The
Portable **E**xtensible **T**oolkit for **S**cientific **C**omputing

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Argonne National Laboratory

Computation Institute
University of Chicago

PETSc Tutorial
Jackson School of Geosciences
University of Texas at Austin, TX September 7, 2011

Outline

Outline

Unit Objectives

- Introduce PETSc
- Download, Configure, Build, and Run an Example
- Empower students to learn more about PETSc

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
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Tutorial Repositories

http://petsc.cs.iit.edu/petsc/tutorials/SimpleTutorial

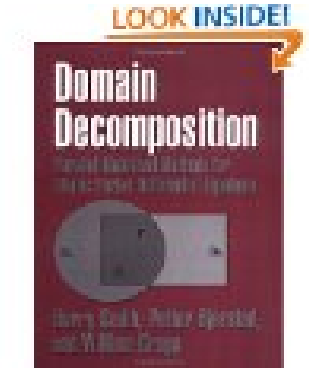
- Very simple
- Shows how to create your own project
- Uses multiple languages

How did PETSc Originate?

PETSc was developed as a Platform for Experimentation

We want to experiment with different

- Models
- Discretizations
- Solvers
- Algorithms
  - which blur these boundaries



The Role of PETSc

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?

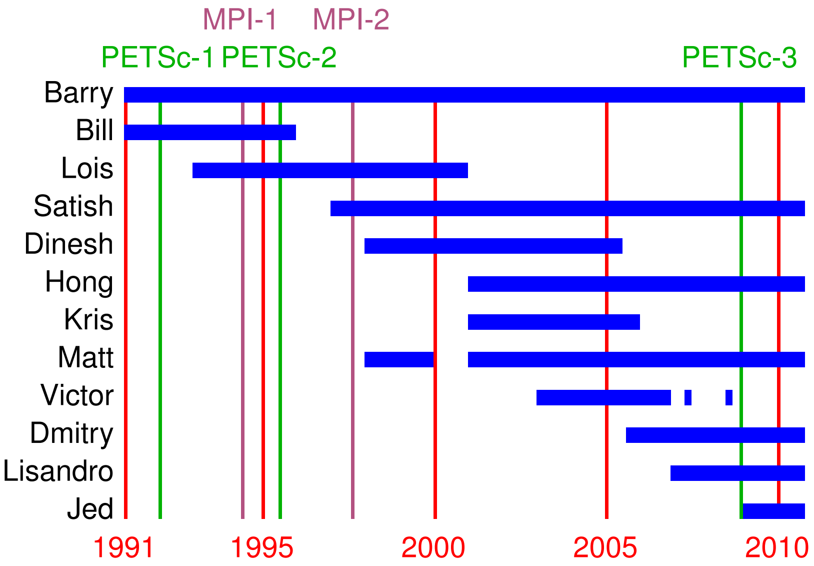
A freely available and supported research code

- 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


MPI-1
MPI-2
PETSc-1
PETSc-2
PETSc-3
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed
1991
1995
2000
2005
2010

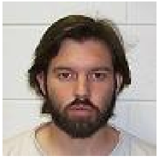
The PETSc Team

Bill Gropp

Barry Smith

Satish Balay

Jed Brown


Matt Knepley

Lisandro Dalcin

Hong Zhang

Victor Eijkhout

Dmitry Karpeev

Outline

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

Who Uses PETSc?

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
- Other Solvers
  - Fast Multipole Method (PetFMM)
  - Radial Basis Function Interpolation (PetRBF)
  - Eigensolvers (SLEPc)
  - Optimization (TAO)

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 290,000 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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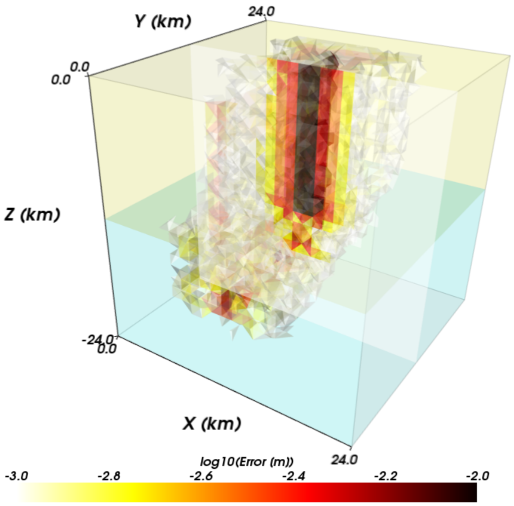
PyLith

- Multiple problems
  - Dynamic rupture
  - Quasi-static relaxation
- Multiple models
  - Nonlinear visco-plastic
  - Finite deformation
  - Fault constitutive models
- Multiple meshes
  - 1D, 2D, 3D
  - Hex and tet meshes
- Parallel
  - PETSc solvers
  - Sieve mesh management

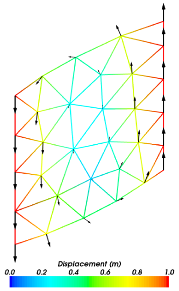


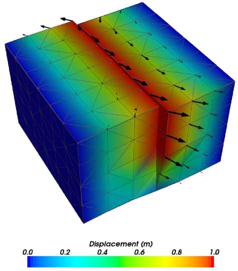
[a]

[a]Aagaard, Knepley, Williams

Multiple Mesh Types

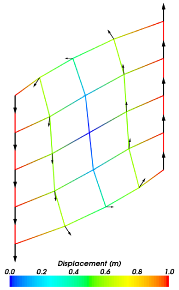
Triangular

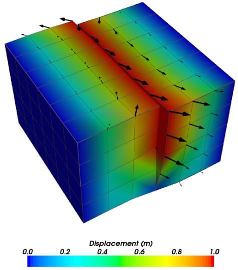




Tetrahedral

Rectangular

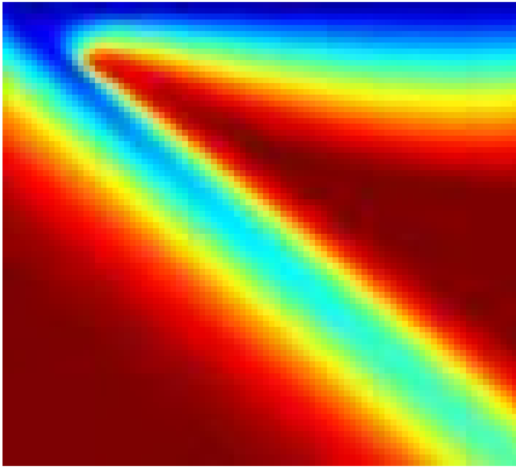




Hexahedral

Magma Dynamics

- Couples scales
  - Subduction
  - Magma Migration
- Physics
  - Incompressible fluid
  - Porous solid
  - Variable porosity
- Deforming matrix
  - Compaction pressure
- Code generation
  - FEniCS
- Multiphysics Preconditioning
  - PETSc FieldSplit



[a]Katz, Speigelman

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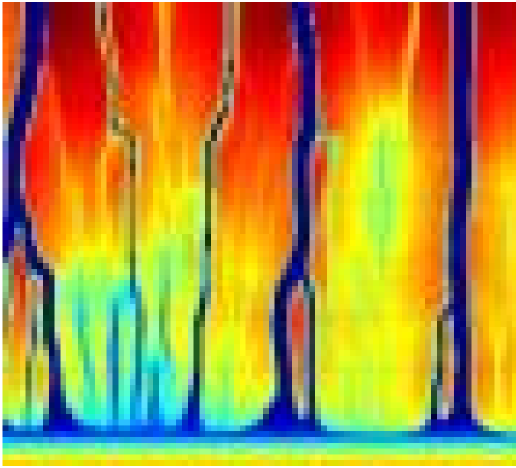
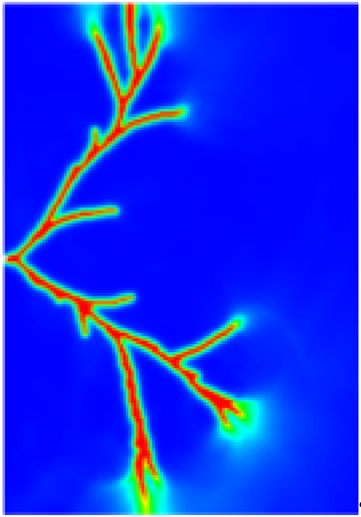


[a]Katz, Speigelman

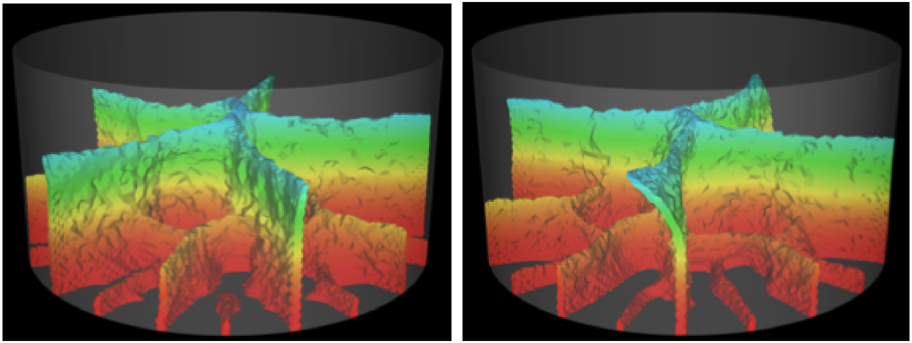
Fracture Mechanics

- Full variational formulation
  - Phase field
  - Linear or Quadratic penalty
- Uses TAO optimization
  - Necessary for linear penalty
  - Backtacking
- No prescribed cracks
  - Arbitrary crack geometry
  - Arbitrary intersections
- Multiple materials
  - Composite toughness

[a]

[a]Bourdin

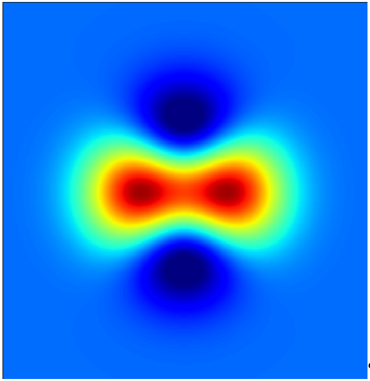
Fracture Mechanics


[1]

[1] Bourdin

Vortex Method
t = 000

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
  - Automatic load balancing
  - Variety of kernels
  - Optimized with templates
- PetRBF
  - Variety of RBFs
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU

[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method
t = 100

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
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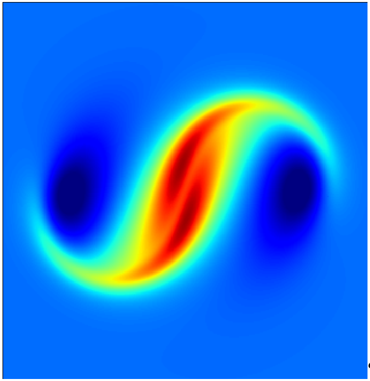[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method
t = 200

- Incompressible Flow
  - Gaussian vortex blobs
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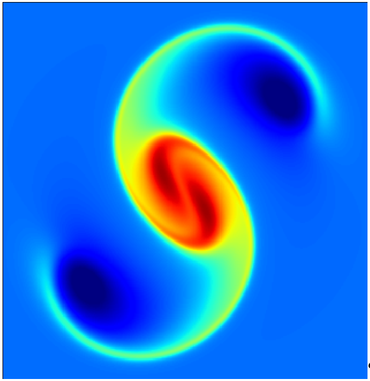[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 300

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
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  - Variety of kernels
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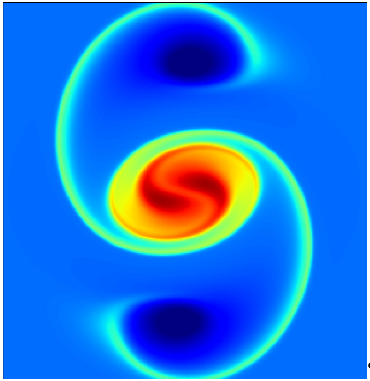
[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 400

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
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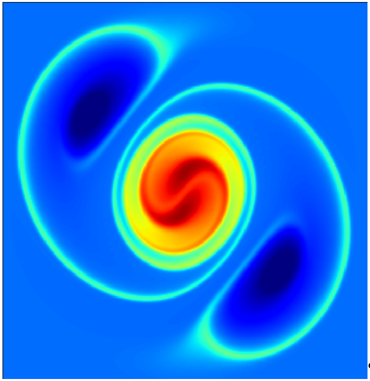[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 500

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
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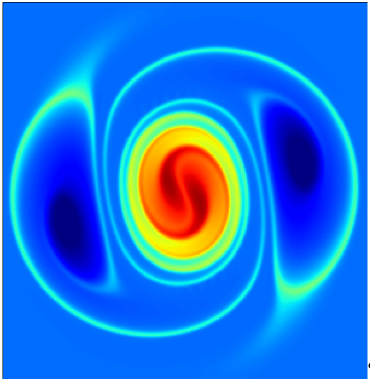
[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 600

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
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  - Automatic load balancing
  - Variety of kernels
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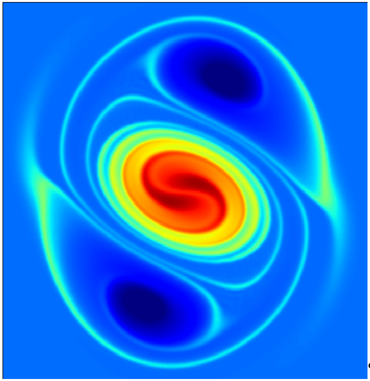[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 700

- Incompressible Flow
  - Gaussian vortex blobs
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- PetFMM
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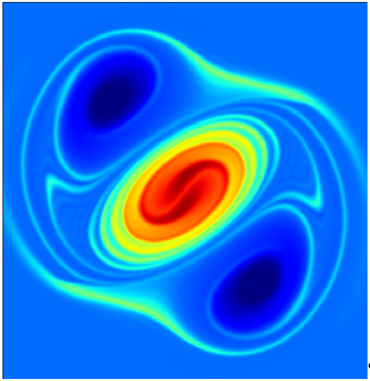
[a]

[a]Cruz, Yokota, Barba, Knepley

Vortex Method
t = 800

- Incompressible Flow
  - Gaussian vortex blobs
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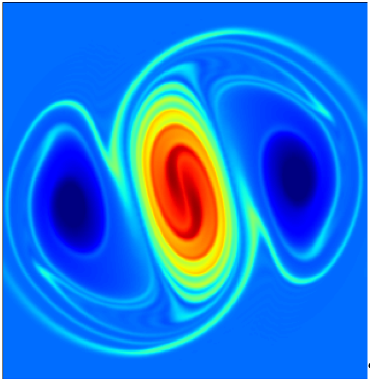
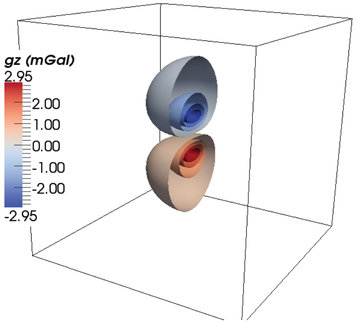

[a]

[a] Cruz, Yokota, Barba, Knepley

Gravity Anomaly Modeling

- Potential Solution
  - Kernel of inverse problem
  - Needs optimal algorithm
- Implementations
  - Direct Summation
  - FEM
  - FMM
- Parallelism
  - MPI
  - 4000+ cores
  - All methods scalable

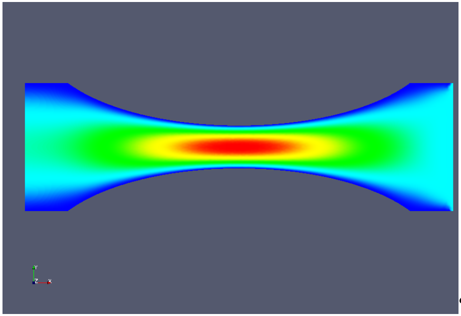


[a]

[a]May, Knepley

FEniCS-Apps
Rheagen

- Rheologies
  - Maxwell
  - Grade 2
  - Oldroyd-B
- Stabilization
  - DG
  - SUPG
  - EVSS
  - DEVSS
  - Macroelement
- Automation
  - FIAT (elements)
  - FFC (weak forms)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[a] Terrel

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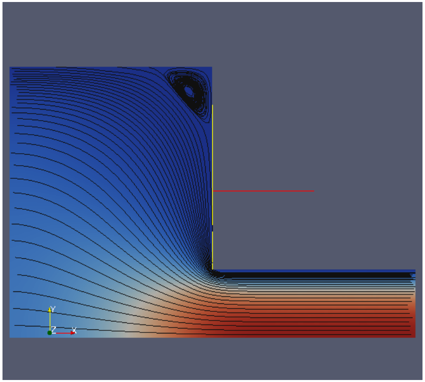
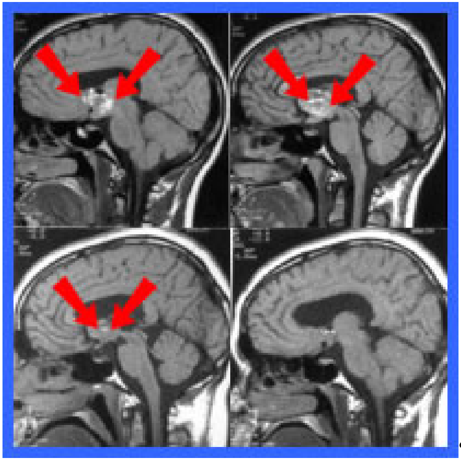


Real-time Surgery

- Brain Surgery
  - Elastic deformation
  - Overlaid on MRI
  - Guides surgeon
- Laser Thermal Therapy
  - PDE constrained optimization
  - Per-patient calibration
  - Thermal inverse problem


[a]

[a]Warfield, Ferrant, et.al.

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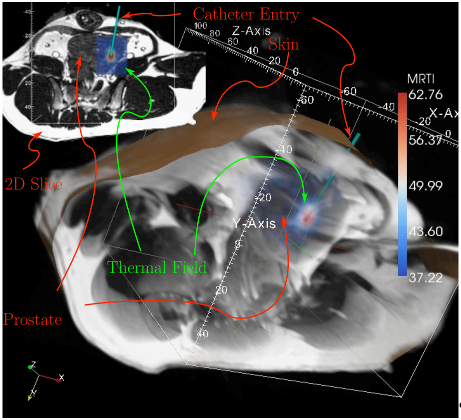


[a]

[a]Fuentes, Oden, et.al.

Outline

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`

Outline

Downloading PETSc

- The latest tarball is on the PETSc site
  - ftp://ftp.mcs.anl.gov/pub/petsc/petsc.tar.gz
  - 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

Unpacking PETSc

- Just clone development repository
  - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
  - `hg clone -rrelease-3.2 petsc-dev petsc-3.2`

or

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

Exercise 1

Download and Unpack PETSc!

Outline

Configuring PETSc

- 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

Configuring PETSc

- You can easily reconfigure with the same options
  - `./$PETSC_ARCH/conf/reconfigure-$PETSC_ARCH.py`
- Can maintain several different configurations
  - `./configure -PETSC_ARCH=linux-fast -with-debugging=0`
- All configuration information is in the logfile
  - `./$PETSC_ARCH/conf/configure.log`
  - ALWAYS send this file with bug reports

Configuring PETSc for Unstructured Meshes

- `-with-clanguage=cxx`
- `-with-shared-libraries -with-dynamic-loading`
- `-download-f-blas-lapack -download-mpich`
- `-download-boost -download-fiat -download-generator`
- `-download-triangle -download-tetgen`
- `-download-chaco -download-parmetis -download-zoltan`
- `-with-sieve`

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.

Outline

Building PETSc

There are three valid ways to build PETSc:

- Using recursive make starting in `cd $PETSC_DIR`
  - `make`
  - `make install` if you configured with `--prefix`
  - Check build when done with `make test`
- Using CMake
  - Same `make`, `make install`, `make test`
  - Automatically enabled if CMake is found by configure
  - Handles dependencies
- Experimental Python build
- `python ./config/builder2.py -help` for Python 2.7
- `./config/builder.py` for older Python
- Handles dependencies

Building PETSc

- Can build multiple configurations
  - `PETSC_ARCH=linux-fast make`
  - Libraries are in `$PETSC_DIR/$PETSC_ARCH/lib/`
- Complete log for each build is in logfile `./$PETSC_ARCH/conf/make.log`
  - ALWAYS send this with bug reports
- (Deprecated) Can also build a subtree with recursive make
  - `cd src/snes; make`
  - `cd src/snes; make ACTION=libfast tree`

Exercise 3

Build your configured PETSc.

Exercise 4

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`

Outline

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`

Running PETSc with Python

- Can run any PETSc example
  - `python ./config/builder2.py check $PETSC_DIR/src/snes/examples/tutorials/ex5.c`
- Checks against test output
  - Ignores if no output is present
- Can specify multiple files
  - `python ./config/builder2.py check [$PETSC_DIR/src/snes/examples/tutorials/ex5.c,extraF`
- Can also run using MPI directly
  - Use `-retain` to keep executable
  - `mpiexec ./$PETSC_ARCH/lib/lib-ex5/ex5 -snes_monitor`

Using MPI

- 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

MPI Concepts

- Communicator
  - A context (or scope) for parallel communication (“Who can I talk to”)
  - There are two defaults:
    - yourself (PETSC_COMM_SELF),
    - and everyone launched (PETSC_COMM_WORLD)
  - Can create new communicators by splitting existing ones
  - Every PETSc object has a communicator
  - Set PETSC_COMM_WORLD to put all of PETSc in a subcomm
- Point-to-point communication
  - Happens between two processes (like in `MatMult()`)
- Reduction or scan operations
  - Happens among all processes (like in `VecDot()`)

Alternative Memory Models

- Single process (address space) model
  - OpenMP and threads in general
  - Fortran 90/95 and compiler-discovered parallelism
  - System manages memory and (usually) thread scheduling
  - Named variables refer to the same storage
- Single name space model
  - HPF, UPC
  - Global Arrays
  - Titanium
  - Variables refer to the coherent values (distribution is automatic)
- Distributed memory (shared nothing)
  - Message passing
  - Names variables in different processes are unrelated

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
  - `-ksp_monitor`, graphically `-ksp_monitor_draw`
- Can disable dynamically
  - `-ksp_monitors_cancel`
- Does not display subsolvers
  - `-snes_monitor`
- Can use the true residual
  - `-ksp_monitor_true_residual`
- Can display different subobjects
  - `-snes_monitor_residual`, `-snes_monitor_solution`, `-snes_monitor_solution_update`
  - `-snes_monitor_range`
  - `-ksp_gmres_krylov_monitor`
- Can display the spectrum
  - `-ksp_monitor_singular_value`

Exercise 5

Run SNES Example 5 using come 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
```

Outline

Getting More Help

- http://www.mcs.anl.gov/petsc
- Hyperlinked documentation
  - Manual
  - Manual pages for evey 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

Outline

Application Integration

- Be willing to experiment with algorithms
  - No optimality without interplay between physics and algorithmics
- Adopt flexible, extensible programming
  - Algorithms and data structures not hardwired
- Be willing to play with the real code
  - Toy models are rarely helpful
- If possible, profile before integration
  - Automatic in PETSc

PETSc Integration

PETSc is a set a library interfaces

- We do not seize `main()`
- We do not control output
- We propagate errors from underlying packages
- We present the same interfaces in:
    - C
    - C++
    - F77
    - F90
    - Python

See Gropp in SIAM, OO Methods for Interop SciEng, '99

Integration Stages

- Version Control
  - It is impossible to overemphasize
  - We use Mercurial
- Initialization
  - Linking to PETSc
- Profiling
  - Profile before changing
  - Also incorporate command line processing
- Linear Algebra
  - First PETSc data structures
- Solvers
  - Very easy after linear algebra is integrated

Initialization

- Call `PetscInitialize()`
  - Setup static data and services
  - Setup MPI if it is not already
- Call `PetscFinalize()`
  - Calculates logging summary
  - Shutdown and release resources
- Checks compile and link

Profiling

- Use `-log_summary` for a performance profile
    - Event timing
    - Event flops
    - Memory usage
    - MPI messages
- Call `PetscLogStagePush()` and `PetscLogStagePop()`
    - User can add new stages
- Call `PetscLogEventBegin()` and `PetscLogEventEnd()`
    - User can add new events

Command Line Processing

- Check for an option
  - `PetscOptionsHasName()`
- Retrieve a value
  - `PetscOptionsGetInt()`, `PetscOptionsGetIntArray()`
- Set a value
  - `PetscOptionsSetValue()`
- Check for unused options
  - `-options_left`
- Clear, alias, reject, etc.
- Modern form uses
  - `PetscOptionsBegin()`, `PetscOptionsEnd()`
  - `PetscOptionsInt()`,`PetscOptionsReal()`
  - Integrates with `-help`

Outline

Vector Algebra

What are PETSc vectors?

- Fundamental objects representing
  - solutions
  - right-hand sides
  - coefficients
- Each process locally owns a subvector of contiguous global data

Vector Algebra

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

Vector Algebra

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**)

Parallel Assembly
Vectors and Matrices

- 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

Vector Assembly

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

```
VecSetValues(Vec v, PetscInt n, PetscInt rows[],
             PetscScalar values[], InsertMode mode)
```

- Mode is either `INSERT_VALUES` or `ADD_VALUES`
- Two phases allow overlap of communication and computation
  - `VecAssemblyBegin(Vec v)`
  - `VecAssemblyEnd(Vec v)`

One Way to Set the Elements of a Vector

```
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);
```

A Better Way to Set the Elements of a Vector

```
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

Function Name	Operation
VecAXPY(Vec y, PetscScalar a, Vec x)	$y = y + a * x$
VecAYPX(Vec y, PetscScalar a, Vec x)	$y = x + a * y$
VecWAYPX(Vec w, PetscScalar a, Vec x, Vec y)	$w = y + a * x$
VecScale(Vec x, PetscScalar a)	$x = a * x$
VecCopy(Vec y, Vec x)	$y = x$
VecPointwiseMult(Vec w, Vec x, Vec y)	$w_i = x_i * y_i$
VecMax(Vec x, PetscInt *idx, PetscScalar *r)	$r = \max r_i$
VecShift(Vec x, PetscScalar r)	$x_i = x_i + r$
VecAbs(Vec x)	$x_i = \|x_i\|$
VecNorm(Vec x, NormType type, PetscReal *r)	$r = \|\|x\|\|$

Working With Local Vectors

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

VecGetArray in C

```
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);
```

VecGetArray in F77

```
#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)
```

VecGetArray in F90

```
#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)
```

VecGetArray in Python

```
with v as a:
  for i in range(len(a)):
    a[i] = 5.0*i
```

Outline

Matrix Algebra

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

Matrix Polymorphism

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
- `MatSetValues(Mat m, m, rows[], n, cols[], values[], mode)`
  - `mode` is either `INSERT_VALUES` or `ADD_VALUES`
  - Logically dense block of values
- Two phase assembly allows overlap of communication and computation
  - `MatAssemblyBegin(Mat m, MatAssemblyType type)`
  - `MatAssemblyEnd(Mat m, MatAssemblyType type)`
  - `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; v[1] = 2.0; v[2] = -1.0;
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_VA
    } 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);
```

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

```
v[0] = -1.0; v[1] = 2.0; 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_VALU
  } 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);
```

Why Are PETSc Matrices That Way?

- 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

Experimentation is Essential!

Proof is not currently enough to examine solvers

- N. M. Nachtigal, S. C. Reddy, and L. N. Trefethen, *How fast are nonsymmetric matrix iterations?*, SIAM J. Matrix Anal. Appl., **13**, pp.778–795, 1992.
- Anne Greenbaum, Vlastimil Ptak, and Zdenek Strakos, *Any Nonincreasing Convergence Curve is Possible for GMRES*, SIAM J. Matrix Anal. Appl., **17** (3), pp.465–469, 1996.

Solver Types

- **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

Linear Solvers
Krylov Methods

- 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` bicgstab

Nonlinear Solvers
Newton and Picard Methods

- 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`

Basic Solver Usage

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)

3rd Party Preconditioners in PETSc

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

Higher Level Abstractions

The PETSc `DA` class is a topology and discretization interface.

- Structured grid interface
  - Fixed simple topology
- Supports stencils, communication, reordering
  - Limited idea of operators
- Nice for simple finite differences

The PETSc `Mesh` class is a topology interface.

- Unstructured grid interface
  - Arbitrary topology and element shape
- Supports partitioning, distribution, and global orders

Higher Level Abstractions

The PETSc `DM` class is a hierarchy interface.

- Supports multigrid
  - `PCMG` combines it with a multigrid preconditioner
- Abstracts the logic of multilevel methods

The `PetscSection` class is a helper class for data layout.

- Functions over unstructured grids
  - Arbitrary layout of degrees of freedom
- Enables distribution and assembly

3 Ways To Use PETSc

User manages all topology (just use `Vec` and `Mat`)

- All indexing is user managed

PETSc manages single topology (use `DM`)

- `DMDA` manages structured grids using (i, j, k) indexing
- `DMMesh` manages unstructured grids using `PetscSection` for indexing
- Communication is setup automatically
- Use `KSPSetDM()` and `SNESSetDM()` to notify solver

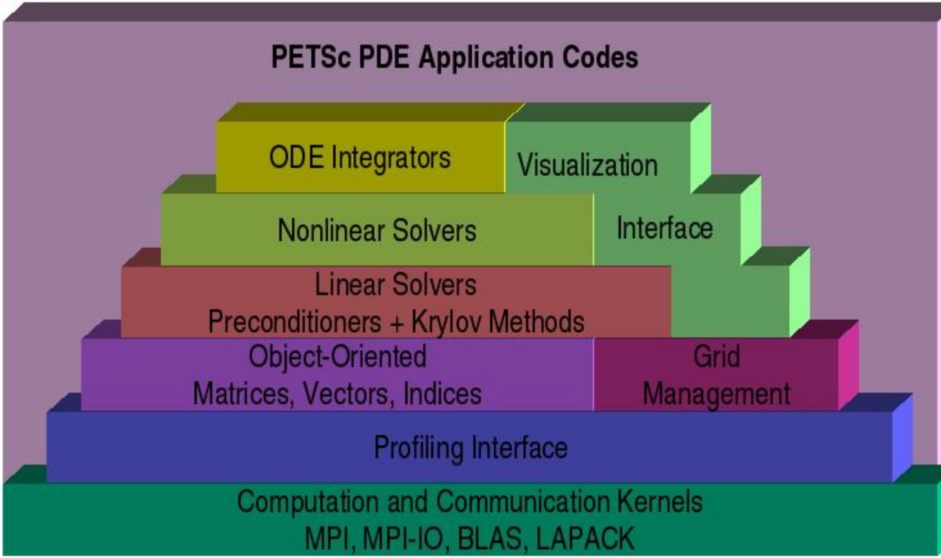
PETSc manages a hierarchy (use `PCMG`)

- Only automated for `DMDA`

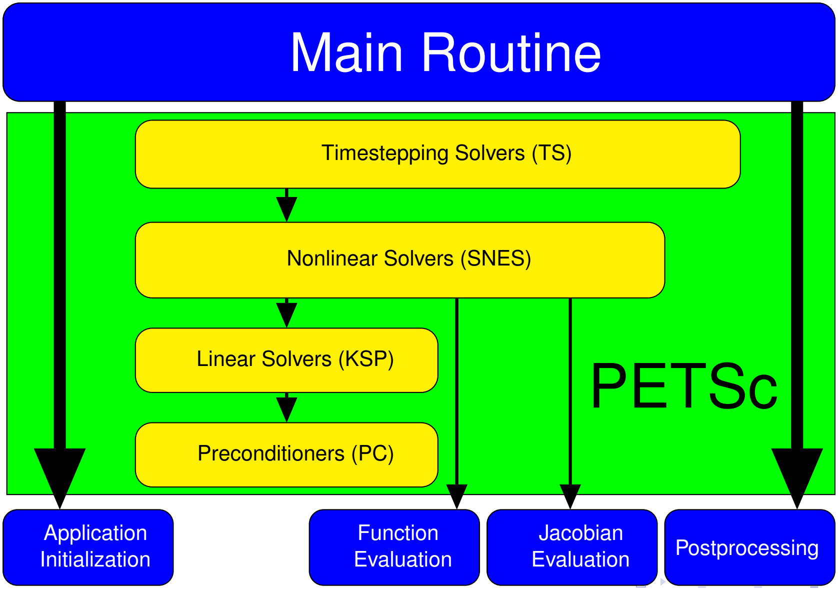
Outline

Outline

PETSc Structure


PETSc PDE Application Codes
ODE Integrators
Visualization
Nonlinear Solvers
Interface
Linear Solvers
Preconditioners + Krylov Methods
Object-Oriented
Matrices, Vectors, Indices
Grid
Management
Profiling Interface
Computation and Communication Kernels
MPI, MPI-IO, BLAS, LAPACK

Flow Control for a PETSc Application



Levels of Abstraction
In Mathematical Software

- Application-specific interface
  - Programmer manipulates objects associated with the application
- High-level mathematics interface
  - Programmer manipulates mathematical objects
    - Weak forms, boundary conditions, meshes
- Algorithmic and discrete mathematics interface
  - Programmer manipulates mathematical objects
    - Sparse matrices, nonlinear equations
  - Programmer manipulates algorithmic objects
    - Solvers
- Low-level computational kernels
  - BLAS-type operations, FFT

Object-Oriented Design

- Design based on operations you perform,
    - rather than the data in the object
- Example: A vector is
    - not a 1d array of numbers
    - an object allowing addition and scalar multiplication
- The efficient use of the computer is an added difficulty
    - which often leads to code generation

What is not in PETSc?

- ~~Unstructured mesh generation and manipulation~~
  - In 3.2, we have `DMMesh` objects
- Discretizations
  - In 3.2, we have an interface to FIAT
  - DealII
- Higher level representations of PDEs
  - FEniCS (FFC/Syfi) and Sundance
- Load balancing
  - Interface to Zoltan
- Sophisticated visualization capabilities
  - Interface to MayaVi2 and Paraview through VTK
- Eigenvalues
  - SLEPc and BLOPEX
- Optimization and sensitivity
  - TAO

Outline

Correctness Debugging

- Automatic generation of tracebacks
- Detecting memory corruption and leaks
- Optional user-defined error handlers

Interacting with the Debugger

- Launch the debugger
  - `-start_in_debugger [gdb,dbx,noxterm]`
  - `-on_error_attach_debugger [gdb,dbx,noxterm]`
- Attach the debugger only to some parallel processes
  - `-debugger_nodes 0,1`
- Set the display (often necessary on a cluster)
  - `-display khan.mcs.anl.gov:0.0`

Debugging Tips

- Put a breakpoint in `PetscError()` to catch errors as they occur
- PETSc tracks memory overwrites at both ends of arrays
  - The `CHKMEMQ` macro causes a check of all allocated memory
  - Track memory overwrites by bracketing them with `CHKMEMQ`
- PETSc checks for leaked memory
  - Use `PetscMalloc()` and `PetscFree()` for all allocation
  - Print unfreed memory on `PetscFinalize()` with `-malloc_dump`
- Simply the best tool today is valgrind
  - It checks memory access, cache performance, memory usage, etc.
  - http://www.valgrind.org
  - Need `-trace-children=yes` when running under MPI

Exercise 7

Use the debugger to find a SEGV
Locate a memory overwrite using CHKMEMQ.

- Get the example
  - `hg clone -r1 http://petsc.cs.iit.edu/petsc/SimpleTutorial`
- Build the example `make`
- Run it and watch the fireworks
  - `mpiexec -n 2 ./bin/ex5 -use_coords`
- Run it under the debugger and correct the error
  - `mpiexec -n 2 ./bin/ex5 -use_coords -start_in_debugger -display :0.0`
  - `hg update -r2`
- Build it and run again smoothly

Outline

Performance Debugging

- PETSc has integrated profiling
    - Option `-log_summary` prints a report on `PetscFinalize()`
- PETSc allows user-defined events
    - Events report time, calls, flops, communication, etc.
    - Memory usage is tracked by object
- Profiling is separated into stages
    - Event statistics are aggregated by stage

Using Stages and Events

- Use `PetscLogStageRegister()` to create a new stage
  - Stages are identifier by an integer handle
- Use `PetscLogStagePush/Pop()` to manage stages
  - Stages may be nested, but will not aggregate in a nested fashion
- Use `PetscLogEventRegister()` to create a new stage
  - Events also have an associated class
- Use `PetscLogEventBegin/End()` to manage events
  - Events may also be nested and will aggregate in a nested fashion
  - Can use `PetscLogFlops()` to log user flops

Adding A Logging Stage
C

```
int stageNum;

PetscLogStageRegister(&stageNum, "name");
PetscLogStagePush(stageNum);

/* Code to Monitor */

PetscLogStagePop();
```

Adding A Logging Stage
Python

```
with PETSc.LogStage('Fluid Stage') as fluidStage:
  # All operations will be aggregated in fluidStage
  fluid.solve()
```

Adding A Logging Event
C

```
static int USER_EVENT;

PetscLogEventRegister(&USER_EVENT, "name", CLS_ID);
PetscLogEventBegin(USER_EVENT,0,0,0,0);

/* Code to Monitor */

PetscLogFlops(user_event_flops);
PetscLogEventEnd(USER_EVENT,0,0,0,0);
```

Adding A Logging Event
Python

```
with PETSc.logEvent('Reconstruction') as recEvent:
  # All operations are timed in recEvent
  reconstruct(sol)
  # Flops are logged to recEvent
  PETSc.Log.logFlops(user_event_flops)
```

Adding A Logging Class

```
static int CLASS_ID;

PetscLogClassRegister(&CLASS_ID, "name");
```

- Class ID identifies a class uniquely
- Must initialize before creating any objects of this type

Matrix Memory Preallocation

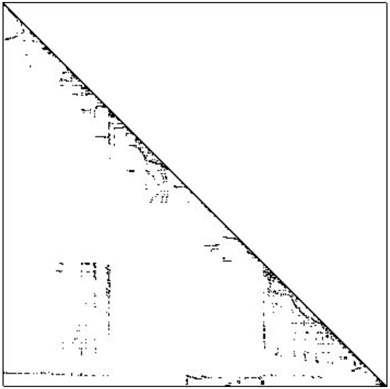
- PETSc sparse matrices are dynamic data structures
  - can add additional nonzeros freely
- Dynamically adding many nonzeros
  - requires additional memory allocations
  - requires copies
  - can kill performance
- Memory preallocation provides
  - the freedom of dynamic data structures
  - good performance
- Easiest solution is to replicate the assembly code
  - Remove computation, but preserve the indexing code
  - Store set of columns for each row
- Call preallocation rourines for all datatypes
  - `MatSeqAIJSetPreallocation()`
  - `MatMPIAIJSetPreallocation()`
  - Only the relevant data will be used

Matrix Memory Preallocation
Sequential Sparse Matrices

```
MatSeqAIJPreallocation(Mat A, int nz, int nnz[])
```

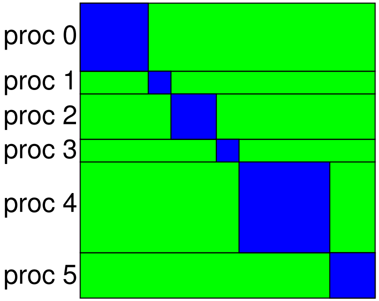
nz: expected number of nonzeros in any row

nnz(i): expected number of nonzeros in row i



Matrix Memory Preallocation
ParallelSparseMatrix

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



🟦 diagonal blocks
🟩 offdiagonal blocks

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

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

Matrix Memory Preallocation

Parallel Sparse Matrices

```
MatMPIAIJPreallocation(Mat A, int dnz, int dnnz[],
int onz, int onnz[])
```

dnz: expected number of nonzeros in any row in the diagonal block

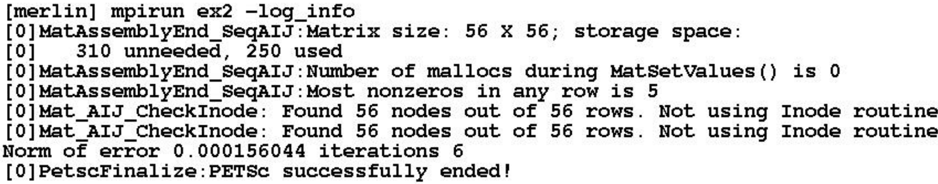
nnz(i): expected number of nonzeros in row i in the diagonal block

onz: expected number of nonzeros in any row in the offdiagonal portion

nnz(i): expected number of nonzeros in row i in the offdiagonal portion

Matrix Memory Preallocation
Verifying Preallocation

- Use runtime option `-info`
- Output:
  ```
  [proc #] Matrix size:  %d X %d; storage space:
  %d unneeded, %d used
  [proc #] Number of mallocs during MatSetValues( )
  is %d
  ```



```
[merlin] mpirun ex2 -log_info
[0]MatAssemblyEnd_SeqAIJ:Matrix size: 56 X 56; storage space:
[0]   310 unneeded, 250 used
[0]MatAssemblyEnd_SeqAIJ:Number of mallocs during MatSetValues() is 0
[0]MatAssemblyEnd_SeqAIJ:Most nonzeros in any row is 5
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routine
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routine
Norm of error 0.000156044 iterations 6
[0]PetscFinalize:PETSc successfully ended!
```

Exercise 8

Return to Execise 7 and add more profiling.

- Update to the next revision
  - `hg update -r3`
- Build, run, and look at the profiling report
  - `make ex5`
  - `./bin/ex5 -use_coords -log_summary`
- Add a new stage for setup
- Add a new event for `FormInitialGuess()` and log the flops
- Build it again and look at the profiling report

Outline

Importance of Computational Modeling

Without a model,
performance measurements are meaningless!

Before a code is written, we should have a model of

- computation
- memory usage
- communication
- bandwidth
- achievable concurrency

This allows us to

- verify the implementation
- predict scaling behavior

Complexity Analysis

The key performance indicator, which we will call the *balance factor* β, is the ratio of flops executed to bytes transfered.

- We will designate the unit $\frac{\mathrm{flop}}{\mathrm{byte}}$ as the *Keyes*
- Using the peak flop rate r_{peak}, we can get the required bandwidth B_{req} for an algorithm

$$B_{\mathrm{req}} = \frac{r_{\mathrm{peak}}}{\beta} \tag{1}$$

- Using the peak bandwidth B_{peak}, we can get the maximum flop rate r_{max} for an algorithm

$$r_{\mathrm{max}} = \beta B_{\mathrm{peak}} \tag{2}$$

Performance Caveats

- The peak flop rate r_{peak} on modern CPUs is attained through the usage of a SIMD multiply-accumulate instruction on special 128-bit registers.
- SIMD MAC operates in the form of 4 simultaneous operations (2 adds and 2 multiplies):

$$c_1 = c_1 + a_1 * b_1 \tag{3}$$

$$c_2 = c_2 + a_2 * b_2 \tag{4}$$

  You will miss peak by the corresponding number of operations you are missing. In the worst case, you are reduced to 25% efficiency if your algorithm performs naive summation or products.
- Memory alignment is also crucial when using SSE, the instructions used to load and store from the 128-bit registers throw very costly alignment exceptions when the data is not stored in memory on 16 byte (128 bit) boundaries.

Analysis of BLAS `axpy()`

$$\vec{y} \leftarrow \alpha\vec{x} + \vec{y}$$

For vectors of length N and b-byte numbers, we have

- Computation
  - $2N$ flops
- Memory Access
  - $(3N+1)b$ bytes

Thus, our balance factor $\beta = \frac{2N}{(3N+1)b} \approx \frac{2}{3b}\text{Keyes}$

Analysis of BLAS `axpy()`

$$\vec{y} \leftarrow \alpha\vec{x} + \vec{y}$$

For Matt's Laptop,

- $r_{\text{peak}} = 1700 \text{MF}/\text{s}$

  implies that
- $B_{\text{req}} = 2550b\ \text{MB}/\text{s}$
  - Much greater than B_{peak}

- $B_{\text{peak}} = 1122 \text{MB}/\text{s}$

  implies that
- $r_{\text{max}} = \frac{748}{b}\ \text{MF}/\text{s}$
  - 5.5% of r_{peak}

STREAM Benchmark

Simple benchmark program measuring sustainable memory bandwidth

- Protoypical operation is Triad (WAXPY): $\mathbf{w} = \mathbf{y} + \alpha \mathbf{x}$
- Measures the memory bandwidth bottleneck (much below peak)
- Datasets outstrip cache

Machine	Peak (MF/s)	Triad (MB/s)	MF/MW	Eq. MF/s
Matt's Laptop	1700	1122.4	12.1	93.5 (5.5%)
Intel Core2 Quad	38400	5312.0	57.8	442.7 (1.2%)
Tesla 1060C	984000	102000.0*	77.2	8500.0 (0.8%)

Table: Bandwidth limited machine performance

http://www.cs.virginia.edu/stream/

Analysis of Sparse Matvec (SpMV)

Assumptions

- No cache misses
- No waits on memory references

Notation

m	Number of matrix rows
nz	Number of nonzero matrix elements
V	Number of vectors to multiply

We can look at bandwidth needed for peak performance

$$\left(8 + \frac{2}{V}\right)\frac{m}{nz} + \frac{6}{V} \text{ byte/flop} \tag{5}$$

or achieveable performance given a bandwith BW

$$\frac{Vnz}{(8V+2)m + 6nz} BW \text{ Mflop/s} \tag{6}$$

Towards Realistic Performance Bounds for Implicit CFD Codes, Gropp, Kaushik, Keyes, and Smith.

Improving Serial Performance

For a single matvec with 3D FD Poisson, Matt's laptop can achieve at most

$$\frac{1}{(8+2)\frac{1}{7}+6} \text{ bytes/flop}(1122.4 \text{ MB/s}) = 151 \text{ MFlops/s}, \tag{7}$$

which is a dismal 8.8% of peak.

Can improve performance by

- Blocking
- Multiple vectors

but operation issue limitations take over.

Improving Serial Performance

For a single matvec with 3D FD Poisson, Matt's laptop can achieve at most

$$\frac{1}{(8+2)\frac{1}{7}+6}\ \mathrm{bytes/flop}(1122.4\ \mathrm{MB/s}) = 151\ \mathrm{MFlops/s}, \tag{7}$$

which is a dismal 8.8% of peak.

Better approaches:

- Unassembled operator application (Spectral elements, FMM)
  - N data, N^2 computation
- Nonlinear evaluation (Picard, FAS, Exact Polynomial Solvers)
  - N data, N^k computation

Performance Tradeoffs

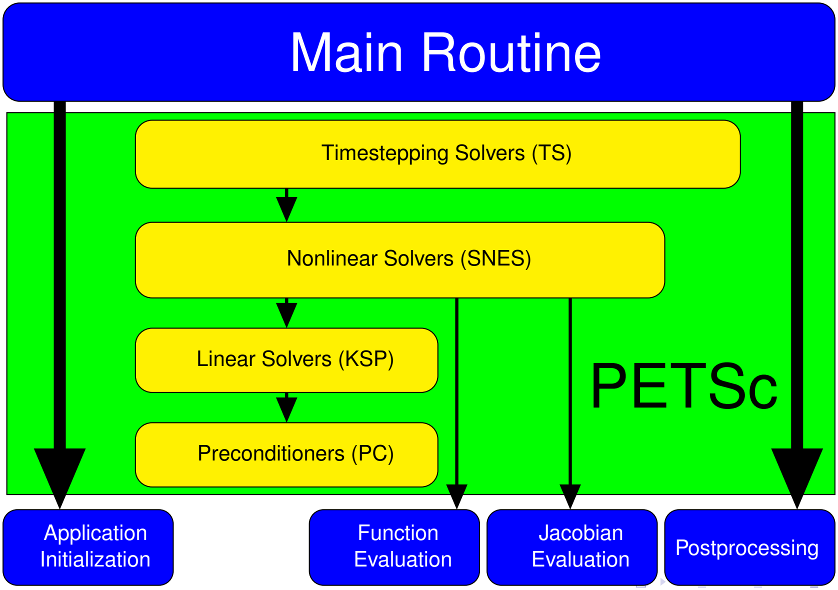
We must balance storage, bandwidth, and cycles

- Assembled Operator Action
  - Trades cycles and storage for bandwidth in application
- Unassembled Operator Action
  - Trades bandwidth and storage for cycles in application
  - For high orders, storage is impossible
  - Can make use of FErari decomposition to save calculation
  - Could storage element matrices to save cycles
- Partial assembly gives even finer control over tradeoffs
  - Also allows introduction of parallel costs (load balance, . . .)

Outline

Outline

Flow Control for a PETSc Application



SNES Paradigm

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

- `DMDA`
  - Abstracts Cartesian grids in any dimension
  - Supports stencils, communication, reordering
  - Nice for simple finite differences
- `DMMesh`
  - Abstracts general topology in any dimension
  - Also supports partitioning, distribution, and global orders
  - Allows aribtrary 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 `PCMG` solver
- `PetscSection`
  - Abstracts functions over a topology
  - Manages allocation and assembly of local and global structures
  - Will merge with `DM` somehow

SNES Function

User provided function calculates the nonlinear residual:

```
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:

```
(*func)(SNES snes,Vec x,Mat *J,Mat *M,MatStructure *flag,void *ctx)
```

`x`: The current solution

`J`: The Jacobian

`M`: The Jacobian preconditioning matrix (possibly J itself)

`ctx`: 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, `-snes_mf`
- finite difference approximation with coloring, `-snes_fd`

SNES Variants

- Line search strategies
- Trust region approaches
- Picard iteration
- Variational inequality approaches

Finite Difference Jacobians

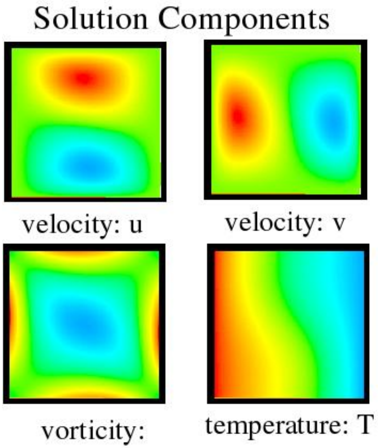
PETSc can compute and explicitly store a Jacobian via 1st-order FD

- 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



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

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

Driven Cavity Application Context

```
typedef struct {
  /*------  basic application data  ------*/
  PetscReal lid_velocity;
  PetscReal prandtl
  PetscReal grashof;
  PetscBool draw_contours;
} AppCtx;
```

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

Driven Cavity Residual Evaluation

```
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;
}
```

Better Driven Cavity Residual Evaluation

```
ResLocal(DMDALocalInfo *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

What is a DMDA?

`DMDA` is a topology interface on structured grids

- Handles parallel data layout
- Handles local and global indices
  - `DMDAGetGlobalIndices()` and `DMDAGetAO()`
- Provides local and global vectors
  - `DMGetGlobalVector()` and `DMGetLocalVector()`
- Handles ghost values coherence
  - `DMGetGlobalToLocal()` and `DMGetLocalToGlobal()`

Function Paradigm

The **DM** interface is based upon *local* callback functions

- `FormFunctionLocal()`
- `FormJacobianLocal()`

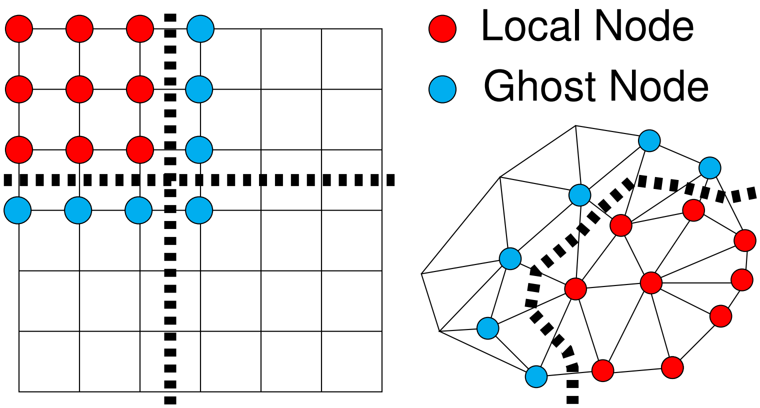
When PETSc needs to evaluate the nonlinear residual **F(x)**,

- Each process evaluates the local residual
- PETSc assembles the global residual automatically
  - Uses `DMLocalToGlobal()` 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



DMDA Global Numberings

Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
15	16	17	18	19
10	11	12	13	14
5	6	7	8	9
0	1	2	3	4
Proc 0			Proc 1	

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

PETSc numbering

DMDA Global vs. Local Numbering

- **Global**: Each vertex has a unique id belongs on a unique process
- **Local**: Numbering includes vertices from neighboring processes
  - These are called ghost vertices

Proc 2			Proc 3	
X	X	X	X	X
X	X	X	X	X
12	13	14	15	X
8	9	10	11	X
4	5	6	7	X
0	1	2	3	X
Proc 0			Proc 1	

Local numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

Global numbering

DMDA Local Function

User provided function calculates the nonlinear residual (in 2D)

```
(*lfunc)(DMDALocalInfo *info, PetscScalar **x, PetscScalar **r, void *ctx)
```

info: All layout and numbering information

x: The current solution
- Notice that it is a multidimensional array

r: The residual

ctx: The user context passed to `DASetLocalFunction()`

The local DMDA function is activated by calling

```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

Bratu Residual Evaluation

$$\Delta u + \lambda e^u = 0$$

```
ResLocal(DMDALocalInfo *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/ex5.c

DMDA Local Jacobian

User provided function calculates the Jacobian (in 2D)

```
(*lfunc)(DMDALocalInfo *info, PetscScalar **x, Mat J, void *ctx)
```

`info`: All layout and numbering information
`x`: The current solution
`J`: The Jacobian
`ctx`: The user context passed to `DASetLocalJacobian()`

The local DMDA function is activated by calling

```
SNESSetJacobian(snes, J, J, SNESDAComputeJacobian, ctx)
```

Bratu Jacobian Evaluation

```
JacLocal(DMDALocalInfo *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);
}}}}
```

$PETCS_DIR/src/snes/examples/tutorials/ex5.c

A DMDA is more than a Mesh

A DMDA contains topology, geometry, and (sometimes) an implicit Q1 discretization.

It is used as a template to create

- Vectors (functions)
- Matrices (linear operators)

DMDA Vectors

- The DMDA 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
  - `DMCreateGlobalVector(DM da, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
  - Each process stores its local portion plus ghost values
  - `DMCreateLocalVector(DM da, Vec *lvec)`
  - includes ghost values!

Updating Ghosts

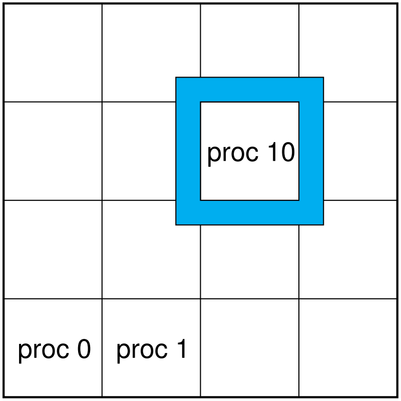
Two-step process enables overlapping computation and communication

- `DMGlobalToLocalBegin(da, gvec, mode, lvec)`
  - `gvec` provides the data
  - `mode` is either `INSERT_VALUES` or `ADD_VALUES`
  - `lvec` holds the local and ghost values
- `DMGlobalToLocalEnd(da, gvec, mode, lvec)`
  - Finishes the communication

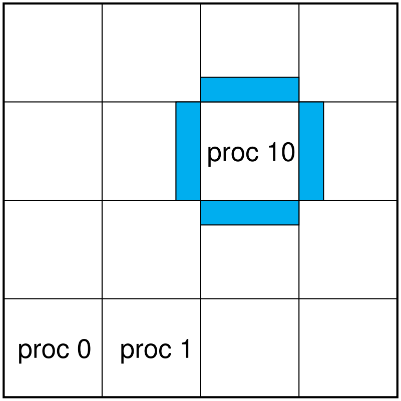
The process can be reversed with `DALocalToGlobal()`.

DMDA Stencils

Both the box stencil and star stencil are available.



Box Stencil



Star Stencil

Setting Values on Regular Grids

PETSc provides

```
MatSetValuesStencil(Mat A, m, MatStencil idxm[], n, MatStencil idxn[],
                    PetscScalar values[], InsertMode mode)
```

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

Creating a DADM

```
DMDACreate2d(comm, bdX, bdY, type, M, N, m, n, dof, s, lm[], ln[], DMDA *c
```

bd: Specifies boundary behavior

- DMDA_BOUNDARY_NONE, DMDA_BOUNDARY_GHOSTED, or DMDA_BOUNDARY_PERIODIC

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

Outline

Things To Check Out

- `PCFieldSplit` for multiphysics
- GPU acceleration for **Vec**, **Mat**, **KSP**
- **PCMG** for multilevel solvers
- **DMMesh** (Sieve) for topology automation
- Deal**II** and FEniCS for FEM automation
- PetFMM and PetRBF for particle methods

Outline

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

MultiPhysics Paradigm

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- extracts functions/operators corresponding to each physics
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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

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly
```

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type additive

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & I \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type multiplicative
-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

$$\begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
-pc_fieldsplit_schur_factorization_type diag
```

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & -\hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
-pc_fieldsplit_schur_factorization_type lower
```

$$\begin{pmatrix} \hat{A} & 0 \\ B^T & \hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
-pc_fieldsplit_schur_factorization_type upper
```

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-pc_fieldsplit_schur_factorization_type full
```

$$\begin{pmatrix} I & 0 \\ B^T A^{-1} & I \end{pmatrix} \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix}$$

Outline

PETSc-GPU

PETSc now has support for Krylov solves on the GPU

- `-with-cuda=1 -with-cusp=1 -with-thrust=1`
  - Also possibly `-with-precision=single`
- New classes `VECCUDA` and `MATAIJCUDA`
  - Just change type on command line, `-vec_type veccuda`
- Uses Thrust and Cusp libraries from Nvidia guys
- Does not communicate vectors during solve

VECCUDA

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

MATAIJCUDA

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

Solvers come for Free

Preliminary Implementation of PETSc Using GPU,
Minden, Smith, Knepley, 2010

- 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

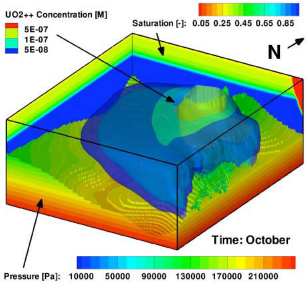
Example
Driven Cavity Velocity-Vorticity with Multigrid

```
ex50 -da_vec_type seqcusp
  -da_mat_type aijcusp -mat_no_inode # Setup types
  -da_grid_x 100 -da_grid_y 100      # Set grid size
  -pc_type none -pc_mg_levels 1      # Setup solver
  -preload off -cuda_synchronize     # Setup run
  -log_summary
```

Example
PFLOTRAN

Flow Solver
$32 \times 32 \times 32$ grid

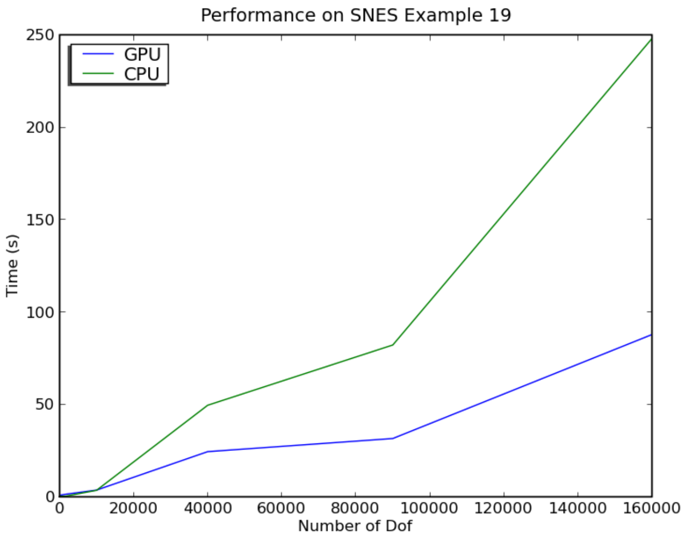
Routine	Time (s)	MFlops	MFlops/s
CPU			
KSPSolve	8.3167	4370	526
MatMult	1.5031	769	512
GPU			
KSPSolve	1.6382	4500	2745
MatMult	0.3554	830	2337


UO2++ Concentration [M]
5E-07
1E-07
5E-08
Saturation [-]: 0.05 0.25 0.45 0.65 0.85
N
Time: October
Pressure [Pa]: 10000 50000 90000 130000 170000 210000

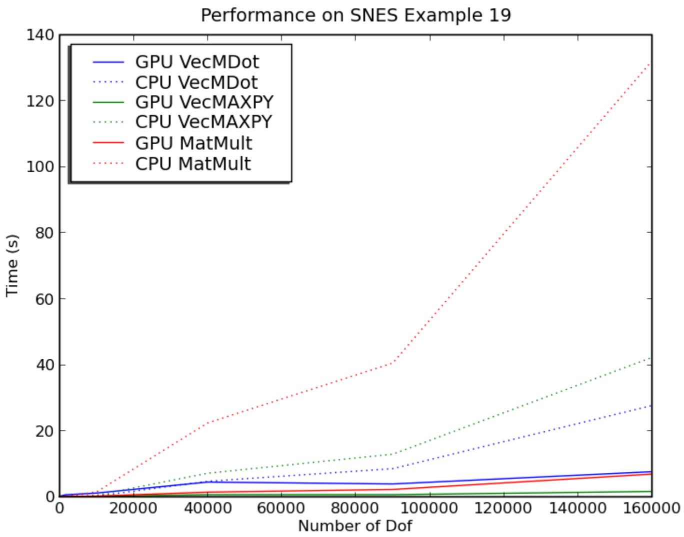
P. Lichtner, G. Hammond, R. Mills, B. Phillip

Serial Performance

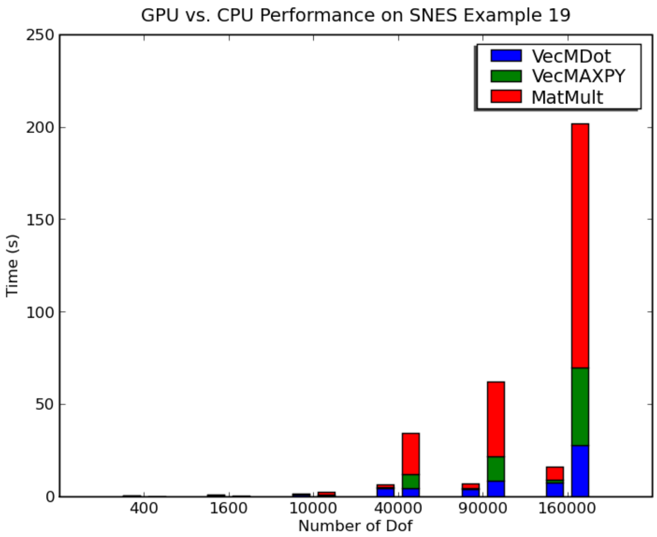
NVIDIA GeForce 9400M



Serial Performance
NVIDIA Tesla M2050



Serial Performance
NVIDIA Tesla M2050



Outline

Multigrid Paradigm

The **DM** interface uses the *local* callback functions to

- assemble global functions/operators from local pieces
- assemble functions/operators on coarse grids

Then **PCMG** organizes

- control flow for the multilevel solve, and
- projection and smoothing operators at each level.

DM Integration with SNES

- DM supplies global residual and Jacobian to SNES
  - User supplies local version to DM
  - The `Rhs_*()` and `Jac_*()` functions in the example
- Allows automatic parallelism
- Allows grid hierarchy
  - Enables multigrid once interpolation/restriction is defined
- Paradigm is developed in unstructured work
  - Solve needs scatter into contiguous global vectors (initial guess)
- Handle Neumann BC using `KSPSetNullSpace()`

Multigrid with DMMG

Allows multigrid with some simple command line options

- `-pc_type mg`, `-pc_mg_levels`
- `-pc_mg_type`, `-pc_mg_cycle_type`, `-pc_mg_galerkin`
- `-mg_levels_1_ksp_type`, `-mg_levels_1_pc_type`
- `-mg_coarse_ksp_type`, `-mg_coarse_pc_type`
- `-ksp_view`

Interface also works with 3rd party packages, like ML from Sandia

Programming with Options

ex55: Allen-Cahn problem in 2D

- constant mobility
- triangular elements

Geometric multigrid method for saddle point variational inequalities:

```
./ex55 -ksp_type fgmres -pc_type mg -mg_levels_ksp_type fgmres
-mg_levels_pc_type fieldsplit -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_pc_fieldsplit_type schur -da_grid_x 65 -da_grid_y 65
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition user
-mg_levels_fieldsplit_1_ksp_type gmres -mg_coarse_ksp_type preonly
-mg_levels_fieldsplit_1_pc_type none   -mg_coarse_pc_type svd
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor    -pc_mg_levels 5
-mg_levels_fieldsplit_0_pc_sor_forward -pc_mg_galerkin
-snes_vi_monitor -ksp_monitor_true_residual -snes_atol 1.e-11
-mg_levels_ksp_monitor -mg_levels_fieldsplit_ksp_monitor
-mg_levels_ksp_max_it 2 -mg_levels_fieldsplit_ksp_max_it 5
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```
./ex55 -ksp_type fgmres -pc_type mg -pc_mg_levels 5
  -da_grid_x 65 -da_grid_y 65
```

Use the Galerkin process to compute the coarse grid operators

```
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```

Programming with Options

ex55: Allen-Cahn problem in 2D

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```

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```
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Smoother: Flexible GMRES (2 iterates) with a Schur complement PC

```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Shur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Smoother: Flexible GMRES (2 iterates) with a Schur complement PC

```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Shur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Programming with Options

ex55: Allen-Cahn problem in 2D

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```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Shur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Programming with Options

ex55: Allen-Cahn problem in 2D

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```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Shur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Outline

Mesh Paradigm

The **DMMesh** interface also uses *local* callback functions

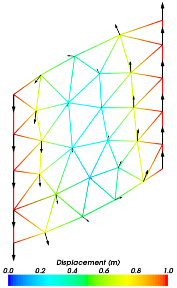
- maps between global Vec and local Vec
- Local vectors are structured using a **PetscSection**

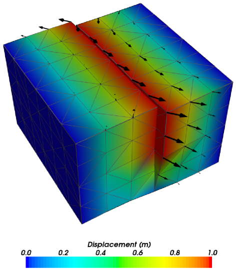
When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Each process evaluates the local residual for each element
- PETSc assembles the global residual automatically
    - `DMLocalToGlobal()` works just as in the structured case

Multiple Mesh Types

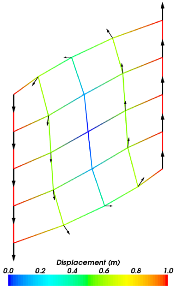
Triangular

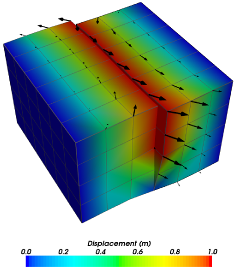




Tetrahedral

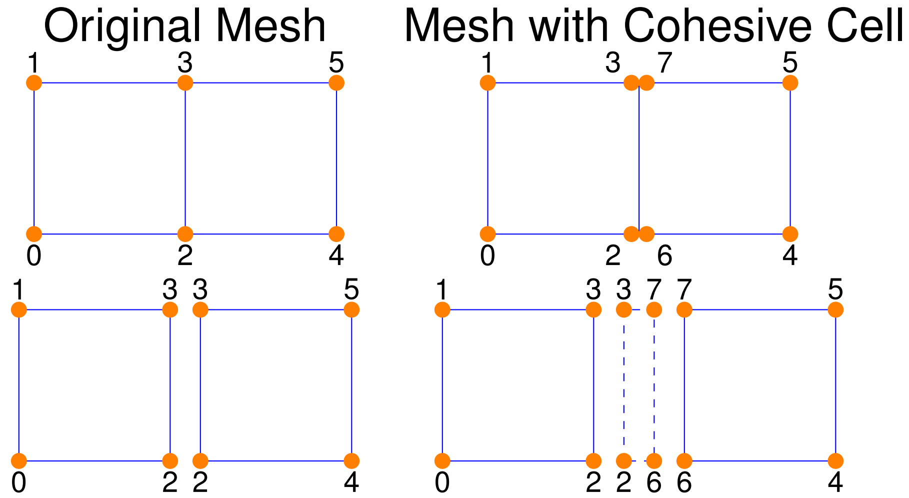
Rectangular





Hexahedral

Cohesive Cells



Exploded view of meshes

Cohesive Cells

Cohesive cells are used to enforce slip conditions on a fault

- Demand complex mesh manipulation
  - We allow specification of only fault vertices
  - Must “sew” together on output
- Use Lagrange multipliers to enforce constraints
  - Forces illuminate physics
- Allow different fault constitutive models
  - Simplest is enforced slip
  - Now have fault constitutive models

Outline

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

`http://www.fenics.org/fiat`

FIAT understands

- Reference element shapes (line, triangle, tetrahedron)
- Quadrature rules
- Polynomial spaces
- Functionals over polynomials (dual spaces)
- Derivatives

User can build arbitrary elements specifying the Ciarlet triple (K, P, P')

FIAT is part of the FEniCS project, as is the PETSc Sieve module

FFC

FFC is a compiler for variational forms by Anders Logg.

Here is a mixed-form Poisson equation:

$$a((\tau, w), (\sigma, u)) = L((\tau, w)) \qquad \forall (\tau, w) \in V$$

where

$$\begin{aligned} a((\tau, w), (\sigma, u)) &= \int_\Omega \tau\sigma - \nabla \cdot \tau u + w \nabla \cdot u \, dx \\ L((\tau, w)) &= \int_\Omega wf \, dx \end{aligned}$$

FFC
Mixed Poisson

```
shape = "triangle"

BDM1 = FiniteElement("Brezzi-Douglas-Marini",shape,1)
DG0  = FiniteElement("Discontinuous Lagrange",shape,0)

element      = BDM1 + DG0
(tau, w)     = TestFunctions(element)
(sigma, u)   = TrialFunctions(element)

a = (dot(tau, sigma) - div(tau)*u + w*div(sigma))*dx

f = Function(DG0)
L = w*f*dx
```

FFC

Here is a discontinuous Galerkin formulation of the Poisson equation:

$$a(v,u) = L(v) \qquad \forall v \in V$$

where

$$\begin{aligned}
a(v,u) &= \int_\Omega \nabla u \cdot \nabla v \, dx \\
&+ \sum_S \int_S - < \nabla v > \cdot [[u]]_n - [[v]]_n \cdot < \nabla u > -(\alpha/h) vu \, dS \\
&+ \int_{\partial\Omega} -\nabla v \cdot [[u]]_n - [[v]]_n \cdot \nabla u - (\gamma/h) vu \, ds \\
L(v) &= \int_\Omega vf \, dx
\end{aligned}$$

FFC
DG Poisson

```
DG1 = FiniteElement("Discontinuous Lagrange",shape,1)
v = TestFunctions(DG1)
u = TrialFunctions(DG1)
f = Function(DG1)
g = Function(DG1)
n = FacetNormal("triangle")
h = MeshSize("triangle")
a = dot(grad(v), grad(u))*dx
  - dot(avg(grad(v)), jump(u, n))*dS
  - dot(jump(v, n), avg(grad(u)))*dS
  + alpha/h*dot(jump(v, n) + jump(u, n))*dS
  - dot(grad(v), jump(u, n))*ds
  - dot(jump(v, n), grad(u))*ds
  + gamma/h*v*u*ds
L = v*f*dx + v*g*ds
```

Outline

FMM Applications

FMM can accelerate both integral and boundary element methods for:

- Laplace
- Stokes
- Elasticity

FMM Applications

FMM can accelerate both integral and boundary element methods for:

- Laplace
- Stokes
- Elasticity

Advantages

- Mesh-free
- $\mathcal{O}(N)$ time
- Distributed and multicore (GPU) parallelism
- Small memory bandwidth requirement

PetFMM

PetFMM is an freely available implementation of the
Fast Multipole Method
http://barbagroup.bu.edu/Barba_group/PetFMM.html

- Leverages PETSc
  - Same open source license
  - Uses Sieve for parallelism
- Extensible design in C++
  - Templated over the kernel
  - Templated over traversal for evaluation
- MPI implementation
  - Novel parallel strategy for anisotropic/sparse particle distributions
  - PetFMM–A dynamically load-balancing parallel fast multipole library
  - 86% efficient strong scaling on 64 procs
- Example application using the Vortex Method for fluids
- (coming soon) GPU implementation

Outline

Conclusions

PETSc can help you

- easily construct a code to test your ideas
  - Lots of code construction, management, and debugging tools
- scale an existing code to large or distributed machines
  - Using `FormFunctionLocal()` and scalable linear algebra
- incorporate more scalable or higher performance algorithms
  - Such as domain decomposition or multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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