

PETSc Tutorial

PETSc Team
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Parallel CFD 2007
Antalya, Turkey
May 21–24, 2007



Enable students to develop new simulations with PETSc.

- Serial and Parallel

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- Linear and Nonlinear

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- Finite Difference and Finite Element

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- Optimal Solvers

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Items in red not finished for tutorial

Outline

- 1 Creating a PETSc Application
- 2 Creating a Simple Mesh
- 3 Defining a Function
- 4 Discretization
- 5 Defining an Operator
- 6 Solving Systems of Equations
- 7 Optimal Solvers
- 8 The Undiscovered Country

Outline

- 1 Creating a PETSc Application
 - What is PETSc?
 - Who uses and develops PETSc?
 - How can I get PETSc?
 - How do I Configure PETSc?
 - How do I Build PETSc?
 - How do I run an example?
 - How do I get more help?
 - Minimal PETSc application

- 2 Creating a Simple Mesh

- 3 Defining a Function

- 4 Discretization

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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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?

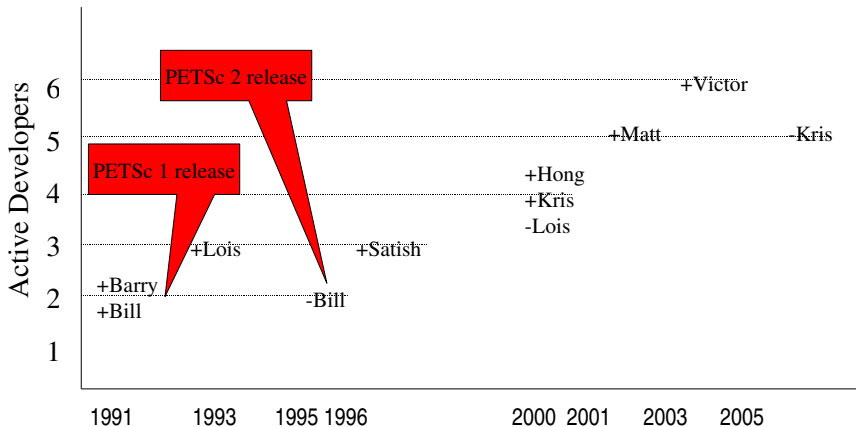
A freely available and supported research code

- 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



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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What Can We Handle?

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- PETSc has run on over **6,000** processors efficiently
 - ftp://info.mcs.anl.gov/pub/tech_reports/reports/P776.ps.Z
- PETSc applications have run at **2 Teraflops**
 - LANL PFLOTRAN code

Who Uses PETSc?

- Computational Scientists
 - PyLith (TECTON), Underworld, Columbia group
- Algorithm Developers
 - Iterative methods and Preconditioning researchers
- Package Developers
 - SLEPc, TAO, 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-2.3.2>

Unpacking PETSc

- Just clone development repository
 - `hg clone http://petsc.cs.iit.edu/petsc/petsc-dev petsc-dev`
 - `hg clone -rRelease-2.3.2 petsc-dev petsc-2.3.2`

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/ParCFD07TutorialCode
```

- Manual download

```
wget ftp://info.mcs.anl.gov/pub/petsc/ParCFD07TutorialCode.tar.gz .
```

Configuring PETSc

- Set `$PETSC_DIR` to the installation root directory
- Run the configuration utility
 - `$PETSC_DIR/config/figure.py`
 - `$PETSC_DIR/config/figure.py --help`
 - `$PETSC_DIR/config/figure.py --download-mpich`
- There are many examples on the installation page
- Configuration files are placed in `$PETSC_DIR/bmake/$PETSC_ARCH`
 - `$PETSC_ARCH` has a default if not specified

Configuring PETSc

- You can easily reconfigure with the same options
 - `./bmake/$PETSC_ARCH/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

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

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 `$PETSC_DIR/lib/$PETSC_ARCH/`
- 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 **M**essage **P**assing **I**nterface 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_xmonitor`
- Can disable dynamically
 - `-ksp_cancelmonitors`
- Does not display subsolvers
 - `-snes_monitor`
- Can use the true residual
 - `-ksp_truemonitor`
- Can display different subobjects
 - `-snes_vecmonitor`, `-snes_vecmonitor_update`,
`-snes_vecmonitor_residual`
 - `-ksp_gmres_krylov_monitor`
- Can display the spectrum
 - `-ksp_singmonitor`

Getting More Help

- <http://www.mcs.anl.gov/petsc>
- Hyperlinked documentation
 - Manual
 - Manual pages for every method
 - HTML of all example code (linked to manual pages)
- FAQ
- Full support at petsc-maint@mcs.anl.gov
- High profile users
 - Lorena Barba
 - David Keyes
 - Xiao-Chuan Cai
 - Richard Katz

Following the Tutorial

Update to each new checkpoint (**r0**):

- `hg clone -r0 ParCFD07TutorialCode 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

1 Creating a PETSc Application

2 Creating a Simple Mesh

- Structured Meshes
- Common PETSc Usage
- Unstructured Meshes
- 3D Meshes

3 Defining a Function

4 Discretization

5 Defining an Operator

6 Solving Systems of Equations

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

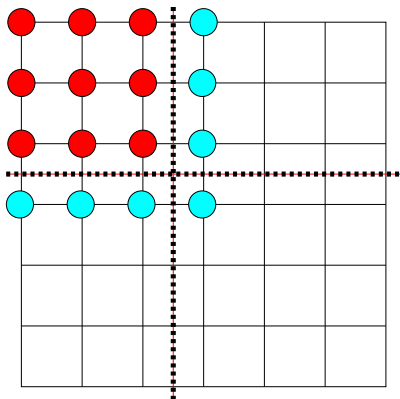
lm/n: Alternative array of local sizes

- Use PETSC_NULL for the default

Ghost Values

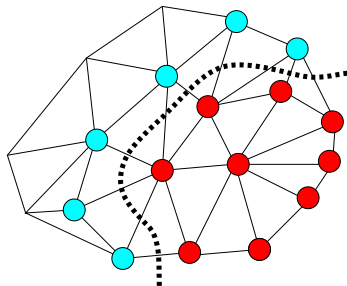
To evaluate a local function $f(x)$, each process requires

- its local portion of the vector x
- its **ghost values**, bordering portions of x owned by neighboring processes



● Local Node

● Ghost Node



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()`

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

Creating the Mesh

- Generic object
 - MeshCreate()
 - MeshSetMesh()
- File input
 - MeshCreatePCICE()
 - MeshCreatePyLith()
- Generation
 - MeshGenerate()
 - MeshRefine()
 - 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`
- `mayavi -d bratu.vtk -m SurfaceMap&`
- `make NP=4 EXTRA_ARGS="--structured 0 -mesh_view_vtk" runbratu`
- Viewable using Mayavi

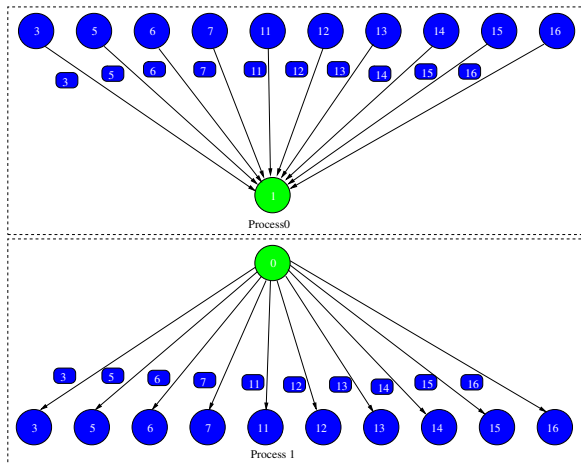
Refining the Mesh

- `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
 - 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

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`
- `mayavi -d bratu.vtk -m SurfaceMap -f UserDefined:vtkExtractEdges`
- `make NP=4 EXTRA_ARGS="-dim 3 -structured 0 -generate -mesh_view_vtk -refinement_limit 0.01" runbratu`

Outline

- 1 Creating a PETSc Application
- 2 Creating a Simple Mesh
- 3 Defining a Function**
 - Vectors
 - Sections
- 4 Discretization
- 5 Defining an Operator
- 6 Solving Systems of Equations
- 7 Optimal Solvers

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

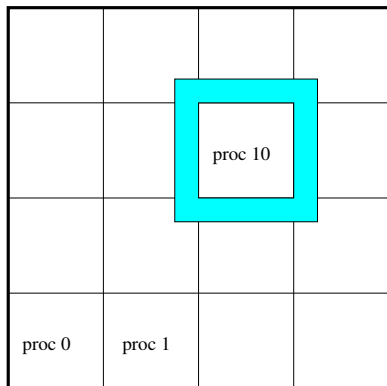
ctx: The user context passed to `DASetLocalFunction()`

The local DA function is activated by calling

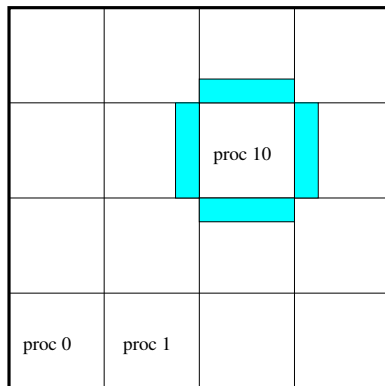
```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

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 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`

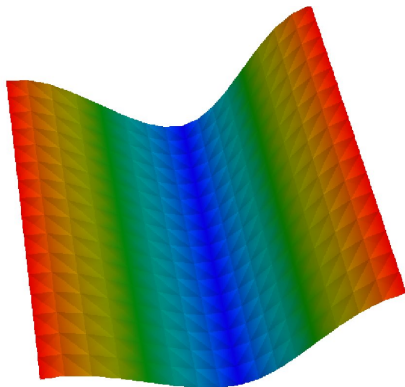
Section can have arbitrary layout

- 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()`

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 `mayavi -d cos.vtk -m SurfaceMap -f WarpScalar`



Outline

- 1 Creating a PETSc Application
- 2 Creating a Simple Mesh
- 3 Defining a Function
- 4 Discretization**
 - Finite Elements
 - Finite Differences
 - Evaluating the Error
- 5 Defining an Operator
- 6 Solving Systems of Equations

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

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

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

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

For this problem, we allow two types of conditions

- Dirichlet

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

- Implemented by constraints on dofs in a Section

- Neumann

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

- Implemented by integration along the boundary (future)

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, apply the corresponding functional N_i to the function g
- Functional application uses `BoundaryCondition::integrateDual()`
- The functionals are generated and set using `BoundaryCondition::setDualIntegrator()`
- `Mesh::setupField()` applies Dirichlet conditions automatically

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

Update to Revision 9

Section Assembly

First we do **local** operations:

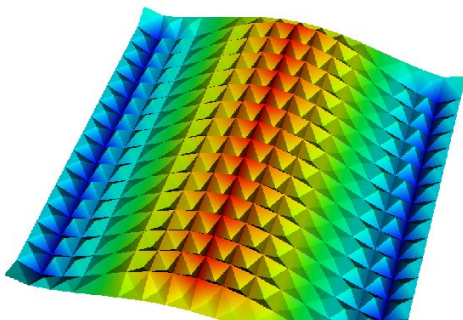
- Loop over cells
- Compute cell geometry
- Integrate each basis function to produce an element vector
- Call `SectionUpdateAdd()`
 - Note that this updates the *closure* of the cell

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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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
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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,

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

The important property for the approximation is *consistency*, meaning

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

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

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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

$$e = \sum_i e_i \phi_i(x) \quad (1)$$

- 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

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

The FE theory predicts a convergence rate for the quantity

$$\|u - \hat{u}\|_2^2 = \sum_T \int_T dA (u - \hat{u})^2 \quad (3)$$

$$= \sum_T \sum_q w_q |J| \left(u(q) - \sum_j \hat{u}_j \phi_j(q) \right)^2 \quad (4)$$

$$(5)$$

The estimate for linear elements is

$$\|u - \hat{u}_h\| < Ch \|u\| \quad (6)$$

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 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" runbratu`

Outline

- 1 Creating a PETSc Application
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- 6 Solving Systems of Equations
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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)
```

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 `MatAssemblyBegin/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`

Update to Revision 14

Operator Assembly

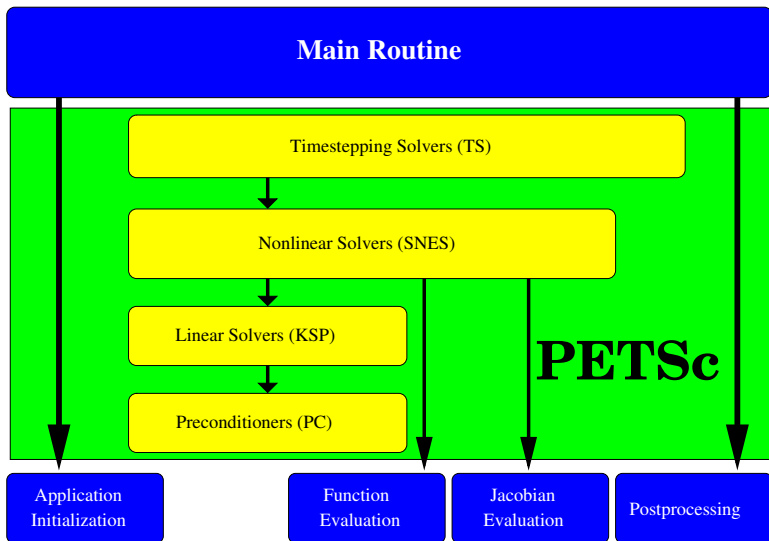
- Full assembly
 - Aggregate along all element interfaces
 - Global sparse matrix
- Stored assembly
 - No aggregation along element interfaces
 - Store element matrices
 - Use a MATSHELL in the solve
- Calculated assembly
 - No aggregation along element interfaces
 - Calculate element matrices on the fly
 - Use a MATSHELL in the solve
- Other alternatives. . .
 - Aggregation along some element interfaces (local?)
 - Custom overlaps
 - Partial calculation

Outline

- 1 Creating a PETSc Application
- 2 Creating a Simple Mesh
- 3 Defining a Function
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- 5 Defining an Operator
- 6 Solving Systems of Equations**
 - Linear Equations
 - Nonlinear Equations

7 Optimal Solvers

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 MatStructure 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

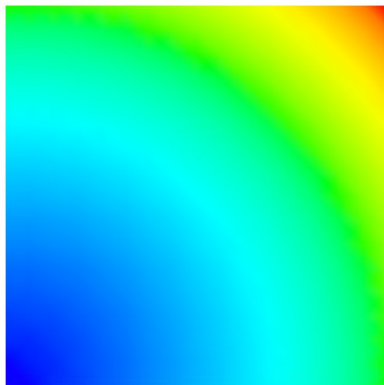
Update to Revision 15

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()`

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 -ksp_monitor -snes_monitor -vec_view_vtk -refinement_limit 0.00125 -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 **default**

Solving the Dirichlet Problem: P_2

- `rm 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 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 19

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 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 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 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_fd" runbratu`

Finding Problems

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

- `rm 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_fd" runbratu`

It works!

Finding Problems

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

- `rm 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_fd" 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 20

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

- 1 Creating a PETSc Application
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- 7 Optimal Solvers**
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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 it 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`

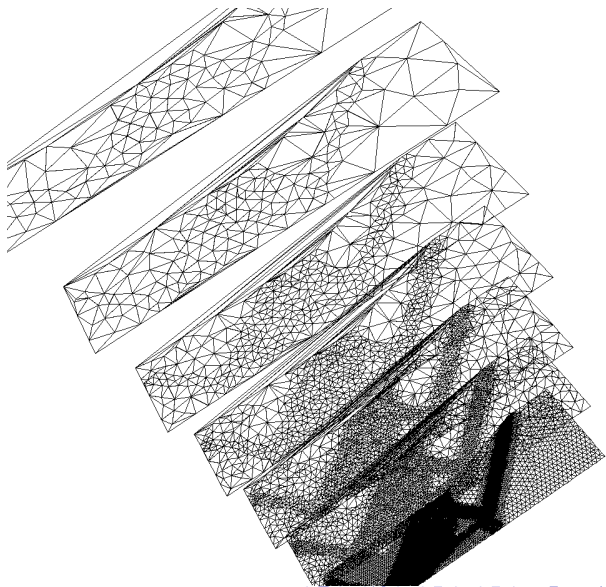
Unstructured Meshes

- 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 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

Coarse Hierarchy



Hierarchy created
using Talmor-Miller
coarsening

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

- 1 Creating a PETSc Application
- 2 Creating a Simple Mesh
- 3 Defining a Function
- 4 Discretization
- 5 Defining an Operator
- 6 Solving Systems of Equations
- 7 Optimal Solvers
- 8 The Undiscovered Country

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 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.