The Portable Extensible Toolkit for Scientific Computing

Matthew Knepley

Computation Institute
University of Chicago

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Short Course on Scientific Computing
GUCAS, Beijing, China

Outline

Unit Objectives

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

What I Need From You

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

Ask Questions!!!

- Helps **me** understand what you are missing
- Helps **you** clarify misunderstandings
- Helps **others** with the same question

How We Can Help at the Tutorial

- Point out relevant documentation
- Answer email at petsc-maint@mcs.anl.gov

How We Can Help at the Tutorial

- Point out relevant documentation
- Quickly answer questions

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How We Can Help at the Tutorial

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- Quickly answer questions
- Help install

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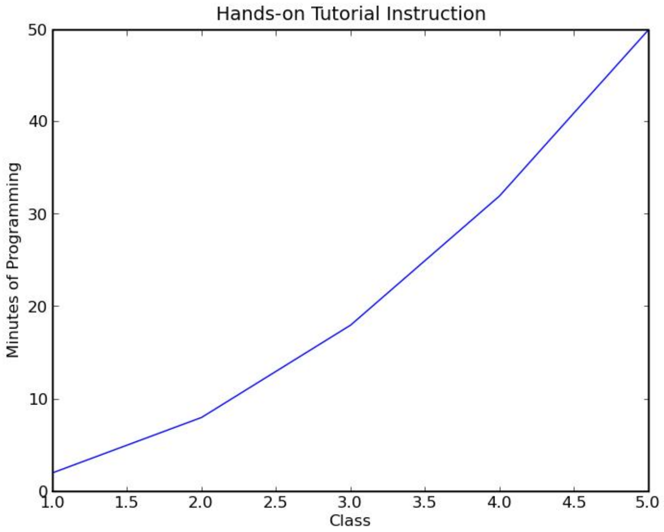
How We Can Help at the Tutorial

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

Hands-on Instruction



Tutorial Repositories

http://petsc.cs.iit.edu/petsc/TutorialExamples

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

http://petsc.cs.iit.edu/petsc/GUCAS09TutorialCode

- Fairly complex
- Shows how to use most PETSc features
- Uses C and C++

How did PETSc Originate?

PETSc was developed as a Platform for Experimentation

We want to experiment with different

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

The Role of PETSc

Developing parallel, nontrivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.

PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver, nor a silver bullet.

— Barry Smith

What is PETSc?

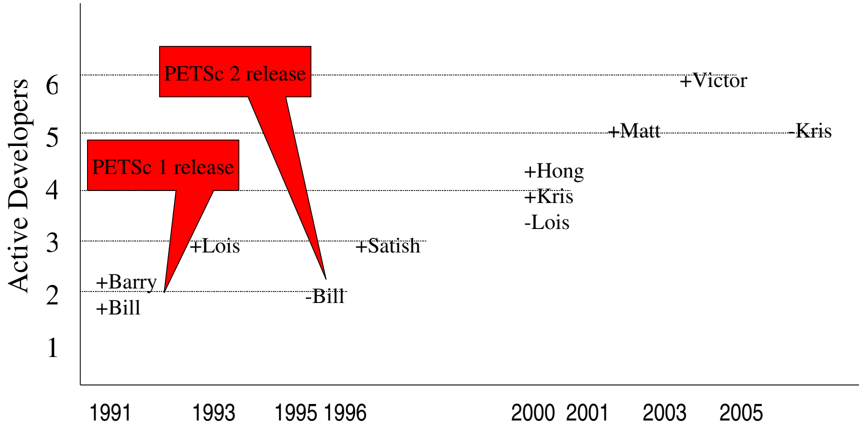
A freely available and supported research code

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

What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems
    - Cray T3E, SGI Origin, IBM SP, HP 9000, Sub Enterprise
  - Loosely coupled systems, such as networks of workstations
    - Compaq,HP, IBM, SGI, Sun, PCs running Linux or Windows
- PETSc History
  - Begun September 1991
  - Over 20,000 downloads since 1995 (version 2)
  - Currently 400 per month
- PETSc Funding and Support
  - Department of Energy
    - SciDAC, MICS Program, INL Reactor Program
  - National Science Foundation
    - CIG, CISE, Multidisciplinary Challenge Program

Timeline


Active Developers
1
2
3
4
5
6
PETSc 2 release
PETSc 1 release
+Barry
+Bill
+Lois
-Bill
+Satish
+Hong
+Kris
-Lois
+Matt
+Victor
-Kris
1991
1993
1995
1996
2000
2001
2003
2005

What Can We Handle?

- PETSc has run implicit problems with over 1 billion unknowns
    - PFLOTRAN for flow in porous media

What Can We Handle?

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- PETSc has run on over 130,000 cores efficiently
  - UNIC on the IBM BG/P Intrepid at ANL
  - PFLOTRAN on the Cray XT5 Jaguar at ORNL

What Can We Handle?

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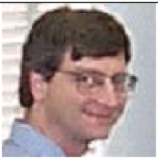
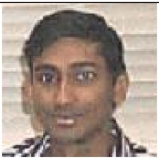
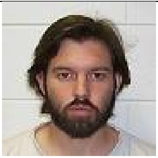
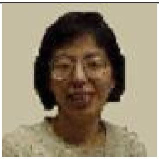
- PETSc applications have run at 3 Teraflops
  - LANL PFLOTRAN code

Who Uses PETSc?

- Computational Scientists
    - PyLith (TECTON), Underworld, Columbia group, PFLOTRAN
- Algorithm Developers
    - Iterative methods and Preconditioning researchers
- Package Developers
    - SLEPc, TAO, PETSc-FEM, MagPar, StGermain, DealII

The PETSc Team

 Bill Gropp	Barry Smith	 Satish Balay
Dinesh Kaushik	Kris Buschelman	 Matt Knepley
 Hong Zhang	Victor Eijkhout	Lois McInnes

Downloading PETSc

- The latest tarball is on the PETSc site
  - ftp://ftp.mcs.anl.gov/pub/petsc/petsc.tar.gz
  - We no longer distribute patches (everything is in the distribution)
- There is a Debian package
- There is a FreeBSD Port
- There is a Mercurial development repository

Cloning PETSc

- The full development repository is open to the public
  - http://petsc.cs.iit.edu/petsc/petsc-dev
  - http://petsc.cs.iit.edu/petsc/BuildSystem
- Why is this better?
  - You can clone to any release (or any specific ChangeSet)
  - You can easily rollback changes (or releases)
  - You can get fixes from us the same day
- We also make release repositories available
  - http://petsc.cs.iit.edu/petsc/petsc-release-3.0.0

Cloning PETSc

- Just clone development repository
  - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
  - `hg clone -rRelease-3.0.0 petsc-dev petsc-3.0.0`

or

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

Exercise 1

Download and Unpack PETSc!

Configuring PETSc

- Set `$PETSC_DIR` to the installation root directory
- Run the configuration utility
  - `$PETSC_DIR/configure`
  - `$PETSC_DIR/configure -help`
  - `$PETSC_DIR/configure -download-mpich`
  - `$PETSC_DIR/configure -prefix=/usr`
- There are many examples on the installation page
- Configuration files are in `$PETSC_DIR/$PETSC_ARCH/conf`
  - Configure header is in `$PETSC_DIR/$PETSC_ARCH/include`
  - `$PETSC_ARCH` has a default if not specified

Configuring PETSc

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

Configuring PETSc for Unstructured Meshes

- `-with-clanguage=cxx -with-fc=g95`
- `-with-shared -with-dynamic`
- `-download-lgrind -download-c2html -download-sowing`
- `-download-f-blas-lapack -download-mpich`
- `-download-boost -download-fiat -download-generator`
- `-download-triangle -download-tetgen`
- `-download-chaco -download-parmetis -download-zoltan`
- `-with-sieve -with-opt-sieve`

Automatic Downloads

- Starting in 2.2.1, some packages are automatically
  - Downloaded
  - Configured and Built (in `$PETSC_DIR/externalpackages`)
  - Installed with PETSc
- Currently works for
  - petsc4py
  - PETSc documentation utilities (Sowing, lgrind, c2html)
  - BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
  - MPICH, MPE, LAM
  - ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
  - MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack, pARMS
  - BLOPEX, FFTW, SPRNG
  - Prometheus, HYPRE, ML, SPAI
  - Sundials
  - Triangle, TetGen
  - FIAT, FFC, Generator
  - Boost

Exercise 2

Configure your downloaded PETSc.

Building PETSc

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

Exercise 3

Build your configured PETSc.

Exercise 4

Reconfigure PETSc to use ParMetis.

1. `linux-gnu-c-debug/conf/reconfigure-linux-gnu-c-debug.py`
    - `-PETSC_ARCH=linux-parmetis`
    - `-download-parmetis`
2. `PETSC_ARCH=linux-parmetis make`
3. `PETSC_ARCH=linux-parmetis make test`

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`

Using MPI

- The Message Passing Interface is:
  - a library for parallel communication
  - a system for launching parallel jobs (mpirun/mpiexec)
  - a community standard
- Launching jobs is easy
  - `mpiexec -n 4 ./ex5`
- You should never have to make MPI calls when using PETSc
  - Almost never

MPI Concepts

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

Alternative Memory Models

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

Common Viewing Options

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

Common Monitoring Options

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

Exercise 5

Run SNES Example 5 using come custom options.

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

Exercise 6

Create a new code based upon SNES Example 5.

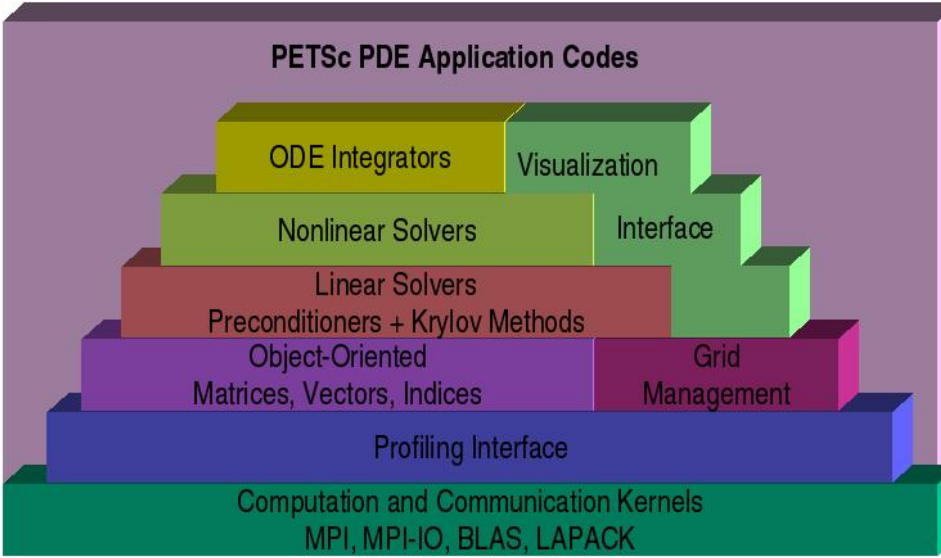
1. Create a new directory
   - `mkdir -p /home/knepley/proj/newsim/src`
2. Copy the source
   - `cp ex5.c /home/knepley/proj/newsim/src`
   - Add `myStuff.c` and `myStuff2.F`
3. Create a PETSc makefile
   - `ex5:  ex5.o myStuff.o myStuff2.o`
   - `  ${CLINKER} -o $@ $^ ${PETSC_SNES_LIB}`
   - `include ${PETSC_DIR}/bmake/common/base`

Getting More Help

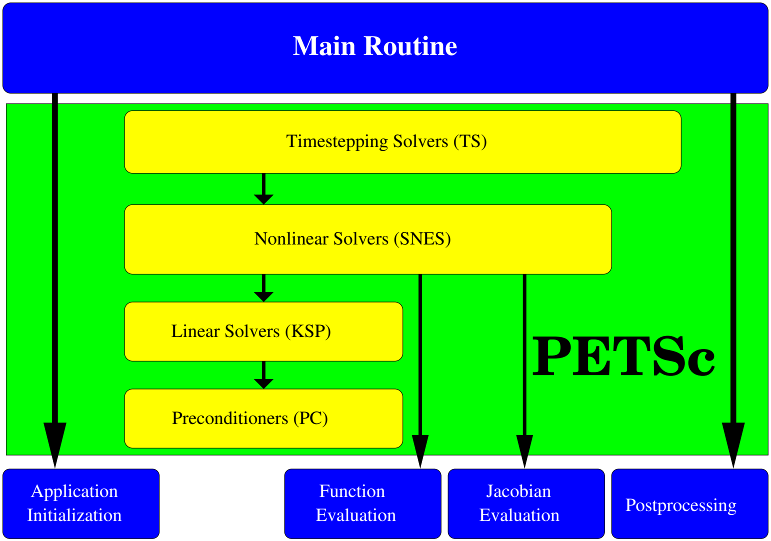
- http://www.mcs.anl.gov/petsc
- Hyperlinked documentation
  - Manual
  - Manual pages for evey method
  - HTML of all example code (linked to manual pages)
- FAQ
- Full support at petsc-maint@mcs.anl.gov
- High profile users
  - David Keyes
  - Marc Spiegelman
  - Richard Katz
  - Brad Aagaard
  - Lorena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

Outline

PETSc Structure


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

Flow Control for a PETSc Application



Levels of Abstraction
In Mathematical Software

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

Object-Oriented Design

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

The PETSc Programming Model

- Goals
    - Portable, runs everywhere
    - High performance
    - Scalable parallelism
- Approach
    - Distributed memory (“shared-nothing”)
    - No special compiler
    - Access to data on remote machines through MPI
    - Hide within objects the details of the communication
    - User orchestrates communication at a higher abstract level

Symmetry Principle

Interfaces to mutable data must be symmetric.

- Creation and query interfaces are paired
    - “No get without a set”
- Fairness
    - “If you can do it, your users will want to do it”
- Openness
    - “If you can do it, your users will want to undo it”

Empiricism Principle

Interfaces must allow easy testing and comparison.

- Swapping different implementations
    - “You will not be smart enough to pick the solver”
- Commonly violated in FE code
    - Elements are hard coded
- Also avoid assuming structure outside of the interface
    - Making continuous fields have discrete structure
    - Temptation to put metadata in a different places

Experimentation is Essential!

Proof is not currently enough to examine solvers

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

Collectivity

- MPI communicators (`MPI_Comm`) specify collectivity
  - Processes involved in a computation
- Constructors are collective over a communicator
  - `VecCreate(MPI_Comm comm, Vec *x)`
  - Use `PETSC_COMM_WORLD` for all processes and `PETSC_COMM_SELF` for one
- Some operations are collective, while others are not
  - collective: `VecNorm()`
  - not collective: `VecGetLocalSize()`
- Sequences of collective calls must be in the same order on each process

What is not in PETSc?

- ~~Unstructured mesh generation and manipulation~~
  - In 3.0, we have `Mesh` objects
- Discretizations
  - DealII
  - In 3.0, we have an interface to FIAT
- Higher level representations of PDEs
  - FEniCS (FFC/Syfi) and Sundance
- Load balancing
  - Interface to Zoltan
- Sophisticated visualization capabilities
  - Interface to MayaVi2 through VTK
- Eigenvalues
  - SLEPc and SIP
- Optimization and sensitivity
  - TAO and Veltisto

Basic `PetscObject` Usage

Every object in PETSc supports a basic interface

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

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

Correctness Debugging

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

Interacting with the Debugger

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

Debugging Tips

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

Exercise 7

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

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

Performance Debugging

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

Using Stages and Events

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

Adding A Logging Stage

```
int stageNum;

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

Code to Monitor

PetscLogStagePop();
```

Adding A Logging Event

```
static int USER_EVENT;

PetscLogEventRegister(&USER_EVENT, "name", CLS_COOKIE)

PetscLogEventBegin(USER_EVENT,0,0,0,0);

Code to Monitor

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

Adding A Logging Class

```
static int CLASS_COOKIE;

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

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

Matrix Memory Preallocation

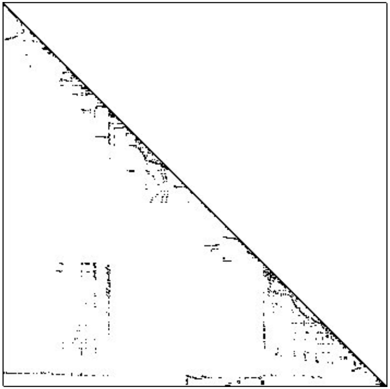
- PETSc sparse matrices are dynamic data structures
  - can add additional nonzeros freely
- Dynamically adding many nonzeros
  - requires additional memory allocations
  - requires copies
  - can kill performance
- Memory preallocation provides
  - the freedom of dynamic data structures
  - good performance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

Matrix Memory Preallocation

Sequential Sparse Matrices

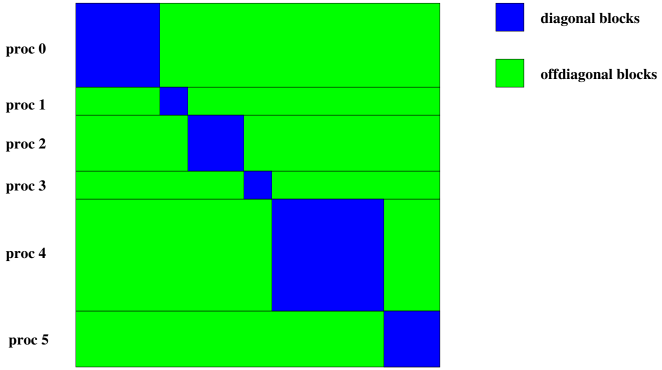
```
MatSeqAIJPreallocation(Mat A, int nz, int nnz[])
```

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



Matrix Memory Preallocation
ParallelSparseMatrix

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



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

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

Matrix Memory Preallocation

Parallel Sparse Matrices

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

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

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

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

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

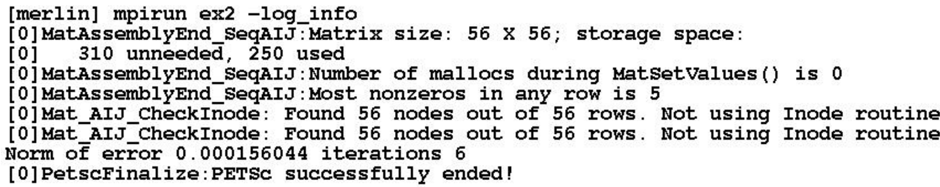
Matrix Memory Preallocation

Verifying Preallocation

- Use runtime option `-info`
- Output:

  `[proc #] Matrix size: %d X %d; storage space: %d unneeded, %d used`

  `[proc #] Number of mallocs during MatSetValues( ) is %d`



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

Exercise 8

Return to Execise 7 and add more profiling.

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

STREAM Benchmark

Simple benchmark program measuring sustainable memory bandwidth

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

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

Table: Bandwidth limited machine performance

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

Analysis of Sparse Matvec (SpMV)

Assumptions

- No cache misses
- No waits on memory references

Notation

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

We can look at bandwidth needed for peak performance

$$\left(8 + \frac{2}{V}\right)\frac{m}{nz} + \frac{6}{V} \text{ byte/flop} \tag{1}$$

or achieveable performance given a bandwith BW

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

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

Improving Serial Performance

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

$$\frac{1}{(8+2)\frac{1}{7}+6} \text{ bytes/flop}(1122.4 \text{ MB/s}) = 151 \text{ MFlops/s}, \tag{3}$$

which is a dismal 8.8% of peak.

Can improve performance by

- Blocking
- Multiple vectors

but operation issue limitations take over.

Improving Serial Performance

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

$$\frac{1}{(8+2)\frac{1}{7}+6}\ \mathrm{bytes/flop}(1122.4\ \mathrm{MB/s}) = 151\ \mathrm{MFlops/s}, \qquad (3)$$

which is a dismal 8.8% of peak.

Better approaches:

- Unassembled operator application (Spectral elements)
  - *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, . . .)

Importance of Computational Modeling

Without a model,
performance measurements are meaningless!

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

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

This allows us to

- verify the implementation
- predict scaling behavior

Outline

Application Integration

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

PETSc Integration

PETSc is a set a library interfaces

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

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

Integration Stages

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

Initialization

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

Profiling

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

Command Line Processing

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

Vector Algebra

What are PETSc vectors?

- Fundamental objects representing field solutions, right-hand sides, etc.
- Each process locally owns a subvector of contiguous global data

How do I create vectors?

- `VecCreate(MPI_Comm, Vec *)`
- `VecSetSizes(Vec, int n, int N)`
- `VecSetType(Vec, VecType typeName)`
- `VecSetFromOptions(Vec)`
  - Can set the type at runtime

Vector Algebra

A PETSc Vec

- Has a direct interface to the values
- Supports all vector space operations
  - `VecDot()`, `VecNorm()`, `VecScale()`
- Has unusual operations, e.g. `VecSqrt()`, `VecWhichBetween()`
- Communicates automatically during assembly
- Has customizable communication (scatters)

Parallel Assembly
Vectors and Matrices

- Processes may set an arbitrary entry
    - Must use proper interface
- Entries need not be generated locally
    - Local meaning the process on which they are stored
- PETSc automatically moves data if necessary
    - Happens during the assembly phase

Vector Assembly

- A three step process
  - Each process sets or adds values
  - Begin communication to send values to the correct process
  - Complete the communication
- `VecSetValues(Vec v, int n, int rows[], PetscScalar values[], mode)`
  - `mode` is either INSERT_VALUES or ADD_VALUES
- Two phase assembly allows overlap of communication and computation
  - `VecAssemblyBegin(Vec v)`
  - `VecAssemblyEnd(Vec v)`

One Way to Set the Elements of a Vector

```
VecGetSize(x, &N);
MPI_Comm_rank(PETSC_COMM_WORLD, &rank);
if (rank == 0) {
  for(i = 0, val = 0.0; i < N; i++, val += 10.0) {
    VecSetValues(x, 1, &i, &val, INSERT_VALUES);
  }
}
/* These routines ensure that the data is distributed
to the other processes */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
```

A Better Way to Set the Elements of a Vector

```
VecGetOwnershipRange(x, &low, &high);
for(i = low,val = low*10.0; i < high; i++,val += 10.0)
{
  VecSetValues(x, 1, &i, &val, INSERT_VALUES);
}
/* These routines ensure that the data is distributed
to the other processes */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
```

Selected Vector Operations

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

Working With Local Vectors

It is sometimes more efficient to directly access local storage of a `Vec`.

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

VecGetArray in C

```
Vec v;
PetscScalar *array;
PetscInt n, i;
PetscErrorCode ierr;

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

VecGetArray in F77

```
#include "finclude/petsc.h"
#include "finclude/petscvec.h"
Vec v;
PetscScalar array(1)
PetscOffset offset
PetscInt n, i
PetscErrorCode ierr

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

VecGetArray in F90

```
#include "finclude/petsc.h"
#include "finclude/petscvec.h"
#include "finclude/petscvec.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)
```

Matrix Algebra

What are PETSc matrices?

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

How do I create matrices?

- `MatCreate(MPI_Comm, Mat *)`
- `MatSetSizes(Mat, int m, int n, int M, int N)`
- `MatSetType(Mat, MatType typeName)`
- `MatSetFromOptions(Mat)`
  - Can set the type at runtime
- `MatSetValues(Mat,...)`
  - **MUST** be used, but does automatic communication

Matrix Polymorphism

The PETSc `Mat` has a single user interface,

- Matrix assembly
  - `MatSetValues()`
- Matrix-vector multiplication
  - `MatMult()`
- Matrix viewing
  - `MatView()`

but multiple underlying implementations.

- AIJ, Block AIJ, Symmetric Block AIJ,
- Dense
- Matrix-Free
- etc.

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

Matrix Assembly

- A three step process
  - Each process sets or adds values
  - Begin communication to send values to the correct process
  - Complete the communication
- `MatSetValues(Mat m, m, rows[], n, cols[], values[], mode)`
  - `mode` is either INSERT_VALUES or ADD_VALUES
  - Logically dense block of values
- Two phase assembly allows overlap of communication and computation
  - `MatAssemblyBegin(Mat m, type)`
  - `MatAssemblyEnd(Mat m, type)`
  - `type` is either MAT_FLUSH_ASSEMBLY or MAT_FINAL_ASSEMBLY

One Way to Set the Elements of a Matrix

Simple 3-point stencil for 1D Laplacian

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
if (rank == 0) {
for(row = 0; row < N; row++) {
  cols[0] = row-1; cols[1] = row; cols[2] = row+1;
  if (row == 0) {
    MatSetValues(A,1,&row,2,&cols[1],&v[1],INSERT_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);
```

A Better Way to Set the Elements of a Matrix

Simple 3-point stencil for 1D Laplacian

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
for(row = start; row < end; row++) {
  cols[0] = row-1; cols[1] = row; cols[2] = row+1;
  if (row == 0) {
    MatSetValues(A,1,&row,2,&cols[1],&v[1],INSERT_VALUES);

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

Why Are PETSc Matrices That Way?

- No one data structure is appropriate for all problems
  - Blocked and diagonal formats provide significant performance benefits
  - PETSc has many formats and makes it easy to add new data structures
- Assembly is difficult enough without worrying about partitioning
  - PETSc provides parallel assembly routines
  - Achieving high performance still requires making most operations local
  - However, programs can be incrementally developed.
  - `MatPartitioning` and `MatOrdering` can help
- Matrix decomposition in contiguous chunks is simple
  - Makes interoperation with other codes easier
  - For other ordering, PETSc provides “Application Orderings” (AO)

Solver Types

- **Explicit**:
  - Field variables are updated using local neighbor information
- **Semi-implicit**:
  - Some subsets of variables are updated with global solves
  - Others with direct local updates
- **Implicit**:
  - Most or all variables are updated in a single global solve

Linear Solvers
Krylov Methods

- Using PETSc linear algebra, just add:
  - `KSPSetOperators(KSP ksp, Mat A, Mat M, MatStructure flag)`
  - `KSPSolve(KSP ksp, Vec b, Vec x)`
- Can access subobjects
  - `KSPGetPC(KSP ksp, PC *pc)`
- Preconditioners must obey PETSc interface
  - Basically just the KSP interface
- Can change solver dynamically from the command line, `-ksp_type`

Nonlinear Solvers
Newton and Picard Methods

- Using PETSc linear algebra, just add:
  - `SNESSetFunction(SNES snes, Vec r, residualFunc, void *ctx)`
  - `SNESSetJacobian(SNES snes, Mat A, Mat M, jacFunc, void *ctx)`
  - `SNESSolve(SNES snes, Vec b, Vec x)`
- Can access subobjects
  - `SNESGetKSP(SNES snes, KSP *ksp)`
- Can customize subobjects from the cmd line
  - Set the subdomain preconditioner to ILU with `-sub_pc_type ilu`

Basic Solver Usage

We will illustrate basic solver usage with `SNES`.

- Use `SNESSetFromOptions()` so that everything is set dynamically
  - Use `-snes_type` to set the type or take the default
- Override the tolerances
  - Use `-snes_rtol` and `-snes_atol`
- View the solver to make sure you have the one you expect
  - Use `-snes_view`
- For debugging, monitor the residual decrease
  - Use `-snes_monitor`
  - Use `-ksp_monitor` to see the underlying linear solver

3rd Party Solvers in PETSc

Complete table of solvers

1. Sequential LU
   - ILUDT (SPARSEKIT2, Yousef Saad, U of MN)
   - EUCLID & PILUT (Hypre, David Hysom, LLNL)
   - ESSL (IBM)
   - SuperLU (Jim Demmel and Sherry Li, LBNL)
   - Matlab
   - UMFPACK (Tim Davis, U. of Florida)
   - LUSOL (MINOS, Michael Saunders, Stanford)
2. Parallel LU
   - MUMPS (Patrick Amestoy, IRIT)
   - SPOOLES (Cleve Ashcroft, Boeing)
   - SuperLU_Dist (Jim Demmel and Sherry Li, LBNL)
3. Parallel Cholesky
   - DSCPACK (Padma Raghavan, Penn. State)
4. XYTlib - parallel direct solver (Paul Fischer and Henry Tufo, ANL)

3rd Party Preconditioners in PETSc

Complete table of solvers

1. Parallel ICC
   - BlockSolve95 (Mark Jones and Paul Plassman, ANL)
2. Parallel ILU
   - BlockSolve95 (Mark Jones and Paul Plassman, ANL)
3. Parallel Sparse Approximate Inverse
   - Parasails (Hypre, Edmund Chow, LLNL)
   - SPAI 3.0 (Marcus Grote and Barnard, NYU)
4. Sequential Algebraic Multigrid
   - RAMG (John Ruge and Klaus Steuben, GMD)
   - SAMG (Klaus Steuben, GMD)
5. Parallel Algebraic Multigrid
   - Prometheus (Mark Adams, PPPL)
   - BoomerAMG (Hypre, LLNL)
   - ML (Trilinos, Ray Tuminaro and Jonathan Hu, SNL)

Higher Level Abstractions

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

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

The PETSc `Mesh` class is a topology interface.

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

Higher Level Abstractions

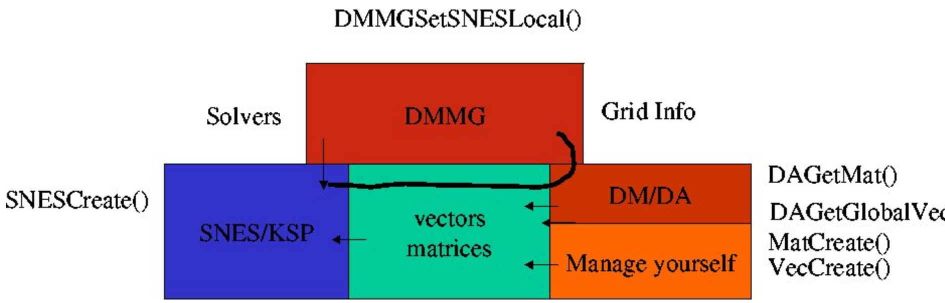
The PETSc `DM` class is a hierarchy interface.

- Supports multigrid
  - `DMMG` combines it with the `MG` preconditioner
- Abstracts the logic of multilevel methods

The PETSc `Section` class is a function interface.

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

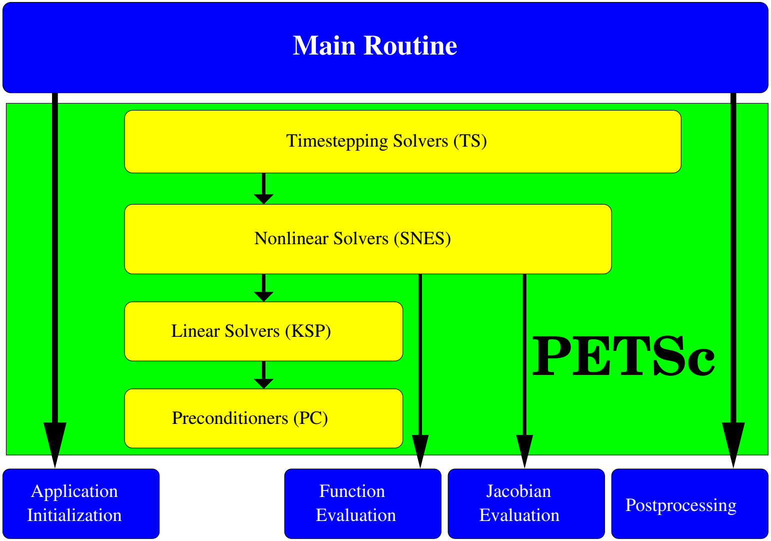
3 Ways To Use PETSc



- User manages all topology (just use Vec and Mat)
- PETSc manages single topology (use DA)
- PETSc manages a hierarchy (use DM)

Outline

Flow Control for a PETSc Application



SNES Paradigm

The SNES interface is based upon callback functions

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

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

- Solver calls the **user's** function
- User function gets application state through the `ctx` variable
    - PETSc never sees application data

Topology Abstractions

- `DA`
  - Abstracts Cartesian grids in any dimension
  - Supports stencils, communication, reordering
  - Nice for simple finite differences
- `Mesh`
  - Abstracts general topology in any dimension
  - Also supports partitioning, distribution, and global orders
  - Allows aribtrary element shapes and discretizations

Assembly Abstractions

- `DM`
  - Abstracts the logic of multilevel (multiphysics) methods
  - Manages allocation and assembly of local and global structures
  - Interfaces to `DMMG` solver
- `Section`
  - Abstracts functions over a topology
  - Manages allocation and assembly of local and global structures
  - Will merge with `DM` somehow

SNES Function

The user provided function which calculates the nonlinear residual has signature

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

`x`: The current solution

`r`: The residual

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

- Use this to pass application information, e.g. physical constants

SNES Jacobian

The user provided function which calculates the Jacobian has signature

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

- `x`: The current solution
- `J`: The Jacobian
- `M`: The Jacobian preconditioning matrix (possibly J itself)
- `ctx`: The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants
- Possible `MatStructure` values are:
  - SAME_NONZERO_PATTERN
  - DIFFERENT_NONZERO_PATTERN

Alternatively, you can use

- a builtin sparse finite difference approximation
- automatic differentiation (ADIC/ADIFOR)

SNES Variants

- Line search strategies
- Trust region approaches
- Pseudo-transient continuation
- Matrix-free variants

Finite Difference Jacobians

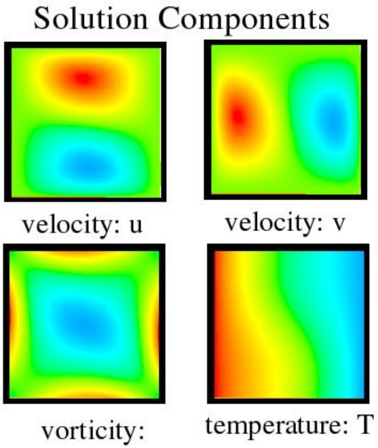
PETSc can compute and explicitly store a Jacobian via 1st-order FD

- Dense
  - Activated by `-snes_fd`
  - Computed by `SNESDefaultComputeJacobian()`
- Sparse via colorings
  - Coloring is created by `MatFDColoringCreate()`
  - Computed by `SNESDefaultComputeJacobianColor()`

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

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

SNES Example
Driven Cavity



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

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

SNES Example
Driven Cavity Application Context

```
typedef struct {
  /*--- basic application data ---*/
  double lid_velocity;
  double prandtl, grashof;
  int mx, my;
  int mc;
  PetscTruth draw_contours;
  /*--- parallel data ---*/
  MPI_Comm comm;
  DA da;
  /* Local ghosted solution and residual */
  Vec localX, localF;
} AppCtx;
```

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

SNES Example

Driven Cavity Residual Evaluation

```
DrivenCavityFunction(SNES snes, Vec X, Vec F, void *ptr) {
  AppCtx *user = (AppCtx *) ptr;
  /* local starting and ending grid points */
  int istart, iend, jstart, jend;
  PetscScalar *f; /* local vector data */
  PetscReal grashof = user->grashof;
  PetscReal prandtl = user->prandtl;
  PetscErrorCode ierr;

  /* Code to communicate nonlocal ghost point data */
  VecGetArray(F, &f);
  /* Code to compute local function components */
  VecRestoreArray(F, &f);
  return 0;
}
```

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

SNES Example
Better Driven Cavity Residual Evaluation

```
PetscErrorCode DrivenCavityFuncLocal(DALocalInfo *info,
  Field **x,Field **f,void *ctx) {
  /* Handle boundaries */
  /* Compute over the interior points */
  for(j = info->ys; j < info->xs+info->xm; j++) {
    for(i = info->xs; i < info->ys+info->ym; i++) {
      /* convective coefficients for upwinding */
      /* U velocity */
      u = x[j][i].u;
      uxx = (2.0*u - x[j][i-1].u - x[j][i+1].u)*hydhx;
      uyy = (2.0*u - x[j-1][i].u - x[j+1][i].u)*hxdhy;
      upw = 0.5*(x[j+1][i].omega-x[j-1][i].omega)*hx
      f[j][i].u = uxx + uyy - upw;
      /* V velocity, Omega, Temperature */
}}}
```

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

What is a DA?

`DA` is a topology interface handling parallel data layout on structured grids

- Handles local and global indices
  - `DAGetGlobalIndices()` and `DAGetAO()`
- Provides local and global vectors
  - `DAGetGlobalVector()` and `DAGetLocalVector()`
- Handles ghost values coherence
  - `DAGetGlobalToLocal()` and `DAGetLocalToGlobal()`

DA Paradigm

The DA interface is based upon local callback functions

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

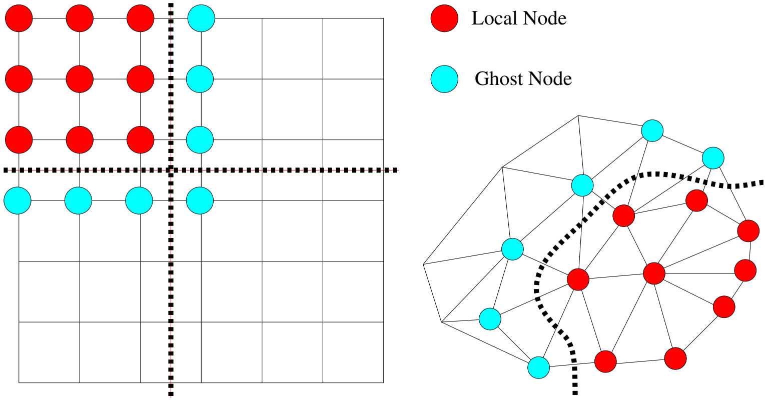
When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Each process evaluates the local residual
- PETSc assembles the global residual automatically

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



DA Global Numberings

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

Natural numbering

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

PETSc numbering

DA Global vs. Local Numbering

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

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

Local numbering

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

Global numbering

DA Local Function

The user provided function which calculates the nonlinear residual in 2D has signature

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

`info`: All layout and numbering information

`x`: The current solution

- Notice that it is a multidimensional array

`r`: The residual

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

The local DA function is activated by calling

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

Bratu Residual Evaluation

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

```
BratuResidualLocal(DALocalInfo *info,Field **x,Field **f)
{
  /* Not Shown: Handle boundaries */
  /* Compute over the interior points */
  for(j = info->ys; j < info->xs+info->ym; j++) {
    for(i = info->xs; i < info->ys+info->xm; i++) {
      u       = x[j][i];
      u_xx    = (2.0*u - x[j][i-1] - x[j][i+1])*hydhx;
      u_yy    = (2.0*u - x[j-1][i] - x[j+1][i])*hxdhy;
      f[j][i] = u_xx + u_yy - hx*hy*lambda*exp(u);
    }
  }
}
```

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

DA Local Jacobian

The user provided function which calculates the Jacobian in 2D has signature

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

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

The local DA function is activated by calling

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

Bratu Jacobian Evaluation

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

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

A DA is more than a Mesh

A DA contains topology, geometry, and an implicit Q1 discretization.

It is used as a template to create

- Vectors (functions)
- Matrices (linear operators)

DA Vectors

- The DA object contains only layout (topology) information
  - All field data is contained in PETSc `Vec`s
- Global vectors are parallel
  - Each process stores a unique local portion
  - `DACreateGlobalVector(DA da, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
  - Each process stores its local portion plus ghost values
  - `DACreateLocalVector(DA da, Vec *lvec)`
  - includes ghost values!

Updating Ghosts

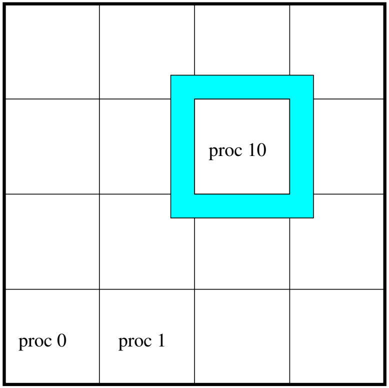
Two-step process enables overlapping computation and communication

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

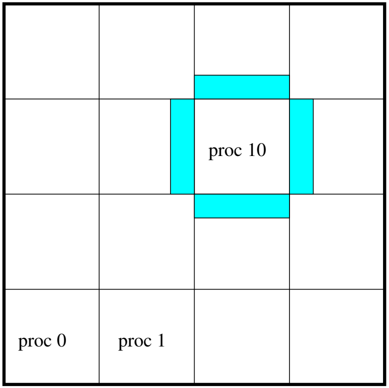
The process can be reversed with `DALocalToGlobal()`.

DA Stencils

Both the box stencil and star stencil are available.



Box Stencil



Star Stencil

Setting Values on Regular Grids

PETSc provides

```
MatSetValuesStencil(Mat A, m, MatStencil idxm[], n,
        MatStencil idxn[], values[], 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 DA

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

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

type: Specifies stencil
- DA_STENCIL_BOX or DA_STENCIL_STAR

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

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

dof: Degrees of freedom per node

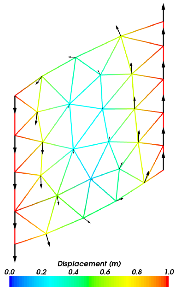
s: The stencil width

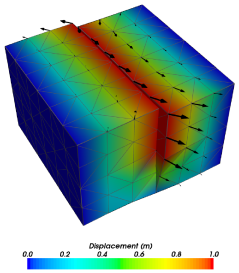
lm/n: Alternative array of local sizes
- Use PETSC_NULL for the default

Outline

Multiple Mesh Types

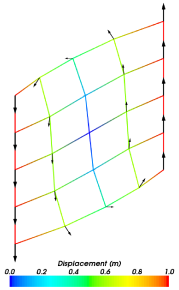
Triangular

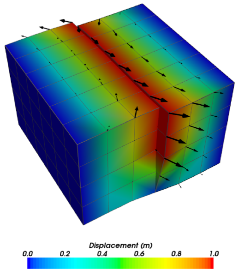




Tetrahedral

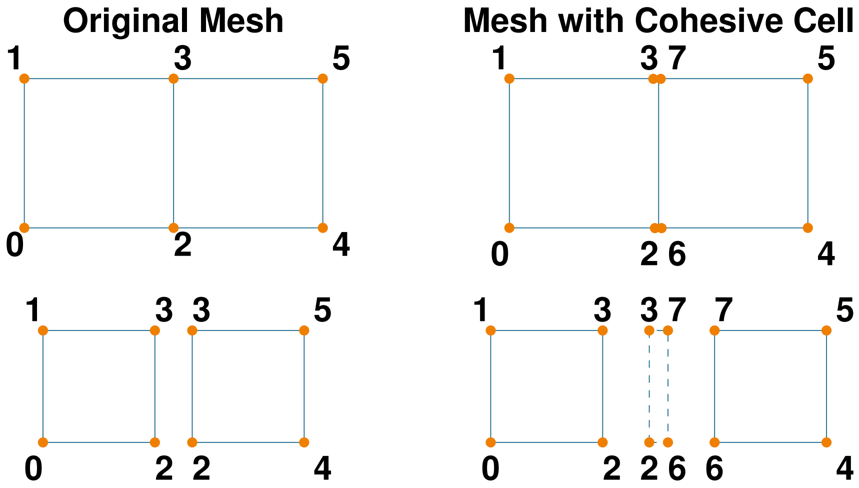
Rectangular





Hexahedral

Cohesive Cells



Exploded view of meshes

Cohesive Cells

Cohesive cells are used to enforce slip conditions on a fault

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

Mesh Paradigm

The Mesh interface also uses *local* callback functions

- maps between global `Vec` and local `Vec` (`Section`)
- provides `Complete()` which generalizes `LocalToGlobal()`

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

- Each process evaluates the local residual for each element
- PETSc assembles the global residual automatically

Higher Level Abstractions

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

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

The PETSc `Mesh` class is a topology interface.

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

Higher Level Abstractions

The PETSc `DM` class is a hierarchy interface.

- Supports multigrid
  - `DMMG` combines it with the `MG` preconditioner
- Abstracts the logic of multilevel methods

The PETSc `Section` class is a function interface.

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

Code Update

Update to Revision 1

Creating a DA

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

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

type: Specifies stencil
- `DA_STENCIL_BOX` or `DA_STENCIL_STAR`

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

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

dof: Degrees of freedom per node

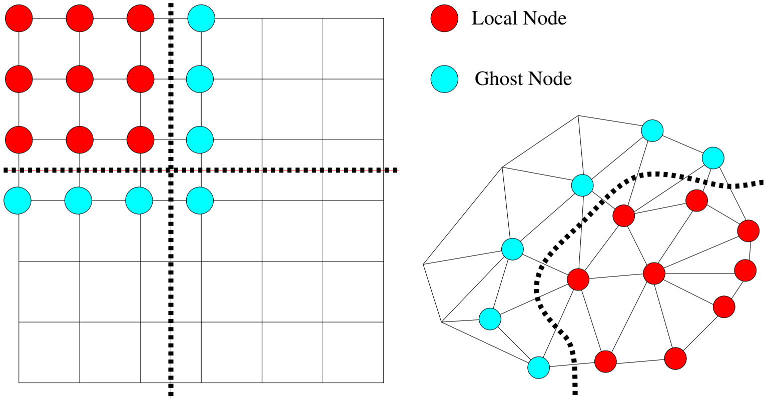
s: The stencil width

lm/n: Alternative array of local sizes
- Use `PETSC_NULL` for the default

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



DA Global Numberings

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

Natural numbering

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

PETSc numbering

DA Global vs. Local Numbering

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

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

Local numbering

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

Global numbering

Viewing the DA

- `make NP=1 EXTRA_ARGS="-da_view_draw -draw_pause -1" runbratu`
- `make NP=1 EXTRA_ARGS="-da_grid_x 10 -da_grid_y 10 -da_view_draw -draw_pause -1" runbratu`
- `make NP=4 EXTRA_ARGS="-da_grid_x 10 -da_grid_y 10 -da_view_draw -draw_pause -1" runbratu`

Correctness Debugging

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

Interacting with the Debugger

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

Debugging Tips

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

Memory Debugging

We can check for unfreed memory using:

```
make EXTRA_ARGS="-malloc_dump" runbratu
```

There is a leak!

All options can be seen using:

```
make EXTRA_ARGS="-help" runbratu
```

Code Update

Update to Revision 2

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`

Code Update

Update to Revision 3

Performance Debugging

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

Using Stages and Events

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

Adding A Logging Stage

```
int stageNum;

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

Code to Monitor

PetscLogStagePop();
```

Adding A Logging Event

```
static int USER_EVENT;

PetscLogEventRegister(&USER_EVENT, "name", CLS_COOKIE)

PetscLogEventBegin(USER_EVENT,0,0,0,0);

Code to Monitor

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

Adding A Logging Class

```
static int CLASS_COOKIE;

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

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

Matrix Memory Preallocation

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

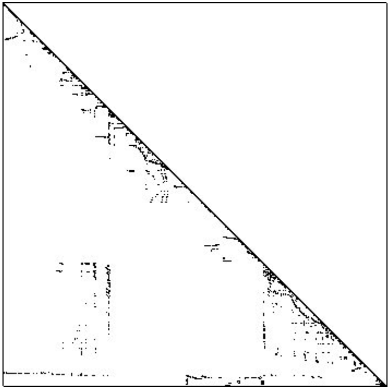
Matrix Memory Preallocation

Sequential Sparse Matrices

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

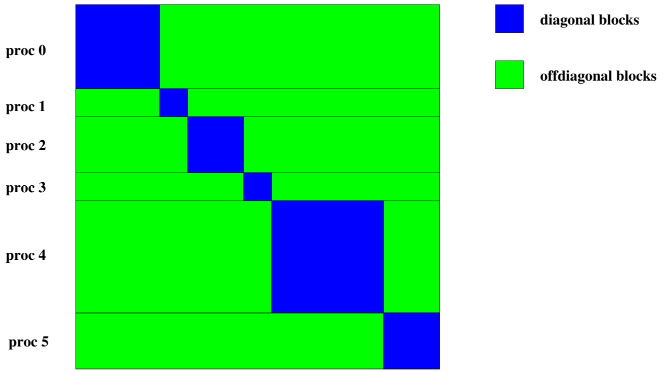
nz: expected number of nonzeros in any row

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



Matrix Memory Preallocation
ParallelSparseMatrix

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



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

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

Matrix Memory Preallocation

Parallel Sparse Matrices

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

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

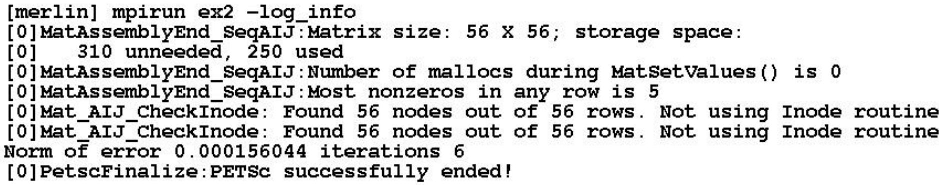
nnz(i): expected number of nonzeros in row i in the diagonal block

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

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

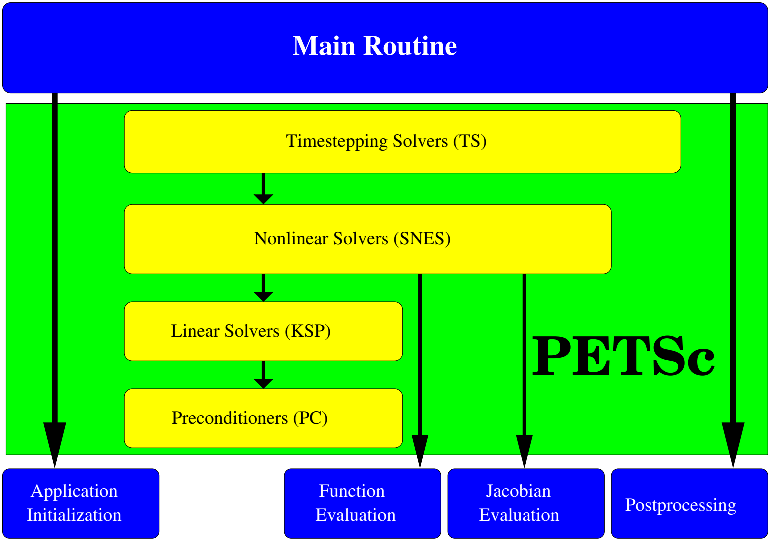
Matrix Memory Preallocation
Verifying Preallocation

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



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

Flow Control for a PETSc Application



Collectivity

- MPI communicators (`MPI_Comm`) specify collectivity
  - Processes involved in a computation
- Constructors are collective over a communicator
  - `VecCreate(MPI_Comm comm, Vec *x)`
  - Use `PETSC_COMM_WORLD` for all processes and `PETSC_COMM_SELF` for one
- Some operations are collective, while others are not
  - collective: `VecNorm()`
  - not collective: `VecGetLocalSize()`
- Sequences of collective calls must be in the same order on each process

Basic `PetscObject` Usage

Every object in PETSc supports a basic interface

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

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

Experimentation is Essential!

Proof is not currently enough to examine solvers

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

Creating the Mesh

- Generic object
  - `MeshCreate()`
  - `MeshSetMesh()`
- File input
  - `MeshCreateExodus()`
  - `MeshCreateDolfin()`
  - `MeshCreatePyLith()`
- Generation
  - `MeshGenerate()`
  - `MeshRefine()`, `MeshCoarsen()`
  - `ALE::MeshBuilder<>::createSquareBoundary()`
- Representation
  - `ALE::SieveBuilder<>::buildTopology()`
  - `ALE::SieveBuilder<>::buildCoordinates()`
- Partitioning and Distribution
  - `MeshDistribute()`
  - `MeshDistributeByFace()`

Code Update

Update to Revision 4

Viewing the Mesh

- `make NP=1 EXTRA_ARGS="-structured 0 -mesh_view_vtk" runbratu`
- `mayavi2 -d bratu.vtk -m Surface&`
- `make NP=4 EXTRA_ARGS="-structured 0 -mesh_view_vtk" runbratu`
- Viewable using Mayavi or Paraview

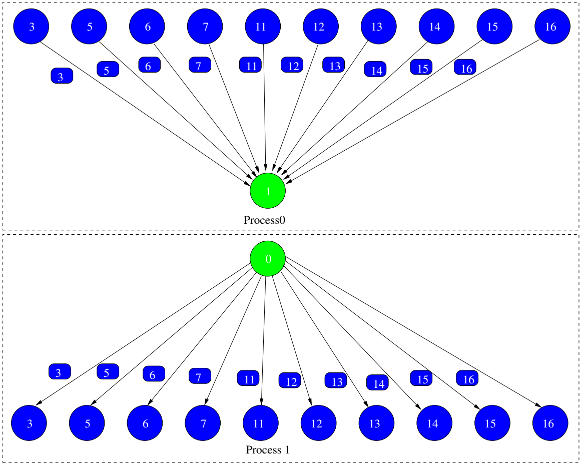
Refining the Mesh

- `make NP=1 EXTRA_ARGS="-structured 0 -generate -mesh_view_vtk" runbratu`
- `make NP=1 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.0625 -mesh_view_vtk" runbratu`
- `make NP=4 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.0625 -mesh_view_vtk" runbratu`

Parallel Sieves

- Sieves use names, not numberings
  - Allows independent adaptation
  - Demanding a global numbering can seriously impact memory scaling
  - Numberings can be constructed on demand
- `Overlaps` relate names on different processes
  - An Overlap can be encoded by a Sieve
- Distribution of a `Section` pushes forward along the Overlap
  - Sieves are distributed as “cone” sections

Overlap for Distribution



- The send overlap is above the receive overlap
- Green points are remote process ranks
- Arrow labels indicate remote process names

Code Update

Update to Revision 5

Viewing the 3d Mesh

- `make NP=1 EXTRA_ARGS="-dim 3 -da_view_draw -draw_pause -1" runbratu`
- `make NP=4 EXTRA_ARGS="-da_grid_x 5 -da_grid_y 5 -da_grid_z 5 -da_view_draw -draw_pause -1" runbratu`
- `make NP=1 EXTRA_ARGS="-dim 3 -structured 0 -generate -mesh_view_vtk" runbratu`
- `mayavi2 -d bratu.vtk -f ExtractEdges -m Surface`
- `make NP=4 EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.01 -mesh_view_vtk" runbratu`

Outline

A DA is more than a Mesh

A DA contains topology, geometry, and an implicit Q1 discretization.

It is used as a template to create

- Vectors (functions)
- Matrices (linear operators)

DA Vectors

- The DA object contains only layout (topology) information
  - All field data is contained in PETSc `Vec`s
- Global vectors are parallel
  - Each process stores a unique local portion
  - `DACreateGlobalVector(DA da, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
  - Each process stores its local portion plus ghost values
  - `DACreateLocalVector(DA da, Vec *lvec)`
  - includes ghost values!

Updating Ghosts

Two-step process enables overlapping computation and communication

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

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

DA Local Function

The user provided function which calculates the nonlinear residual in 2D has signature

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

`info`: All layout and numbering information

`x`: The current solution

- Notice that it is a multidimensional array

`r`: The residual

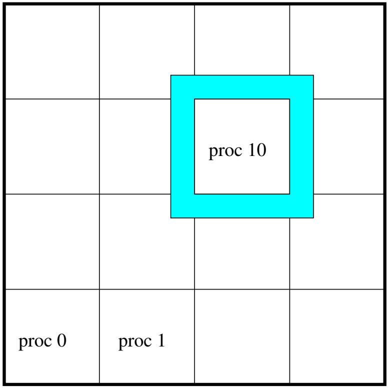
`ctx`: The user context passed to `DASetLocalFunction()`

The local DA function is activated by calling

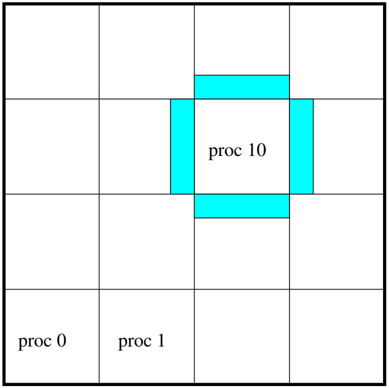
```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

DA Stencils

Both the box stencil and star stencil are available.



Box Stencil



Star Stencil

Setting Values on Regular Grids

PETSc provides

```
MatSetValuesStencil(Mat A, m, MatStencil idxm[], n,
        MatStencil idxn[], values[], 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

Code Update

Update to Revision 6

Structured Functions

- Functions takes 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

-
  ```
  make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1"
  runbratu
  ```

Sections

Sections associate data to submeshes

- Name comes from section of a fiber bundle
  - Generalizes linear algebra paradigm
- Define `restrict()`,`update()`
- Define `complete()`
- Assembly routines take a `Sieve` and several `Section`s
  - This is called a `Bundle`

Section Types

Section can contain arbitrary values

- C interface has two value types
  - `SectionReal`
  - `SectionInt`
- C++ interface is templated over value type

Section can have arbitrary layout

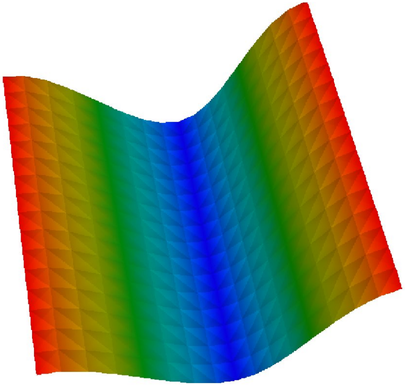
- C interface has default layouts
  - `MeshGetVertexSectionReal()`
  - `MeshGetCellSectionReal()`
- C++ interface can place dof on any Mesh entity (Sieve point)
  - `Mesh::setupField()` allows layout on a hierarchy
  - It is parametrized by `Discretization` and `BoundaryCondition`

Code Update

Update to Revision 7

Viewing the Section

- `make EXTRA_ARGS="-run test -structured 0 -vec_view_vtk" runbratu`
  - Produces linear.vtk and cos.vtk
- Viewable with MayaVi, exactly as with the mesh.
- `make NP=2 EXTRA_ARGS="-run test -structured 0 -vec_view_vtk -generate -refinement_limit 0.003125" runbratu`
  - Use `mayavi2 -d cos.vtk -f WarpScalar -m Surface`



Outline

Weak Forms

A weak form is the pairing of
a *function* with an element of the *dual space*.

- Produces a number (by definition of the dual)
- Can be viewed as a “function” of the dual vector
- Used to define finite element solutions
- Require a dual space and integration rules

For example, for $f \in V$, we have the weak form

$$\int_\Omega \phi(\mathbf{x}) f(\mathbf{x}) dx \qquad \phi \in V^*$$

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

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

FIAT understands

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

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

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

Maps

We are interested in nonlinear maps $F : \mathbb{R}^n \longrightarrow \mathbb{R}^n$.

- Can contain the action of differential operators
- Encapsulated in `Rhs_*()` methods
- Will later be used to form the residual of our system

Code Update

Update to Revision 8

FIAT Integration

The `quadrature.fiat` file contains:

- An element (usually a family and degree) defined by FIAT
- A quadrature rule

It is run

- automatically by `make`, or
- independently by the user

It can take arguments

- `-element_family` and `-element_order`, or
- `make` takes variables `ELEMENT` and `ORDER`

Then `make` produces `bratu_quadrature.h` with:

- Quadrature points and weights
- Basis function and derivative evaluations at the quadrature points
- Integration against dual basis functions over the cell
- Local dofs for Section allocation

Boundary Conditions

Dirichlet conditions may be expressed as

$$u|_\Gamma = g$$

and implemented by constraints on dofs in a Section

- The user provides a function.

Neumann conditions may be expressed as

$$\nabla u \cdot \hat{n}|_\Gamma = h$$

and implemented by explicit integration along the boundary

- The user provides a weak form.

Assembly with Dirichlet Conditions

The original equation may be partitioned into

- unknowns in the interior (I)
- unknowns on the boundary (Γ)

so that we obtain

$$\begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} u_I \\ u_\Gamma \end{pmatrix} = \begin{pmatrix} f_I \\ f_\Gamma \end{pmatrix}$$

However u_Γ is known, so we may reduce this to

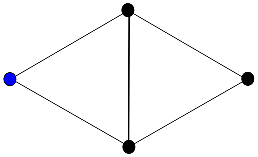
$$A_{II} u_I = f_I - A_{I\Gamma} u_\Gamma$$

We will show that our scheme automatically constructs this extra term.

Assembly with Dirichlet Conditions

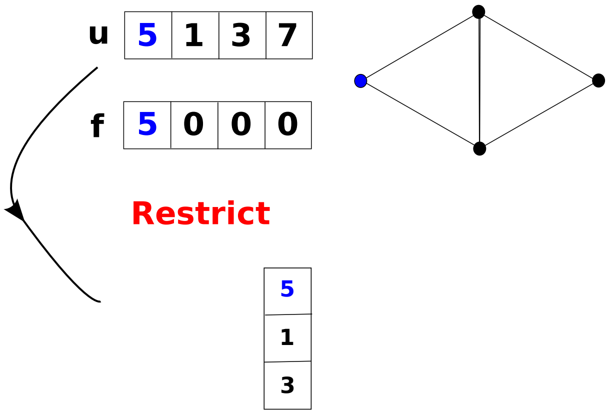
Residual Assembly

u	**5**	**1**	**3**	**7**
f	**5**	**0**	**0**	**0**



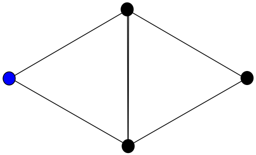
Assembly with Dirichlet Conditions

Residual Assembly



Assembly with Dirichlet Conditions
Residual Assembly

u	5	1	3	7
f	5	0	0	0

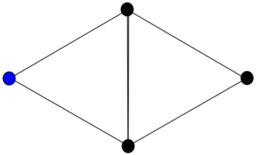


Compute

$$\begin{bmatrix} 0.5 & 0.0 & -0.5 \\ 0.0 & 0.5 & -0.5 \\ -0.5 & -0.5 & 1.0 \end{bmatrix} \begin{bmatrix} 5 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

Assembly with Dirichlet Conditions
Residual Assembly

u	5	1	3	7
f	5	0	0	0

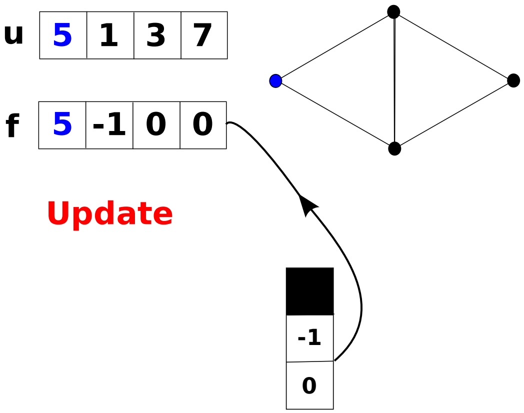


Compute

$$\begin{bmatrix} A_{\Gamma\Gamma} & A_{\Gamma I} \\ A_{I\Gamma} & A_{II} \end{bmatrix} \begin{bmatrix} 5 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \Bigg\} \text{This piece contains rhs interior values}$$

Assembly with Dirichlet Conditions

Residual Assembly



Dirichlet Conditions (Essential BC)

- Explicit limitation of the approximation space
- Idea:
  - Maintain the same FEM interface (`restrict()`, `update()`)
  - Allow direct access to reduced problem (contiguous storage)
- Implementation
  - Ignored by `size()` and `update()`, but `restrict()` works normally
  - Use `updateBC()` to define the boundary values
  - Use `updateAll()` to define both boundary and regular values
  - Points have a negative fiber dimension **or**
  - Dof are specified as constrained

Dirichlet Values

- Topological boundary is marked during generation
- Cells bordering boundary are marked using `markBoundaryCells()`
- To set values:
  1. Loop over boundary cells
  2. Loop over the element closure
  3. For each boundary point i, apply the functional N_i to the function g
- The functionals are generated with the quadrature information
- Section allocation applies Dirichlet conditions automatically
  - Values are stored in the Section
  - `restrict()` behaves normally, `update()` ignores constraints

Dual Basis Application

We would like the action of a dual basis vector (functional)

$$< \mathcal{N}_i, f >= \int_{\mathrm{ref}} N_i(x) f(x) dV$$

- Projection onto $\mathcal{P}$
- Code is generated from FIAT specification
  - Python code generation package inside PETSc
- Common interface for all elements

Section Assembly

First we do local operations:

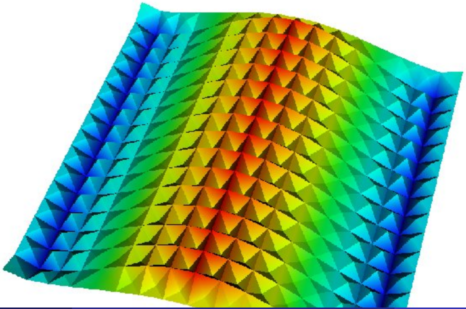
- Loop over cells
- Compute cell geometry
- Integrate each basis function to produce an element vector
- Call `SectionUpdateAdd()`
    - Note that this updates the closure of the cell

Then we do global operations:

- `SectionComplete()` exchanges data across overlap
    - C just adds nonlocal values (C++ is flexible)
- C++ also allows completion over arbitrary overlaps

Viewing a Mesh Weak Form

- We use finite elements and a Galerkin formulation
  - We calculate the residual $F(u) = -\Delta u - f$
  - Correct basis/derivatives table chosen by `setupQuadrature()`
  - Could substitute exact integrals for quadrature
- `make NP=2 EXTRA_ARGS="-run test -structured 0 -vec_view_vtk -generate -refinement_limit 0.003125" runbratu`
- `make EXTRA_ARGS="-run test -dim 3 -structured 0 -generate -vec_view_vtk" runbratu`



Global and Local

Local (analytical)

Global (topological)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions

Global (topological)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Difference Approximations

With finite differences, we approximate differential operators with difference quotients,

$$\frac{\partial u(x)}{\partial x} \approx \frac{u(x+h)-u(x-h)}{2h}$$
$$\frac{\partial^2 u(x)}{\partial x^2} \approx \frac{u(x+h)-2u(x)+u(x-h)}{h^2}$$

The important property for the approximation is consistency, meaning

$$\lim_{h\to 0} \frac{\partial u(x)}{\partial x} - \frac{u(x+h)-u(x-h)}{2h} = 0$$

and in fact,

$$\frac{\partial^2 u(x)}{\partial x^2} - \frac{u(x+h)-2u(x)+u(x-h)}{h^2} \in \mathcal{O}(h^2)$$

Code Update

Update to Revision 9

Viewing FD Operator Actions

We cannot currently visualize the 3D results,

- `make EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" runbratu`
- `make EXTRA_ARGS="-run test -da_grid_x 10 -da_grid_y 10 -vec_view_draw -draw_pause -1" runbratu`
- `make EXTRA_ARGS="-run test -dim 3 -vec_view" runbratu`

but can check the ASCII output if necessary.

Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" debugbratu`

Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" debugbratu`
- Spawns one debugger window per process

Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" debugbratu`
- Spawns one debugger window per process
- SEGV on access to ghost coordinates

Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" debugbratu`
- Spawns one debugger window per process
- SEGV on access to ghost coordinates
- Fix by using a local ghosted vector
  - Update to Revision 10

Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-run test -vec_view_draw -draw_pause -1" debugbratu`
- Spawns one debugger window per process
- SEGV on access to ghost coordinates
- Fix by using a local ghosted vector
  - Update to Revision 10
- Notice
  - we already use ghosted assembly (completion) for FEM
  - FD does not need ghosted assembly

Representations of the Error

- A single number, the norm itself
- A number per element, the element-wise norm
- Injection into the finite element space

$$e = \sum_i e_i \phi_i(x)$$

  - We calculate e_i by least-squares projection into $\mathcal{P}$

Interpolation Pitfalls

Comparing solutions on different meshes can be problematic.

- Picture our solutions as functions defined over the entire domain
  - For FEM, $\hat{u}(x) = \sum_i u_i \phi_i(x)$
- After interpolation, the interpolant might not be the same function
- We often want to preserve thermodynamic bulk properties
  - Energy, stress energy, incompressibility, ...
- Can constrain interpolation to preserve desirable quantities
  - Usually produces a saddlepoint system

Calculating the L_2 Error

We begin with a continuum field $u(x)$ and an FEM approximation

$$\hat{u}(x) = \sum_i \hat{u}_i \phi_i(x)$$

The FE theory predicts a convergence rate for the quantity

$$||u - \hat{u}||_2^2 = \sum_T \int_T dA (u - \hat{u})^2 \tag{4}$$

$$= \sum_T \sum_q w_q |J| \left(u(q) - \sum_j \hat{u}_j \phi_j(q) \right)^2 \tag{5}$$

The estimate for linear elements is

$$||u - \hat{u}_h|| < Ch||u||$$

Code Update

Update to Revision 11

Calculating the Error

- Added `CreateProblem()`
  - Define the global section
  - Setup exact solution and boundary conditions
- Added `CreateExactSolution()` to project the solution function
- Added `CheckError()` to form the error norm
  - Finite differences calculates a pointwise error
  - Finite elements calculates a normwise error
- Added `CheckResidual()` which uses our previous functionality

Checking the Error

- `make NP=2 EXTRA_ARGS="-run full -da_grid_x 10 -da_grid_y 10" runbratu`
- `make EXTRA_ARGS="-run full -dim 3" runbratu`
- `make EXTRA_ARGS="-run full -structured 0 -generate" runbratu`
- `make NP=2 EXTRA_ARGS="-run full -structured 0 -generate" runbratu`
- `make EXTRA_ARGS="-run full -structured 0 -generate -refinement_limit 0.03125" runbratu`
- `make EXTRA_ARGS="-run full -dim 3 -structured 0 -generate -refinement_limit 0.01" runbratu`

Notice that the FE error does not always vanish, since we are using information across the entire element. We can enrich our FE space:

- `rm bratu_quadrature.h; make ORDER=2`
- `make EXTRA_ARGS="-run full -structured 0 -generate -refinement_limit 0.03125" runbratu`
- `make EXTRA_ARGS="-run full -dim 3 -structured 0 -generate -refinement_limit 0.01" runbratu`

Outline

DA Local Jacobian

The user provided function which calculates the Jacobian in 2D has signature

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

`info`: All layout and numbering information

`x`: The current solution

`J`: The Jacobian

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

The local DA function is activated by calling

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

Code Update

Update to Revision 12

DA Operators

- Evaluate only the local portion
  - No nice local array form without copies
- Use `MatSetValuesStencil()` to convert `(i,j,k)` to indices
- `make NP=2 EXTRA_ARGS="-run test -da_grid_x 10 -da_grid_y 10 -mat_view_draw -draw_pause -1" runbratu`
- `make NP=2 EXTRA_ARGS="-run test -dim 3 -da_grid_x 5 -da_grid_y 5 -da_grid_z 5 -mat_view_draw -draw_pause -1" runbratu`

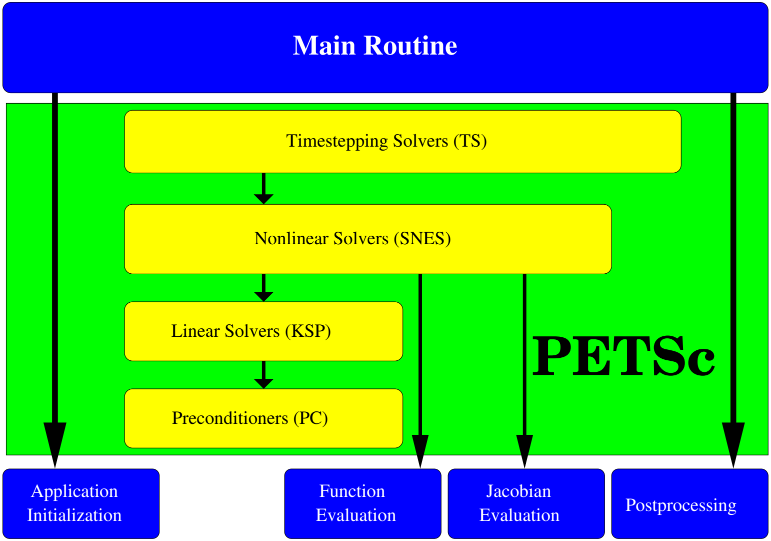
Mesh Operators

- We evaluate the local portion just as with functions
- Notice we use J^{-1} to convert derivatives
- Currently `updateOperator()` uses `MatSetValues()`
  - We need to call `MatAssembleyBegin/End()`
  - We should properly have `OperatorComplete()`
  - Also requires a Section, for layout, and a global variable order for PETSc index conversion

- `make EXTRA_ARGS="-run test -structured 0 -mat_view_draw -draw_pause -1 -generate" runbratu`
- `make NP=2 EXTRA_ARGS="-run test -structured 0 -mat_view_draw -draw_pause -1 -generate -refinement_limit 0.03125" runbratu`
- `make EXTRA_ARGS="-run test -dim 3 -structured 0 -mat_view_draw -draw_pause -1 -generate" runbratu`

Outline

Flow Control for a PETSc Application



SNES Paradigm

The SNES interface is based upon callback functions

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

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

- Solver calls the **user's** function
- User function gets application state through the `ctx` variable
  - PETSc never sees application data

SNES Function

The user provided function which calculates the nonlinear residual has signature

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

`x`: The current solution

`r`: The residual

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

- Use this to pass application information, e.g. physical constants

SNES Jacobian

The user provided function which calculates the Jacobian has signature

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

`x`: The current solution

`J`: The Jacobian

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

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

- Use this to pass application information, e.g. physical constants

- Possible `MatStructure` values are:
  - SAME_NONZERO_PATTERN
  - DIFFERENT_NONZERO_PATTERN

Alternatively, you can use

- a builtin sparse finite difference approximation
- automatic differentiation (ADIC/ADIFOR)

SNES Variants

- Line search strategies
- Trust region approaches
- Pseudo-transient continuation
- Matrix-free variants

Finite Difference Jacobians

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

- Dense
  - Activated by `-snes_fd`
  - Computed by `SNESDefaultComputeJacobian()`
- Sparse via colorings
  - Coloring is created by `MatFDColoringCreate()`
  - Computed by `SNESDefaultComputeJacobianColor()`

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

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

Code Update

Update to Revision 13

DMMG Integration with SNES

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

DM Interface

- Allocation and layout
  - `createglobalvector(DM, Vec *)`
  - `createlocalvector(DM, Vec *)`
  - `getmatrix(DM, MatType, Mat *)`
- Intergrid transfer
  - `getinterpolation(DM, DM, Mat *, Vec *)`
  - `getaggregates(DM, DM, Mat *)`
  - `getinjection(DM, DM, VecScatter *)`

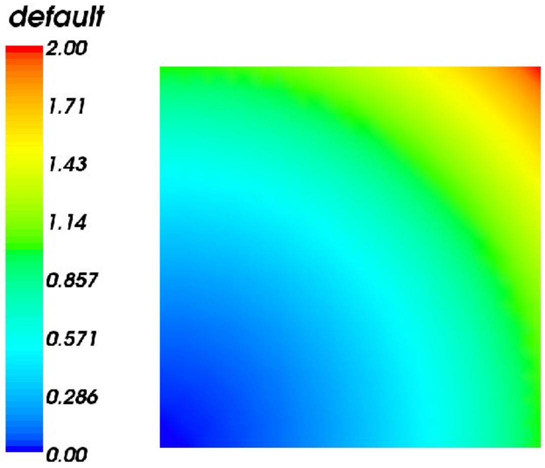
DM Interface

- Grid creation
  - `refine(DM, MPI_Comm, DM *)`
  - `coarsen(DM, MPI_Comm, DM *)`
  - `refinehierarchy(DM, PetscInt, DM **)`
  - `coarsenhierarchy(DM, PetscInt, DM **)`
- Mapping (completion)
  - `globaltolocalbegin/end(DM, Vec, InsertMode, Vec)`
  - `localtoglobal(DM, Vec, InsertMode, Vec)`

Solving the Dirichlet Problem: P_1

- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- The linear basis cannot represent the quadratic solution exactly
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -ksp_monitor -snes_monitor -vec_view_vtk -ksp_rtol 1.0e-9" runbratu`
- The error decreases with h
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -ksp_monitor -snes_monitor -vec_view_vtk -ksp_rtol 1.0e-9" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- Notice that the preconditioner is weaker in parallel

Solving the Dirichlet Problem: P_1



Solving the Dirichlet Problem: P_2

- `rm bratu_quadrature.h; make ORDER=2`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- Here we get the exact solution
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- Notice that the solution is only as accurate as the KSP tolerance
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- Again the preconditioner is weaker in parallel
- Currently we have no system for visualizing higher order solutions

Solving the Dirichlet Problem: FD

- `make EXTRA_ARGS="-snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_draw -draw_pause -1" runbratu`
- Notice that we converge at the vertices, despite the quadratic solution
- `make EXTRA_ARGS="-snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -da_grid_x 40 -da_grid_y 40 -vec_view_draw -draw_pause -1" runbratu`
- `make NP=2 EXTRA_ARGS="-snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -da_grid_x 40 -da_grid_y 40 -vec_view_draw -draw_pause -1" runbratu`
- Again the preconditioner is weaker in parallel
- `make NP=2 EXTRA_ARGS="-dim 3 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -da_grid_x 10 -da_grid_y 10 -da_grid_z 10" runbratu`

Solving the Neumann Problem: P_1

- `make EXTRA_ARGS="-structured 0 -generate -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`
- The error decreases with *h*
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_vtk" runbratu`

Solving the Neumann Problem: P_3

- `rm bratu_quadrature.h; make ORDER=3`
- `make EXTRA_ARGS="-structured 0 -generate -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- Here we get the exact solution
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9" runbratu`

The Bratu Problem

$$\Delta u + \lambda e^{u} = f \quad \text{in} \quad \Omega \tag{6}$$
$$u = g \quad \text{on} \quad \partial\Omega \tag{7}$$

- Also called the Solid-Fuel Ignition equation
- Can be treated as a nonlinear eigenvalue problem
- Has two solution branches until $\lambda \cong 6.28$

Nonlinear Equations

We will have to alter

- The residual calculation, `Rhs_*()`
- The Jacobian calculation, `Jac_*()`
- The forcing function to match our chosen solution, `CreateProblem()`

Code Update

Update to Revision 14

Solving the Bratu Problem: FD

- `make EXTRA_ARGS="-snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_draw -draw_pause -1 -lambda 0.4" runbratu`
- Notice that we converge at the vertices, despite the quadratic solution
- `make NP=2 EXTRA_ARGS="-da_grid_x 40 -da_grid_y 40 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -vec_view_draw -draw_pause -1 -lambda 6.28" runbratu`
- Notice the problem is more nonlinear near the bifurcation
- `make NP=2 EXTRA_ARGS="-dim 3 -da_grid_x 10 -da_grid_y 10 -da_grid_z 10 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`

Finding Problems

We switch to quadratic elements so that our FE solution will be exact

- `rm bratu_quadrature.h; make ORDER=2`

-
  ```
  make EXTRA_ARGS="-structured 0 -generate -snes_monitor
  -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4" runbratu
  ```

Finding Problems

We switch to quadratic elements so that our FE solution will be exact

- `rm bratu_quadrature.h; make ORDER=2`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4" runbratu`

We do not converge!

Finding Problems

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  ```
  make EXTRA_ARGS="-structured 0 -generate -snes_monitor
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We do not converge!

- Residual is zero, so the Jacobian could be wrong (try FD)

-
  ```
  make EXTRA_ARGS="-structured 0 -generate -snes_monitor
  -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_mf" runbratu
  ```

Finding Problems

We switch to quadratic elements so that our FE solution will be exact

- `rm bratu_quadrature.h; make ORDER=2`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4" runbratu`

We do not converge!

- Residual is zero, so the Jacobian could be wrong (try FD)
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_mf" runbratu`

It works!

Finding Problems

Investigating the Jacobian directly,

- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_max_it 3 -mat_view" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_fd -mat_view" runbratu`

Finding Problems

Investigating the Jacobian directly,

- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_max_it 3 -mat_view" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4 -snes_fd -mat_view" runbratu`
- Entries are too big, we forgot to initialize the matrix

Code Update

Update to Revision 15

Solving the Bratu Problem: P_2

- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`

Solving the Bratu Problem: P_1

- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 0.4" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.01 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.28" runbratu`

Outline

What Is Optimal?

I will define *optimal* as an $\mathcal{O}(N)$ solution algorithm

These are generally hierarchical, so we need

- hierarchy generation
- assembly on subdomains
- restriction and prolongation

Payoff

Why should I care?

1. Current algorithms do not efficiently utilize modern machines

Payoff

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3. Multicore processors are the future
4. Optimal multilevel solvers are necessary

Claim: Hierarchical operations can be handled by a single interface

Why Optimal Algorithms?

- The more powerful the computer,
  the greater the importance of optimality
- Example:
  - Suppose Alg_1 solves a problem in time CN^2, N is the input size
  - Suppose Alg_2 solves the same problem in time CN
  - Suppose Alg_1 and Alg_2 are able to use 10,000 processors
- In constant time compared to serial,
  - Alg1 can run a problem 100X larger
  - Alg2 can run a problem 10,000X larger
- Alternatively, filling the machine's memory,
  - Alg1 requires 100X time
  - Alg2 runs in constant time

Multigrid

Multigrid is *optimal* in that is does $\mathcal{O}(N)$ work for $||r|| < \epsilon$

- Brandt, Briggs, Chan & Smith
- Constant work per level
    - Sufficiently strong solver
    - Need a constant factor decrease in the residual
- Constant factor decrease in dof
    - Log number of levels

Linear Convergence

Convergence to $||r|| < 10^{-9}||b||$ using GMRES(30)/ILU

Elements	Iterations
128	10
256	17
512	24
1024	34
2048	67
4096	116
8192	167
16384	329
32768	558
65536	920
131072	1730

Linear Convergence

Convergence to $||r|| < 10^{-9}||b||$ using GMRES(30)/MG

Elements	Iterations
128	5
256	7
512	6
1024	7
2048	6
4096	7
8192	6
16384	7
32768	6
65536	7
131072	6

DMMG Paradigm

The DMMG interface uses the *local* DA/Mesh callback functions to

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

DMMG relies upon DM to organize the

- assembly
- coarsening/refinement

while it organizes the control flow for the multilevel solve.

DMMG Integration with SNES

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

Structured Meshes

The `DMMG` allows multigrid which some simple options

- `-dmmg_nlevels`, `-dmmg_view`
- `-pc_mg_type`, `-pc_mg_cycle_type`
- `-mg_levels_1_ksp_type`, `-dmmg_levels_1_pc_type`
- `-mg_coarse_ksp_type`, `-mg_coarse_pc_type`

Solving with Structured Multigrid

- `make EXTRA_ARGS="-dmmg_nlevels 2 -dmmg_view -snes_monitor -ksp_monitor -ksp_rtol 1e-9" runbratu`
- Notice that the solver on each level can be customized
- number of KSP iterations is approximately constant
- `make EXTRA_ARGS="-da_grid_x 10 -da_grid_y 10 -dmmg_nlevels 8 -dmmg_view -snes_monitor -ksp_monitor -ksp_rtol 1e-9" runbratu`
    - Notice that there are over 1 million unknowns!
- Coarsening is not currently implemented

AMG

Why not use AMG?

AMG

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- Of course we will try AMG

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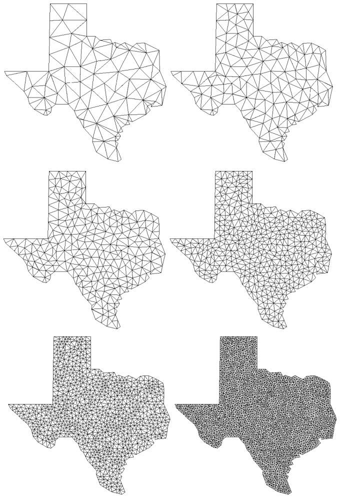
- Geometric aspects to the problem
  - Material property variation

AMG

Why not use AMG?

- Of course we will try AMG
    - BoomerAMG, ML, SAMG, ASA
- Problems with vector character
- Geometric aspects to the problem
    - Material property variation
    - Faults

Coarsening



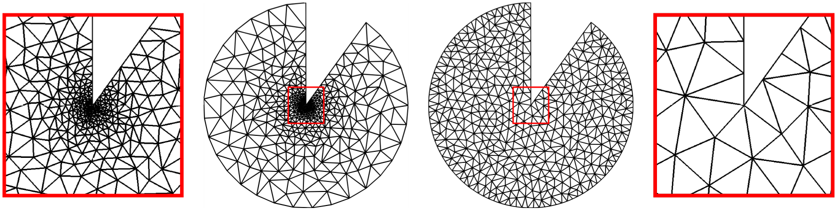
- Users want to control the mesh
- Developed efficient, topological coarsening
  - Miller, Talmor, Teng algorithm
- Provably well-shaped hierarchy

A Priori refinement

For the Poisson problem, meshes with reentrant corners have a length-scale requirement in order to maintain accuracy:

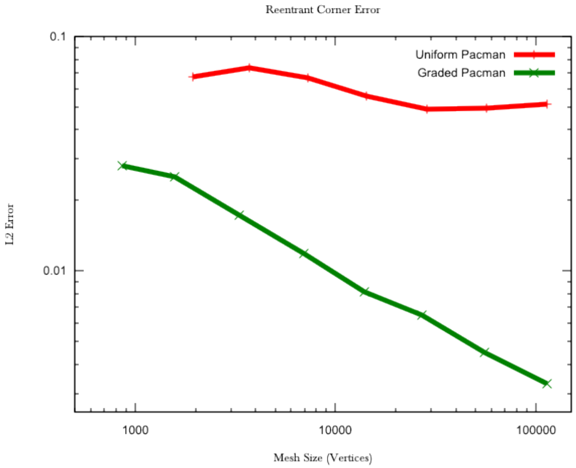
$$C_{low} r^{1-\mu} \leq h \leq C_{high} r^{1-\mu}$$

$$\mu \leq \frac{\pi}{\theta}$$



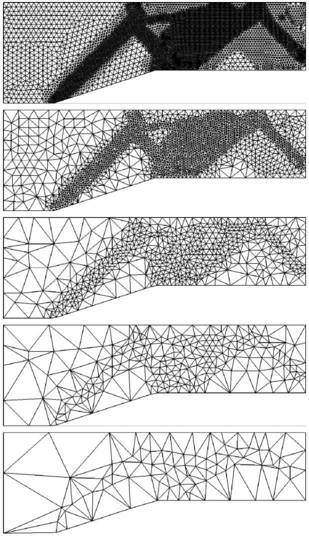
The Folly of Uniform Refinement

uniform refinement may fail to eliminate error



Geometric Multigrid

- We allow the user to refine for fidelity
- Coarse grids are created automatically
- Could make use of AMG interpolation schemes



Requirements of Geometric Multigrid

- Sufficient conditions for optimal-order convergence:
  - $|M_c| < 2|M_f|$ in terms of cells
  - any cell in M_c overlaps a bounded # of cells in M_f
  - monotonic increase in cell length-scale

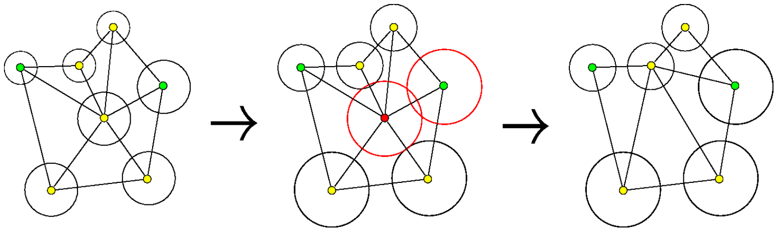
Requirements of Geometric Multigrid

- Sufficient conditions for optimal-order convergence:
  - $|M_c| < 2|M_f|$ in terms of cells
  - any cell in M_c overlaps a bounded # of cells in M_f
  - monotonic increase in cell length-scale
- Each M_k satisfies the **quasi-uniformity** condition:

$$C_1 h_k \leq h_K \leq C_2 \rho_K$$

  - h_K is the length-scale (longest edge) of any cell K
  - h_k is the maximum length-scale in the mesh M_k
  - ρ_K is the diameter of the inscribed ball in K

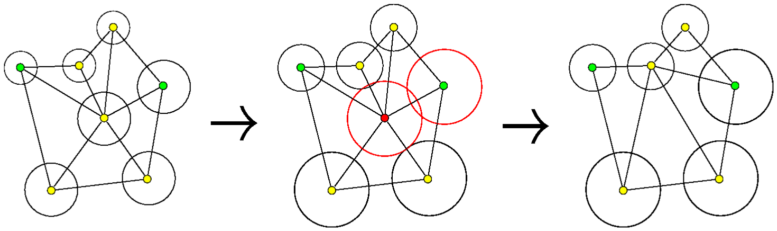
Miller-Talmor-Teng Algorithm



Simple Coarsening

1. Compute a spacing function f for the mesh (Koebe)

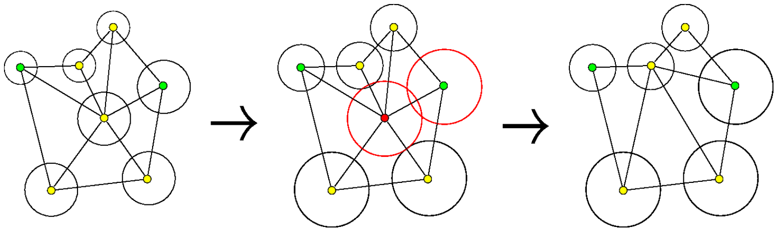
Miller-Talmor-Teng Algorithm



Simple Coarsening

1. Compute a spacing function f for the mesh (Koebe)
2. Scale f by a factor $C > 1$

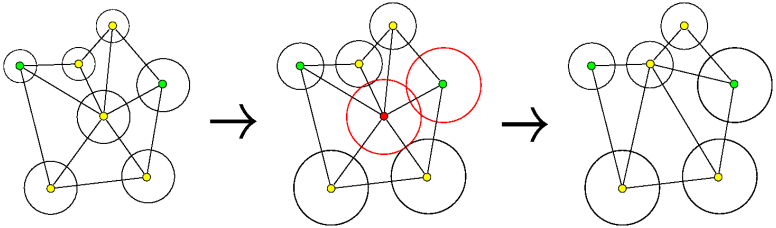
Miller-Talmor-Teng Algorithm



Simple Coarsening

1. Compute a spacing function f for the mesh (Koebe)
2. Scale f by a factor $C > 1$
3. Choose a maximal independent set of vertices for new f

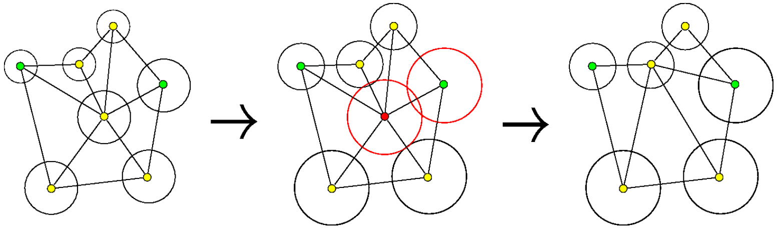
Miller-Talmor-Teng Algorithm



Simple Coarsening

1. Compute a spacing function *f* for the mesh (Koebe)
2. Scale *f* by a factor $C > 1$
3. Choose a maximal independent set of vertices for new *f*
4. Retriangulate

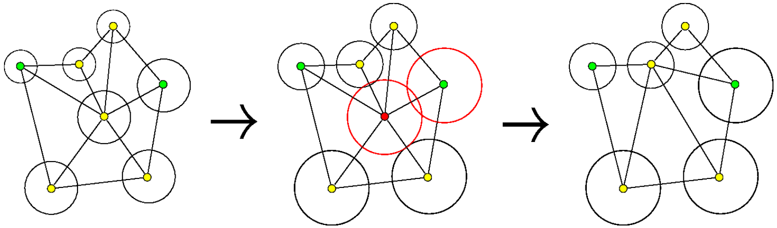
Miller-Talmor-Teng Algorithm



Caveats

1. Must generate coarsest grid in hierarchy first

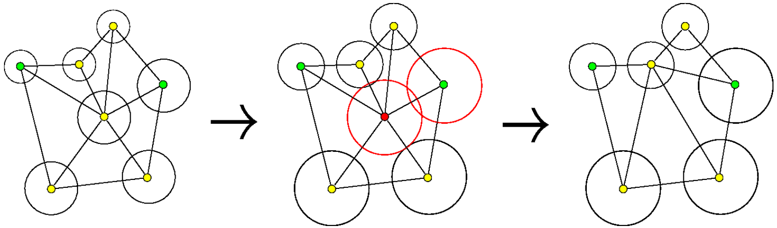
Miller-Talmor-Teng Algorithm



Caveats

1. Must generate coarsest grid in hierarchy first
2. Must choose boundary vertices first (and protect boundary)

Miller-Talmor-Teng Algorithm

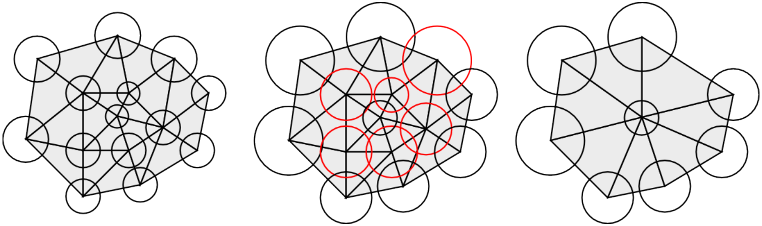


Caveats

1. Must generate coarsest grid in hierarchy first
2. Must choose boundary vertices first (and protect boundary)
3. Must account for boundary geometry

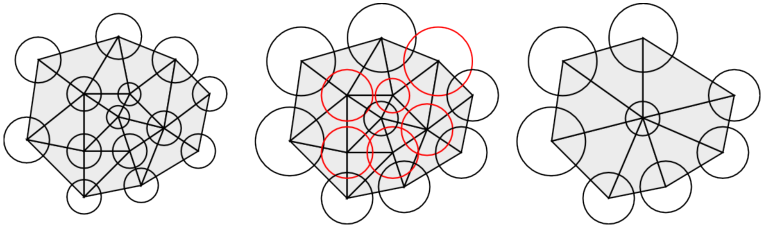
Function Based Coarsening

- (Miller, Talmor, Teng; 1997)
- triangulated planar graphs $\equiv$ disk-packings (Koebe; 1934)
- define a spacing function S() over the vertices
- obvious one: $S(v) = \frac{dist(NN(v),v)}{2}$



Function Based Coarsening

- pick a subset of the vertices such that $\beta(S(v) + S(w)) > dist(v, w)$
- for all $v, w \in M$, with $\beta > 1$
- dimension independent
- provides guarantees on the size/quality of the resulting meshes



Decimation Algorithm

- Loop over the vertices
  - include a vertex in the new mesh

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  - **every** vertex is either included or removed
  - bounded degree mesh $\Rightarrow O(n)$ time

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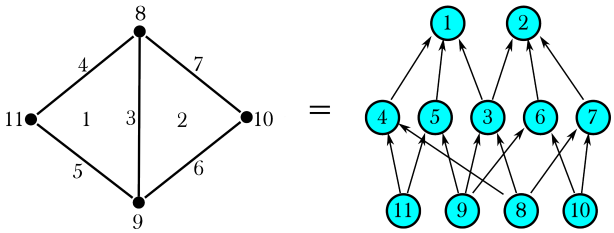
- Eventually we have that
  - **every** vertex is either included or removed
  - bounded degree mesh $\Rightarrow O(n)$ time
- Remeshing may be performed either during or after coarsening
  - local Delaunay remeshing can be done in 2D and 3D
  - faster to connect edges and remesh later

Implementation in *Sieve*

Peter Brune, 2008

- vertex neighbors: $cone(support(v)) \setminus v$
- vertex link: $closure(star(v)) \setminus star(closure(v))$



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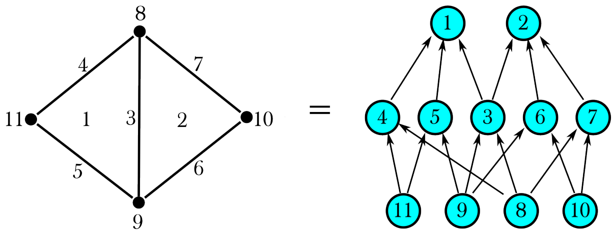
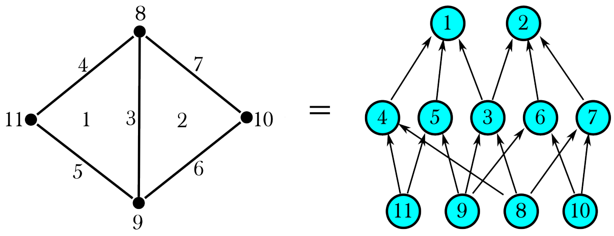


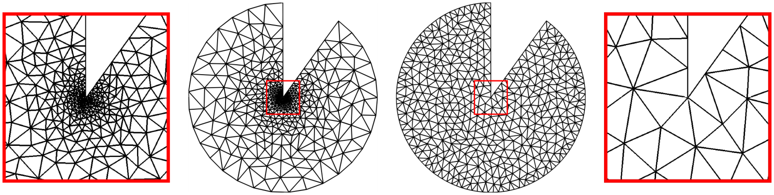
Implementation in *Sieve*
Peter Brune, 2008

- vertex neighbors: $cone(support(v)) \setminus v$
- vertex link: $closure(star(v)) \setminus star(closure(v))$
- connectivity graph induced by limiting sieve depth
- remeshing can be handled as local modifications on the sieve
- meshing operations, such as *cone construction* easy



Reentrant Problems

- Reentrant corners need nonnuiform refinement to maintain accuracy
- Coarsening preserves accuracy in MG without user intervention



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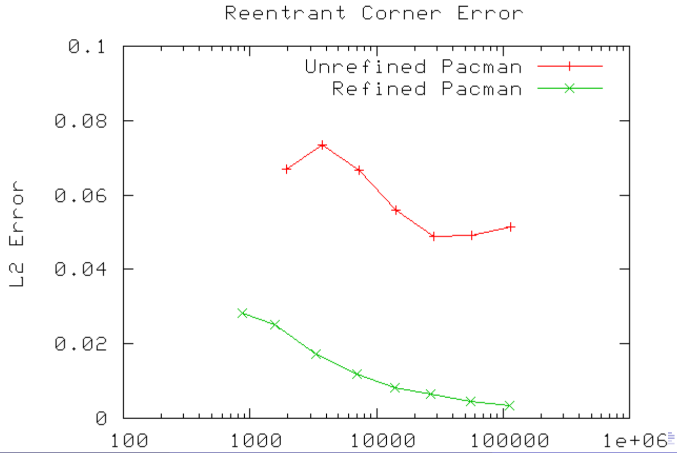
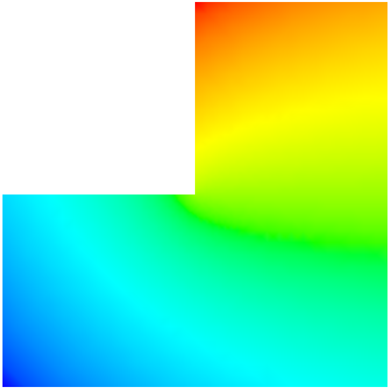
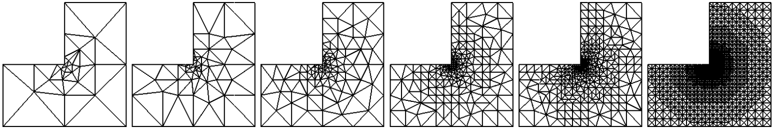


Reentrant Problems

Exact Solution for reentrant problem: $u(x, y) = r^{\frac{2}{3}} sin(\frac{2}{3}\theta)$





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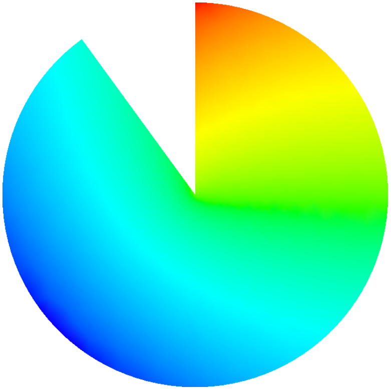
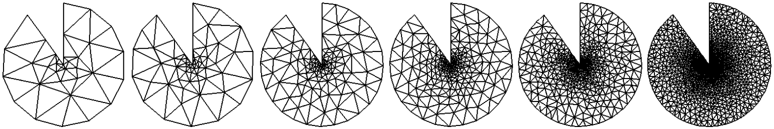
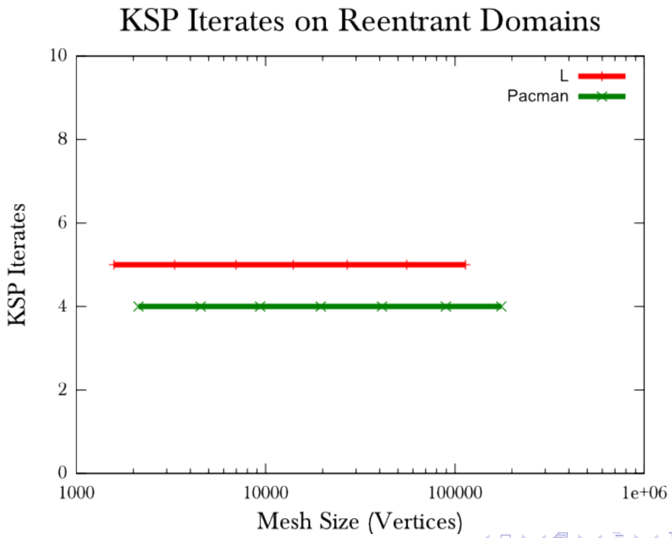




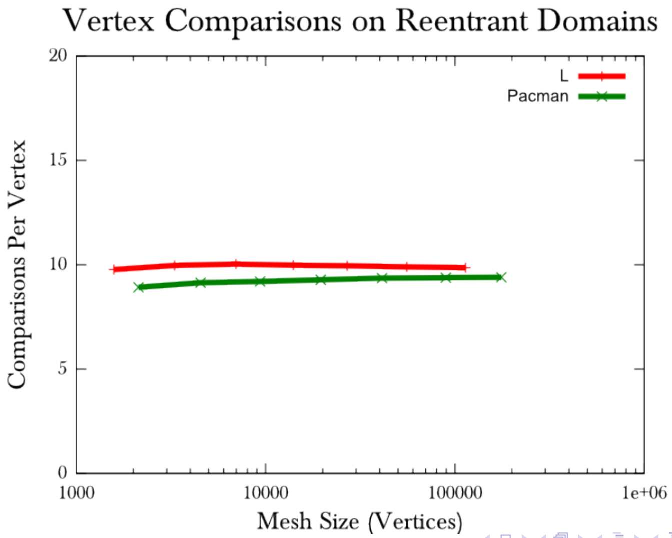
GMG Performance

Linear solver iterates are constant as system size increases:



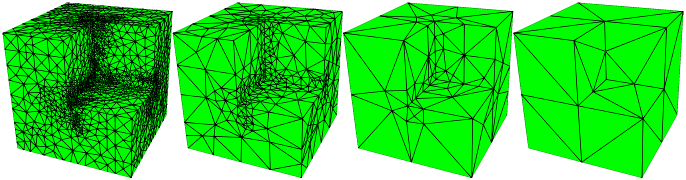
GMG Performance

Work to build the preconditioner is constant as system size increases:



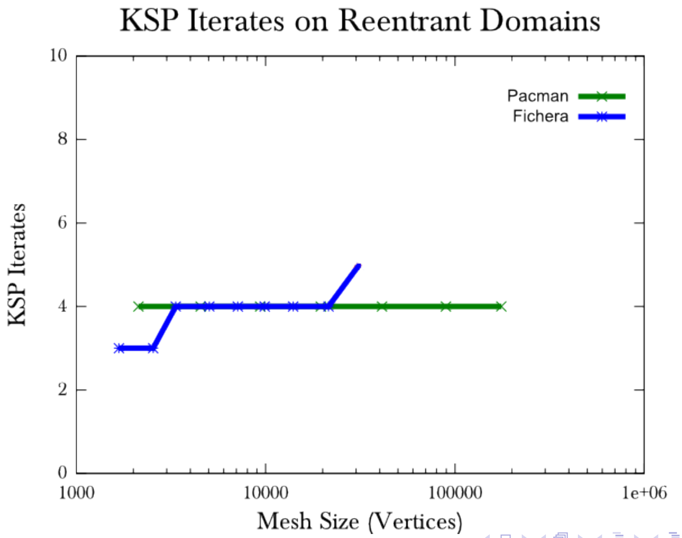
3D Test Problem

- $\Omega_{fichera}$
- $-\Delta u = f$
- $f(x, y, z) = 3\sin(x + y + z)$
- Exact Solution: $u(x, y, z) = \sin(x + y + z)$



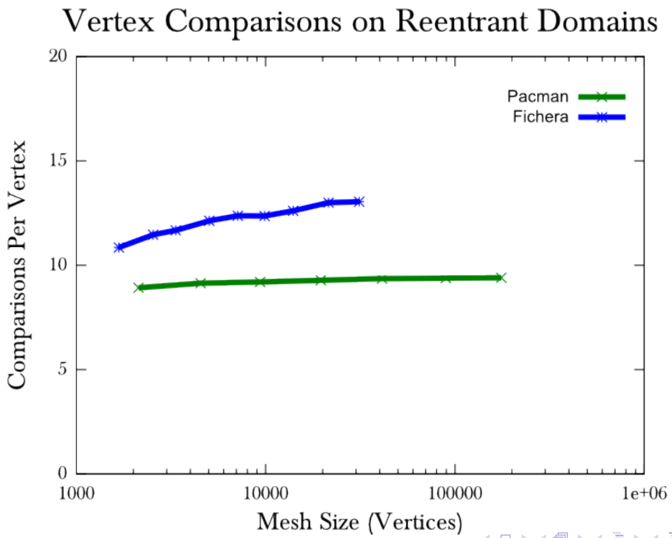
GMG Performance

Linear solver iterates are nearly as system size increases:



GMG Performance

Coarsening work is nearly constant as system size increases:



Quality Experiments

Table: Hierarchy quality metrics - 2D

Pacman Mesh, $\beta = 1.45$						
level	cells	vertices	$\frac{min(h_K)}{h_k}$	max $\frac{h_K}{\rho_K}$	$\min(h_K)$	max. overlap
0	19927	10149	0.020451	4.134135	0.001305	-
1	5297	2731	0.016971	4.435928	0.002094	23
2	3028	1572	0.014506	4.295703	0.002603	14
3	1628	856	0.014797	5.295322	0.003339	14
4	863	464	0.011375	6.403574	0.003339	14
5	449	250	0.022317	6.330512	0.007979	13

Unstructured Meshes

- Same `DMMG` options as the structured case
- Mesh refinement
  - Ruppert algorithm in Triangle and TetGen
- Mesh coarsening
  - Talmor-Miller algorithm in PETSc
- More advanced options
  - `-dmmg_refine`
  - `-dmmg_hierarchy`
- Current version only works for linear elements

Outline

Things To Check Out

- PCFieldSplit for multiphysics
- Deal**II** and FEniCS for FEM automation
- PetFMM for particle methods

MultiPhysics Paradigm

The PCFieldSplit interface uses the `VecScatter` objects to

- extract functions/operators corresponding to each physics
- assemble functions/operators over all physics

Notice that this works in exactly the same manner for

- multiple resolutions (MG, Wavelets)
- multiple domains (Domain Decomposition)
- multiple dimensions (ADI)

Preconditioning

Several varieties of preconditioners can be supported:

- Block Jacobi or Block Gauss-Siedel
- Schur complement
- Block ILU (approximate coupling and Schur complement)
- Dave May's implementation of Elman-Wathen type PCs

which only require actions of individual operator blocks

Notice also that we may have any combination of

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

since we have access to an algebraic interface

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

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

FIAT understands

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

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

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

FFC

FFC is a compiler for variational forms by Anders Logg.

Here is a mixed-form Poisson equation:

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

where

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

FFC

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

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

f = Function(DG0)

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

FFC

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Here is a discontinuous Galerkin formulation of the Poisson equation:

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

where

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

FFC

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

PetFMM

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

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

Outline

Conclusions

PETSc can help you

- easily construct a code to test your ideas
- scale an existing code to large or distributed machines
- incorporate more scalable or higher performance algorithms
- tune your code to new architectures

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PETSc can help you

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- incorporate more scalable or higher performance algorithms
  - Such as domain decomposition or multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

References

- Documentation: http://www.mcs.anl.gov/petsc/docs
  - PETSc Users manual
  - Manual pages
  - Many hyperlinked examples
  - FAQ, Troubleshooting info, installation info, etc.
- Publications: http://www.mcs.anl.gov/petsc/publications
  - Research and publications that make use PETSc
- MPI Information: http://www.mpi-forum.org
- **Using MPI** (2nd Edition), by Gropp, Lusk, and Skjellum
- **Domain Decomposition**, by Smith, Bjorstad, and Gropp

Experimentation is Essential!

Proof is not currently enough to examine solvers

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

Quiz

1. How are PETSc matrices divided in parallel, by rows or by columns?
2. What is a PETSc KSP object?
3. What PETSc class represents a structured grid?
4. What command line option changes the type of linear solver?
5. Is VecDot() a collective operation?