The Portable Extensible Toolkit for Scientific Computing

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PETSc Tutorial
CEMRACS Summer School
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Never believe *anything*,

unless you can run it.
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unless you can run it.
The PETSc Team

Bill Gropp
Barry Smith
Satish Balay
Jed Brown
Matt Knepley
Lisandro Dalcin
Hong Zhang
Mark Adams
Toby Issac
Timeline (Old People)

PETSc-1
Barry
Bill
Lois
Satish
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Hong
Kris
Matt
Victor
Dmitry
PETSc-2
1991
1995
MPI-1
MPI-2
2000
PETSc-3
2005
2010
2015
PETSc
Timeline (Young People)

PETSc-3

Lisandro
Jed
Shri
Peter
Jason
Mark
Patrick
Michael
Toby
Karl
Stefano
Dave

What I Need From You

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

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

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

2 PETSc Integration

3 DM

4 Advanced Solvers
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
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
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 for the parallel solution of nonlinear algebraic equations**

**Free**
- Free for everyone, including industrial users

**Supported**
- 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, Matlab, Julia, and Python
What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems
    - Cray XT6, BG/Q, NVIDIA Fermi, K Computer
  - 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
  - ECP, AMR Program, SciDAC, MICS Program, INL Reactor Program
- National Science Foundation
  - SI2, CIG, CISE, Multidisciplinary Challenge Program
- Intel Parallel Computing Center
Outline

1 Getting Started with PETSc
   - Who uses PETSc?
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     - How do I run an example?
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Who Uses PETSc?

Computational Scientists

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

- **Subsurface Flow and Porous Media**
  - STOMP (DOE)
  - PFLOTRAN (DOE)
Computational Scientists

- CFD
  - Firedrake
  - Fluidity
  - OpenFOAM
  - freeCFD
  - OpenFVM

- MicroMagnetics
  - MagPar

- Fusion
  - XGC
  - BOUT++
  - 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
  - libMesh
  - MOOSE
  - PETSc-FEM
  - Deal II
  - OOFEM

- Other Solvers
  - Fast Multipole Method (PetFMM)
  - Radial Basis Function Interpolation (PetRBF)
  - Eigensolvers (SLEPc)
  - Optimization (TAO)
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 1,500,000 cores efficiently
- Gordon Bell Prize Mantle Convection on IBM BG/Q Sequoia

PETSc applications have run at 23% of peak (600 Teraflops)
- Jed Brown on NERSC Edison
- HPGMG 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
  - DMProx mesh management

\[ ^a \text{Aagaard, Knepley, Williams} \]
Multiple Mesh Types

- Triangular
- Rectangular
- Tetrahedral
- 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

$^{aKatz}$
Magma Dynamics

- Couples scales
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- Physics
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- Code generation
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Katz, Speigelman
Fracture Mechanics

- Full variational formulation
  - Phase field
  - Linear or Quadratic penalty

- Uses TAO optimization
  - Necessary for linear penalty
  - Backtacking

- No prescribed cracks (movie)
  - Arbitrary crack geometry
  - Arbitrary intersections

- Multiple materials
  - Composite toughness

*a*Bourdin

Matt (Rice)

PETSc

K2I 24 / 225
Fracture Mechanics

1 Bourdin

Matt (Rice)  PETSc  K2I  24 / 225
Vortex Method

$\text{t = 000}$

- **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

$^a$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
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\[a\]Cruz, Yokota, Barba, Knepley
Incompressible Flow
- Gaussian vortex blobs
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PetRBF
- Variety of RBFs
- Uses PETSc solvers
- Scalable preconditioner

Parallelism
- MPI
- GPU

*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

\(^a\text{Cruz, Yokota, Barba, Knepley}\)
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

\(^a\text{Cruz, Yokota, Barba, Knepley}\)
Vortex Method

- 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

\(^a\)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

\(^a\)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

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\(^a\)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

\[ ^a \text{Cruz, Yokota, Barba, Knepley} \]
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* May, Knepley
Rheologies
- Maxwell
- Grade 2
- Oldroyd-B

Stabilization
- DG
- SUPG
- EVSS
- DEVSS
- Macroelement

Automation
- FIAT (elements)
- FFC (weak forms)
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

\textsuperscript{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
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\[a\] Fuentes, Oden, et.al.
Outline

1. Getting Started with 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`
Getting Started with 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?
The latest tarball is on the PETSc site:  
http://www.mcs.anl.gov/petsc/download

There is a Debian package (aptitude install petsc-dev)

There is a Git development repository
Cloning PETSc

- The full development repository is open to the public
  - https://bitbucket.org/petsc/petsc/
- 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
  - You can easily submit changes using a pull request
- All releases are just tags:
  - Source at tag v3.7.2
Unpacking PETSc

- Just clone development repository
  - `git clone http://bitbucket.org/petsc/petsc.git`
  - `git checkout -rv3.7.2`

- or

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

Download and Unpack PETSc!
Getting Started with 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
- Config files in \$PETSC_DIR/\$PETSC_ARCH/lib/petsc/conf
- Config header in \$PETSC_DIR/\$PETSC_ARCH/include
- \$PETSC_ARCH\ has a default if not specified
You can easily reconfigure with the same options

- ./${PETSC_ARCH}/lib/petsc/conf/reconfigure-${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}/lib/petsc/conf/configure.log

ALWAYS send this file with bug reports
$PETSC_DIR/configure
  –download-triangle –download-ctetgen –download-p4est
  –download-chaco –download-metis –download-parmetis
  –download-pragmatic
  –download-hdf5 –download-netcdf –download-exodusii
  –download-gmp –download-mpfr
Configuring PETSc for FEM

$PETSC_DIR/configure
   –download-triangle –download-ctetgen –download-p4est
   –download-chaco  –download-metis  –download-parmetis
   –download-pragmatic
   –download-hdf5   –download-netcdf  –download-exodusii
   –download-gmp    –download-mpfr
$PETSC_DIR/configure

–download-triangle
–download-ctetgen
–download-p4est
–download-chaco
–download-metis
–download-parmetis
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  –download-pragmatic
  –download-hdf5  –download-netcdf  –download-exodusii
  –download-gmp  –download-mpfr
Configuring PETSc for Accelerators

```
$PETSC_DIR/configure
  --with-cuda
  --with-cudac='nvcc -m64' --with-cuda-arch=sm_10
  --with-cuda-only
  --with-opencl
  --with-opencl-include=/System/Library/Frameworks/OpenCL.framework/Headers/
  --with-opencl-lib=/System/Library/Frameworks/OpenCL.framework/OpenCL
  --with-precision=single
```
Configuring PETSc for Accelerators

$PETSC_DIR/configure
   --with-cuda
   --with-cudac='nvcc -m64' --with-cuda-arch=sm_10
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  --with-precision=single
$PETSC_DIR$/configure

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      --with-opencl-lib=/System/Library/Frameworks/OpenCL.framework/OpenCL
   --with-precision=single
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  --with-cuda-only
  --with-opencl
  --with-opencl-include=/System/Library/Frameworks/OpenCL.framework/Headers/
  --with-opencl-lib=/System/Library/Frameworks/OpenCL.framework/OpenCL
  --with-precision=single
Getting Started with PETSc

How do I Configure PETSc?

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, mpi4py
- PETSc documentation utilities (Sowing, c2html)
- BLAS, LAPACK, Elemental, ScaLAPACK
- MPICH, OpenMPI
- ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
- SuiteSparse, MUMPS, SuperLU, SuperLU_Dist, PaStiX, Pardiso
- HYPRE, ML
- BLOPEX, FFTW, STRUMPACK, SPAI, CUSP, Sundials
- Triangle, TetGen, p4est, Pragmatic
- HDF5, NetCDF, ExodusII
- AfterImage, gifLib, libjpeg, opengl
- GMP, MPFR
- ConcurrencyKit, hwloc
Configure your downloaded PETSc.
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There is now One True Way to build PETSc:

- make
- make install if you configured with --prefix
- Check build when done with make test

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/lib/petsc/conf/make.log
- ALWAYS send this with bug reports
Build your configured PETSc.
Exercise 4

Reconfigure PETSc to use ParMetis.

1. `linux-debug/lib/petsc/conf/reconfigure-linux-debug.py`
   - `--PETSC_ARCH=linux-parmetis`
   - `--download-metis --download-parmetis`

2. `PETSC_ARCH=linux-parmetis make`

3. `PETSC_ARCH=linux-parmetis make test`
Getting Started with PETSc

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Running PETSc

- Try running PETSc examples first
  - `cd $PETSC_DIR/src/snes/examples/tutorials`
- Build examples using make targets
  - `make ex5`
- Run examples using the make target
  - `make runex5`
- Can also run using MPI directly
  - `mpirun ./ex5 -snes_max_it 5`
  - `mpiexec ./ex5 -snes_monitor`
Running PETSc with Python

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

How do I run an example?

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
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:sol.bin::, -vec_view ::matlab, -vec_view socket`
- Sometimes provides extra information
  - `-mat_view ::ascii_info, -mat_view ::ascii_info_detailed`
- Use `-help` to see all options
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`
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Getting More Help

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

1. Getting Started with PETSc

2. PETSc Integration
   - Initial Operations
   - Vector Algebra
   - Matrix Algebra
   - Algebraic Solvers
   - Debugging PETSc
   - Profiling PETSc
   - Serial Performance

3. DM

4. Advanced Solvers
OUTLINE

2. PETSc Integration
   - Initial Operations
   - Vector Algebra
   - Matrix Algebra
   - Algebraic Solvers
   - Debugging PETSc
   - Profiling PETSc
   - Serial Performance
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 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

Integration Stages

- **Version Control**
  - It is impossible to overemphasize
  - We use Git

- **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
Profilers

- 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
PETSc Integration

Initial Operations

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
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What are PETSc vectors?

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

- Each process locally owns a subvector of contiguous global data
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
A PETSc Vec

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

`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(v)`
- `VecAssemblyEnd(v)`
One Way to Set the Elements of a Vector

```c
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

```c
VecGetOwnershipRange(x, &low, &high);
val = low*10.0;
for (i = low; i < high; ++i) {
    VecSetValues(x, 1, &i, &val, INSERT_VALUES);
    val += 10.0;
}
/* No data will be communicated here */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
```
## Selected Vector Operations

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

- PETSc allows you to access the local storage with
  
  VecGetArray(Vec, double *[])

- You must return the array to PETSc when you finish
  
  VecRestoreArray(Vec, double *[])

- Allows PETSc to handle data structure conversions
  
  Commonly, these routines are fast and do not involve a copy
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

```c
#include "finCLUDE/petsc.h"

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

call VecGetArray(v, array, offset, ierr)
call VecGetLocalSize(v, n, ierr)
do i=1,n
    array(i+offset) = array(i+offset) + rank
end do
call VecRestoreArray(v, array, offset, ierr)
```
VecGetArray in F90

```c
#include "finclude/petsc.h90"

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

call VecGetArrayF90(v, array, ierr)
call VecGetLocalSize(v, n, ierr)
do i=1,n
    array(i) = array(i) + rank
end do
call VecRestoreArrayF90(v, array, ierr)
```
with v as a:
    for i in range(len(a)):
        a[i] = 5.0*i
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);
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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[])
- **MatXAIJPreallocation**(Mat, bs, dnz[], onz[], dnzu[], onzu[])
- **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()
  - MatGetLocalSubMatrix()
- 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(Matm, 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(Matm, MatAssemblyType type)
- MatAssemblyEnd(Matm, 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

```c
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_VALUES);
        } else if (row == N-1) {
            MatSetValues(A, 1, &row, 2, cols, v, INSERT_VALUES);
        } else {
            MatSetValues(A, 1, &row, 3, cols, v, INSERT_VALUES);
        }
    }
}
MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
```
Parallel Sparse Matrix Layout

- **proc 0**
  - diagonal blocks
  - offdiagonal blocks

- **proc 1**
  - diagonal blocks

- **proc 2**
  - diagonal blocks

- **proc 3**
  - diagonal blocks

- **proc 4**
  - diagonal blocks

- **proc 5**
  - diagonal blocks
  - offdiagonal blocks
A Better Way to Set the Elements of a Matrix
Simple 3-point stencil for 1D Laplacian

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

\[ \text{MatGetOwnershipRange}(A, \& \text{start}, \& \text{end}); \]

\[ \text{for} \ (\text{row} = \text{start}; \ \text{row} < \text{end}; \ \text{row}++) \ { \]
\[ \quad \text{cols}[0] = \text{row}-1; \quad \text{cols}[1] = \text{row}; \quad \text{cols}[2] = \text{row}+1; \]
\[ \quad \text{if} \ (\text{row} == 0) \ { \]
\[ \quad \quad \text{MatSetValues}(A,1,\& \text{row},2,\& \text{cols}[1],\& v[1],\text{INSERT_VALUES}); \]
\[ \quad } \]
\[ \quad } \]
\[ \quad \text{else if} \ (\text{row} == \text{N}-1) \ { \]
\[ \quad \quad \text{MatSetValues}(A,1,\& \text{row},2,\text{cols},v,\text{INSERT_VALUES}); \]
\[ \quad } \]
\[ \quad } \]
\[ \quad \text{else} \ { \]
\[ \quad \quad \text{MatSetValues}(A,1,\& \text{row},3,\text{cols},v,\text{INSERT_VALUES}); \]
\[ \quad } \]
\[ } \]
\[ \text{MatAssemblyBegin}(A, \text{MAT_FINAL_ASSEMBLY}); \]
\[ \text{MatAssemblyEnd}(A, \text{MAT_FINAL_ASSEMBLY}); \]
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
  - It's better to partition and reorder the underlying grid
- Matrix decomposition in contiguous chunks is simple
  - Makes interoperation with other codes easier
  - For other ordering, PETSc provides “Application Orderings” (AO)
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Proof is not currently enough to examine solvers

Using PETSc linear algebra, just add:

- `KSPSetOperators(KSP ksp, Mat A, Mat M, Mat Structure 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

Using PETSc linear algebra, just add:

- `SNESSetFunction(SNESsnes, Vecr, residualFunc, void *ctx)`
- `SNESSetJacobian(SNESsnes, MatA, MatM, jacFunc, void *ctx)`
- `SNESSSolve(SNESsnes, Vecb, Vecx)`

Can access subobjects

- `SNESGetKSP(SNESsnes, 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)
- 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
3rd Party Solvers in PETSc

Complete table of solvers

- **Sequential LU**
  - ESSL (IBM)
  - SuperLU (Sherry Li, LBNL)
  - Suitesparse (Tim Davis, U. of Florida)
  - LUSOL (MINOS, Michael Saunders, Stanford)
  - PILUT (Hypre, David Hysom, LLNL)

- **Parallel LU**
  - Elemental/Clique (Jack Poulson, Google)
  - MUMPS (Patrick Amestoy, IRIT)
  - SuperLU_Dist (Jim Demmel and Sherry Li, LBNL)
  - Pardiso (MKL, Intel)
  - STRUMPACK (Pieter Ghysels, LBNL)

- **Parallel Cholesky**
  - Elemental (Jack Poulson, Google)
  - DSCPACK (Padma Raghavan, Penn. State)
  - MUMPS (Patrick Amestoy, Toulouse)
Complete table of solvers

- Parallel Algebraic Multigrid
  - GAMG (Mark Adams, LBNL)
  - BoomerAMG (Hypre, LLNL)
  - ML (Trilinos, Ray Tuminaro and Jonathan Hu, SNL)
- Parallel BDDC (Stefano Zampini, KAUST)
- Parallel ILU, PaStiX (Faverge Mathieu, INRIA)
- Parallel Redistribution (Dave May, Oxford)
- Parallel Sparse Approximate Inverse
  - Parasails (Hypre, Edmund Chow, LLNL)
  - SPAI 3.0 (Marcus Grote and Barnard, NYU)
### User Solve

```c
MPI_Comm comm;
SNES snes;
DM dm;
Vec u;

SNESCreate(comm, &snes);
SNESSetDM(snes, dm);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNESolve(snes, NULL, u);
```
Solver use in SNES ex62

Solver code does not change for different algorithms:

```c
SNES snes;
DM dm;
Vec u;
PetscErrorCode ierr;

ierr = SNESCreate(PETSC_COMM_WORLD, &snes);CHKERRQ(ierr);
ierr = SNESSetDM(snes, dm);CHKERRQ(ierr);
/* Specify residual computation */
ierr = SNESSetFromOptions(snes);CHKERRQ(ierr); /* Configure solver */
ierr = DMCreateGlobalVector(dm, &u);CHKERRQ(ierr);
ierr = SNES Solve(snes, PETSC_NULL, u);CHKERRQ(ierr);
```

- Never recompile! all configuration is dynamic
- **DM** controls data layout and communication
- Type of nested solvers can be changed at runtime
Solver use in SNES ex62

I will omit error checking and declarations:

```c
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, dm);
/* Specify residual computation */
SNESSetFromOptions(snes); /* Configure solver */
DMCreateGlobalVector(dm, &u);
SNESSolve(snes, PETSC_NULL, u);
```
Solver use in SNES ex62

The configuration API can also be used:

```c
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, dm);
/* Specify residual computation */
SNESNGMRESSetRestartType(snes, SNES_NGMRES_RESTART_PERIODIC);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNESolve(snes, PETSC_NULL, u);
```

- Ignored when not applicable (no ugly check)
- Type safety of arguments is retained
- No downcasting
Adding a prefix namespaces command line options:

```c
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, dm);
/* Specify residual computation */
SNESSetOptionsPrefix(snes, "stokes_");
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
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);
SNESSetDM(snes, dm);
DMCreateGlobalVector(dm, &r);
SNESSetFunction(snes, r, FormFunction, &user);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNESolve(snes, PETSC_NULL, u);
```

\[ r = F(u) \]

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

Algebraic Solvers

Solver use in SNES ex62

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

```c
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, dm);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNESolve(snes, PETSC_NULL, u);

DMSNESSetLocalFunction(dm, FormFunctionLocal);
```

- Code looks serial to the user
- PETSc handles global residual assembly
- Also works for unstructured meshes
Solver use in SNES ex62

Optionally, the user can also provide a Jacobian:

```c
SNESCreate(PETSC_COMM_WORLD, &snes);
SNESSetDM(snes, dm);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNES_solve(snes, PETSC_NULL, u);

DMSNESSetLocalFunction(dm, FormFunctionLocal);
DMSNESSetLocalJacobian(dm, 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:

```c
CreateMesh(PETSC_COMM_WORLD, &user, &dm);
DMCreateLocalVector(dm, &lu);
DMCreateGlobalVector(dm, &u);
DMCreateMatrix(dm, &J);
```

- DM can create local and global vectors
- Matrices are correctly preallocated
- Easy supported for discretization
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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 \texttt{PetscError()} to catch errors as they occur.
- PETSc tracks memory overwrites at both ends of arrays.
  - The \texttt{CHKMEMQ} macro causes a check of all allocated memory.
  - Track memory overwrites by bracketing them with \texttt{CHKMEMQ}.
- PETSc checks for leaked memory.
  - Use \texttt{PetscMalloc()} and \texttt{PetscFree()} for all allocation.
  - Print unfreed memory on \texttt{PetscFinalize()} with \texttt{-malloc_dump}.
- Simply the best tool today is \texttt{valgrind}.
  - It checks memory access, cache performance, memory usage, etc.
  - \texttt{http://www.valgrind.org}
  - Need \texttt{--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
  - hg update -r2

- Build it and run again smoothly
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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 identified 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
```c
int stageNum;
PetscLogStageRegister(&stageNum, "name");
PetscLogStagePush(stageNum);

/* Code to Monitor */
PetscLogStagePop();
```
with PETSc.LogStage('Fluid Stage') as fluidStage:
    # All operations will be aggregated in fluidStage
    fluid.solve()
Adding A Logging Event

C

```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);
```
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)
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 routines for all datatypes
  - \texttt{MatSeqAIJSetPreallocation()}
  - \texttt{MatMPIAIJSetPreallocation()}
  - Only the relevant data will be used
Matrix Memory Preallocation
Sequential Sparse Matrices

\texttt{MatSeqAIJPreallocation(MatA, int nz, int nnz[])}

- **nz**: expected number of nonzeros in any row
- **nnz(i)**: expected number of nonzeros in row i
Matrix Memory Preallocation

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

- MatGetOwnershipRange(MatA, 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(MatA, 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:

\[ \text{proc #] Matrix size: } \%d \times \%d; \text{ storage space: } \%d \text{ unneeded, } \%d \text{ used} \]

\[ \text{proc #] Number of mallocs during MatSetValues( ) is } \%d \]

```bash
[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 Exercise 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

2 PETSc Integration
- Initial Operations
- Vector Algebra
- Matrix Algebra
- Algebraic Solvers
- Debugging PETSc
- Profiling PETSc
- Serial Performance
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* $\beta$, is the ratio of flops executed to bytes transferred.

- We will designate the unit $\frac{\text{flop}}{\text{byte}}$ as the *Keyes*
- Using the peak flop rate $r_{\text{peak}}$, we can get the required bandwidth $B_{\text{req}}$ for an algorithm
  \[ B_{\text{req}} = \frac{r_{\text{peak}}}{\beta} \]  
  \[ (1) \]
- Using the peak bandwidth $B_{\text{peak}}$, we can get the maximum flop rate $r_{\text{max}}$ for an algorithm
  \[ r_{\text{max}} = \beta B_{\text{peak}} \]
  \[ (2) \]
Performance Caveats

- The peak flop rate $r_{\text{peak}}$ 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):

$$c_1 = c_1 + a_1 \times b_1$$
$$c_2 = c_2 + a_2 \times b_2$$

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 $\text{axpy}()$

\[
\vec{y} \leftarrow \alpha \vec{x} + \vec{y}
\]

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

- **Computation**
  - $2N$ flops

- **Memory Access**
  - $(3N + 1)b$ bytes

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

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

For Matt’s Laptop,

- $r_{\text{peak}} = 1700 \text{MF/s}$
  - implies that
- $B_{\text{req}} = 2550b \text{ MB/s}$
  - Much greater than $B_{\text{peak}}$

- $B_{\text{peak}} = 1122 \text{MB/s}$
  - implies that
- $r_{\text{max}} = \frac{748}{b} \text{ MF/s}$
  - 5.5% of $r_{\text{peak}}$
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

<table>
<thead>
<tr>
<th>Machine</th>
<th>Peak (MF/s)</th>
<th>Triad (MB/s)</th>
<th>MF/MW</th>
<th>Eq. MF/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matt’s Laptop</td>
<td>1700</td>
<td>1122.4</td>
<td>12.1</td>
<td>93.5 (5.5%)</td>
</tr>
<tr>
<td>Intel Core2 Quad</td>
<td>38400</td>
<td>5312.0</td>
<td>57.8</td>
<td>442.7 (1.2%)</td>
</tr>
<tr>
<td>Tesla 1060C</td>
<td>984000</td>
<td>102000.0*</td>
<td>77.2</td>
<td>85000.0 (0.8%)</td>
</tr>
</tbody>
</table>

**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

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

or achievable performance given a bandwidth $BW$

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

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

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

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

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

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, . . . )
Consider the Gram-Schmidt Orthogonalization process. Starting with a set of vectors \( \{v_i\} \), create a set of orthonormal vectors \( \{n_i\} \).

\[
\begin{align*}
n_1 &= \frac{v_1}{\|v_1\|} \\
n_2 &= \frac{w_2}{\|w_2\|} \quad \text{where} \quad w_2 = v_2 - (n_1 \cdot v_2)n_1 \\
n_k &= \frac{w_k}{\|w_k\|} \quad \text{where} \quad w_k = v_k - \sum_{j<k} (n_j \cdot v_k)n_j
\end{align*}
\]

What is
1. the balance factor \( \beta \) for this algorithm?
2. the bandwidth required to run at peak \( (B_{\text{req}}) \) on your computer?
3. the maximum achievable flop rate \( (r_{\text{max}}) \) on your computer?

Extra Credit: Can this algorithm be improved?
Run SNES ex5 for a variety of solver and preconditioner combinations. Plot the total number of linear iterations against the problem size.
DM Interface

- **Allocation**
  - DMCreateGlobalVector(DM, Vec *)
  - DMCreateLocalVector(DM, Vec *)
  - DMCreateMatrix(DM, MatType, Mat *)

- **Mapping**
  - DMGlobalToLocalBegin/End(DM, Vec, InsertMode, Vec)
  - DMLocalToGlobalBegin/End(DM, Vec, InsertMode, Vec)
  - DMGetLocalToGlobalMapping(DM, IS *)
Geometry
- DMGetCoordinateDM(DM, DM *)
- DMGetCoordinates(DM, Vec *)
- DMGetCoordinatesLocal(DM, Vec *)

Layout
- DMGetDefaultSection(DM, PetscSection *)
- DMGetDefaultGlobalSection(DM, PetscSection *)
- DMGetDefaultSF(DM, PetscSF *)
DM Interface

- **Hierarchy**
  - `DMRefine(DM, MPI_Comm, DM *)`
  - `DMCoarsen(DM, MPI_Comm, DM *)`
  - `DMGetSubDM(DM, MPI_Comm, DM *)`

- **Intergrid transfer**
  - `DMGetInterpolation(DM, DM, Mat *, Vec *)`
  - `DMGetAggregates(DM, DM, Mat *)`
  - `DMGetInjection(DM, DM, VecScatter *)`
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.
Outline

3 DM

- Structured Meshes (DMDA)
- Unstructured Meshes (DMPIlex/DMForest)
**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
  - `DMGlobalToLocalBegin/End()` and `DMLocalToGlobalBegin/End()`
Residual Evaluation

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

- FormFunctionLocal()
- FormJacobianLocal()

Callbacks are registered using

- SNESSetDM(), TSSetDM()
- DMSNESetFunctionLocal(), DMTSSetJacobianLocal()

When PETSc needs to evaluate the nonlinear residual $\mathbf{F}(\mathbf{x})$,

- 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

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

**Natural numbering**

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

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

**PETSc 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

<table>
<thead>
<tr>
<th>Proc 2</th>
<th>Proc 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>X X X X</td>
<td>X X</td>
</tr>
<tr>
<td>X X X</td>
<td>X X</td>
</tr>
<tr>
<td>12 13 14</td>
<td>15 X</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Proc 0</th>
<th>Proc 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 1 2</td>
<td>3 X</td>
</tr>
</tbody>
</table>

**Local numbering**

<table>
<thead>
<tr>
<th>Proc 2</th>
<th>Proc 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>21 22 23</td>
<td>28 29</td>
</tr>
<tr>
<td>18 19 20</td>
<td>26 27</td>
</tr>
<tr>
<td>15 16 17</td>
<td>24 25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Proc 0</th>
<th>Proc 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 7 8</td>
<td>13 14</td>
</tr>
<tr>
<td>3 4 5</td>
<td>11 12</td>
</tr>
<tr>
<td>0 1 2</td>
<td>9 10</td>
</tr>
</tbody>
</table>

**Global numbering**
DMDA Local Function

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

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

**info:** All layout and numbering information  
**x:** The current solution (a multidimensional array)  
**r:** The residual  
**ctx:** The user context passed to \text{DMDASNES}SetFunctionLocal()

The local DMDA function is activated by calling

\[
\text{DMDASNES}SetFunctionLocal(dm, \text{INSERT\_VALUES}, \text{lf}func, \ &ctx)
\]
Bratu Residual Evaluation

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

```c
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] = 2.0*(hydhx+hxdhy)*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);
    }
  }
}
```

$PETSC_DIR/src/snes/examples/tutorials/ex5.c$
DMDA Local Jacobian

User provided function calculates the Jacobian (in 2D)

\begin{verbatim}
(* ljac *)(DMDALocalInfo *info, PetscScalar**x, Mat J, void *ctx)
\end{verbatim}

**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

\begin{verbatim}
DMDASNESSetJacobianLocal(dm, ljac, &ctx)
\end{verbatim}
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);
            }
        }
    }
}
```

$PETSC_DIR/src/snes/examples/tutorials/ex5.c
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
  - \texttt{DMCreateGlobalVector(DM da, Vec *gvec)}

Local vectors are sequential (and usually temporary)
- Each process stores its local portion plus ghost values
  - \texttt{DMCreateLocalVector(DM da, Vec *lvec)}
- includes ghost and boundary 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 **DALocalToGlobalBegin/End()**.
Both the **box** stencil and **star** stencil are available.

### Box Stencil

```
proc 0   proc 1
```

### Star Stencil

```
proc 0   proc 1
```

**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 DMDA

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

**bd**: Specifies boundary behavior

- **DM_BOUNDARY_NONE**, **DM_BOUNDARY_GHOSTED**, or **DM_BOUNDARY_PERIODIC**

**type**: Specifies stencil

- **DMDA_STENCIL_BOX** or **DMDA_STENCIL_STAR**

**M/N**: Number of grid points in x/y-direction

**m/n**: Number of processes in x/y-direction

**dof**: Degrees of freedom per node

**s**: The stencil width

**lm/n**: Alternative array of local sizes

- Use **NULL** for the default
Viewing the DA

We use **SNES ex5**

- `ex5 -dm_view`
  - Shows both the DA and coordinate DA:
    - `ex5 -dm_view draw -draw_pause -1`
    - `ex5 -da_grid_x 10 -da_grid_y 10 -dm_view draw -draw_pause -1`

- `${PETSC_ARCH}/bin/mpiexec -n 4 ex5 -da_grid_x 10 -da_grid_y 10 -dm_view draw -draw_pause -1`
  - Shows PETSc numbering
DA Operators

- Evaluate only the local portion
  - No nice local array form without copies
- Use `MatSetValuesStencil()` to convert \((i,j,k)\) to indices

Also use **SNES ex48**

- `mpiexec -n 2
  ./ex5 -da_grid_x 10 -da_grid_y 10 -mat_view draw -draw_pause -1`

- `mpiexec -n 3
  ./ex48 -mat_view draw -draw_pause 1 -da_refine 3 -mat_type aij`
Viewing FD Operator Actions

We cannot currently visualize the 3D results,

- make runbratu EXTRA_ARGS="-run_test -vec_view_draw -draw_pause -1"
- make runbratu EXTRA_ARGS="-run_test -da_grid_x 10 -da_grid_y 10 -vec_view_draw -draw_pause -1"
- make runbratu EXTRA_ARGS="-run_test -dim 3 -vec_view"

but can check the ASCII output if necessary.
On two processes, I get a **SEGV**!

So we try running with:

- `make NP=2 debugbratu`  
  `EXTRA_ARGS="-run_test -vec_view_draw -draw_pause -1"`
- Spawns one debugger window per process
- SEGV on access to ghost coordinates
- Fix by using a local ghosted vector
  - Update to fixed version
- Notice
  - we already use ghosted assembly (completion) for FEM
  - FD does not need ghosted assembly
On two processes, I get a **SEGV**!

So we try running with:

- `make NP=2 debugbratu EXTRA_ARGS="-run\_test\_vec\_view\_draw\_draw\_pause\_1"

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So we try running with:

1. `make NP=2 debugbratu`
   
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2. Spawns one debugger window per process
3. **SEGV on access to ghost coordinates**
4. Fix by using a local ghosted vector
   
   - Update to fixed version

**Notice**

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Debugging Assembly

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Structured Functions

- Functions take values at the DA vertices
- Used as approximations to functions on the continuous domain
  - Values are really coefficients of linear basis
- User only constructs the local portion

```bash
cmpiexec -n 2 ./ex5 -run test -vec_view_draw -draw_pause -1```
Outline

3 DM

- Structured Meshes (DMDA)
- Unstructured Meshes (DMStuff/DMForest)
Problem

Traditional PDE codes cannot:

- Compare different discretizations
  - Different orders, finite elements
  - Finite volume vs. finite element

- Compare different mesh types
  - Simplicial, hexahedral, polyhedral

- Run 1D, 2D, and 3D problems

- Enable an optimal solver
  - Fields, auxiliary operators
Problem

Traditional Mesh/Solver Interface is Too **General**: 

- Solver not told about discretization data, e.g. fields
- Cannot take advantage of problem structure
  - blocking
  - saddle point structure
- Cannot use auxiliary data
  - Eigen-estimates
  - null spaces
Problem

Traditional Mesh/Solver Interface is Too **Specific**:

- Assembly code specialized to each discretization
  - dimension
  - cell shape
  - approximation space

- Explicit references to element type
  - `getVertices(faceID)`, `getAdjacency(edgeID, VERTEX)`, `getAdjacency(edgeID, dim = 0)`

- No interface for transitive closure
  - Awkward nested loops to handle different dimensions
Mesh Representation

We represent each mesh as a **Hasse Diagram**:

- Can represent any CW complex
- Can be implemented as a Directed Acyclic Graph
- Reduces mesh information to a single *covering* relation
- Can discover dimension, since meshes are ranked posets

We use an abstract *topological* interface to organize traversals for:

- discretization integrals
- solver size determination
- computing communication patterns

Mesh geometry is treated as just another mesh function.
Sample Meshes
Interpolated triangular mesh

Vertices
- 7
- 8
- 9
- 10

Edges
- 2
- 3
- 4
- 5
- 6

Cells
- 0
- 1

Depth
- Depth 0: 7, 8, 9, 10
- Depth 1: 2, 3, 4, 5, 6
- Depth 2: 0, 1
Sample Meshes
Optimized triangular mesh

Vertices: 2, 3, 4, 5
Cells: 0, 1
Depth 0: 2, 0, 3, 1, 4, 5
Depth 1: 0, 1

DM Unstructured Meshes (DMplex/DMForest)
Sample Meshes
Interpolated quadrilateral mesh
Sample Meshes
Optimized quadrilateral mesh

Vertices
2 3 4 5 6 7

Cells
0 1

Depth 0

Depth 1
Sample Meshes
Interpolated tetrahedral mesh

Vertices
18
19
20
21
22

Edges
9
10
11
12
13
14
15
16
17

Faces
2
3
4
5
6
7
8

Cells
0
1

Depth 0
Depth 1
Depth 2
Depth 3
Mesh Interface

By focusing on the key topological relations, the interface can be both concise and quite general

- Single relation
- Dual is obtained by reversing arrows
- Can associate functions with DAG points
  - Dual operation gives the support of the function

We begin with the basic covering relation, 
cone(0) = \{2, 3, 4\}
Basic Operations

Support

reverse arrows to get the dual operation,
support(9) = {3, 4, 6}
Basic Operations

Closure

add the transitive closure of the relation,

closure(0) = \{0, 2, 3, 4, 7, 8, 9\}
and the transitive closure of the dual,

\[
\text{star}(7) = \{7, 2, 3, 0\}
\]
and augment with lattice operations.
meet(0, 1) = \{4\}
and augment with lattice operations.

\[ \text{join}(8, 9) = \{4\} \]
Residual Evaluation

I developed a single residual evaluation routine independent of spatial dimension, cell geometry, and finite element:

$$F(\vec{u}) = 0$$

<table>
<thead>
<tr>
<th>Dim</th>
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<tr>
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<td>H(div) FEM*</td>
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† Peter Brune, ANL
* FEniCS Project
‡ Blaise Bourdin, LSU

We have also implemented a polyhedral FVM.
I developed a single residual evaluation routine independent of spatial dimension, cell geometry, and finite element:

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Dim   | Cell Types       | Discretizations          
---    |------------------|--------------------------
1      | Simplex          | Lagrange FEM            
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6†     | Prism            | DG FEM *†               

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We have also implemented a polyhedral FVM.
We consider weak forms dependent only on fields and gradients,
\[\int_{\Omega} \phi \cdot f_0(u, \nabla u) + \nabla \phi : \vec{f}_1(u, \nabla u) = 0.\] (11)

Discretizing we have
\[\sum_e \mathcal{E}_e^T \left[ B^T W^q f_0(u^q, \nabla u^q) + \sum_k D_k^T W^q \vec{f}_1^k(u^q, \nabla u^q) \right] = 0 \] (12)

\(f_n\) pointwise physics functions
\(u^q\) field at a quad point
\(W^q\) diagonal matrix of quad weights
\(B, D\) basis function matrices which reduce over quad points
\(\mathcal{E}\) assembly operator
DMplexComputeResidualFEM(dm, X, F, user)
{
    VecSet(F, 0.0);
    <Put boundary conditions into local input vector>
    <Extract coefficients and geometry for batch>
    <Integrate batch of elements>
    <Insert batch of element vectors into global vector>
}
Batch Integration
Set boundary conditions

DM::DMComputeResidualFEM(dm, X, F, user)
{
    VecSet(F, 0.0);
    DM::DMProjectFunctionLocal(dm, numComponents, bcFuncs, INSERT_BC_VALUES, X);
    <Extract coefficients and geometry for batch>
    <Integrate batch of elements>
    <Insert batch of element vectors into global vector>
}
Batch Integration
Extract coefficients and geometry

```c
DMPlexComputeResidualFEM(dm, X, F, user) {
    VecSet(F, 0.0);
    <Put boundary conditions into local input vector>

    DMPlexGetHeightStratum(dm, 0, &cStart, &cEnd);
    for (c = cStart; c < cEnd; ++c) {
        DMPlexComputeCellGeometry(dm, c, &v0[c*dim],
                                   &J[c*dim*dim], &invJ[c*dim*dim], &detJ[c]);
        DMPlexVecGetClosure(dm, NULL, X, c, NULL, &x);
        for (i = 0; i < cellDof; ++i) u[c*cellDof+i] = x[i];
        DMPlexVecRestoreClosure(dm, NULL, X, c, NULL, &x);
    }
    <Integrate batch of elements>
    <Insert batch of element vectors into global vector>
}
```
Batch Integration
Integrate element batch

```c
DMPushComputeResidualFEM(dm, X, F, user)
{
    VecSet(F, 0.0);
    <Put boundary conditions into local input vector>
    <Extract coefficients and geometry for batch>
    for (field = 0; field < numFields; ++field) {
        (*mesh->integrateResidualFEM)(Ne, numFields, field,
                                      quad, u,
                                      v0, J, invJ, detJ,
                                      f0, f1, elemVec);
        (*mesh->integrateResidualFEM)(Nr, ...);
    }
    <Insert batch of element vectors into global vector>
}
```
Batch Integration
Insert element vectors

DMplexComputeResidualFEM(dm, X, F, user)
{
    VecSet(F, 0.0);
    <Put boundary conditions into local input vector>
    <Extract coefficients and geometry for batch>
    <Integrate batch of elements>
    for (c = cStart; c < cEnd; ++c) {
        DMPlexVecSetClosure(dm, NULL, F, c, &elemVec[c*cellDof], ADD_VALUES);
    }
}
FEMIntegrateResidualBatch(Ne, numFields, field, 
quad[], coefficients[], 
v0s[], jacobians[], jacobianInv[], jacobianDet[], 
f0_func, f1_func)
{
<Loop over batch of elements (e)>
<Loop over quadrature points (q)>
<Make x_q>
<Make u_q and gradU_q>
<Call f_0 and f_1>
<Loop over element vector entries (f, fc)>
<Add contributions from f_0 and f_1>
}
Element Integration
Calculate \( x_q \)

\[
\text{FEMIntegrateResidualBatch}(\ldots)
\{
\quad \text{<Loop over batch of elements (e)>}
\quad \text{<Loop over quadrature points (q)>}
\quad \text{for } (d = 0; d < \text{dim}; ++d) \{
\quad \quad x[d] = v0[d];
\quad \quad \text{for } (d2 = 0; d2 < \text{dim}; ++d2) \{
\quad \quad \quad x[d] += J[d*\text{dim}+d2]*(\text{quadPoints}[q*\text{dim}+d2]+1);
\quad \quad \}
\quad \}
\quad \text{<Make } x_q \text{>}
\quad \text{<Make } u_q \text{ and } \text{gradU}_q \text{>}
\quad \text{<Call } f_0 \text{ and } f_1 \text{>}
\quad \text{<Loop over element vector entries (f, fc)>}
\quad \text{<Add contributions from } f_0 \text{ and } f_1 \text{>}
\}
Element Integration

Calculate $u_q$ and $\nabla u_q$

FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
  <Loop over quadrature points (q)>
   <Make x_q>
     for (f = 0; f < numFields; ++f) {
       for (b = 0; b < Nb; ++b) {
         for (comp = 0; comp < Ncomp; ++comp) {
           u[comp] += coefficients[cidx]\times basis[q+cidx];
           for (d = 0; d < dim; ++d) {
             <Transform derivative to real space>
             gradU[comp\times dim+d] +=
               coefficients[cidx]\times realSpaceDer[d];
           }
         }
       }
     }
  }
  <Call f_0 and f_1>
  <Loop over element vector entries (f, fc)>
Element Integration

Calculate $u_q$ and $\nabla u_q$

FEMIntegrateResidualBatch(...)
{
    <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
    <Make $x_q$>
    for (f = 0; f < numFields; ++f) {
        for (b = 0; b < Nb; ++b) {
            for (comp = 0; comp < Ncomp; ++comp) {
                u[comp] += coefficients[cidx]*basis[q+cidx];
                for (d = 0; d < dim; ++d) {
                    realSpaceDer[d] = 0.0;
                    for (g = 0; g < dim; ++g) {
                        realSpaceDer[d] +=
                            invJ[g*dim+d]*basisDer[(q+cidx)*dim+g];
                    }
                    gradU[comp*dim+d] +=
                        coefficients[cidx]*realSpaceDer[d];
                }
            }
        }
    }
}
Element Integration

Call $f_0$ and $f_1$

FEMIntegrateResidualBatch(...)
{
    <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
    <Make $x_q$>
    <Make $u_q$ and $\text{grad}U_q$>
    $f_0\_func(u, \text{grad}U, x, &f_0[q*N\text{comp}])$;
    for (i = 0; i < N\text{comp}; ++i) {
        $f_0[q*N\text{comp}+i] \ast= \text{det}J*\text{quadWeights}[q];$
    }
    $f_1\_func(u, \text{grad}U, x, &f_1[q*N\text{comp}*\text{dim}])$;
    for (i = 0; i < N\text{comp}*\text{dim}; ++i) {
        $f_1[q*N\text{comp}*\text{dim}+i] \ast= \text{det}J*\text{quadWeights}[q];$
    }
    <Loop over element vector entries ($f$, $fc$)>
    <Add contributions from $f\_0$ and $f\_1$>
}
FEMIntegrateResidualBatch(...)
{
    <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
        <Make x_q>
        <Make u_q and gradU_q>
        <Call f_0 and f_1>
    <Loop over element vector entries (f, fc)>
        for (q = 0; q < Nq; ++q) {
            elemVec[cidx] += basis[q+cidx]*f0[q+comp];
            for (d = 0; d < dim; ++d) {
                <Transform derivative to real space>
                elemVec[cidx] +=
                    realSpaceDer[d]*f1[(q+comp)*dim+d];
            }
        }
}
Adaptive Mesh Refinement

- DM interface with p4est package from Burstedde and Isaac
- PETSc solvers can be used seamlessly
- 2015 Gordon Bell Winner for Mantle Convection Simulation
- Inversion for basal traction on the full Antarctic ice sheet
Adaptive Mesh Refinement

- DM interface with p4est package from Burstedde and Isaac
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- 2015 Gordon Bell Winner for Mantle Convection Simulation
- Inversion for basal traction on the full Antarctic ice sheet

Observed surface flow velocity (Rignot et al., 2011)

Antarctic Ice sheet inversion for the basal friction parameter field using InSAR surface velocity measurements

Isaac
What does a DM do?

- **Problem Definition**
  - Discretization/Dof mapping (**PetscSection**)  
  - Residual calculation

- **Decomposition**
  - Partitioning, **DMCreateSubDM()**
  - **Vec** and **Mat** creation
  - Global ⇐⇒ Local mapping

- **Hierarchy**
  - **DMCoarsen()** and **DMRefine()**
  - **DMInterpolate()** and **DMRestrict()**
  - Hooks for resolution-dependent data
PetscSection
What Is It?

Similar to **PetscLayout**, maps point $\rightarrow$ (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 **DMPlenx**
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, FVM, 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.
High Level Interface

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

<table>
<thead>
<tr>
<th>Discretization</th>
<th>Dof/Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_1 - P_0$</td>
<td>[3 0 0 0</td>
</tr>
<tr>
<td>$Q_2 - Q_1$</td>
<td>[3 3 3 3</td>
</tr>
<tr>
<td>$Q_2 - P_1^{\text{disc}}$</td>
<td>[3 3 3 3</td>
</tr>
</tbody>
</table>
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);
**DMPllex** 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
The operations used in SNES ex62 get and set values from a Vec, organized by the DM and PetscSection.

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

- Element vector on cell
- Coordinates on cell vertices

Used in FormFunctionLocal(),

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

    DMplexVecGetClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
    for (PetscInt i = 0; i < cellDof; ++i) {
        u[c*cellDof+i] = x[i];
    }
    DMplexVecRestoreClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
}
```
The operations used in SNES ex62 get and set values from a Vec, organized by the DM and PetscSection

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        u[c*cellDof+i] = x[i];
    }
    DMVecRestoreClosure(dm, PETSC_NULL, X, c, PETSC_NULL, &x);
}
The operations used in SNES ex62 get and set values from a Vec, organized by the DM and PetscSection

DMplexVecSetClosure(
    DM dm, PetscSection section, Vec v, PetscInt point,
    const PetscScalar values[], InsertMode mode)

DMplexMatSetClosure(
    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) {
    DMplexMatSetClosure(dm, PETSC_NULL, PETSC_NULL, JacP, c,
        &elemMat[c*cellDof*cellDof], ADD_VALUES);
}
The operations used in SNES ex62 get and set values from a Vec, organized by the DM and PetscSection

DMVecSetClosure(
  DM dm, PetscSection section, Vec v, PetscInt point,
  const PetscScalar values[], InsertMode mode)

DMMatSetClosure(
  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) {
  DMVecSetClosure(dm, PETSC_NULL, PETSC_NULL, JacP, c,
  &elemMat[c*cellDof*cellDof], ADD_VALUES);
}
The functions above are built upon

DM::GetTransitiveClosure(
    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
Naively, we have

\[ cl(\text{cell}) = \begin{bmatrix} f e_0 e_1 e_2 & v_0 & v_1 & v_2 \end{bmatrix} \]

\[ x(\text{cell}) = \begin{bmatrix} u_{e_0} & v_{e_0} & u_{e_1} & v_{e_1} & u_{e_2} & v_{e_2} \\ u v_0 & v v_0 & u v_1 & v v_1 & p v_1 & u v_2 & v v_2 & p v_2 \end{bmatrix} \]
$P_2 - P_1$ Stokes Example

We reorder so that fields are contiguous

$$x'(\text{cell}) = \begin{bmatrix} u_{e_0} v_{e_0} u_{e_1} v_{e_1} u_{e_2} v_{e_2} \\ u_{v_0} v_{v_0} u_{v_1} v_{v_1} u_{v_2} v_{v_2} \\ p_{v_0} p_{v_1} p_{v_2} \end{bmatrix}$$
Outline

1. Getting Started with PETSc
2. PETSc Integration
3. DM
4. Advanced Solvers
   - Fieldsplit
   - Multigrid
   - Timestepping
5. More Stuff
Outline

4 Advanced Solvers

- Fieldsplit
- Multigrid
- Timestepping
FieldSplit Preconditioner

- **Analysis**
  - Use ISes to define fields
  - Decouples PC from problem definition

- **Synthesis**
  - Additive, Multiplicative, Schur
  - Commutes with Multigrid
FieldSplit Customization

**Analysis**
- `-pc_fieldsplit_<split num>_fields 2,1,5`
- `-pc_fieldsplit_detect_saddle_point`

**Synthesis**
- `-pc_fieldsplit_type <additive, multiplicative, schur>`
- `-pc_fieldsplit_diag_use_amat`
  - `-pc_fieldsplit_off_diag_use_amat`
  
  Use diagonal blocks of operator to build PC

**Schur complements**
- `-pc_fieldsplit_schur_precondition <user,all,full,self,selfp>`
  
  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
Solver Configuration: No New Code

ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$
**ex62**: $P_2/P_1$ Stokes Problem on Unstructured Mesh


-ksp_type gmres -pc_type fieldsplit -pc_fieldsplit_type additive
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi

$$
\begin{pmatrix}
A & 0 \\
0 & I
\end{pmatrix}
$$
Solver Configuration: No New Code

**ex62:** $P_2/P_1$ Stokes Problem on Unstructured Mesh


```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type additive
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
-fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type Jacobi
```

$$
\begin{pmatrix}
\hat{A} & 0 \\
0 & I
\end{pmatrix}
$$
ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh


-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type multiplicative
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
-fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi

\[
\begin{pmatrix}
\hat{A} & B \\
0 & I
\end{pmatrix}
\]
**Solver Configuration: No New Code**

**ex62**: $P_2/P_1$ Stokes Problem on Unstructured Mesh


```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type multiplicative
    -pc_fieldsplit_0_fields 1 -pc_fieldsplit_1_fields 0
    -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
    -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi
```

\[
\begin{pmatrix}
I & B^T \\
0 & \tilde{A}
\end{pmatrix}
\]
ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh


-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type diag
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
-fieldsplit_pressure_ksp_type minres -fieldsplit_pressure_pc_type none

\[
\begin{pmatrix}
\hat{A} & 0 \\
0 & -\hat{S}
\end{pmatrix}
\]
Solver Configuration: No New Code

ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

Lower Schur Complement, May and Moresi, PEPI, 2008.

-ksp_type fgmres  -pc_type fieldsplit  -pc_fieldsplit_type schur
   -pc_fieldsplit_schur_factorization_type lower
   -fieldsplit_velocity_ksp_type preonly  -fieldsplit_velocity_pc_type gamg
   -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type none

\[
\begin{pmatrix}
\hat{A} & 0 \\
B^T & \hat{S}
\end{pmatrix}
\]
**Solver Configuration: No New Code**

**ex62**: $P_2/P_1$ Stokes Problem on Unstructured Mesh


```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
  -pc_fieldsplit_schur_factorization_type upper
  -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
  -fieldsplit_pressure_ksp_type minres -fieldsplit_pressure_pc_type none

(\hat{A} \quad B)
\begin{pmatrix}
\hat{S}
\end{pmatrix}
```
ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

Uzawa Iteration, Uzawa, 1958

-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type upper
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_ksp_type richardson
-fieldsplit_pressure_ksp_max_its 1

$$\begin{pmatrix} A & B \\ \hat{S} & \end{pmatrix}$$
**Solver Configuration: No New Code**

---

**ex62**: $P_2/P_1$ Stokes Problem on Unstructured Mesh

Full Schur Complement, Schur, 1905.

-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-_pc_fieldsplit_schur_factorization_type full
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi

\[
\begin{pmatrix}
I & 0 \\
B^T A^{-1} & I
\end{pmatrix}
\begin{pmatrix}
A & 0 \\
0 & S
\end{pmatrix}
\begin{pmatrix}
I & A^{-1} B \\
0 & I
\end{pmatrix}
\]
**Solver Configuration: No New Code**

**ex62**: $P_2/P_1$ Stokes Problem on Unstructured Mesh


```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-kpc_fieldsplit_schur_factorization_type full
-fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
- fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi
-fieldsplit_pressure_inner_ksp_type preonly
- fieldsplit_pressure_inner_pc_type jacobi
- fieldsplit_pressure_upper_ksp_type preonly
- fieldsplit_pressure_upper_pc_type jacobi
```

\[
\begin{pmatrix}
I & 0 \\
B^T A^{-1} & I
\end{pmatrix}
\begin{pmatrix}
A & 0 \\
0 & B^T D_A^{-1} B
\end{pmatrix}
\begin{pmatrix}
I & D_A^{-1} B \\
0 & I
\end{pmatrix}
\]
ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh


-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
-pc_fieldsplit_schur_precondition self
-fieldsplit_velocity_ksp_type gmres -fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_ksp_rtol 1e-5 -fieldsplit_pressure_pc_type lsc
Solver Configuration: No New Code

ex31: $P_2/P_1$ Stokes Problem with Temperature on Unstructured Mesh


-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type additive
-nc Fieldsplit 0,1 -pc_fieldsplit 1 Fieldsplit
-nc Fieldsplit 0_ksp_type fgmres -nc Fieldsplit 0_pc_type fieldsplit
-nc Fieldsplit 0_pc_fieldsplit_type schur
-nc Fieldsplit 0_pc_fieldsplit_schur_factorization_type full
-nc Fieldsplit 0 Fieldsplit_velocity_ksp_type preonly
-nc Fieldsplit 0 Fieldsplit_velocity_pc_type lu
-nc Fieldsplit 0 Fieldsplit_pressure_ksp_rtol 1e-10
-nc Fieldsplit 0 Fieldsplit_pressure_pc_type jacobi
-nc Fieldsplit_temperature_ksp_type preonly
-nc Fieldsplit_temperature_pc_type lu

\[
\begin{bmatrix}
I & 0 \\
B^T A^{-1} & I \\
0 & \hat{A} & 0 \\
0 & 0 & \hat{S} & 0 \\
0 & 0 & 0 & \hat{L}
\end{bmatrix}
\]
ex31: $P_2/P_1$ Stokes Problem with Temperature on Unstructured Mesh

Upper Schur Comp. + Full Schur Comp. + Least-Squares Comm.

-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_0_fields 0,1 -pc_fieldsplit_1_fields 2
-pc_fieldsplit_schur_factorization_type upper
-fieldsplit_0_ksp_type fgmres -fieldsplit_0_pc_type fieldsplit
-fieldsplit_0_pc_fieldsplit_type schur
-fieldsplit_0_pc_fieldsplit_schur_factorization_type full
-fieldsplit_0_fieldsplit_velocity_ksp_type preonly
-fieldsplit_0_fieldsplit_velocity_pc_type lu
-fieldsplit_0_fieldsplit_pressure_ksp_rtol 1e-10
-fieldsplit_0_fieldsplit_pressure_pc_type jacobi
-fieldsplit_temperature_ksp_type gmres
-fieldsplit_temperature_pc_type lsc

$$
\begin{pmatrix}
I & 0 \\
B^T A^{-1} & I \\
0 & \hat{S}
\end{pmatrix}
\begin{pmatrix}
\hat{A} & 0 \\
0 & \hat{S}
\end{pmatrix}
\begin{pmatrix}
I & A^{-1} B \\
0 & I
\end{pmatrix}
G
\hat{S}_{LSC}
$$
SNES ex62
Preconditioning

Jacobi

ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -vel_petsc_space_order 2 -pres_petsc_space_order 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
    -vel_petscspace_order 2 -pres_petscspace_order 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
- vel_petscspace_order 2 - pres_petscspace_order 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 multiplicative
- 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
- vel_petscspace_order 2 -pres_petscspace_order 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
  -vel_petscspace_order 2 -pres_petscspace_order 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

```bash
ex62
- run_type full - bc_type dirichlet - show_solution 0
- refinement_limit 0.00625 - interpolate 1
- vel_petscspace_order 2 - pres_petscspace_order 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
-vel_petscspace_order 2 -pres_petscspace_order 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
```
**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
```
**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
```
ex55: Allen-Cahn problem in 2D

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```bash
./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

```bash
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```bash
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```
**ex55: Allen-Cahn problem in 2D**

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```sh
./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

```sh
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```sh
-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

```bash
./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

```bash
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```bash
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```
ex55: Allen-Cahn problem in 2D

Smoothers: 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`

Schur 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`  

**Schur 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

Smother: 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>`

Schur 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>`
ex55: Allen-Cahn problem in 2D

Smusher: 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

Schur 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
Null spaces

For a single matrix, use

\[ \texttt{MatSetNullSpace}(J, \text{nullSpace}); \]

to alter the \textbf{KSP}, and

\[ \texttt{MatSetNearNullSpace}(J, \text{nearNullSpace}); \]

to set the coarse basis for AMG.

But this will not work for dynamically created operators.
For a single matrix, use

\texttt{MatSetNullSpace(J, nullSpace);} 

to alter the \texttt{KSP}, and

\texttt{MatSetNearNullSpace(J, nearNullSpace);} 

to set the coarse basis for AMG.

But this will not work for dynamically created operators.
Null spaces
Field Split

Can attach a nullspace to the IS that creates a split,

```
PetscObjectCompose(pressureIS, "nullspace",
                   (PetscObject) nullSpacePres);
```

If the DM makes the IS, use

```
PetscObject pressure;

DMGetField(dm, 1, &pressure);
PetscObjectCompose(pressure, "nullspace",
                    (PetscObject) nullSpacePres);
```
Outline

4 Advanced Solvers

- Fieldsplit
- Multigrid
- Timestepping
Why not use AMG?

- Of course we will try AMG
  - GAMG, -pc_type gamg
  - ML, -download-ml, -pc_type ml
  - BoomerAMG, -download-hypre, -pc_type hypre
    - pc_hypre_type boomeramg

- Problems with
  - vector character
  - anisotropy
  - scalability of setup time
Why not use AMG?

- Of course we will try AMG
  - GAMG, `pc_type` gamg
  - ML, `download`-ml, `pc_type` ml
  - BoomerAMG, `download`-hypre, `pc_type` hypre
    - `pc_hypre_type` boomeramg

- Problems with
  - vector character
  - anisotropy
  - scalability of setup time
Why not use AMG?

- Of course we will try AMG
  - GAMG, \(-\text{pc\_type} \ \text{gamg}\)
  - ML, \(-\text{download-ml, -pc\_type} \ \text{ml}\)
  - BoomerAMG, \(-\text{download-hypre, -pc\_type} \ \text{hypre}\)
    - \(-\text{pc\_hypre\_type} \ \text{boomeramg}\)

- Problems with
  - vector character
  - anisotropy
  - scalability of setup time
Multigrid with DM

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`
- `da_refine`, `ksp_view`

Interface also works with GAMG and 3rd party packages like ML
A 2D Problem

Problem has:
- 1,640,961 unknowns (on the fine level)
- 8,199,681 nonzeros

Options

<table>
<thead>
<tr>
<th>Option</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>./ex5 -da_grid_x 21 -da_grid_y 21</td>
<td>Original grid is 21x21</td>
</tr>
<tr>
<td>-ksp_rtol 1.0e-9</td>
<td>Solver tolerance</td>
</tr>
<tr>
<td>-da_refine 6</td>
<td>6 levels of refinement</td>
</tr>
<tr>
<td>-pc_type mg</td>
<td>4 levels of multigrid</td>
</tr>
<tr>
<td>-pc_mg_levels 4</td>
<td></td>
</tr>
<tr>
<td>-snes_monitor -snes_view</td>
<td>Describe solver</td>
</tr>
</tbody>
</table>
**A 3D Problem**

Problem has:

- **1,689,600 unknowns** (on the fine level)
- **89,395,200 nonzeros**

<table>
<thead>
<tr>
<th>Options</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>/ex48 -M 5 -N 5</code></td>
<td>Coarse problem size</td>
</tr>
<tr>
<td><code>-da_refine 5</code></td>
<td>5 levels of refinement</td>
</tr>
<tr>
<td><code>-ksp_rtol 1.0e-9</code></td>
<td>Solver tolerance</td>
</tr>
<tr>
<td><code>-thi_mat_type baij</code></td>
<td>Needs SOR</td>
</tr>
<tr>
<td><code>-pc_type mg</code></td>
<td>4 levels of multigrid</td>
</tr>
<tr>
<td><code>-pc_mg_levels 4</code></td>
<td></td>
</tr>
<tr>
<td><code>-snes_monitor -snes_view</code></td>
<td>Describe solver</td>
</tr>
</tbody>
</table>
The Full Multigrid algorithm (FMG)

- V-cycle at each level,
- then interpolate to the next finer grid
- Can solve to discretization error with a single iteration
Full Multigrid Work

\[ C_{FMG} = \left( 1 + \frac{1}{2^d} + \frac{1}{2^{2d}} + \cdots \right) C_V \]

\[ = \sum_{n=0}^{\infty} \frac{1}{2^{nd}} C_V \]

\[ = \frac{2^d}{2^d - 1} C_V \]

\[ = \left( \frac{2^d}{2^d - 1} \right)^2 C_{\text{twolevel}} \cdot \]

1D FMG is \( 2 \times C_V \), 3D FMG is \( \frac{8}{7} \times C_V \)
Full Multigrid Work

\[ C_{FMG} = \left( 1 + \frac{1}{2^d} + \frac{1}{2^{2d}} + \cdots \right) C_V \]

\[ = \sum_{n=0}^{\infty} \frac{1}{2^{nd}} C_V \]

\[ = \frac{2^d}{2^d - 1} C_V \]

\[ = \left( \frac{2^d}{2^d - 1} \right)^2 C_{\text{twolevel}}. \]

1D FMG is \( 2 \times C_V \), 3D FMG is \( \frac{8}{7} \times C_V \).
Suppose we have an order $\alpha$ method,

$$\|x - x_h\| < Ch^\alpha$$

FD and $P_1$ both have $\alpha = 2$
Full Multigrid Accuracy

$E_d$  Discretization Error

$E_a$  Algebraic Error

Choose iterative tolerance so that

$$E_a = rE_d \quad r < 1$$

and

$$E \leq E_d + E_a = (1 + r)Ch^\alpha$$
Suppose

- Finish V-cycle for $2h$ grid,
- Use as coarse correction for $h$ grid
- Perform final V-cycle for $h$ grid
- Need V-cycle error reduction factor $\eta$ to get $r$ reduction in $E_a$
Full Multigrid Accuracy

\[ \eta E_a < rCh^\alpha \]
\[ \eta (E - E_d) < rCh^\alpha \]
\[ \eta ((1 + r)C(2h)^\alpha - Ch^\alpha) < rCh^\alpha \]
\[ \eta ((1 + r)2^\alpha - 1) < r \]
\[ \eta < \frac{1}{2^\alpha + \frac{2^\alpha - 1}{r}}. \]

If \( \alpha = 2 \) and \( r = \frac{1}{2} \), then \( \eta < \frac{1}{10} \).
Full Multigrid Experiment
V-cycle

./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
-ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short

gives

0 SNES Function norm 0.0287773
  0 KSP Residual norm 0.793727
1 KSP Residual norm 0.00047526
2 KSP Residual norm 4.18007e-06
3 KSP Residual norm 1.668e-07
4 KSP Residual norm 3.25952e-09
5 KSP Residual norm 7.274e-11
1 SNES Function norm 2.251e-10
N: 625 error l2 1.21529e-13 inf 9.53484e-12
Full Multigrid Experiment
V-cycle

./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
-ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short

and it changes little if we refine six more times

0 SNES Function norm 0.000455131
  0 KSP Residual norm 50.6842
  1 KSP Residual norm 0.00618427
  2 KSP Residual norm 9.87833e-07
  3 KSP Residual norm 2.99517e-09
1 SNES Function norm 2.83358e-09
N: 2362369 error l2 1.28677e-15 inf 7.68693e-12
Full Multigrid Experiment

FMG

./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1 -ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short -pc_mg_type full

We do not seem to see the convergence acceleration

0 SNES Function norm 0.0287773
  0 KSP Residual norm 0.799687
1 KSP Residual norm 6.95292e-05
2 KSP Residual norm 1.50836e-06
3 KSP Residual norm 2.62524e-08
4 KSP Residual norm 6.184e-10
5 KSP Residual norm 1.275e-11
1 SNES Function norm 3.757e-11
N: 625 error l2 2.1428e-14 inf 1.80611e-12
Full Multigrid Experiment

FMG

./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1 -ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short -pc_mg_type full

although its a little more apparent as we refine,

0 SNES Function norm 0.000455131
  0 KSP Residual norm 51.2
  1 KSP Residual norm 2.92416e-06
  2 KSP Residual norm 3.76404e-09
1 SNES Function norm 8.50096e-09
N: 2362369 error l2 1.70304e-15 inf 6.22476e-11
#!/usr/bin/env python
import argparse
import subprocess
import numpy as np

parser = argparse.ArgumentParser(
    description = 'CAAM 519 FMG',
    epilog = 'For more information, visit http://www.mcs.anl.gov/petsc',
    formatter_class = argparse.ArgumentDefaultsHelpFormatter)
parser.add_argument('--kmax', type=int, default=5,
    help='The number of doublings to test')
parser.add_argument('--save', action='store_true', default=False,
    help='Save the figures')
args = parser.parse_args()

sizesA = []
sizesB = []
errorA = []
errorB = []
for k in range(args.kmax):
    options = ['-snes_type', 'newtonls', '-snes_max_it', '1', '-da_refine',
               '-par', '0.0', '-ksp_atol', '1e-1', '-mms', '1',
               '-pc_type', 'mg', '-pc_mg_type', 'multiplicative',
               '-mg_levels_ksp_max_it', '5']
    cmd = './ex5 ' + ' '.join(options)
    out = subprocess.check_output(['./ex5'] + options).split(' ')
    # This is l_2, out[6] is l_infty
    sizesA.append(int(out[1]))
    errorA.append(float(out[4]))
for k in range(args.kmax):
    options = ['-snes_type', 'newtonls', '-snes_max_it', '1', '-da_refine',
               '-par', '0.0', '-ksp_atol', '1e-1', '-mms', '1',
               '-pc_type', 'mg', '-pc_mg_type', 'full',
               '-mg_levels_ksp_max_it', '5']
    cmd = './ex5 ' + ' '.join(options)
    out = subprocess.check_output(['./ex5'] + options).split(' ')
    # This is l_2, out[6] is l_infty
    sizesB.append(int(out[1]))
    errorB.append(float(out[4]))
SA = np.array(sizesA)
SB = np.array(sizesB)

from pylab import legend, plot, loglog, show, title, xlabel, ylabel, savefig

loglog(SA, errorA, 'r', SA, 5e-6 * SA ** -0.5, 'r--',
       SB, errorB, 'g', SB, 5e-6 * SB ** -1., 'g--')
title('SNES ex5')
xlabel('Problem size $N$')
ylabel('Error $\|u - u^*\|$')
legend(["GMRES/GMG", "$h = N\{-1/2\}$", "GMRES/FMG", "$h^2 = N\{-1\}$"],
       'upper right', shadow = True)

if args.save:
    savefig('fmg.png')
else:
    show()
Full Multigrid Experiment

Comparison

SNES ex5

- GMRES/GMG
- $h = N^{-1/2}$
- GMRES/FGM
- $h^2 = N^{-1}$

Problem size $N$ vs. error $|u - u^*|$
Outline

4 Advanced Solvers
   • Fieldsplit
   • Multigrid
   • Timestepping
What about TS?

Time Integration in PETSc Has Made a Quantum Leap

and is now a premier library in the field, thanks to Jed, Emil, and Peter
What about TS?

Time Integration in PETSc Has Made a Quantum Leap

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What about TS?

Time Integration in PETSc Has Made a Quantum Leap

and is now a premier library in the field,

thanks to Jed, Emil, and Peter
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)
**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()`
Stiff linear advection-reaction test problem

Equations

TS ex22.c

\[ u_t + a_1 u_x = -k_1 u + k_2 v + s_1 \]
\[ v_t + a_2 v_x = k_1 u - k_2 v + s_2 \]

Upstream boundary condition:

\[ u(0, t) = 1 - \sin(12t)^4 \]
Stiff linear advection-reaction test problem

Equations

\[ u_t + a_1 u_x = -k_1 u + k_2 v + s_1 \]
\[ v_t + a_2 v_x = k_1 u - k_2 v + s_2 \]

FormIFunction(TS ts, PetscReal t, Vec X, Vec Xdot, Vec F, void *ptr) {
    TSGetDM(ts, &da);
    DMDAGetLocalInfo(da, &info);
    DMDAVecGetArray(da, X, &x);
    DMDAVecGetArray(da, Xdot, &xdot);
    DMDAVecGetArray(da, F, &f);
    /* Compute function over the locally owned part of the grid */
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        f[i][0] = xdot[i][0] + k[0]*x[i][0] - k[1]*x[i][1] - s[0];
        f[i][1] = xdot[i][1] - k[0]*x[i][0] + k[1]*x[i][1] - s[1];
    }
    DMDAVecRestoreArray(da, X, &x);
    DMDAVecRestoreArray(da, Xdot, &xdot);
    DMDAVecRestoreArray(da, F, &f);
}
Stiff linear advection-reaction test problem

Equations

\[ u_t + a_1 u_x = -k_1 u + k_2 v + s_1 \]
\[ v_t + a_2 v_x = k_1 u - k_2 v + s_2 \]

FormIJacobian(TS ts, PetscReal t, Vec X, Vec Xdot, PetscReal a, Mat *J, Mat *Jpre, MatStructure *str, void *ptr) {
  for (i = info.xs; i < info.xs+info.xm; ++i) {
    PetscScalar v[2][2];
    v[0][0] = a + k[0]; v[0][1] = -k[1];
    v[1][0] = -k[0]; v[1][1] = a+k[1];
    MatSetValuesBlocked(*Jpre, 1, &i, 1, &i, &v[0][0], INSERT_VALUES);
  }
  MatAssemblyBegin(*Jpre, MAT_FINAL_ASSEMBLY);
  MatAssemblyEnd(*Jpre, MAT_FINAL_ASSEMBLY);
  if (*J != *Jpre) {
    MatAssemblyBegin(*J, MAT_FINAL_ASSEMBLY);
    MatAssemblyEnd(*J, MAT_FINAL_ASSEMBLY);
  }
}

Matt (Rice)
Stiff linear advection-reaction test problem

Equations

**TS ex22.c**

\[
\begin{align*}
\frac{\partial u}{\partial t} + a_1 \frac{\partial u}{\partial x} &= -k_1 u + k_2 v + s_1 \\
\frac{\partial v}{\partial t} + a_2 \frac{\partial v}{\partial x} &= k_1 u - k_2 v + s_2
\end{align*}
\]

FormRHSFunction(TS ts, PetscReal t, Vec X, Vec F, void *ptr) {
    PetscReal u0t[2] = {1.0 - PetscPowScalar(sin(12.0*t), 4.), 0};
    DMGetLocalVector(da, &Xloc);
    DMGlobalToLocalBegin(da, X, INSERT_VALUES, Xloc);
    DMGlobalToLocalEnd(da, X, INSERT_VALUES, Xloc);
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        /* CALCULATE RESIDUAL f[i][j] */
    }
}
Stiff linear advection-reaction test problem

Equations

\[ u_t + a_1 u_x = -k_1 u + k_2 v + s_1 \]
\[ v_t + a_2 v_x = k_1 u - k_2 v + s_2 \]

for (i = info.xs; i < info.xs+info.xm; ++i) {
    for (j = 0; j < 2; ++j) {
        const PetscReal a = a[j]/hx;
        if (i == 0)
            f[i][j] = a*(1/3*u0t[j] + 1/2*x[i][j] - x[i+1][j] + 1/6*x[i+2][j]);
        else if (i == 1)
            f[i][j] = a*(-1/12*u0t[j] + 2/3*x[i-1][j] - 2/3*x[i+1][j] + 1/12*x[i+2][j]);
        else if (i == info.mx-2)
            f[i][j] = a*(-1/6*x[i-2][j] + x[i-1][j] - 1/2*x[i][j] - 1/3*x[i+1][j]);
        else if (i == info.mx-1)
            f[i][j] = a*(-x[i][j] + x[i-1][j]);
        else
            f[i][j] = a*(-1/12*x[i-2][j] + 2/3*x[i-1][j] - 2/3*x[i+1][j] + 1/12*x[i+2][j]);
    }
}
Stiff linear advection-reaction test problem

Parameters

$$\begin{align*}
a_1 &= 1, & k_1 &= 10^6, & s_1 &= 0, \\
a_2 &= 0, & k_2 &= 2k_1, & s_2 &= 1
\end{align*}$$

TS ex22.c

Matt (Rice)
**Stiff linear advection-reaction test problem**

**Initial conditions**

\[
u(x, 0) = 1 + s_2 x
\]

\[
\nu(x, 0) = \frac{k_0}{k_1} u(x, 0) + \frac{s_1}{k_1}
\]

**PetscErrorCode** FormInitialSolution(TS ts, Vec X, void *ctx) {
    TSGetDM(ts, &da);
    DMDAGetLocalInfo(da, &info);
    DMDAVecGetArray(da, X, &x);
    /* Compute function over the locally owned part of the grid */
    for (i = info.xs; i < info.xs + info.xm; ++i) {
        PetscReal r = (i+1)*hx;
        PetscReal ik = user->k[1] != 0.0 ? 1.0/user->k[1] : 1.0;
        x[i][0] = 1 + user->s[1]*r;
        x[i][1] = user->k[0]*ik*x[i][0] + user->s[1]*ik;
    }
    DMDAVecRestoreArray(da, X, &x);
}
Stiff linear advection-reaction test problem

Initial conditions

\[ u(x, 0) = 1 + s_2 x \]
\[ v(x, 0) = \frac{k_0}{k_1} u(x, 0) + \frac{s_1}{k_1} \]

**PetscErrorCode** FormInitialSolution(\textbf{TS} ts, \textbf{Vec} X, \textbf{void} *ctx) {
  TSGetDM(ts, &da);
  DMDAGetLocalInfo(da, &info);
  DMDAVecGetArray(da, X, &x);
  /* Compute function over the locally owned part of the grid */
  for (i = info.xs; i < info.xs+info.xm; ++i) {
    PetscReal r = (i+1)*hx;
    PetscReal ik = user->k[1] != 0.0 ? 1.0/user->k[1] : 1.0;
    x[i][0] = 1 + user->s[1]*r;
    x[i][1] = user->k[0]*ik*x[i][0] + user->s[1]*ik;
  }
  DMDAVecRestoreArray(da, X, &x);
}
**Stiff linear advection-reaction test problem**

**Examples**

**TS ex22.c**

- `./ex22 -da_grid_x 200 -ts_monitor_draw_solution -ts_arkimex_type 4 -ts_adapt_type none`
- `./ex22 -da_grid_x 200 -ts_monitor_draw_solution -ts_type rosw -ts_dt 1e-3 -ts_adapt_type none`
- `./ex22 -da_grid_x 200 -ts_monitor_draw_solution -ts_type rosw -ts_rosw_type sandu3 -ts_dt 5e-3 -ts_adapt_type none`
- `./ex22 -da_grid_x 200 -ts_monitor_draw_solution -ts_type rosw -ts_rosw_type ra34pw2 -ts_adapt_monitor`

**PETSc**

Matt (Rice)  K2I  218 / 225
1D Brusselator reaction-diffusion

Equations

TS ex25.c

\[ u_t - \alpha u_{xx} = A - (B + 1)u + u^2v \]
\[ v_t - \alpha v_{xx} = Bu - u^2v \]

Boundary conditions:

\[ u(0, t) = u(1, t) = 1 \]
\[ v(0, t) = v(1, t) = 3 \]
1D Brusselator reaction-diffusion Equations

**TS ex25.c**

\[
\begin{align*}
    u_t - \alpha u_{xx} &= A - (B + 1)u + u^2v \\
    v_t - \alpha v_{xx} &= Bu - u^2v
\end{align*}
\]

```c
FormIFunction(TS ts, PetscReal t, Vec X, Vec Xdot, Vec F, void *ptr) {
    DMGlobalToLocalBegin(da, X, INSERT_VALUES, Xloc);
    DMGlobalToLocalEnd(da, X, INSERT_VALUES, Xloc);
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        if (i == 0) {
            f[i].u = hx * (x[i].u - uleft);
            f[i].v = hx * (x[i].v - vleft);
        } else if (i == info.mx-1) {
            f[i].u = hx * (x[i].u - uright);
            f[i].v = hx * (x[i].v - vright);
        } else {
            f[i].u = hx * xdot[i].u - alpha * (x[i-1].u - 2.*x[i].u + x[i+1].u) / hx;
            f[i].v = hx * xdot[i].v - alpha * (x[i-1].v - 2.*x[i].v + x[i+1].v) / hx;
        }
    }
}
```
1D Brusselator reaction-diffusion Equations

**TS ex25.c**

\[ u_t - \alpha u_{xx} = A - (B + 1)u + u^2v \]
\[ v_t - \alpha v_{xx} = Bu - u^2v \]

FormIJacobian(TS ts, PetscReal t, Vec X, Vec Xdot, PetscReal a, Mat *J, Mat *Jpre, MatStructure *str, void *ptr) {
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        if (i == 0 || i == info.mx-1) {
            const PetscInt row = i, col = i;
            const PetscScalar vals[2][2] = {{hx,0},{0,hx}};
            MatSetValuesBlocked(*Jpre,1,&row,1,&col,&vals[0][0],INSERT_VALUES);
        } else {
            const PetscInt row = i, col[] = {i-1,i,i+1};
            const PetscScalar dL = -a/hx, dC = 2*a/hx, dR = -a/hx;
            const PetscScalar v[2][3][2] = {{dL,0},{a*hx+dC,0},{dR,0}},
                {{0,dL},{0,a*hx+dC},{0,dR}};
            MatSetValuesBlocked(*Jpre,1,&row,3,col,&v[0][0][0],INSERT_VALUES);
        }
    }
}

Matt (Rice)
1D Brusselator reaction-diffusion Equations

TS ex25.c

\[ u_t - \alpha u_{xx} = A - (B + 1)u + u^2v \]
\[ v_t - \alpha v_{xx} = Bu - u^2v \]

FormRHSFunction(TS ts, PetscReal t, Vec X, Vec F, void *ptr) {
    TSGetDM(ts, &da);
    DMDAGetLocalInfo(da, &info);
    DMDAVecGetArray(da, X, &x);
    DMDAVecGetArray(da, F, &f);
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        PetscScalar u = x[i].u, v = x[i].v;
        f[i].u = hx*(A - (B+1)*u + u*u*v);
        f[i].v = hx*(B*u - u*u*v);
    }
    DMDAVecRestoreArray(da, X, &x);
    DMDAVecRestoreArray(da, F, &f);
}
1D Brusselator reaction-diffusion

Parameters

\[ A = 1, \quad B = 3, \quad \alpha = 1/50 \]

TS ex25.c
1D Brusselator reaction-diffusion

Initial conditions

\[ u(x, 0) = 1 + \sin(2\pi x) \]
\[ v(x, 0) = 3 \]

**PetscErrorCode** FormInitialSolution(TS ts, Vec X, void *ctx) {
    TSGetDM(ts, &da);
    DMDAGetLocalInfo(da, &info);
    DMDAVecGetArray(da, X, &x);
    /* Compute function over the locally owned part of the grid */
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        PetscReal xi = i*hx;
        x[i].u = uleft*(1-xi) + uright*xi + sin(2*PETSC_PI*xi);
        x[i].v = vleft*(1-xi) + vright*xi;
    }
    DMDAVecRestoreArray(da, X, &x);
}
**1D Brusselator reaction-diffusion**

### Initial conditions

**TS ex25.c**

\[
\begin{align*}
    u(x, 0) &= 1 + \sin(2\pi x) \\
    v(x, 0) &= 3
\end{align*}
\]

```c
PetscErrorCode FormInitialSolution(TS ts, Vec X, void *ctx) {
    TSGetDM(ts, &da);
    DMDAGetLocalInfo(da, &info);
    DMDAVecGetArray(da, X, &x);
    /* Compute function over the locally owned part of the grid */
    for (i = info.xs; i < info.xs+info.xm; ++i) {
        PetscReal xi = i*hx;
        x[i].u = uleft*(1-xi) + uright*xi + sin(2*PETSC_PI*xi);
        x[i].v = vleft*(1-xi) + vright*xi;
    }
    DMDAVecRestoreArray(da, X, &x);
}
```
1D Brusselator reaction-diffusion
Examples

**TS ex25.c**

- ./ex25 -da_grid_x 20 -ts_monitor_draw_solution -ts_type rosw 
  -ts_dt 5e-2 -ts_adapt_type none

- ./ex25 -da_grid_x 20 -ts_monitor_draw_solution -ts_type rosw 
  -ts_rosw_type 2p -ts_dt 5e-2

- ./ex25 -da_grid_x 20 -ts_monitor_draw_solution -ts_type rosw 
  -ts_rosw_type 2p -ts_dt 5e-2 -ts_adapt_type none
TS ex11.c

MESH_DIR = $PETSC_DIR/share/petsc/datafiles/meshes

./ex11 -f $MESH_DIR/sevenside.exo
./ex11 -f $MESH_DIR/sevenside-quad-15.exo
./ex11 -f $MESH_DIR/sevenside.exo -ts_type rosw
TS ex11.c

./ex11  -f -grid_size 2,1 -grid_bounds -1,1.,0.,1 -grid_skew_60
-physics euler -bc_wall 1,2,3,4 -eu_type iv_shock -ufv_cfl 10
 -eu_alpha 60. -eu_gamma 1.4 -eu_amach 2.02 -eu_rho2 3.
-dm_type p4est -dm_forest_partition_overlap 1
 -dm_forest_maximum_refinement 6 -dm_forest_minimum_refinement 2
 -dm_forest_initial_refinement 2
-petscfv_type leastsquares -petscfv_compute_gradients 0
-petsclimiter_type minmod
-ts_final_time 1 -ts_ssp_type rks2 -ts_ssp_nstages 10
-ufv_use_amr -ufv_refine_tol 0.5 -ufv_coarsen_tol 1.e-2
 -ufv_vtk_interval 1 -monitor density,energy
-ufv_view_initial_refinement
Outline

1. Getting Started with PETSc
2. PETSc Integration
3. DM
4. Advanced Solvers
5. More Stuff
Things I Will Not Talk About

- Communication abstractions
  - PetscSF and VecScatter

- Finite elements and finite volumes
  - PetscFE and PetscFV

- Non-nested geometric multigrid
  - Uses DMPlEx and Pragmatic

- Timestepping for second order systems and stiff systems
  - TSALPHA2 and TSBDF