
  - MPICH, MPE, OpenMPI
  - ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
  - MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack, pARMS
  - BLOPEX, FFTW, SPRNG
  - Prometheus, HYPRE, ML, SPAI
  - Sundials
  - Triangle, TetGen
  - FIAT, FFC, Generator
  - Boost
Exercise 2

Configure your downloaded PETSc.
1 Introduction

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Building PETSc

- Uses recursive make starting in `cd $PETSC_DIR`
  - `make`
  - `make install` if you configured with `--prefix`
  - Check build when done with `make test`
- Or `./config/builder.py` which handles dependencies
- Complete log for each build is in logfile
  - `./$PETSC_ARCH/conf/make.log`
  - ALWAYS send this with bug reports
- Can build multiple configurations
  - `PETSC_ARCH=linux-fast make`
  - Libraries are in `$PETSC_DIR/$PETSC_ARCH/lib/`
- Can also build a subtree
  - `cd src/snes; make`
  - `cd src/snes; make ACTION=libfast tree`
Exercise 3

Build your configured PETSc.
Reconfigure PETSc to use ParMetis.

1. `linux-c-debug/conf/reconfigure-linux-c-debug.py`
   - `-PETSC_ARCH=linux-parmetis`
   - `-download-parmetis`

2. `PETSC_ARCH=linux-parmetis make`

3. `PETSC_ARCH=linux-parmetis make test`
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Running PETSc

- Try running PETSc examples first
  - `cd $PETSC_DIR/src/snes/examples/tutorials`
- Build examples using make targets
  - `make ex5`
- Run examples using the make target
  - `make runex5`
- Can also run using MPI directly
  - `mpirun ./ex5 -snes_max_it 5`
  - `mpiexec ./ex5 -snes_monitor`
The **Message Passing Interface** is:
- a library for parallel communication
- a system for launching parallel jobs (mpirun/mpiexec)
- a community standard

Launching jobs is easy
- `mpiexec -n 4 ./ex5`

You should never have to make MPI calls when using PETSc
- Almost never
Common Viewing Options

- Gives a text representation
  - `vec_view`
- Generally views subobjects too
  - `snes_view`
- Can visualize some objects
  - `mat_view_draw`
- Alternative formats
  - `vec_view_binary`, `vec_view_matlab`, `vec_view_socket`
- Sometimes provides extra information
  - `mat_view_info`, `mat_view_info_detailed`
Common Monitoring Options

- Display the residual
  - \texttt{-ksp_monitor}, \texttt{graphically \ -ksp_monitor_draw}
- Can disable dynamically
  - \texttt{-ksp_monitors_cancel}
- Does not display subsolvers
  - \texttt{-snes_monitor}
- Can use the true residual
  - \texttt{-ksp_monitor_true_residual}
- Can display different subobjects
  - \texttt{-snes_monitor_residual, \ -snes_monitor_solution,}
    \texttt{-snes_monitor_solution_update}
  - \texttt{-snes_monitor_range}
  - \texttt{-ksp_gmres_krylov_monitor}
- Can display the spectrum
  - \texttt{-ksp_monitor_singular_value}
Exercise 5

Run SNES Example 5 using some custom options.

1. `cd $PETSC_DIR/src/snes/examples/tutorials`
2. `make ex5`
3. `mpiexec ./ex5 -snes_monitor -snes_view`
4. `mpiexec ./ex5 -snes_type tr -snes_monitor -snes_view`
5. `mpiexec ./ex5 -ksp_monitor -snes_monitor -snes_view`
6. `mpiexec ./ex5 -pc_type jacobi -ksp_monitor -snes_monitor -snes_view`
7. `mpiexec ./ex5 -ksp_type bicg -ksp_monitor -snes_monitor -snes_view`
Exercise 6

Create a new code based upon SNES Example 5.

1. Create a new directory
   - `mkdir -p /home/knepley/proj/newsim/src`

2. Copy the source
   - `cp ex5.c /home/knepley/proj/newsim/src`
   - Add `myStuff.c` and `myStuff2.F`

3. Create a PETSc makefile
   - `bin/ex5: src/ex5.o src/myStuff.o src/myStuff2.o`
   - `${CLINKER} -o $@ $^ ${PETSC_SNES_LIB}`
   - `include ${PETSC_DIR}/conf/variables`
   - `include ${PETSC_DIR}/conf/rules`

To get the project ready-made

`hg clone http://petsc.cs.iit.edu/petsc/tutorials/SimpleTutorial newsim`
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Getting More Help

- http://www.mcs.anl.gov/petsc
- Hyperlinked documentation
  - Manual
  - Manual pages for every method
  - HTML of all example code (linked to manual pages)
- FAQ
- Full support at petsc-maint@mcs.anl.gov
- High profile users
  - David Keyes
  - Marc Spiegelman
  - Richard Katz
  - Brad Aagaard
  - Aron Ahmadia
Outline

1. Introduction
2. Version Control
3. Vector Algebra
4. Matrix Algebra
5. Algebraic Solvers
6. SNES
7. DA
8. PCFieldSplit
9. PETSc-GPU
Version Control
  - Mercurial, Git, Subversion

Hosting
  - BitBucket, GitHub, Launchpad

Community involvement
  - arXiv, PubMed
CVS/SVN manage a single repository
- Versioned data
- Local copy for modification and checkin

Mercurial manages many repositories
- Identified by URLs
- No one *Master*

Repositories communicate by *ChangeSets*
- Use *push* and *pull* to move changesets
- Can move arbitrary changes with *patch queues*
Figure: Single Repository
Project Workflow

Figure: Master Repository with User Clones
Project Workflow

Master → Release

User → Bugfix

Figure: Project with Release and Bugfix Repositories
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What are PETSc vectors?

- Fundamental objects representing
  - solutions
  - right-hand sides
  - coefficients

- Each process locally owns a subvector of contiguous global data
How do I create vectors?

- `VecCreate(MPI_Comm, Vec *)`
- `VecSetSizes(Vec, PetscInt n, PetscInt N)`
- `VecSetType(Vec, VecType typeName)`
- `VecSetFromOptions(Vec)`

  - Can set the type at runtime
A PETSc Vec

- Supports all vector space operations
  - VecDot(), VecNorm(), VecScale()
- Has a direct interface to the values
  - VecGetArray(), VecGetArrayF90()
- Has unusual operations
  - VecSqrtAbs(), VecStrideGather()
- Communicates automatically during assembly
- Has customizable communication (VecScatter)
Processes may set an arbitrary entry
  - Must use proper interface
Entries need not be generated locally
  - Local meaning the process on which they are stored
**PETSc automatically moves data if necessary**
  - Happens during the assembly phase
A three step process
- Each process sets or adds values
- Begin communication to send values to the correct process
- Complete the communication

\[
\text{VecSetValues}(\text{Vec } v, \text{PetscInt } n, \text{PetscInt } \text{rows}[], \text{PetscScalar } \text{values}[], \text{InsertMode } \text{mode})
\]

Mode is either \text{INSERT \_VALUES} or \text{ADD \_VALUES}

Two phases allow overlap of communication and computation
- \text{VecAssemblyBegin}(\text{Vec } v)
- \text{VecAssemblyEnd}(\text{Vec } v)
VecGetSize(x, &N);
MPI_Comm_rank(PETSC_COMM_WORLD, &rank);
if (rank == 0) {
    val = 0.0;
    for (i = 0; i < N; ++i) {
        VecSetValues(x, 1, &i, &val, INSERT_VALUES);
        val += 10.0;
    }
}

/* These routines ensure that the data is distributed to the other processes */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
VecGetOwnershipRange(x, &low, &high);
val = low*10.0;
for(i = low; i < high; ++i) {
    VecSetValues(x, 1, &i, &val, INSERT_VALUES);
    val += 10.0;
}
/* No data will be communicated here */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
## Selected Vector Operations

<table>
<thead>
<tr>
<th>Function Name</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>VecAXPY(Vec y, PetscScalar a, Vec x)</td>
<td>( y = y + a \times x )</td>
</tr>
<tr>
<td>VecAYPX(Vec y, PetscScalar a, Vec x)</td>
<td>( y = x + a \times y )</td>
</tr>
<tr>
<td>VecWAYPX(Vec w, PetscScalar a, Vec x, Vec y)</td>
<td>( w = y + a \times x )</td>
</tr>
<tr>
<td>VecScale(Vec x, PetscScalar a)</td>
<td>( x = a \times x )</td>
</tr>
<tr>
<td>VecCopy(Vec y, Vec x)</td>
<td>( y = x )</td>
</tr>
<tr>
<td>VecPointwiseMult(Vec w, Vec x, Vec y)</td>
<td>( w_i = x_i \times y_i )</td>
</tr>
<tr>
<td>VecMax(Vec x, PetscInt *idx, PetscScalar *r)</td>
<td>( r = \max r_i )</td>
</tr>
<tr>
<td>VecShift(Vec x, PetscScalar r)</td>
<td>( x_i = x_i + r )</td>
</tr>
<tr>
<td>VecAbs(Vec x)</td>
<td>( x_i =</td>
</tr>
<tr>
<td>VecNorm(Vec x, NormType type, PetscReal *r)</td>
<td>( r =</td>
</tr>
</tbody>
</table>
It is sometimes more efficient to directly access local storage of a Vec. 

- PETSc allows you to access the local storage with
  - `VecGetArray(Vec, double *[])`
- You must return the array to PETSc when you finish
  - `VecRestoreArray(Vec, double *[])`
- Allows PETSc to handle data structure conversions
  - Commonly, these routines are fast and do not involve a copy
Vec v;
PetscScalar *array;
PetscInt n, i;
PetscErrorCode ierr;

VecGetArray(v, &array);
VecGetLocalSize(v, &n);
PetscSynchronizedPrintf(PETSC_COMM_WORLD, "First element of local array is %f\n", array[0]);
PetscSynchronizedFlush(PETSC_COMM_WORLD);
for (i = 0; i < n; ++i) {
    array[i] += (PetscScalar) rank;
}
VecRestoreArray(v, &array);
```c
#include "finclude/petsc.h"

Vec v;
PetscScalar array(1)
PetscOffset offset
PetscInt n, i
PetscErrorCode ierr

call VecGetArray(v, array, offset, ierr)
call VecGetLocalSize(v, n, ierr)
do i=1,n
   array(i+offset) = array(i+offset) + rank
end do

call VecRestoreArray(v, array, offset, ierr)
```
```c
#include "finclude/petsc.h90"

Vec v;
PetscScalar pointer :: array(:)
PetscInt n, i
PetscErrorCode ierr

call VecGetArrayF90(v, array, ierr)
call VecGetLocalSize(v, n, ierr)
do i=1,n
    array(i) = array(i) + rank
end do
call VecRestoreArrayF90(v, array, ierr)
```
with v as a:

    for i in range(len(a)):
        a[i] = 5.0*i
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M. Knepley (UW '11 62 / 118)
What are PETSc matrices?

- Fundamental objects for storing stiffness matrices and Jacobians
- Each process locally owns a contiguous set of rows
- Supports many data types
  - AIJ, Block AIJ, Symmetric AIJ, Block Matrix, etc.
- Supports structures for many packages
  - MUMPS, Spooles, SuperLU, UMFPack, DSCPack
How do I create matrices?

- **MatCreate**(`MPI_Comm`, `Mat *`)
- **MatSetSizes**(`Mat`, `PetscInt m`, `PetscInt n`, `M`, `N`)
- **MatSetType**(`Mat`, `MatType` `typeName`)
- **MatSetFromOptions**(`Mat`)

  - Can set the type at runtime
- **MatSeqAIJPreallocation**(`Mat`, `PetscInt nz`, `const PetscInt nnz[]`)
- **MatMPIAIJPreallocation**(`Mat`, `dnz`, `dnz[]`, `onz`, `onz[]`)
- **MatSetValues**(`Mat`, `m`, `rows[]`, `n`, `cols[]`, `values[]`, `InsertMode`)

  - **MUST** be used, but does automatic communication
The PETSc Mat has a single user interface,
- Matrix assembly
  - MatSetValues()
- Matrix-vector multiplication
  - MatMult()
- Matrix viewing
  - MatView()
but multiple underlying implementations.
- AIJ, Block AIJ, Symmetric Block AIJ,
- Dense
- Matrix-Free
- etc.

A matrix is defined by its interface, not by its data structure.
Matrix Assembly

- A three step process
  - Each process sets or adds values
  - Begin communication to send values to the correct process
  - Complete the communication

\[ \text{MatSetValues}(\text{Mat } m, m, \text{rows}[], n, \text{cols}[], \text{values}[], \text{mode}) \]

  \[ \text{mode is either INSERT\_VALUES or ADD\_VALUES} \]
  - Logically dense block of values

- Two phase assembly allows overlap of communication and computation

\[ \text{MatAssemblyBegin}(\text{Mat } m, \text{MatAssemblyType } \text{type}) \]
\[ \text{MatAssemblyEnd}(\text{Mat } m, \text{MatAssemblyType } \text{type}) \]

  \[ \text{type is either MAT\_FLUSH\_ASSEMBLY or MAT\_FINAL\_ASSEMBLY} \]
One Way to Set the Elements of a Matrix
Simple 3-point stencil for 1D Laplacian

\[ v[0] = -1.0; \quad v[1] = 2.0; \quad v[2] = -1.0; \]

```c
if (rank == 0) {
    for (row = 0; row < N; row++) {
        cols[0] = row-1; cols[1] = row; cols[2] = row+1;
        if (row == 0) {
            MatSetValues(A, 1, &row, 2, &cols[1], &v[1], INSERT_VALUES);
        } else if (row == N-1) {
            MatSetValues(A, 1, &row, 2, cols, v, INSERT_VALUES);
        } else {
            MatSetValues(A, 1, &row, 3, cols, v, INSERT_VALUES);
        }
    }
    MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
    MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
}
```

Matrix Storage Layout

- 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
A Better Way to Set the Elements of a Matrix
Simple 3-point stencil for 1D Laplacian

\[ v[0] = -1.0; \quad v[1] = 2.0; \quad v[2] = -1.0; \]

MatGetOwnershipRange(A, &start, &end);

for (row = start; row < end; row++) {
    cols[0] = row - 1; cols[1] = row; cols[2] = row + 1;
    if (row == 0) {
        MatSetValues(A, 1, &row, 2, &cols[1], &v[1], INSERT_VALUES);
    } else if (row == N - 1) {
        MatSetValues(A, 1, &row, 2, cols, v, INSERT_VALUES);
    } else {
        MatSetValues(A, 1, &row, 3, cols, v, INSERT_VALUES);
    }
}

MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
No one data structure is appropriate for all problems
- Blocked and diagonal formats provide performance benefits
- PETSc has many formats
- Makes it easy to add new data structures

Assembly is difficult enough without worrying about partitioning
- PETSc provides parallel assembly routines
- High performance still requires making most operations local
- However, programs can be incrementally developed.
  - `MatPartitioning` and `MatOrdering` can help

Matrix decomposition in contiguous chunks is simple
- Makes interoperation with other codes easier
- For other ordering, PETSc provides “Application Orderings” (AO)
Outline

1. Introduction
2. Version Control
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4. Matrix Algebra
5. Algebraic Solvers
6. SNES
7. DA
8. PCFieldSplit

M. Knepley (PETSc)
Explicit:
- Field variables are updated using local neighbor information

Semi-implicit:
- Some subsets of variables are updated with global solves
- Others with direct local updates

Implicit:
- Most or all variables are updated in a single global solve
Using PETSc linear algebra, just add:
- `KSPSetOperators(KSP ksp, Mat A, Mat M, MatStructure flag)`
- `KSPSolve(KSP ksp, Vec b, Vec x)`

Can access subobjects
- `KSPGetPC(KSP ksp, PC *pc)`

Preconditioners must obey PETSc interface
- Basically just the KSP interface

Can change solver dynamically from the command line
- `-ksp_type biconjugate_gradient_stabilized`
Using PETSc linear algebra, just add:

- `SNESSetFunction(SNES snes, Vec r, residualFunc, void *ctx)`
- `SNESSetJacobian(SNES snes, Mat A, Mat M, jacFunc, void *ctx)`
- `SNESSolve(SNES snes, Vec b, Vec x)`

Can access subobjects

`SNESGetKSP(SNES snes, KSP *ksp)`

Can customize subobjects from the cmd line

Set the subdomain preconditioner to ILU with `-sub_pc_type ilu`
Use `SNESSetFromOptions()` so that everything is set dynamically

- Set the type
  - Use `-snes_type` (or take the default)
- Override the tolerances
  - Use `-snes_rtol` and `-snes_atol`
- View the solver to make sure you have the one you expect
  - Use `-snes_view`
- For debugging, monitor the residual decrease
  - Use `-snes_monitor`
  - Use `-ksp_monitor` to see the underlying linear solver
### 3rd Party Solvers in PETSc

#### Complete table of solvers

1. **Sequential LU**
   - ILUDT (SPARSEKIT2, Yousef Saad, U of MN)
   - EUCLID & PILUT (Hypre, David Hysom, LLNL)
   - ESSL (IBM)
   - SuperLU (Jim Demmel and Sherry Li, LBNL)
   - Matlab
   - UMFPACK (Tim Davis, U. of Florida)
   - LUSOL (MINOS, Michael Saunders, Stanford)

2. **Parallel LU**
   - MUMPS (Patrick Amestoy, IRIT)
   - SPOOLES (Cleve Ashcroft, Boeing)
   - SuperLU_Dist (Jim Demmel and Sherry Li, LBNL)

3. **Parallel Cholesky**
   - DSCPACK (Padma Raghavan, Penn. State)
   - MUMPS (Patrick Amestoy, Toulouse)
   - CHOLMOD (Tim Davis, Florida)

4. **XYTlib - parallel direct solver** (Paul Fischer and Henry Tufo, ANL)
Complete table of solvers

1. Parallel ICC
   - BlockSolve95 (Mark Jones and Paul Plassman, ANL)

2. Parallel ILU
   - PaStiX (Faverge Mathieu, INRIA)

3. Parallel Sparse Approximate Inverse
   - Parasails (Hypre, Edmund Chow, LLNL)
   - SPAI 3.0 (Marcus Grote and Barnard, NYU)

4. Sequential Algebraic Multigrid
   - RAMG (John Ruge and Klaus Steuben, GMD)
   - SAMG (Klaus Steuben, GMD)

5. Parallel Algebraic Multigrid
   - Prometheus (Mark Adams, PPPL)
   - BoomerAMG (Hypre, LLNL)
   - ML (Trilinos, Ray Tuminaro and Jonathan Hu, SNL)
Outline

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M. Knepley ()

PETSc

UW '11 77 / 118
Flow Control for a PETSc Application

Main Routine

- Timestepping Solvers (TS)
- Nonlinear Solvers (SNES)
- Linear Solvers (KSP)
- Preconditioners (PC)

Application

- Initialization
- Function Evaluation
- Jacobian Evaluation
- Postprocessing

PETSc
The SNES interface is based upon callback functions

- `FormFunction()`, set by `SNESSetFunction()`
- `FormJacobian()`, set by `SNESSetJacobian()`

When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Solver calls the **user's** function

- User function gets application state through the `ctx` variable
  - PETSc **never** sees application data
Topology Abstractions

- **DA**
  - Abstracts Cartesian grids in any dimension
  - Supports stencils, communication, reordering
  - Nice for simple finite differences

- **Mesh**
  - Abstracts general topology in any dimension
  - Also supports partitioning, distribution, and global orders
  - Allows arbitrary element shapes and discretizations
Assembly Abstractions

- **DM**
  - Abstracts the logic of multilevel (multiphysics) methods
  - Manages allocation and assembly of local and global structures
  - Interfaces to \texttt{DMMG} solver

- **Section**
  - Abstracts functions over a topology
  - Manages allocation and assembly of local and global structures
  - Will merge with \texttt{DM} somehow
User provided function calculates the nonlinear residual:

```c
PetscErrorCode (*func)(SNES snes, Vec x, Vec r, void *ctx)
```

- **x**: The current solution
- **r**: The residual
- **ctx**: The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants
SNES Jacobian

User provided function calculates the Jacobian:

\[(\ast \text{func})(\text{SNES } \text{snes}, \text{Vec } x, \text{Mat } *J, \text{Mat } *M, \text{MatStructure } *\text{flag}, \text{void } *\text{ctx})\]

\[x: \text{ The current solution}\]
\[J: \text{ The Jacobian}\]
\[M: \text{ The Jacobian preconditioning matrix (possibly J itself)}\]
\[ctx: \text{ The user context passed to SNESSetJacobian()}\]

- Use this to pass application information, e.g. physical constants
- Possible MatStructure values are:
  - SAME_NONZERO_PATTERN
  - DIFFERENT_NONZERO_PATTERN

Alternatively, you can use
- matrix-free finite difference approximation, \(-\text{snes_mf}\)
- finite difference approximation with coloring, \(-\text{snes_fd}\)
SNES Variants

- Line search strategies
- Trust region approaches
- Picard iteration
- Variational inequality approaches
PETSc can compute and explicitly store a Jacobian via 1st-order FD

- **Dense**
  - Activated by `-snes_fd`
  - Computed by `SNESDefaultComputeJacobian()`

- **Sparse via colorings**
  - Coloring is created by `MatFDColoringCreate()`
  - Computed by `SNESDefaultComputeJacobianColor()`

Can also use Matrix-free Newton-Krylov via 1st-order FD

- Activated by `-snes_mf` without preconditioning
- Activated by `-snes_mf_operator` with user-defined preconditioning
  - Uses preconditioning matrix from `SNESSetJacobian()`
SNES Example
Driven Cavity

Solution Components

- Velocity-vorticity formulation
- Flow driven by lid and/or bouyancy
- Logically regular grid
  - Parallelized with DA
- Finite difference discretization
- Authored by David Keyes

$\text{PETCS_DIR/src/snes/examples/tutorials/ex19.c}$
typedef struct {
    /*----- basic application data ------*/
    PetscReal lid_velocity;
    PetscReal prandtl;
    PetscReal grashof;
    PetscBool draw_contours;
} AppCtx;

$PETCS_DIR/src/snes/examples/tutorials/ex19.c
Residual(SNES snes, Vec X, Vec F, void *ptr) {
    AppCtx *user = (AppCtx *) ptr;

    /* local starting and ending grid points */
    PetscInt istart, iend, jstart, jend;
    PetscScalar *f; /* local vector data */
    PetscReal grashof = user->grashof;
    PetscReal prandtl = user->prandtl;
    PetscErrorCode ierr;

    /* Code to communicate nonlocal ghost point data */
    VecGetArray(F, &f);
    /* Code to compute local function components */
    VecRestoreArray(F, &f);
    return 0;
}
ResLocal(DALocalInfo *info, 
  PetscScalar **x, PetscScalar **f, void *ctx)
{
  for (j = info->ys; j < info->ys+info->ym; ++j) {
    for (i = info->xs; i < info->xs+info->xm; ++i) {
      u = x[j][i];
      if (i==0 || j==0 || i == M || j == N) {
        f[j][i] = u; continue;
      }
      u_xx = (2.0 *u - x[j][i-1] - x[j][i+1])*hydhx;
      u_yy = (2.0 *u - x[j-1][i] - x[j+1][i])*hxdhy;
      f[j][i] = u_xx + u_yy - hx*hy*lambda*exp(u);
    }
  }
}

$PETCS_DIR/src/snes/examples/tutorials/ex19.c
Outline

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DA is a topology interface on structured grids

- Handles parallel data layout
- Handles local and global indices
  - `DAGetGlobalIndices()` and `DAGetAO()`
- Provides local and global vectors
  - `DAGetGlobalVector()` and `DAGetLocalVector()`
- Handles ghost values coherence
  - `DAGetGlobalToLocal()` and `DAGetLocalToGlobal()`
The DA interface is based upon *local* callback functions

- `FormFunctionLocal()`, set by `DASetLocalFunction()`
- `FormJacobianLocal()`, set by `DASetLocalJacobian()`

When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Each process evaluates the local residual
- PETSc assembles the global residual automatically
  - *Uses* `DALocalToGlobal()` method
Ghost Values

To evaluate a local function $f(x)$, each process requires
- its local portion of the vector $x$
- its **ghost values**, bordering portions of $x$ owned by neighboring processes

![Diagram showing local and ghost nodes](image)
### DA Global Numberings

<table>
<thead>
<tr>
<th>Proc 2</th>
<th>Proc 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 26 27</td>
<td>28 29</td>
</tr>
<tr>
<td>20 21 22</td>
<td>23 24</td>
</tr>
<tr>
<td>15 16 17</td>
<td>18 19</td>
</tr>
<tr>
<td>10 11 12</td>
<td>13 14</td>
</tr>
<tr>
<td>5 6 7</td>
<td>8 9</td>
</tr>
<tr>
<td>0 1 2</td>
<td>3 4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Proc 0</th>
<th>Proc 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural numbering</td>
<td></td>
</tr>
</tbody>
</table>

### PETSc numbering

<table>
<thead>
<tr>
<th>Proc 2</th>
<th>Proc 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>21 22 23</td>
<td>28 29</td>
</tr>
<tr>
<td>18 19 20</td>
<td>26 27</td>
</tr>
<tr>
<td>15 16 17</td>
<td>24 25</td>
</tr>
<tr>
<td>6 7 8</td>
<td>13 14</td>
</tr>
<tr>
<td>3 4 5</td>
<td>11 12</td>
</tr>
<tr>
<td>0 1 2</td>
<td>9 10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Proc 0</th>
<th>Proc 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETSc numbering</td>
<td></td>
</tr>
</tbody>
</table>
**Global**: Each vertex has a unique id belongs on a unique process

**Local**: Numbering includes vertices from neighboring processes

These are called *ghost* vertices
The user provided function which calculates the nonlinear residual in 2D has signature

\[(\text{DA}\text{LocalInfo} \ \text{info}, \ \text{PetscScalar} \ **x, \ \text{PetscScalar} \ **r, \ \text{void} \ *\text{ctx})\]

- \textbf{info}: All layout and numbering information
- \textbf{x}: The current solution
  - Notice that it is a multidimensional array
- \textbf{r}: The residual
- \textbf{ctx}: The user context passed to \texttt{DASetLocalFunction()}

The local DA function is activated by calling

\texttt{SNESSetFunction(snes, r, SNESDADAFormFunction, ctx)}
\[ \Delta u + \lambda e^u = 0 \]

\[
\text{ResLocal}(\text{DAInfo} \ast \text{info}, \\
\text{PetscScalar} \ast \ast \text{x}, \text{PetscScalar} \ast \ast \text{f}, \text{void} \ast \text{ctx}) \\
\{
\text{for} (j = \text{info->ys}; j < \text{info->ys+info->ym}; ++j) \{ \\
\text{for} (i = \text{info->xs}; i < \text{info->xs+info->xm}; ++i) \{ \\
\text{u} = \text{x}[j][i]; \\
\text{if} \ (i==0 \ || \ j==0 \ || \ i == \text{M} \ || \ j == \text{N}) \{ \\
\text{f}[j][i] = \text{u}; \text{ continue}; \\
\}
\text{u} \_\text{xx} = (2.0 \ast \text{u} - \text{x}[j][i-1] - \text{x}[j][i+1]) \ast \text{hydhx}; \\
\text{u} \_\text{yy} = (2.0 \ast \text{u} - \text{x}[j-1][i] - \text{x}[j+1][i]) \ast \text{hxdhy}; \\
\text{f}[j][i] = \text{u} \_\text{xx} + \text{u} \_\text{yy} - \text{hx} \ast \text{hy} \ast \text{lambda} \ast \exp(\text{u}); \\
\}
\}
\]

$\text{PETCS_DIR/src/snes/examples/tutorials/ex5.c$
The user provided function which calculates the Jacobian in 2D has signature

\((*lfunc)(DA\text{LocalInfo} \,*info, \, \text{PetscScalar} \, **x, \, \text{Mat} \, J, \, \text{void} \, *ctx)\)

- **info**: All layout and numbering information
- **x**: The current solution
- **J**: The Jacobian
- **ctx**: The user context passed to \text{DASetLocalJacobian}()

The local DA function is activated by calling

\text{SNESSetJacobian}(\text{snes}, \, J, \, J, \, \text{SNESDADebugComputeJacobian}, \, \text{ctx})
Bratu Jacobian Evaluation

JacLocal(DALocalInfo *info, PetscScalar **x, Mat jac, void *ctx) {
    for (j = info->ys; j < info->ys + info->ym; j++) {
        for (i = info->xs; i < info->xs + info->xm; i++) {
            row.j = j; row.i = i;
            if (i == 0 || j == 0 || i == mx-1 || j == my-1) {
                v[0] = 1.0;
                MatSetValuesStencil(jac, 1, &row, 1, &row, v, INSERT_VALUES);
            } else {
                v[0] = -(hx/hy); col[0].j = j-1; col[0].i = i;
                v[1] = -(hy/hx); col[1].j = j; col[1].i = i-1;
                v[2] = 2.0*(hy/hx+hx/hy)
                    - hx*hy*lambda*PetscExpScalar(x[j][i]);
                v[3] = -(hy/hx); col[3].j = j; col[3].i = i+1;
                v[4] = -(hx/hy); col[4].j = j+1; col[4].i = i;
                MatSetValuesStencil(jac, 1, &row, 5, col, v, INSERT_VALUES);
            }
        }
    }
}
A DA is more than a Mesh

A DA contains topology, geometry, and an implicit Q1 discretization. It is used as a template to create
- Vectors (functions)
- Matrices (linear operators)
The DA object contains only layout (topology) information
- All field data is contained in PETSc Vecs

Global vectors are parallel
- Each process stores a unique local portion
- DACreateGlobalVector(DA da, Vec *gvec)

Local vectors are sequential (and usually temporary)
- Each process stores its local portion plus ghost values
- DACreateLocalVector(DA da, Vec *lvec)
- includes ghost values!
Updating Ghosts

Two-step process enables overlapping computation and communication

- DAGlobalToLocalBegin(da, gvec, mode, lvec)
  - gvec provides the data
  - mode is either INSERT_VALUES or ADD_VALUES
  - lvec holds the local and ghost values

- DAGlobalToLocalEnd(da, gvec, mode, lvec)
  - Finishes the communication

The process can be reversed with DALocalToGlobal().
Both the box stencil and star stencil are available.

Box Stencil

Star Stencil
PETSc provides

\[ \text{MatSetValuesStencil} \left( \text{Mat} \ A, \ m, \ \text{MatStencil} \ \text{idxm}[], \ n, \ \text{MatStencil} \ \text{idxn}[], \ \text{PetscScalar} \ \text{values}[], \ \text{InsertMode} \ \text{mode} \right) \]

- Each row or column is actually a \text{MatStencil}
  - This specifies grid coordinates and a component if necessary
  - Can imagine for unstructured grids, they are \textit{vertices}
- The values are the same logically dense block in row/col
Creating a DA

```
DACreate2d(comm, wrap, type, M, N, m, n, dof, s, lm[], ln[], DA *da)
```

**wrap**: Specifies periodicity
- DA_NONPERIODIC, DA_XPERIODIC, DA_YPERIODIC, or DA_XYPERIODIC

**type**: Specifies stencil
- DA_STENCIL_BOX or DA_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

**lm/n**: Alternative array of local sizes
- Use PETSC_NULL for the default
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MultiPhysics Paradigm

The **PCFieldSplit** interface

- extracts functions/operators corresponding to each physics
  - *VecScatter* and *MatGetSubMatrix()* for efficiency
- assemble functions/operators over all physics
  - Generalizes *LocalToGlobal()* mapping
- is composable with **ANY** PETSc solver and preconditioner
  - This can be done recursively
The **PCFieldSplit** interface

- extracts functions/operators corresponding to each physics
  - `VecScatter` and `MatGetSubMatrix()` for efficiency

- assemble functions/operators over all physics
  - Generalizes `LocalToGlobal()` mapping

- is composable with **ANY** PETSc solver and preconditioner
  - This can be done recursively

FieldSplit provides the **buildings blocks** for multiphysics preconditioning.
MultiPhysics Paradigm

The **PCFieldSplit** interface

- extracts functions/operators corresponding to each physics
  - *VecScatter* and *MatGetSubMatrix()* for efficiency

- assemble functions/operators over all physics
  - Generalizes *LocalToGlobal()* mapping

- is composable with ANY PETSc solver and preconditioner
  - This can be done recursively

Notice that this works in exactly the same manner as

- multiple resolutions (MG, FMM, Wavelets)

- multiple domains (Domain Decomposition)

- multiple dimensions (ADI)
Preconditioning

Several varieties of preconditioners can be supported:

- Block Jacobi or Block Gauss-Siedel
- Schur complement
- Block ILU (approximate coupling and Schur complement)
- Dave May’s implementation of Elman-Wathen type PCs which only require actions of individual operator blocks

Notice also that we may have any combination of

- “canned” PCs (ILU, AMG)
- PCs needing special information (MG, FMM)
- custom PCs (physics-based preconditioning, Born approximation)

since we have access to an algebraic interface
Outline

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Thrust is a CUDA library of parallel algorithms

- Interface similar to C++ Standard Template Library
- Containers (vector) on both host and device
- Algorithms: sort, reduce, scan
- Freely available, part of PETSc configure (-with-thrust-dir)
Cusp is a CUDA library for sparse linear algebra and graph computations

- Builds on data structures in Thrust
- Provides sparse matrices in several formats (CSR, Hybrid)
- Includes some preliminary preconditioners (Jacobi, SA-AMG)
- Freely available, part of PETSc configure \(-\text{with-cusp-dir}\)
Strategy: Define a new `Vec` implementation

- Uses **Thrust** for data storage and operations on GPU
- Supports full PETSc `Vec` interface
- Inherits PETSc scalar type
- Can be activated at runtime, `-vec_type cuda`
- PETSc provides memory coherence mechanism
PETSc Objects now hold a coherence flag

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETSC_CUDA_UNALLOCATED</td>
<td>No allocation on the GPU</td>
</tr>
<tr>
<td>PETSC_CUDA_GPU</td>
<td>Values on GPU are current</td>
</tr>
<tr>
<td>PETSC_CUDA_CPU</td>
<td>Values on CPU are current</td>
</tr>
<tr>
<td>PETSC_CUDA_BOTH</td>
<td>Values on both are current</td>
</tr>
</tbody>
</table>

**Table:** Flags used to indicate the memory state of a PETSc CUDA Vec object.
Also define new `Mat` implementations

- Uses `Cusp` for data storage and operations on GPU
- Supports full PETSc `Mat` interface, some ops on CPU
- Can be activated at runtime, `-mat_type aijcuda`
- Notice that parallel matvec necessitates off-GPU data transfer
Solvers come for Free

- All linear algebra types work with solvers
- Entire solve can take place on the GPU
  - Only communicate scalars back to CPU
- GPU communication cost could be amortized over several solves
- Preconditioners are a problem
  - Cusp has a promising AMG
PETSc only needs

# Turn on CUDA
--with-cuda

# Specify the CUDA compiler
--with-cudac='nvcc -m64'

# Indicate the location of packages
# --download-* will also work soon
--with-thrust-dir=/PETSc3/multicore/thrust
--with-cusp-dir=/PETSc3/multicore/cusp

# Can also use double precision
--with-precision=single
Example
Driven Cavity Velocity-Vorticity with Multigrid

```
ex19 -da_vec_type seqcuda -da_mat_type aijcuda -mat_no_inode -da_grid_x 100 -da_grid_y 100 -pc_type none -dmmg_nlevels 1 -preload off -cuda_synchronize -log_summary
```

# Setup types
# Set grid size
# Setup solver
# Setup run
### Flow Solver

32 × 32 × 32 grid

<table>
<thead>
<tr>
<th>Routine</th>
<th>Time (s)</th>
<th>MFlops</th>
<th>MFlops/s</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CPU</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>KSPSolve</td>
<td>8.3167</td>
<td>4370</td>
<td>526</td>
</tr>
<tr>
<td>MatMult</td>
<td>1.5031</td>
<td>769</td>
<td>512</td>
</tr>
<tr>
<td><strong>GPU</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>KSPSolve</td>
<td>1.6382</td>
<td>4500</td>
<td>2745</td>
</tr>
<tr>
<td>MatMult</td>
<td>0.3554</td>
<td>830</td>
<td>2337</td>
</tr>
</tbody>
</table>

P. Lichtner, G. Hammond, R. Mills, B. Phillip