# PETSc Tutorial

PETSc Team
Presented by Matthew Knepley

Mathematics and Computer Science Division
Argonne National Laboratory

First Latin-American SCAT Workshop and Summer School
Universidad Técnica Federico Santa María
January 10, 2007



# Disclaimer

This PETSc Tutorial is still New!

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear
- Finite Difference and Finite Element

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear
- Finite Difference and Finite Element
- Structured and Unstructured

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear
- Finite Difference and Finite Element
- Structured and Unstructured
- Triangles and Hexes

# Tutorial Goal

Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear
- Finite Difference and Finite Element
- Structured and Unstructured
- Triangles and Hexes
- Optimal Solvers

# Tutorial Goal

## Enable students to develop new simulations with PETSc.

- Serial and Parallel
- Linear and Nonlinear
- Finite Difference and Finite Element
- Structured and Unstructured
- Triangles and Hexes
- Optimal Solvers

Items in red not finished for tutorial

# Outline

# Part I

# Creating a PETSc Application

# 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

# How Can We Help?

- Provide documentation
- Quickly answer questions

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

# How Can We Help?

- Provide documentation
- Quickly answer questions
- Help install

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

# 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.*

# What is PETSc?

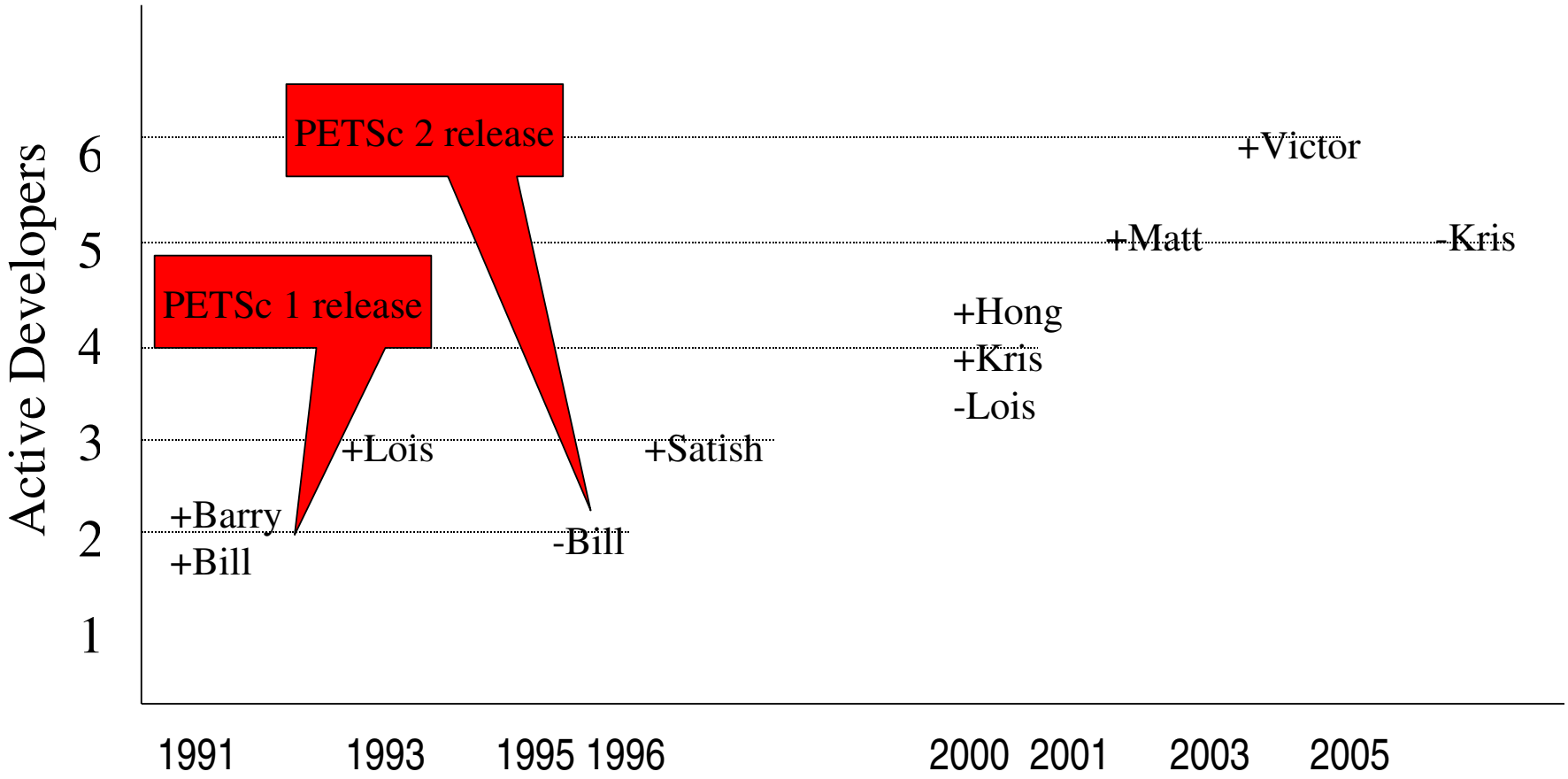
A freely available and supported research code

- 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 8,500 downloads since 1995 (version 2), currently 250 per month
- PETSc Funding and Support
  - Department of Energy
    - SciDAC, MICS Program
  - National Science Foundation
    - CIG, CISE, Multidisciplinary Challenge Program

# Timeline


Active Developers
6
5
4
3
2
1
PETSc 2 release
PETSc 1 release
+Victor
+Matt
-Kris
+Hong
+Kris
-Lois
+Lois
+Satish
+Barry
+Bill
-Bill
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

# 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 6,000 processors efficiently
  - ftp://info.mcs.anl.gov/pub/tech_reports/reports/P776.ps.Z

# 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 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

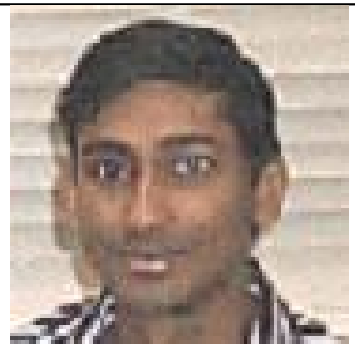
# Who Uses PETSc?

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

# The PETSc Team

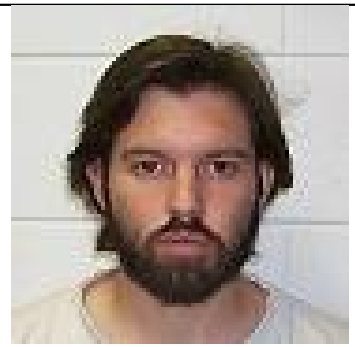

Bill Gropp


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

# 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/Columbia06TutorialCode
```

- Manual download

```
wget ftp://info.mcs.anl.gov/pub/petsc/Columbia06TutorialCode.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 `$PETSC_DIR/bmake/$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
  - MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack
  - 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 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_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 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 Columbia06TutorialCode 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()`
- 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

Part II

# Creating a Simple 2D Mesh

# 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

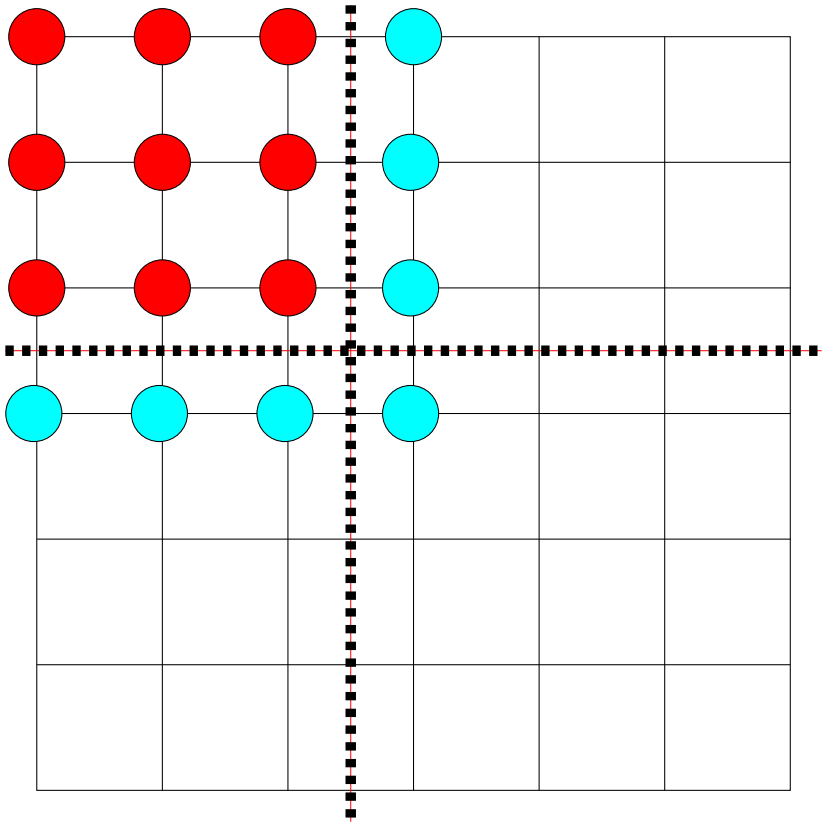
`s`: The stencil width

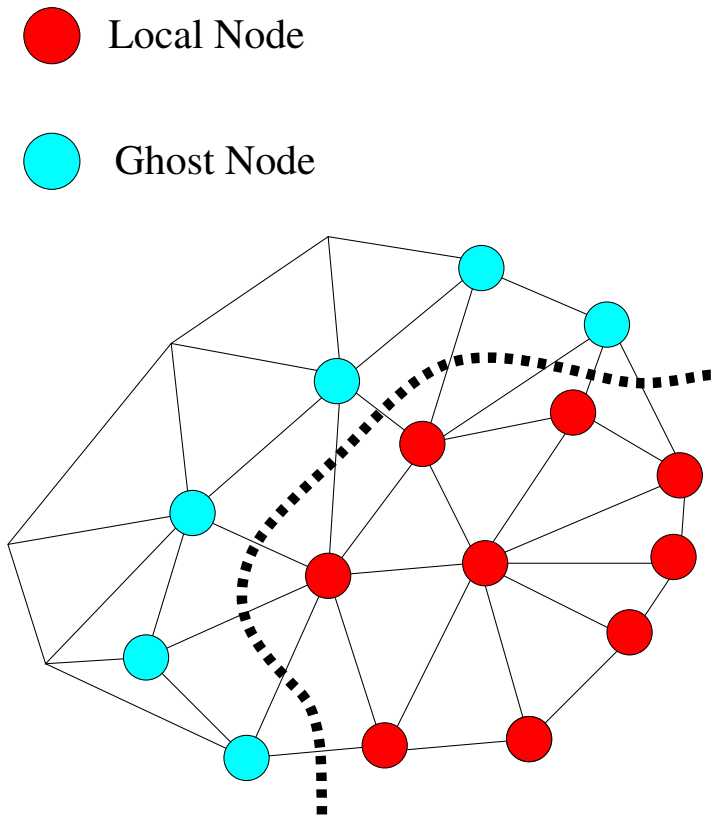
`lm/n`: Alternative array of local sizes
- Use `PETSC_NULL` for the default

# 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()`

# Memory Debugging

We can check for unfreed memory using:

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

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()`
- Clear, alias, reject, etc.

# Code Update

## Update to Revision 3

# Creating the Mesh

- File input
  - `MeshCreatePCICE()`
  - `MeshCreatePyLith()`
- Generation
  - `ALE::Generator::generateMesh()`
  - `ALE::Generator::refineMesh()`
- Partitioning and Distribution
  - `MeshDistribute()`

# 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`

Part III

# Defining a Function

# 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
- `DAGlobalToLocal End(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

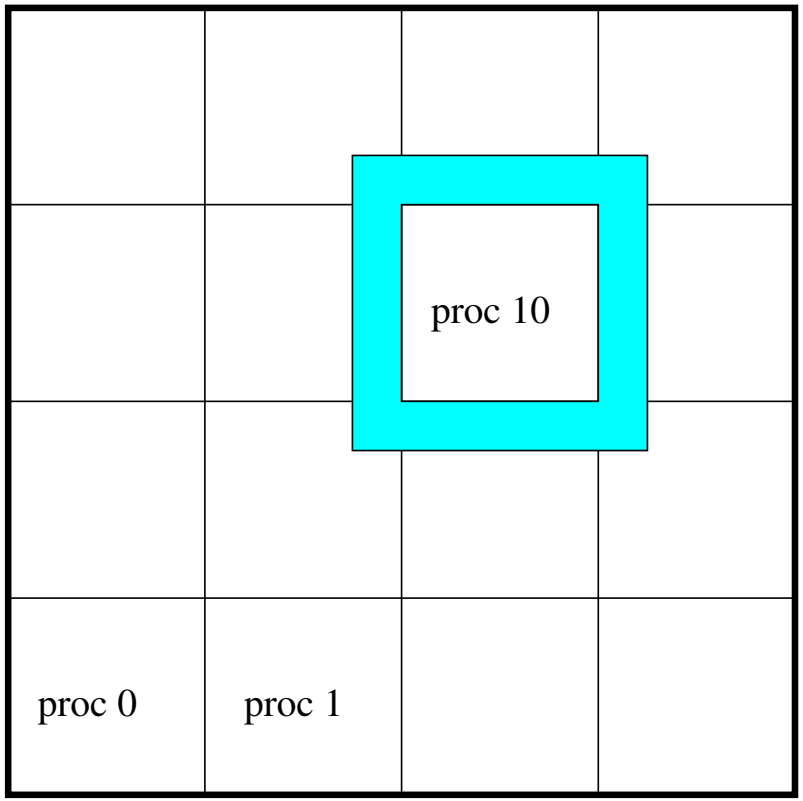
`ctx`: The user context passed to `DASetLocalFunction()`

The local DA function is activated by calling

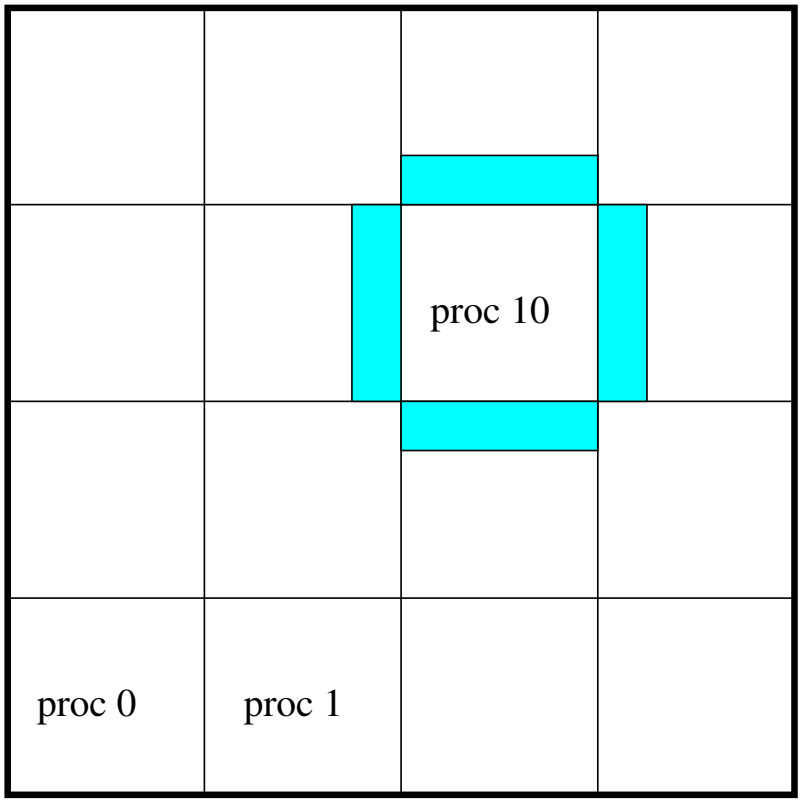
```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

# 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 5

# 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="-test 1 -vec_view_draw -draw_pause -1" runbratu`

# Code Update

Update to Revision 6

# 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 `Topology` 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 three value types
  - `SectionReal`
  - `SectionInt`
  - `SectionPair`

Section can have arbitrary layout

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

# Viewing the Section

- `make EXTRA_ARGS="-test 1 -structured 0 -vec_view_vtk" runbratu`
  - Produces linear.vtk and cos.vtk
- Viewable with MayaVi, exactly as with the mesh.
- `make EXTRA_ARGS="-test 1 -structured 0 -vec_view_vtk -generate -refinement_limit 0.003125" runbratu`
  - Use `mayavi -d cos.vtk -m SurfaceMap -f WarpScalar`

# 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

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

# Code Update

## Update to Revision 7

# FIAT Integration

Finite Element Integrator and Tabulator by Rob Kirby

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

The `quadrature.fiat` file contains:

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

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

- Quadrature points and weights
- Basis function evaluations at the quadrature points
- Basis function derivative evaluations at the quadrature points

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

# Code Update

## Update to Revision 8

# Viewing a DA Weak Form

- We use Q1 finite elements and a *Galerkin* formulation
  - Uses a linear basis in each dimension
  - Should really use a fast tensor evaluation routine
- Could substitute exact integrals for quadrature
- `make EXTRA_ARGS="-test 1 -vec_view_draw -draw_pause -1" runbratu`
- `make EXTRA_ARGS="-test 1 -vec_view_draw -draw_pause -1 -da_grid_x 20 -da_grid_y 20" runbratu`

# Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-test 1 -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="-test 1 -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="-test 1 -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="-test 1 -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 9

# Debugging Assembly

On two processes, I get a SEGV!

So we try running with:

- `make NP=2 EXTRA_ARGS="-test 1 -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 9
- Notice that we were already using ghosted assembly
  - Could eliminate this by reorganizing element traversal

# Code Update

## Update to Revision 10

# 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++ interface allow completion over arbitrary overlaps

```
make NP=2 EXTRA_ARGS="-test 1 -structured 0 -vec_view_vtk" runbratu
```

# Viewing a Mesh Weak Form

- We use P1 finite elements and a *Galerkin* formulation
  - Uses a linear basis in each dimension
  - Correct FIAT table is chosen at runtime
- Could substitute exact integrals for quadrature
- `make EXTRA_ARGS="-test 1 -structured 0 -vec_view_vtk" runbratu`
- `make EXTRA_ARGS="-test 1 -structured 0 -vec_view_vtk -generate -refinement_limit 0.003125" runbratu`

# Global and Local

Local (analytical)

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

# Global and Local

Local (analytical)

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

Largely dim dependent
(e.g. quadrature)

# Global and Local

Local (analytical)

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

Largely dim dependent
(e.g. quadrature)

Global (topological)

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

# Global and Local

Local (analytical)

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

Largely dim dependent
(e.g. quadrature)

Global (topological)

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

Largely dim independent
(e.g. mesh traversal)

Part IV

# Defining an Operator

# Update to Revision 11

# DA Operators

- Evaluate again only the local portion
  - No nice local array form without copies
- Use `MatSetValuesStencil()` to convert `(i,j,k)` to indices
- Notice we use $J^{-1}$ to convert derivatives
- `make NP=1 EXTRA_ARGS="-test 1 -mat_view_draw -draw_pause -1" runbratu`

# DA Local Jacobian

The user provided function which calculates the nonlinear residual 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)
```

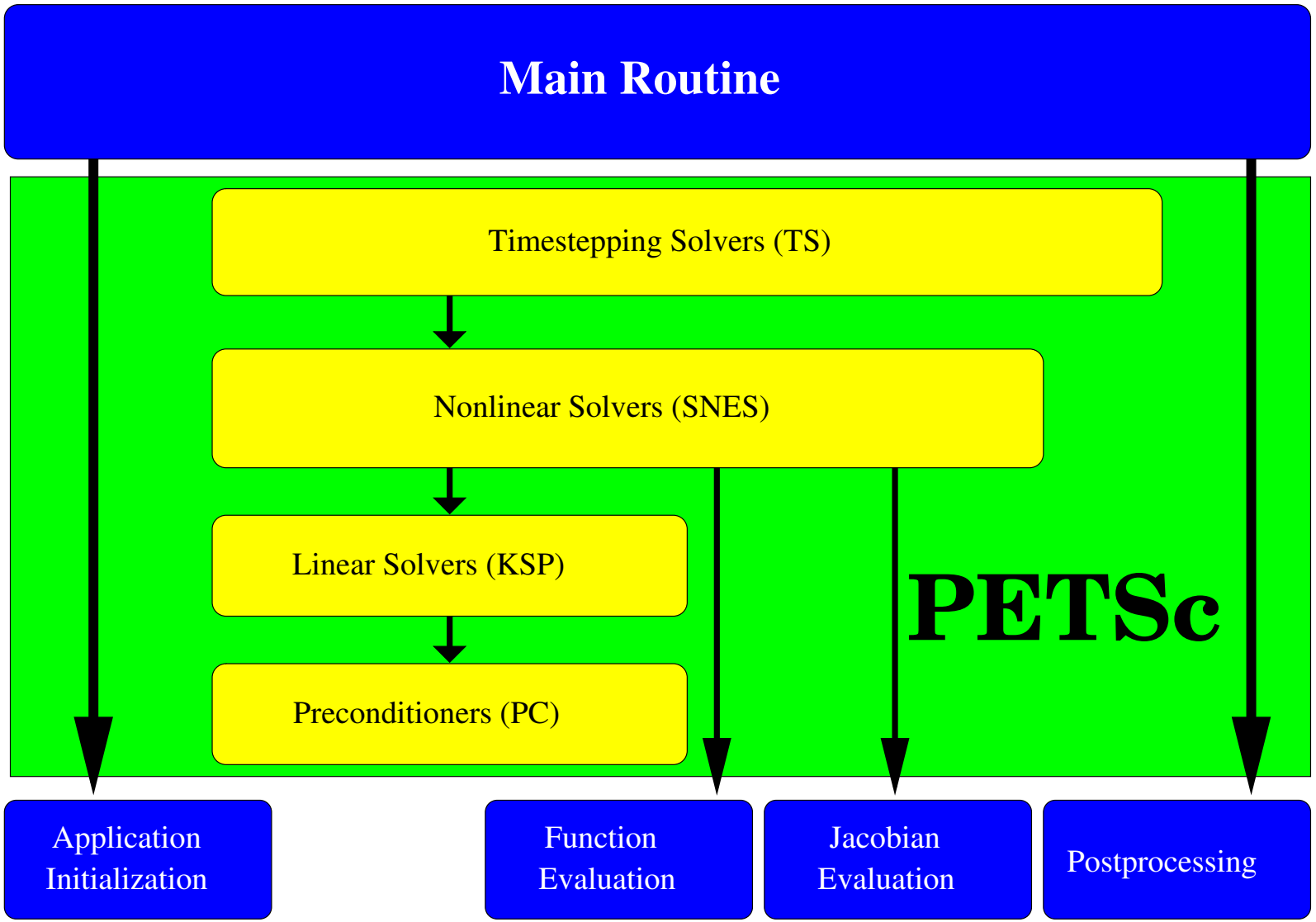
# Mesh Operators

- We evaluate the local portion just as with functions
- 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 NP=1 EXTRA_ARGS="-test 1 -structured 0 -mat_view_draw -draw_pause -1" runbratu`

Part V

# Solving Systems of Equations

# 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()`

# Update to Revision 12

# 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 Neumann Problem

- `make NP=1 EXTRA_ARGS="-vec_view_draw -mat_view_draw -draw_pause -1 -snes_monitor -ksp_monitor" runbratu`
- `make NP=1 EXTRA_ARGS="-vec_view_vtk -mat_view_draw -draw_pause -1 -snes_monitor -ksp_monitor -structured 0" runbratu`

Part VI

# Boundary Conditions

# 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
  - Elements have a negative fiber dimension
  - Ignored by `size()` and `update()`, but `restrict()` works normally
  - Use `updateBC()` to define the boundary values

# Update to Revision 13

# Solving the Dirichlet Problem

We are using the exact solution $u^* = x^2 + y^2$,so that $f = -4$

- `make NP=1 EXTRA_ARGS="-structured 0 -generate -bc_type dirichlet -vec_view -vec_view_vtk -snes_monitor -ksp_monitor" runbratu`
  - Notice that the only variable is the middle point, which is 0.5
- `make NP=1 EXTRA_ARGS="-structured 0 -generate -refinement_limit 0.003125 -bc_type dirichlet -vec_view_vtk -snes_monitor -ksp_monitor" runbratu`
- `mayavi -d sol.vtk -m SurfaceMap -f WarpScalar`

Part VII

# Out of Flatland

# Update to Revision 14

# Structured Mesh Conversion

- Added new constructor call
- Added new local evaluation routines
  - `Rhs_Structured_3d()` and `Jac_Structured_3d()`
- Added new 3D source term

# Unstructured Mesh Conversion

- Added new quadrature rule
- No need to change evaluation routines
  - Just need to pick the correct quadrature
- Added new 3D mesh files
  - Interfaces to TetGen (and soon TUMBLE) mesh generator

# Solving the 3D Problem

- `make NP=1 EXTRA_ARGS="-dim 3 -snes_monitor -ksp_monitor" runbratu`
  - We currently have no way to visualize this solution
- `make NP=1 EXTRA_ARGS="-dim 3 -structured 0 -snes_monitor -ksp_monitor" runbratu`
- `make NP=1 EXTRA_ARGS="-dim 3 -structured 0 -generate -refinement_limit 0.003125 -bc_type dirichlet -vec_view_vtk -snes_monitor -ksp_monitor" runbratu`

Part VIII

# Optimal Solvers

# 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

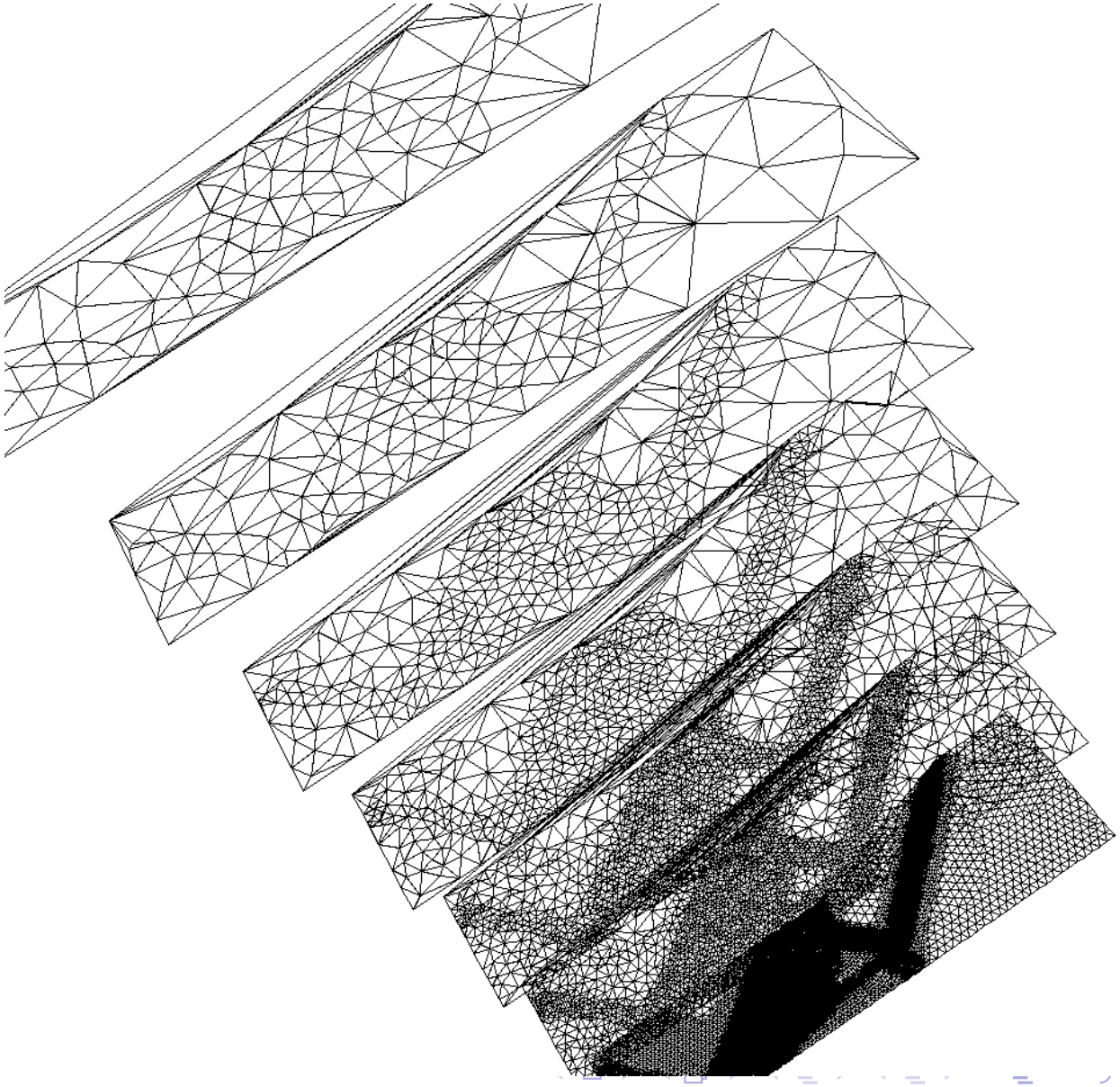
# Unstructured Meshes

- Same `DMMG` options as the structured case
- Mesh refinement
  - Ruppert algorithm in Triangle and TetGen
- Mesh coarsening
  - Talmor-Miller algorithm in PETSc

# Solving with Multigrid

- `make NP=1 EXTRA_ARGS="-da_grid_x 10 -da_grid_y 10 -ksp_rtol 1e-8 -dmmg_nlevels 8 -dmmg_view -snes_monitor -ksp_monitor" runbratu`
  - Notice that there are over 1 million unknowns!
- `make NP=1 EXTRA_ARGS="-structured 0 -ksp_rtol 1e-8 -dmmg_nlevels 2 -dmmg_view -snes_monitor -ksp_monitor" runbratu`

# Coarse Hierarchy



Hierarchy created using Talmor-Miller coarsening

Part IX

# The Undiscovered Country

# What We Have Not Covered

- Unstructured hexes
- Nonlinearity
- Error Estimation
- Semi-Lagrangian Schemes

# 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.