The Portable Extensible Toolkit for Scientific Computing

Matthew Knepley

Mathematics and Computer Science Division
Argonne National Laboratory

Computation Institute
University of Chicago

PETSc Tutorial
13th Workshop on the DOE ACTS Collection
LBNL, Berkeley, CA August 14–17, 2012

Main Point

Never believe *anything*,

unless you can run it.

Main Point

Never believe *anything*,

unless you can run it.

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
- Answer email at petsc-maint@mcs.anl.gov

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

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

How We Can Help at the Tutorial

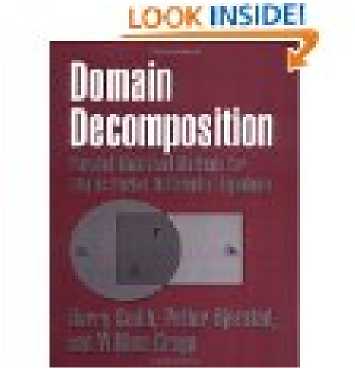
- Point out relevant documentation
- Quickly answer questions
- Help install
- Guide design of large scale codes
- Answer email at petsc-maint@mcs.anl.gov

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

Advice from Bill Gropp

You want to think about how you decompose your data structures, how you think about them globally. [...] If you were building a house, you'd start with a set of blueprints that give you a picture of what the whole house looks like. You wouldn't start with a bunch of tiles and say. "Well I'll put this tile down on the ground, and then I'll find a tile to go next to it." But all too many people try to build their parallel programs by creating the smallest possible tiles and then trying to have the structure of their code emerge from the chaos of all these little pieces. You have to have an organizing principle if you're going to survive making your code parallel.

(http://www.rce-cast.com/Podcast/rce-28-mpich2.html)

What is PETSc?

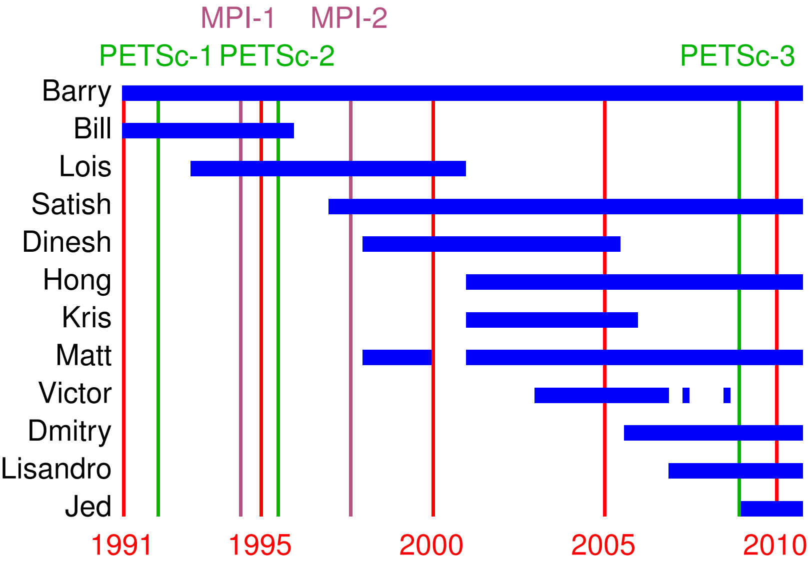
A freely available and supported research code

- 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

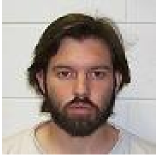
The PETSc Team

Bill Gropp

Barry Smith

Satish Balay

Jed Brown



Matt Knepley

Lisandro Dalcin

Hong Zhang

Victor Eijkhout

Dmitry Karpeev

Outline

1. Getting Started with PETSc
   - What is PETSc?
   - Who uses 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?

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
  - Fluidity
  - 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

What Can We Handle?

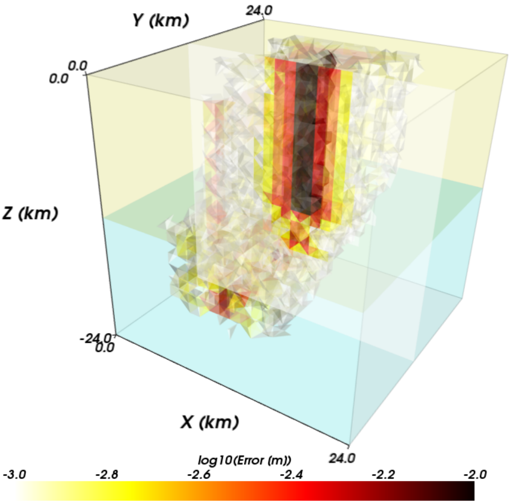
- PETSc has run implicit problems with over 500 billion unknowns
  - UNIC on BG/P and XT5
  - PFLOTRAN for flow in porous media
- PETSc has run on over 290,000 cores efficiently
  - UNIC on the IBM BG/P Intrepid at ANL
  - PFLOTRAN on the Cray XT5 Jaguar at ORNL
- PETSc applications have run at 22 Teraflops
  - Kaushik on XT5
  - LANL PFLOTRAN code

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

PyLith

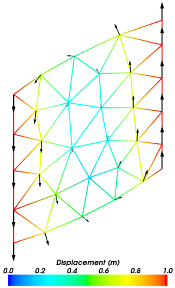
- Multiple problems
  - Dynamic rupture
  - Quasi-static relaxation
- Multiple models
  - Nonlinear visco-plastic
  - Finite deformation
  - Fault constitutive models
- Multiple meshes
  - 1D, 2D, 3D
  - Hex and tet meshes
- Parallel
  - PETSc solvers
  - Sieve mesh management

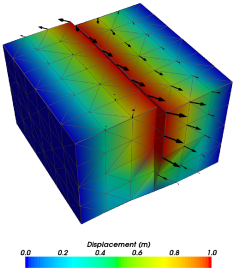


[a] Aagaard, Knepley, Williams

Multiple Mesh Types

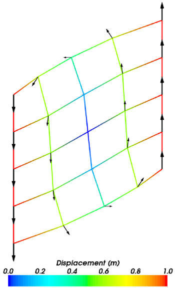
Triangular

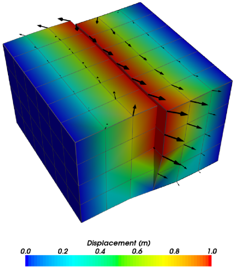




Tetrahedral

Rectangular

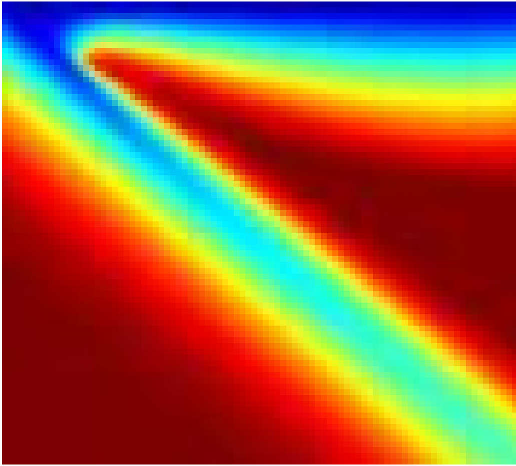




Hexahedral

Magma Dynamics

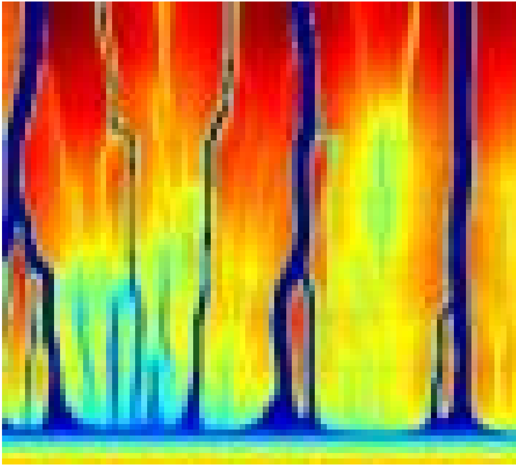
- Couples scales
  - Subduction
  - Magma Migration
- Physics
  - Incompressible fluid
  - Porous solid
  - Variable porosity
- Deforming matrix
  - Compaction pressure
- Code generation
  - FEniCS
- Multiphysics Preconditioning
  - PETSc FieldSplit



[a] Katz, Speigelman

Magma Dynamics

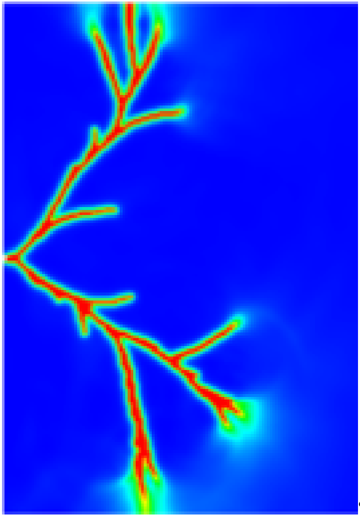
- Couples scales
  - Subduction
  - Magma Migration
- Physics
  - Incompressible fluid
  - Porous solid
  - Variable porosity
- Deforming matrix
  - Compaction pressure
- Code generation
  - FEniCS
- Multiphysics Preconditioning
  - PETSc FieldSplit



[a] Katz, Speigelman

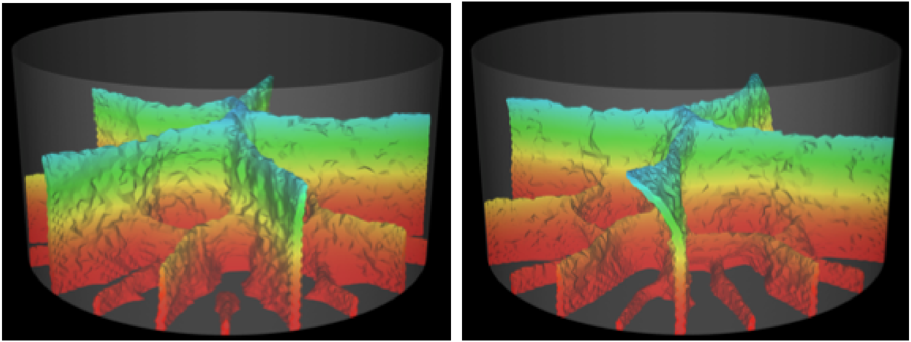
Fracture Mechanics

- 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

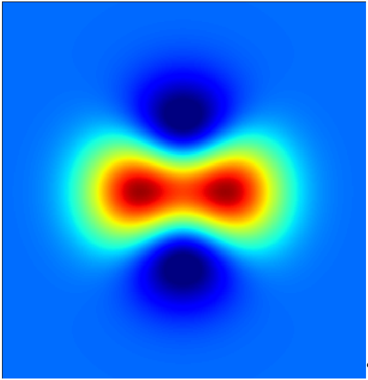

[1]

[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

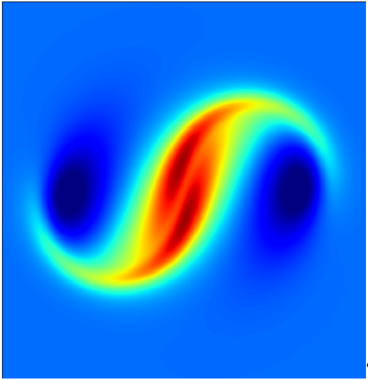
 [a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 100

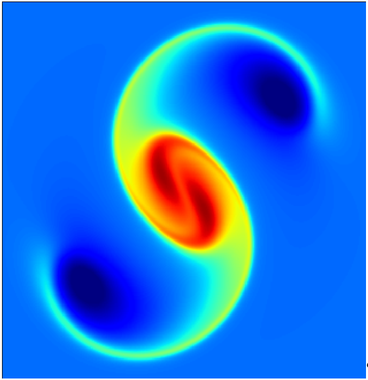
- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
  - Automatic load balancing
  - Variety of kernels
  - Optimized with templates
- PetRBF
  - Variety of RBFs
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU

[a]

[a] Cruz, Yokota, Barba, Knepley

# Vortex Method
t = 200

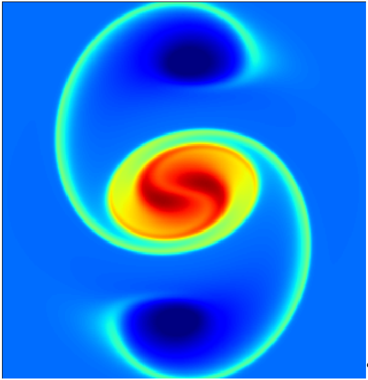
- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
  - Automatic load balancing
  - Variety of kernels
  - Optimized with templates
- PetRBF
  - Variety of RBFs
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU


[a]

[a] Cruz, Yokota, Barba, Knepley

# Vortex Method
t = 300

- 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

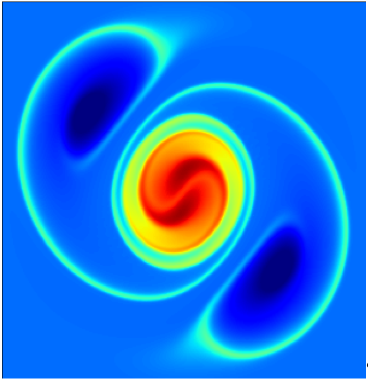
[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 400

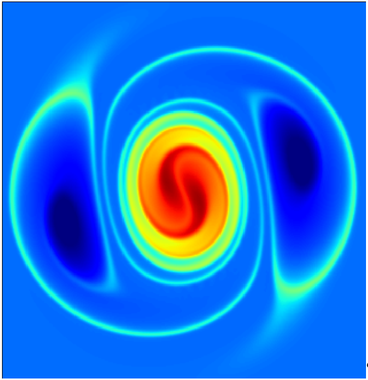
- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
  - Automatic load balancing
  - Variety of kernels
  - Optimized with templates
- PetRBF
  - Variety of RBFs
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU

[a]

[a] Cruz, Yokota, Barba, Knepley

# Vortex Method
t = 500

- 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

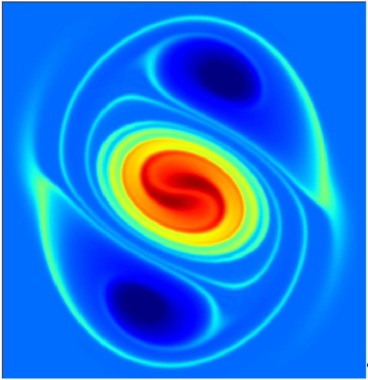

[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 600

- 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

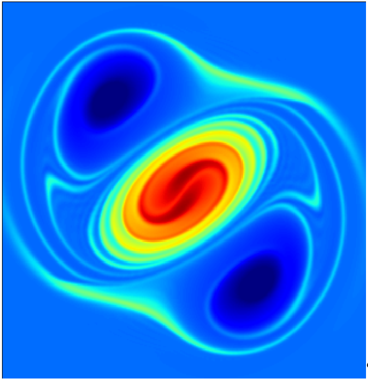
[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 700

- 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

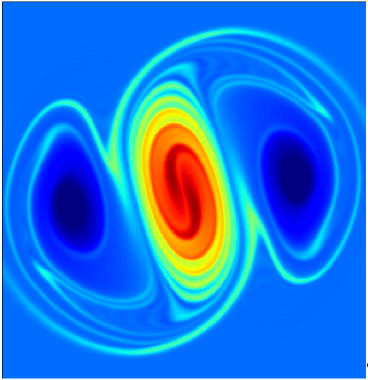
[a]

[a] Cruz, Yokota, Barba, Knepley

Vortex Method

t = 800

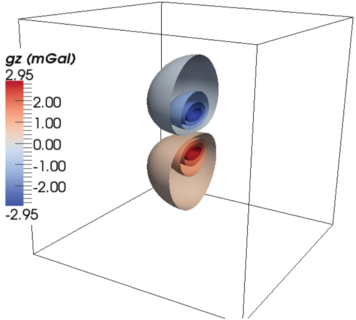
- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
- PetFMM
  - 2D/3D domains
  - Automatic load balancing
  - Variety of kernels
  - Optimized with templates
- PetRBF
  - Variety of RBFs
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU


[a]

[a] Cruz, Yokota, Barba, Knepley

Gravity Anomaly Modeling

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

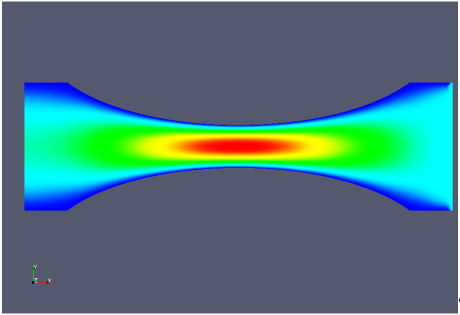


[a]

[a] May, Knepley

FEniCS-Apps
Rheagen

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

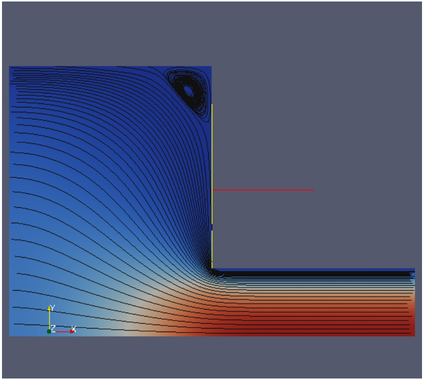

[a]

[a] Terrel

FEniCS-Apps

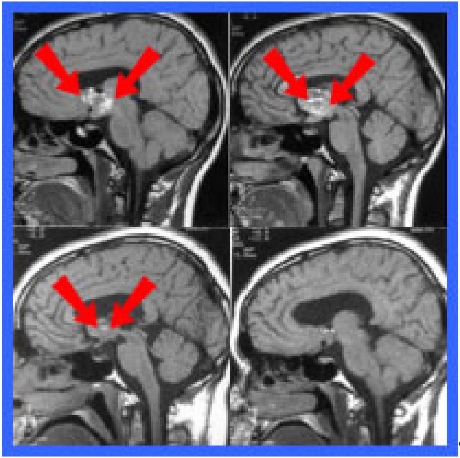
Rheagen

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



Real-time Surgery

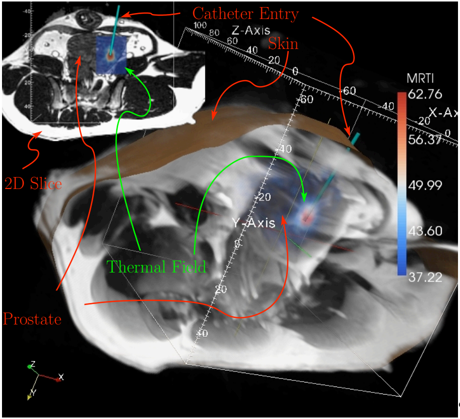
- Brain Surgery
  - Elastic deformation
  - Overlaid on MRI
  - Guides surgeon
- Laser Thermal Therapy
  - PDE constrained optimization
  - Per-patient calibration
  - Thermal inverse problem

[a]

[a] Warfield, Ferrant, et.al.

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]Fuentes, Oden, et.al.

Outline

1. Getting Started with PETSc
   - What is PETSc?
   - Who uses 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?

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

1. Getting Started with PETSc
   - What is PETSc?
   - Who uses 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?

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-3.3
  - http://petsc.cs.iit.edu/petsc/releases/BuildSystem-3.3

Unpacking PETSc

- Just clone development repository
  - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
  - `hg clone -rrelease-3.3 petsc-dev petsc-3.3`

or

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

Exercise 1

Download and Unpack PETSc!

Outline

1. Getting Started with PETSc
   - What is PETSc?
   - Who uses 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?

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 FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen

–download-chaco –download-parmetis

–download-scientificpython –download-fiat –download-generator

–with-cuda

–with-cudac='nvcc -m64' –with-cuda-arch=sm_10

–with-cusp-dir=/PETSc3/multicore/cusp

–with-thrust-dir=/PETSc3/multicore/thrust

–with-cuda-only

–with-precision=single

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()`)

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`

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

SNES ex62
Formulation

The isoviscous Stokes problem

$$\begin{aligned} \Delta\vec{u} \quad - \quad \nabla p &= \vec{f} \\ \nabla\cdot\vec{u} \qquad\qquad &= 0 \end{aligned}$$

on the square domain $\Omega = [0, 1]^2$.

The sides of the box may have

- Dirichlet, or
- homogeneous Neumann

boundary conditions.

SNES ex62
Discretization

We discretize using finite elements on an unstructured mesh:

$$\begin{aligned}(\nabla \vec{v}, \nabla \vec{u}) \quad - \quad (\nabla \cdot \vec{v}, p) &= -(\vec{v}, \vec{f}) \\ (q, \nabla \cdot \vec{u}) \qquad\qquad\qquad\qquad &= 0\end{aligned}$$

A finite element basis tabulation header is generated using

```
bin/pythonscripts/PetscGenerateFEMQuadrature.py
  dim order dim 1 laplacian   dim order 1 1 gradient   ex62.h
```

dim The spatial dimension

order The order of the Lagrange element

The code should be capable of using any FIAT element,
but has not yet been tested for this.

Outline

Outline

3 Solvers
- Objects
- Design

Typical PetscObject

```
SNES snes;

SNESCreate(comm, &snes);
SNESSetOptionsPrefix(snes, "foo_");
SNESSetFromOptions(snes);
/* Use snes */
SNESView(snes, PETSC_VIEWER_DRAW_WORLD);
SNESDestroy(snes);
```

- `SNES` is an opaque object (pointer to incomplete type)
  - Assignment, comparison, etc, are cheap
- What's up with this *Options* stuff?
  - Allows the type to be set at runtime: `-foo_snes_type qn`
  - Inversion of Control similar to service locator pattern, related to dependency injection
  - Other options (performance and semantics) can be changed at runtime under `-foo_snes_`

Basic `PetscObject` Usage

Every object in PETSc supports a basic interface

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

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

Ways to set options

- Command line
- Filename in the third argument of `PetscInitialize()`
- `~/.petscrc`
- `$PWD/.petscrc`
- `$PWD/petscrc`
- `PetscOptionsInsertFile()`
- `PetscOptionsInsertString()`
- `PETSC_OPTIONS` environment variable
- command line option `-options_file [file]`

Outline

3 Solvers
- Objects
- Design

Always use **SNES**

Always use **SNES** instead of **KSP**:

- No more costly than linear solver
- Can accomodate unanticipated nonlinearities
- Automatic iterative refinement
- Callback interface can take advantage of problem structure

Jed actually recommends **TS**. . .

Always use **SNES**

Always use **SNES** instead of **KSP**:

- No more costly than linear solver
- Can accomodate unanticipated nonlinearities
- Automatic iterative refinement
- Callback interface can take advantage of problem structure

Jed actually recommends **TS**. . .

What about TS?

Didn't Time Integration Suck in PETSc?

Yes, it did . . .

until Jed, Emil, and Peter rewrote it $\Longrightarrow$

What about TS?

Didn't Time Integration Suck in PETSc?

Yes, it did . . .

until Jed, Emil, and Peter rewrote it $\Longrightarrow$

What about TS?

Didn't Time Integration Suck in PETSc?

Yes, it did . . .

until Jed, Emil, and Peter rewrote it $\Longrightarrow$

IMEX time integration in PETSc

Additive Runge-Kutta IMEX methods

$$G(t, x, \dot{x}) = F(t, x)$$
$$J_\alpha = \alpha G_{\dot{x}} + G_x$$

User provides:

- `FormRHSFunction(ts,t,x,F,void *ctx)`
- `FormIFunction(ts,t,x,xdot,G,void *ctx)`
- `FormIJacobian(ts,t,x,xdot,alpha,J,J_p,mstr,void *ctx)`

- Single step interface so user can have own time loop
- Choice of explicit method, e.g. SSP
- L-stable DIRK for stiff part G
- Orders 2 through 5, embedded error estimates
- Dense output, hot starts for Newton
- More accurate methods if G is linear, also Rosenbrock-W
- Can use preconditioner from classical “semi-implicit” methods
- Extensible adaptive controllers, can change order within a family
- Easy to register new methods: `TSARKIMEXRegister()`

Some TS methods

TSSSPRK104 10-stage, fourth order, low-storage, optimal explicit SSP Runge-Kutta $c_{\text{eff}} = 0.6$ (Ketcheson 2008)

TSARKIMEX2E second order, one explicit and two implicit stages, *L*-stable, optimal (Constantinescu)

TSARKIMEX3 (and 4 and 5), *L*-stable (Kennedy and Carpenter, 2003)

TSROSWRA3PW three stage, third order, for index-1 PDAE, *A*-stable, $R(\infty) = 0.73$, second order strongly *A*-stable embedded method (Rang and Angermann, 2005)

TSROSWRA34PW2 four stage, third order, *L*-stable, for index 1 PDAE, second order strongly *A*-stable embedded method (Rang and Angermann, 2005)

TSROSWLLSSP3P4S2C four stage, third order, *L*-stable implicit, SSP explicit, *L*-stable embedded method (Constantinescu)

TS Examples

- 1D nonlinear hyperbolic conservation laws
  - `src/ts/examples/tutorials/ex9.c`
  - `./ex9 -da_grid_x 100 -initial 1 -physics shallow -limit minmod -ts_ssp_type rks2 -ts_ssp_nstages 8 -ts_monitor_solution`
- Stiff linear advection-reaction test problem
  - `src/ts/examples/tutorials/ex22.c`
  - `./ex22 -da_grid_x 200 -ts_monitor_solution -ts_type rosw -ts_rosw_type ra34pw2 -ts_adapt_monitor`
- 1D Brusselator (reaction-diffusion)
  - `src/ts/examples/tutorials/ex25.c`
  - `./ex25 -da_grid_x 40 -ts_monitor_solution -ts_type rosw -ts_rosw_type 2p -ts_adapt_monitor`

New methods in SNES

LS, TR	Newton-type with line search and trust region
NRichardson	Nonlinear Richardson, usually preconditioned
VIRS, VISS	reduced space and semi-smooth methods for variational inequalities
QN	Quasi-Newton methods like BFGS
NGMRES	Nonlinear GMRES
NCG	Nonlinear Conjugate Gradients
SORQN	SOR quasi-Newton
GS	Nonlinear Gauss-Seidel sweeps
FAS	Full approximation scheme (nonlinear multigrid)
MS	Multi-stage smoothers (in FAS for hyperbolic problems)
Shell	Your method, often used as a (nonlinear) preconditioner

Recent PETSc functionality: Indicated by blue

Time Integrators

Pseudo-Timestepping	Runge-Kutta	Strong Stability Preserving
General Linear	IMEX	Rosenbrock-W

Nonlinear Algebraic Solvers

Line Search Newton	Quasi-Newton (BFGS)	Nonlinear Gauss-Seidel	Nonlinear MG (FAS)
Trust Region Newton	Successive Substitutions	Nonlinear CG	Active Set VI

Krylov Subspace Solvers

Richardson	GMRES	Hierarchical Krylov		BiCG Stabilized
Chebychev	TFQMR	LSQR	SYMMLQ	CG IBCGS

Preconditioners

Blocks (by field)	Additive Schwarz	ILU/ICC
Schur Complement	Algebraic Multigrid	Geometric Multigrid

Matrices

Compressed Sparse Row (AIJ)	Block AIJ	Matrix Blocks (MatNest)
Symmetric Block AIJ	Dense	GPU & PThread Matrices

Vectors **Index Sets**

In PETSc, objects at higher levels of abstraction use lower-level objects.

Solver use in SNES ex62

Solver code does not change for different algorithms:

```
SNES           snes;
Vec            u, r;
PetscErrorCode ierr;

ierr = SNESCreate(PETSC_COMM_WORLD, &snes);CHKERRQ(ierr);
/* Specify residual computation */
ierr = SNESSetFromOptions(snes);CHKERRQ(ierr); /* Configure solver */
ierr = SNESSolve(snes, PETSC_NULL, u);CHKERRQ(ierr);
```

- Never recompile! all configuration is dynamic
- Factories are hidden from the user
- Type of nested solvers can be changed at runtime

Solver use in SNES ex62

I will omit error checking and declarations:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
/* Specify residual computation */
SNESSetFromOptions(snes); /* Configure solver */
SNESSolve(snes, PETSC_NULL, u);
```

Solver use in SNES ex62

The configuration API can also be used:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
/* Specify residual computation */
SNESNGMRESSetRestartType(snes, SNES_NGMRES_RESTART_PERIODIC);
SNESSetFromOptions(snes);
SNESSolve(snes, PETSC_NULL, u);
```

- Ignored when not applicable (no ugly check)
- Type safety of arguments is retained
- No downcasting

Solver use in SNES ex62

Adding a prefix namespaces command line options:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
/* Specify residual computation */
SNESSetOptionsPrefix(snes, "stokes_");
SNESSetFromOptions(snes);
SNESSolve(snes, PETSC_NULL, u);
```

`-stokes_snes_type qn` changes the solver type,

whereas `-snes_type qn` does not

Solver use in SNES ex62

User provides a function to compute the residual:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetFunction(snes, r, FormFunction, &user);
SNESSetFromOptions(snes);
SNESSolve(snes, PETSC_NULL, u);
```

$$r = F(u)$$

- User handles parallel communication
- User handles domain geometry and discretization

Solver use in SNES ex62

DM allows the user to compute only on a local patch:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, user.dm);
SNESSetFunction(snes, r, SNESDMComputeFunction, &user);
SNESSetFromOptions(snes);
SNESSolve(snes, PETSC_NULL, u);

DMSetLocalFunction(user.dm, (DMLocalFunction1) FormFunctionLocal);
```

- Code looks serial to the user
- PETSc handles global residual assembly

Solver use in SNES ex62

Optionally, the user can also provide a Jacobian:

```
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, user.dm);
SNESSetFunction(snes, r, SNESDMComputeFunction, &user);
SNESSetJacobian(snes, A, J, SNESDMComputeJacobian, &user);
SNESSetFromOptions(snes);
SNESSolve(snes, PETSC_NULL, u);

DMSetLocalFunction(user.dm, (DMLocalFunction1) FormFunctionLocal);
DMSetLocalJacobian(user.dm, (DMLocalJacobian1) FormJacobianLocal);
```

SNES ex62 allows both

- finite difference (JFNK), and
- FEM action

versions of the Jacobian.

Solver use in SNES ex62

The **DM** also handles storage:

```
CreateMesh(PETSC_COMM_WORLD, &user, &user.dm);
DMCreateGlobalVector(user.dm, &u);
VecDuplicate(u, &r);
DMCreateMatrix(user.dm, MATAIJ, &J);
```

- DM can create local and global vectors
- Matrices are correctly preallocated

Basic Solver Usage

Use `SNESSetFromOptions()` so that everything is set dynamically

- Set the type
  - Use `-snes_type` (or take the default)
- Set the preconditioner
  - Use `-npc_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

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

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

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

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

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

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
```

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

The Great Solver Schism: Monolithic or Split?

Monolithic

- Direct solvers
- Coupled Schwarz
- Coupled Neumann-Neumann (need unassembled matrices)
- Coupled multigrid

X Need to understand local spectral and compatibility properties of the coupled system

Split

- Physics-split Schwarz (based on relaxation)
- Physics-split Schur (based on factorization)
  - approximate commutators SIMPLE, PCD, LSC
  - segregated smoothers
  - Augmented Lagrangian
  - “parabolization” for stiff waves

X Need to understand global coupling strengths

- Preferred data structures depend on which method is used.
- Interplay with geometric multigrid.

FieldSplit Preconditioner

- Analysis
  - Use **IS**es to define fields
  - Decouples **PC** from problem definition
- Synthesis
  - Additive, Multiplicative, Schur
  - Commutes with Multigrid

FieldSplit Options

- Analysis
  - `-pc_fieldsplit_<split num>_fields 2,1,5`
  - `-pc_fieldsplit_detect_saddle_point`
- Synthesis
  - `-pc_fieldsplit_type`
  - `-pc_fieldsplit_real_diagonal`
    Use diagonal blocks of operator to build PC
- Schur complements
  - `-pc_fieldsplit_schur_precondition <self,user,diag>`
    How to build preconditioner for S
  - `-pc_fieldsplit_schur_factorization_type <diag,lower,upper,full>`
    Which off-diagonal parts of the block factorization to use

Stokes example

The common block preconditioners for Stokes require only options:

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

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
```

PC

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

Cohouet & Chabard, Some fast 3D finite element solvers for the generalized Stokes problem, 1988.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type multiplic

-fieldsplit_0_pc_type hypre
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

PC

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

Elman, Multigrid and Krylov subspace methods for the discrete Stokes equations, 1994.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type diag
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.
Olshanskii, Peters, and Reusken, Uniform preconditioners for a parameter dependent saddle point problem with application to generalized Stokes interface equations, 2006.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type lower
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type upper
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type lsc
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type upper
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.
Kay, Loghin and Wathen, A Preconditioner for the Steady-State N-S Equations, 2002.
Elman, Howle, Shadid, Shuttleworth, and Tuminaro, Block preconditioners based on approximate commutators, 2006.

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
```

PC

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

FEM Setup

```
./bin/pythonscripts/PetscGenerateFEMQuadrature.py
  2 2 2 1 laplacian
  2 1 1 1 gradient
  src/snes/examples/tutorials/ex62.h
```

Jacobi

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_gmres_restart 100 -ksp_rtol 1.0e-9
    -ksp_monitor_short
  -pc_type jacobi
```

Block diagonal

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type additive
  -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_pc_type jacobi
```

Block triangular

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type multiplicati
  -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_pc_type jacobi
```

Diagonal Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type diag
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Upper triangular Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type upper
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Lower triangular Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type lower
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Full Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type full
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Outline

Outline

5 DM
- PetscSection and DMComplex
- Vec and Mat Particulars

What does a DM do?

- Problem Definition
  - Discretization/Dof mapping (**PetscSection**)
  - Residual calculation
- Decomposition
  - Partitioning, `DMCreateSubDM()`
  - **Vec** and **Mat** creation
  - Global $\Longleftrightarrow$ Local mapping
- Hierarchy
  - `DMCoarsen()` and `DMRefine()`
  - `DMInterpolate()` and `DMRestrict()`
  - Hooks for resolution-dependent data

PetscSection
What Is It?

Similar to **PetscLayout**, maps point $\longrightarrow$ (size, offset)

- Processes are replaced by points
  - Also what we might use for multicore **PetscLayout**
- Boundary conditions are just another **PetscSection**
  - Map points to number of constrained dofs
  - Offsets into integer array of constrained local dofs
- Fields are just another PetscSection
  - Map points to number of field dofs
  - Offsets into array with all fields
- Usable by all **DM** subclasses
  - Structured grids with **DMDA**
  - Unstructured grids with **DMComplex**

PetscSection
Why Use It?

PETSc Solvers only understand Integers

Decouples Mesh From Discretization

- Mesh does not need to know how dofs are generated, just how many are attached to each point.
- It does not matter whether you use FD, FV, FEM, etc.

Decouples Mesh from Solver

- Solver gets the data layout and partitioning from **Vec** and **Mat**, nothing else from the mesh.
- Solver gets restriction/interpolation matrices from **DM**.

Decouples Discretization from Solver

- Solver only gets the field division, nothing else from discretization.

PetscSection
How Do I Build One?

High Level Interface

```
DMComplexCreateSection(
    DM dm, PetscInt dim, PetscInt numFields,
      PetscInt numComp[], PetscInt numDof[],
    PetscInt numBC, PetscInt bcField[], IS bcPoints[],
    PetscSection *section);
```

Discretization	Dof/Dimension
$P_1 - P_0$	[2 0 0 0 | 0 0 0 1]
$Q_2 - Q_1$	[2 2 0 0 | 1 0 0 0]
$Q_2 - P_1^{\mathrm{disc}}$	[2 2 0 0 | 0 0 0 4]

PetscSection
How Do I Build One?

Low Level Interface

```
PetscSectionCreate(PETSC_COMM_WORLD, &s);
PetscSectionSetNumFields(s, 2);
PetscSectionSetFieldComponents(s, 0, 3);
PetscSectionSetFieldComponents(s, 1, 1);
PetscSectionSetChart(s, cStart, vEnd);
for(PetscInt v = vStart; v < vEnd; ++v) {
  PetscSectionSetDof(s, v, 3);
  PetscSectionSetFieldDof(s, v, 0, 3);
}
for(PetscInt c = cStart; c < cEnd; ++c) {
  PetscSectionSetDof(s, c, 1);
  PetscSectionSetFieldDof(s, c, 1, 1);
}
PetscSectionSetUp(s);
```

DMComplex
What is It?

DMComplex stands for a DM modeling a CW Complex

- Handles any kind of mesh
  - Simplicial
  - Hex
  - Hybrid
  - Non-manifold
- Small interface
  - Simple to input a mesh using the API
- Accepts mesh generator input
  - ExodusII, Triangle, TetGen, LaGriT, Cubit

DMComplex
How Do I Use It?

The operations used in SNES ex62 get and set values from a **Vec**, organized by the **DM** and **PetscSection**

```
DMComplexVecGetClosure(
  DM dm, PetscSection section, Vec v, PetscInt point,
  PetscInt *csize, const PetscScalar *values[])
```

- Element vector on cell
- Coordinates on cell vertices

Used in `FormFunctionLocal()`,

```
for(c = cStart; c < cEnd; ++c) {
  const PetscScalar *x;

  DMComplexVecGetClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
  for(PetscInt i = 0; i < cellDof; ++i) {
    u[c*cellDof+i] = x[i];
  }
  DMComplexVecRestoreClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
}
```

DMComplex
How Do I Use It?

The operations used in SNES ex62 get and set values from a **Vec**, organized by the **DM** and **PetscSection**

```
DMComplexVecGetClosure(
  DM dm, PetscSection section, Vec v, PetscInt point,
  PetscInt *csize, const PetscScalar *values[])
```

- Element vector on cell
- Coordinates on cell vertices

Used in `FormFunctionLocal()`,

```
for(c = cStart; c < cEnd; ++c) {
  const PetscScalar *x;

  DMComplexVecGetClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
  for(PetscInt i = 0; i < cellDof; ++i) {
    u[c*cellDof+i] = x[i];
   }
  DMComplexVecRestoreClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
}
```

DMComplex
How Do I Use It?

The operations used in SNES ex62 get and set values from a **Vec**, organized by the **DM** and **PetscSection**

```
DMComplexVecSetClosure(
  DM dm, PetscSection section, Vec v, PetscInt point,
  const PetscScalar values[], InsertMode mode)
DMComplexMatSetClosure(
  DM dm, PetscSection section, PetscSection globalSection, Mat A, PetscInt
  PetscScalar values[], InsertMode mode)
```

- Element vector and matrix on cell

Used in `FormJacobianLocal()`,

```
for(c = cStart; c < cEnd; ++c) {
  DMComplexMatSetClosure(dm, PETSC_NULL, PETSC_NULL, JacP, c,
                         &elemMat[c*cellDof*cellDof], ADD_VALUES);
}
```

DMComplex
How Do I Use It?

The operations used in SNES ex62 get and set values from a **Vec**, organized by the **DM** and **PetscSection**

```
DMComplexVecSetClosure(
  DM dm, PetscSection section, Vec v, PetscInt point,
  const PetscScalar values[], InsertMode mode)
DMComplexMatSetClosure(
  DM dm, PetscSection section, PetscSection globalSection, Mat A, PetscInt
  PetscScalar values[], InsertMode mode)
```

- Element vector and matrix on cell

Used in `FormJacobianLocal()`,

```
for(c = cStart; c < cEnd; ++c) {
  DMComplexMatSetClosure(dm, PETSC_NULL, PETSC_NULL, JacP, c,
                         &elemMat[c*cellDof*cellDof], ADD_VALUES);
}
```

DMComplex
How Do I Use It?

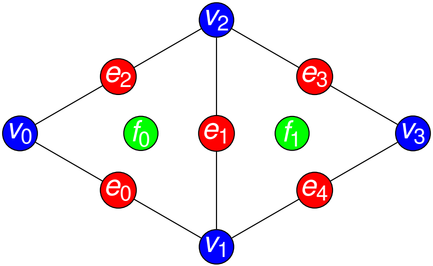
The functions above are built upon

```
DMComplexGetTransitiveClosure(
  DM dm, PetscInt p, PetscBool useCone,
  PetscInt *numPoints, PetscInt *points[])
```

- Returns points *and* orientations
- Iterate over points to stack up the data in the array

DMComplex
SNES ex62

$P_2 - P_1$ Stokes Example

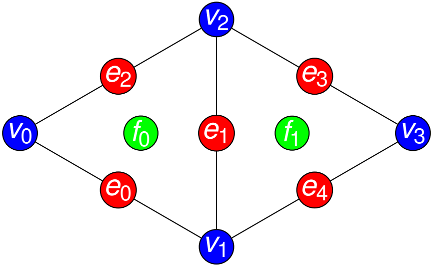


Naively, we have

$$\mathrm{cl}(\mathrm{cell}) = [f e_0\, e_1\, e_2\, v_0\, v_1\, v_2]$$
$$x(\mathrm{cell}) = [u_{e_0}\, v_{e_0}\, u_{e_1}\, v_{e_1}\, u_{e_2}\, v_{e_2}\; u_{v_0}\, v_{v_0}\, p_{v_0}\, u_{v_1}\, v_{v_1}\, p_{v_1}\, u_{v_2}\, v_{v_2}\, p_{v_2}]$$

DMComplex
SNES ex62

$P_2 - P_1$ Stokes Example



We reorder so that fields are contiguous

$$x'(\text{cell}) = \begin{array}{l}[u_{e_0} v_{e_0} u_{e_1} v_{e_1} u_{e_2} v_{e_2} \\ u_{v_0} v_{v_0} u_{v_1} v_{v_1} u_{v_2} v_{v_2} \\ p_{v_0} p_{v_1} p_{v_2} \qquad\qquad]\end{array}$$

DMComplex
Basic Operations

- Cone
  - edge $\longrightarrow$ endpoints
  - cell $\longrightarrow$ faces
- Support
  - vertex $\longrightarrow$ edges
  - face $\longrightarrow$ cells
- Transitive Closure
  - cell $\longrightarrow$ faces, edges, vertices
- Meet
  - cells $\longrightarrow$ shared face
- Join
  - vertices $\longrightarrow$ shared cell

Outline

5 DM
- PetscSection and DMComplex
- Vec and Mat Particulars

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;

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
```

DMDAVecGetArray in C

```
DM             da;
Vec            v;
DMDALocalInfo *info;
PetscScalar  **array;

DMDAVecGetArray(da, v, &array);
for(j = info->ys; j < info->ys+info->ym; ++j) {
  for(i = info->xs; i < info->xs+info->xm; ++i) {
    u       = x[j][i];
    uxx     = (2.0*u - x[j][i-1] - x[j][i+1])*hydhx;
    uyy     = (2.0*u - x[j-1][i] - x[j+1][i])*hxdhy;
    f[j][i] = uxx + uyy;
  }
}
DMDAVecRestoreArray(da, v, &array);
```

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, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations