PETSc Tutorial

PETSc Team
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Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel

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- Linear and Nonlinear

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- Optimal Solvers

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- Triangles and Hexes
- Optimal Solvers

Items in red not finished for tutorial

Outline

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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)

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

How Can We Help?

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

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- Quickly answer questions

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- Help install

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How Can We Help?

- Provide documentation
- Quickly answer questions
- Help install
- Guide large scale flexible code development
- Answer email at petsc-maint@mcs.anl.gov

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?

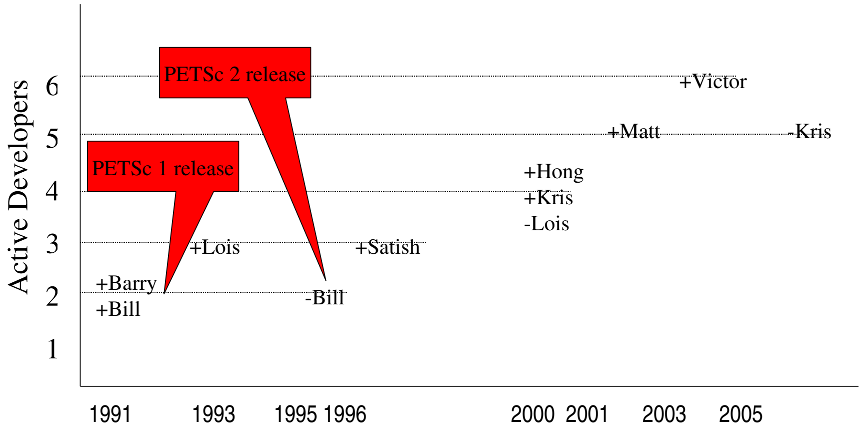
A freely available and supported research code

- 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 300 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 problems with over 500 million unknowns
    - http://www.scconference.org/sc2004/schedule/pdfs/pap111.pdf

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    - PFLOTRAN on the Cray XT4 Jaguar at ORNL

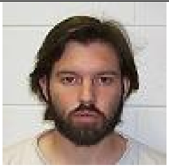
What Can We Handle?

- PETSc has run problems with over 500 million unknowns
  - http://www.scconference.org/sc2004/schedule/pdfs/pap111.pdf
- PETSc has run on over 27,580 processors efficiently
  - PFLOTRAN on the Cray XT4 Jaguar at ORNL
- 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, Deal**II**

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-2.3.3

Unpacking PETSc

- Just clone development repository
  - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
  - `hg clone -rRelease-2.3.3 petsc-dev petsc-2.3.3`

or

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

Getting the Source

You will need the Developer copy of PETSc:

- Using Mercurial

```
hg clone http://petsc.cs.iit.edu/petsc/petsc-dev
cd petsc-dev/python
hg clone http://petsc.cs.iit.edu/petsc/BuildSystem
```

- Manual download

```
wget ftp://info.mcs.anl.gov/pub/petsc/petsc-dev.tar.gz .
```

and the tutorial source code:

- Using Mercurial

```
hg clone http://petsc.cs.iit.edu/petsc/TACC08TutorialCode
```

- Manual download

```
wget ftp://info.mcs.anl.gov/pub/petsc/TACC08TutorialCode.tar.gz .
```

Configuring PETSc

- Set `$PETSC_DIR` to the installation root directory
- Run the configuration utility
  - `$PETSC_DIR/config/configure.py`
  - `$PETSC_DIR/config/configure.py --help`
  - `$PETSC_DIR/config/configure.py --download-mpich`
- There are many examples on the installation page
- Configuration files are placed in `$PETSC_DIR/$PETSC_ARCH/conf`
  - Configure header is in `$PETSC_DIR/$PETSC_ARCH/include`

Configuring PETSc

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

Configuring Sieve

- `--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 in PETSc
- Currently works for
  - 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

Building PETSc

- Uses recursive make starting in `cd $PETSC_DIR`
  - `make`
  - Check build when done with `make test`
- Complete log for each build in `make_log_$PETSC_ARCH`
  - 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`

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 -np 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
- 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
  - Named 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_monitor_cancel`
- Does not display subsolvers
  - `-snes_monitor`
- Can use the true residual
  - `-ksp_monitor_true_residual`
- Can display different subobjects
  - `-snes_monitor_solution`, `-snes_monitor_solution_update`, `-snes_monitor_residual`
  - `-ksp_gmres_krylov_monitor`
- Can display the spectrum
  - `-ksp_monitor_singular_value`

PETSc Example

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`

User Example

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`
3. Create a PETSc makefile
   - Add a link target
   - `${CLINKER} -o $@ $^ ${PETSC_SNES_LIB}`
   - `${FLINKER} -o $@ $^ ${PETSC_SNES_LIB}`
   - `include ${PETSC_DIR}/conf/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
    - Lorena Barba
    - David Keyes
    - Xiao-Chuan Cai
    - Richard Katz

Following the Tutorial

Update to each new checkpoint (r0):

- `hg clone -r0 TACC08TutorialCode code-test`

or

- `hg update 0`

Build the executable with `make`, and then run:

- `make runbratu`
- `make debugbratu`
- `make valbratu`
- `make NP=2 runbratu`
- `make EXTRA_ARGS="-pc_type jacobi" runbratu`

Code Update

Update to Revision 0

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

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.

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

Outline

Higher Level Abstractions

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

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

The PETSc `Mesh` class is a topology interface.

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

Higher Level Abstractions

The PETSc `DM` class is a hierarchy interface.

- Supports multigrid
  - `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

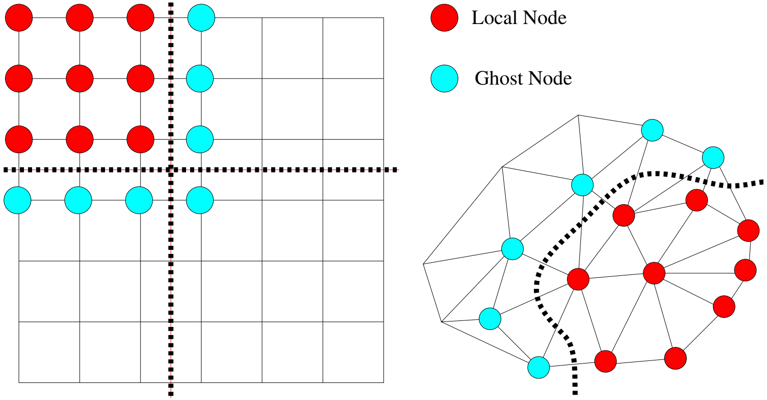
`lm/n`: Alternative array of local sizes

- 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 belongs to a unique process and has a unique id
- **Local**: Numbering includes ghost vertices from neighboring processes

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

- Putting a breakpoint in `PetscError()` can catch errors as they occur
- PETSc tracks memory overwrites at the beginning and end 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
  - Option `-malloc_dump` will print unfreed memory on `PetscFinalize()`
- Simply the best tool today is valgrind
  - It checks memory access, cache performance, memory usage, etc.
  - http://www.valgrind.org

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.

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 and will 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", CLASS_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
- Initialization must happen before any objects of this type are created

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

Efficient Matrix Creation

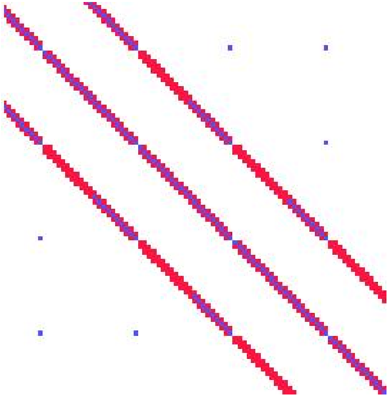
- Create matrix with `MatCreate()`
- Set type with `MatSetType()`
- Determine the number of nonzeros in each row
  - loop over the grid for finite differences
  - loop over the elements for finite elements
  - need only local+ghost information
- Preallocate matrix
  - `MatSeqAIJSetPreallocation()`
  - `MatMPIAIJSetPreallocation()`

Indicating Expected Nonzeros

Sequential Sparse Matrices

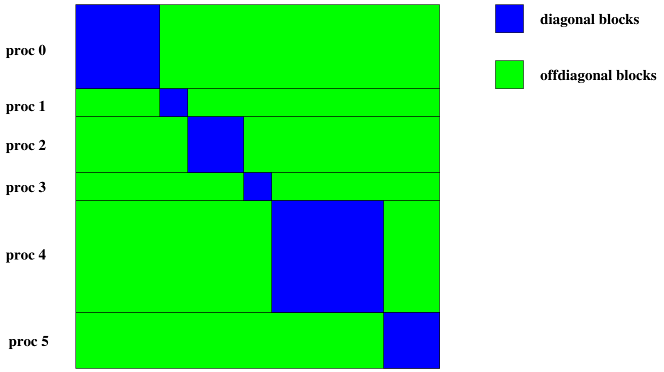
`MatSeqAIJPreallocation(Mat A, int nz, int nnz[])`

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



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

Indicating Expected Nonzeros
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

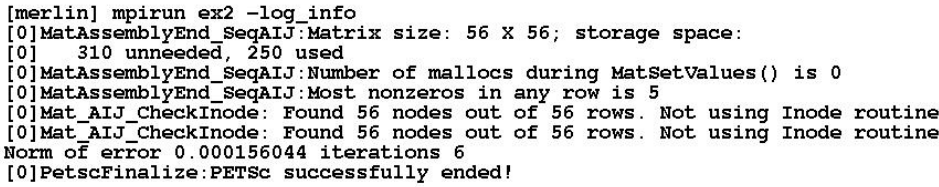
nnz(i): expected number of nonzeros in row i in the diagonal block

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

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!
```

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

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
  - Now we have `Mesh` objects
- Discretizations
  - Now we have an interface to FIAT
  - Deal**II**
- Higher level representations of PDEs
  - Unstructured mesh generation and manipulation
  - FEniCS (FFC/Syfi) and Sundance
- Load balancing
- Sophisticated visualization capabilities
  - MayaVi2
- 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 line
`SetUp()`	preform other initialization
`View()`	view the object
`Destroy()`	cleanup object allocation

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

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

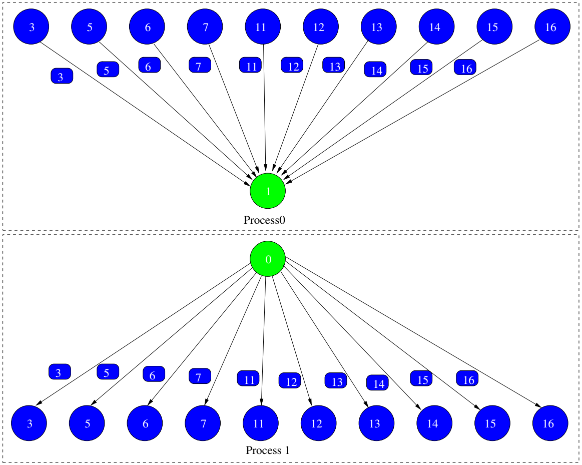
Refining the Mesh

- `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 `Vecs`
- Global vectors are parallel
  - Each process stores a unique local portion
  - `DACreateGlobalVector(DA da, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
  - Each process stores its local portion plus ghost values
  - `DACreateLocalVector(DA da, Vec *lvec)`
  - includes ghost values!

Updating Ghosts

Two-step process enables overlapping computation and communication

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

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

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)
```

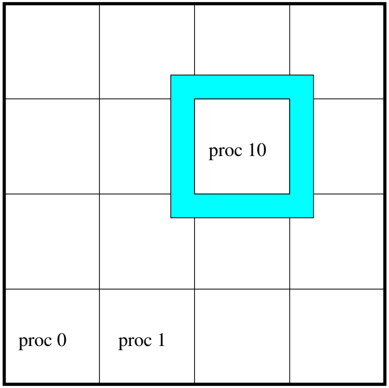
`info`:	All layout and numbering information
`x`:	The current solution • Notice that it is a multidimensional array
`r`:	The residual
`ctx`:	The user context passed to `DASetLocalFunction()`

The local DA function is activated by calling

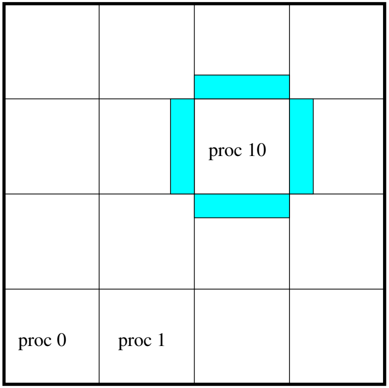
```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

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 rows and columns

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 `Sections`
    - This is called a `Bundle`

Section Types

Section can contain arbitrary values

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

Section can have arbitrary layout

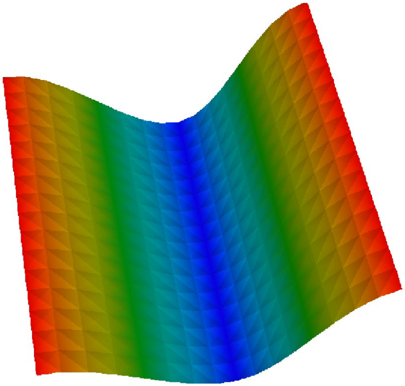
- C++ interface can place unknowns on any Mesh entity (Sieve point)
    - `Mesh::setupField()` parametrized by `Discretization` and `BoundaryCondition`
- C interface has default layouts
    - `MeshGetVertexSectionReal()`
    - `MeshGetCellSectionReal()`

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 by specifying the Ciarlet triple (K, P, P')

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

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 `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

Neumann conditions may be expressed as

Boundary Conditions

Dirichlet conditions may be expressed as

$$u|_{\Gamma} = g$$

Neumann conditions may be expressed as

Boundary Conditions

Dirichlet conditions may be expressed as

$$u|_\Gamma = g$$

and implemented by constraints on dofs in a Section

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Neumann conditions may be expressed as

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and implemented by explicit integration along the boundary

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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.

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

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 9

Section Assembly

First we do local operations:

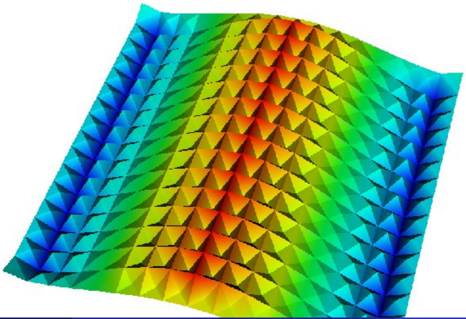
- Loop over cells
- Compute cell geometry
- Integrate each basis function to produce an element vector
- Call `SectionUpdateAdd()`
    - Note that this updates the *closure* of the cell

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)

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

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Largely dim dependent
(e.g. quadrature)

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

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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,

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

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 10

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 11

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 11
- 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

$$e = \sum_i e_i \phi_i(x) \tag{1}$$

  - 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 a finite element approximation

$$\hat{u}(x) = \sum_i \hat{u}_i \phi_i(x) \tag{2}$$

The FE theory predicts a convergence rate for the quantity

$$\begin{align} ||u - \hat{u}||_2^2 &= \sum_T \int_T dA (u - \hat{u})^2 \tag{3} \\ &= \sum_T \sum_q w_q |J| \left(u(q) - \sum_j \hat{u}_j \phi_j(q) \right)^2 \tag{4} \\ & \tag{5} \end{align}$$

The estimate for linear elements is

$$||u - \hat{u}_h|| < Ch||u|| \tag{6}$$

Code Update

Update to Revision 12

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 Jacboian 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 13

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`

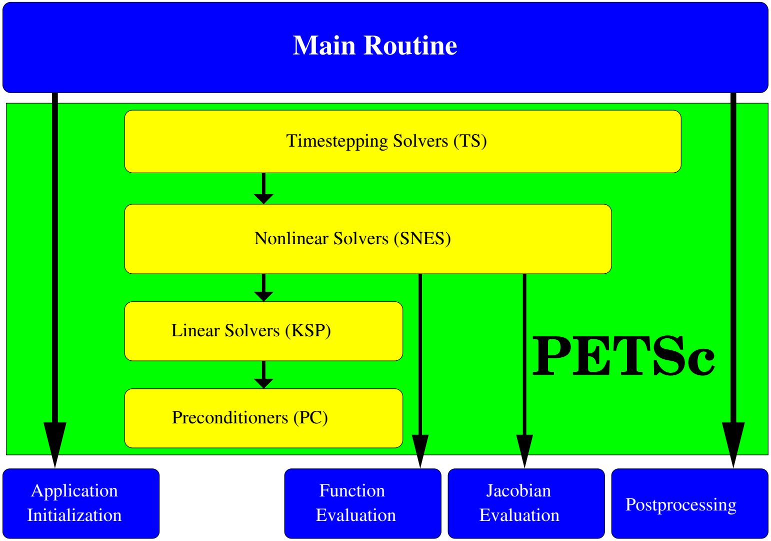
Mesh Operators

- 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



SNESCallbacks

The SNES interface is based upon callback functions

- `SNESSetFunction()`
- `SNESSetJacobian()`

When PETSc needs to evaluate the nonlinear residual $F(x)$, the solver calls the user's function inside the application.

The user function get 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 `MatrStructure` values are:
    - SAME_NONZERO_PATTERN, DIFFERENT_NONZERO_PATTERN, ...

Alternatively, you can use

- a builtin sparse finite difference approximation
- automatic differentiation
    - AD support via ADIC/ADIFOR (P. Hovland and B. Norris from ANL)

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 14

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
    - Notice we have to scatter into contiguous global vectors (initial guess)
- Handle Neumann BC using `DMMGSetNullSpace()`

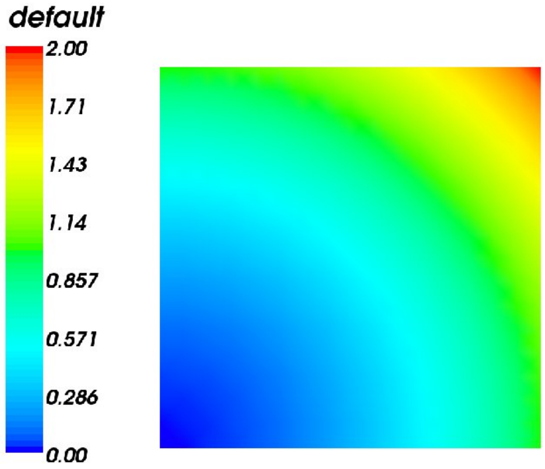
DM Interface

- 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 *)`
- 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

Alternative Assembly

- `make EXTRA_ARGS="-structured 0 -generate -ksp_monitor -snes_monitor -ksp_rtol 1.0e-9 -assembly_type full -pc_type none" runbratu`
- Since we cannot precondition without a matrix, we turn it off for comparison
- `make EXTRA_ARGS="-structured 0 -generate -ksp_monitor -snes_monitor -ksp_rtol 1.0e-9 -assembly_type stored -pc_type none" runbratu`
- Here we store all the element matrices
- `make EXTRA_ARGS="-structured 0 -generate -ksp_monitor -snes_monitor -ksp_rtol 1.0e-9 -assembly_type calculated -pc_type none" runbratu`
- This reduces storage, but increases computation

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 Louisville-Bratu-Gelfand Problem

$$-\Delta u - \lambda e^u = f \tag{7}$$

- Simplification of the Solid-Fuel Ignition Problem
- Also a nonlinear eigenproblem
- Exhibits a bifurcation at $\lambda \approx 6.8$
- We will use Dirichlet conditions

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 15

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 6.8" 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 6.8" 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

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`

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

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!

- `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 16

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 6.8" runbratu`
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.8" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.8" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.8" 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 6.8" runbratu`
- `make NP=2 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.00125 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.8" runbratu`
- `make EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.01 -snes_monitor -ksp_monitor -ksp_rtol 1.0e-9 -lambda 6.8" 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

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

Structured Meshes

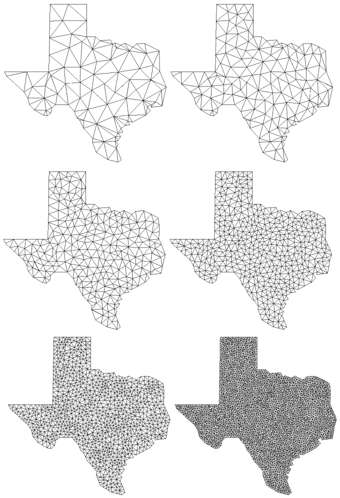
The DMMG allows multigrid which some simple options

- -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

Coarsening



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

Mesh Coarsening

- Easy in structured case, but unstructured is more subtle
- Delaunay coarsening is popular
    - M_{coarse} is a nonadjacent vertex subset of M_{fine}
    - Reduces to maximal independent set over edges
    - Enforces a spacing increase for well-shaped meshes
    - Mesh degradation from repeated coarsenings

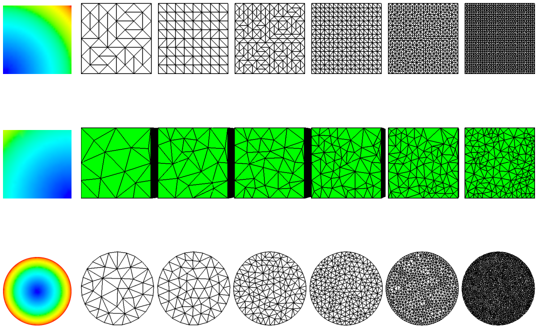
Function-Based Coarsening

G. Miller, D. Talmor, S.-H. Teng, *Optimal Coarsening of Unstructured Meshes*, J. Algorithms, 31 (1999), pp. 29-65

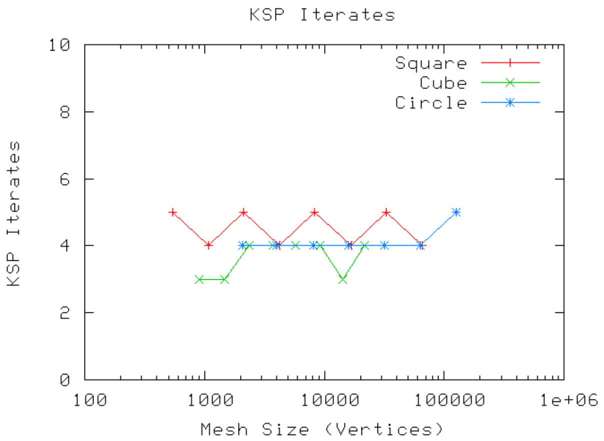
- Vertex *spacing function*
  - For example, nearest neighbor distance
- Expand the spacing function by some factor C
- Prune the mesh until expanded function is satisfied
  - Remove nodes until spheres of diameter $C * dist_{NN}$ are disjoint
- Guaranteed vertex spacing and cell shape
- Works in any dimension

Convex Domains

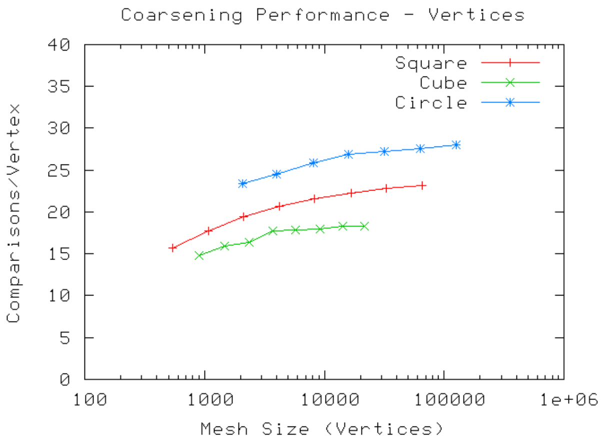
- $\Omega_{square} = [0,1] \times [0,1] (\times [0,1])$
- $\Omega_{circle} = \{p(x,y) : x^2 + y^2 <= 1\}$
- $\Delta u = f$
- $f(x,y) = -4$
- Exact Solution: $u(x,y) = x^2 + y^2$



KSP Performance

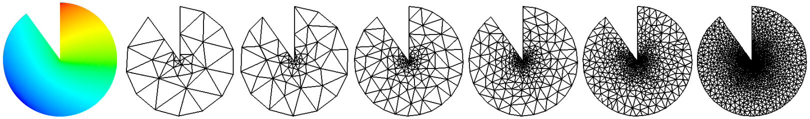


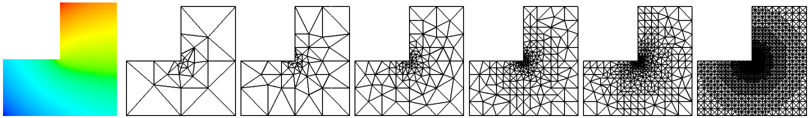
Coarsening Performance



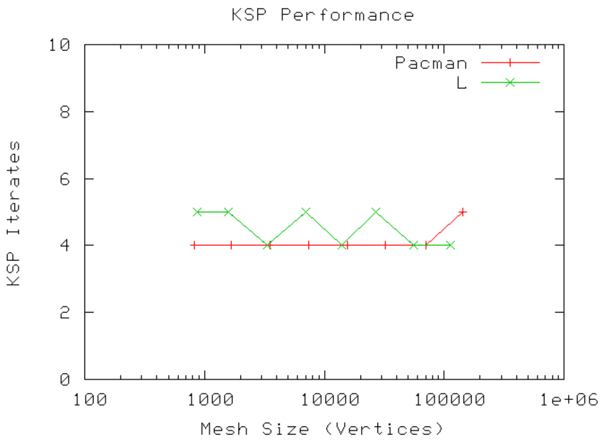
Domains with Reentrant Corners and Refinement

- $\Omega_{pacman} = \{p(x,y) \rightarrow p(r,\theta) : [0,1] \times [0,.9*2\pi]\}$
- $\Omega_L = [0,1] \times [-1,1] \setminus [-1,0] \times [-1,0]$
- $\Delta u = f$
- $f(x,y) = 0$
- Exact Solution: $u(x,y) = r^{\frac{2}{3}} sin(\frac{2}{3}\theta)$

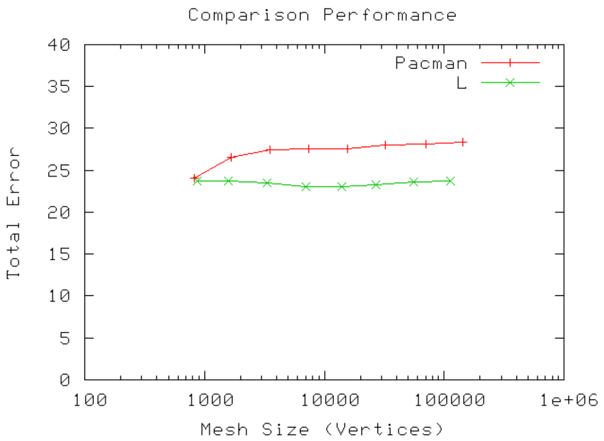




KSP Performance



Coarsening Performance



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

Solving with Unstructured Multigrid

- `make EXTRA_ARGS="-structured 0 -generate -bc_type neumann -dmmg_nlevels 2 -dmmg_view -snes_monitor -ksp_monitor -ksp_rtol 1e-9 -vec_view" runbratu`
- Compare to explicitly refined solution
- `make EXTRA_ARGS="-structured 0 -generate -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1e-9 -refinement_limit 0.0625 -vec_view" runbratu`
- We would really like to coarsen an existing mesh
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.03125 -bc_type neumann -dmmg_nlevels 3 -dmmg_refine 0 -dmmg_hierarchy -dmmg_view -snes_monitor -ksp_monitor -ksp_rtol 1e-9 -vec_view" runbratu`
- `make EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.03125 -bc_type neumann -snes_monitor -ksp_monitor -ksp_rtol 1e-9 -vec_view" runbratu`
- Notice that here we refine both meshes to the same level

Outline

What We Have Not Covered

- Unstructured hexes
    - Structured hex FEM
- *a posteriori* Error Estimation
- Exotic elements
- Semi-Lagrangian Schemes

What We Have Not Focused On

- Linear and Nonlinear Solvers
    - MANY other PETSc tutorials on this
- Unstructured mesh framework
    - Several preprints on Sieve architecture
- Structure of multilevel methods
    - Barry's talk from SIAM PP 2006
- Preconditioning
    - Very problem dependent (best left to applications?)
- Scalability and Performance
    - Coming soon. . .

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 currrently 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.