Building Robust Scientific Codes

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HPC^3: Workshop on High Performance Computing
and Hybrid Programming Concepts for Hyperbolic PDE Codes
KAUST, Saudi Arabia, March 2011

What I Need From You

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

Ask Questions!!!

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

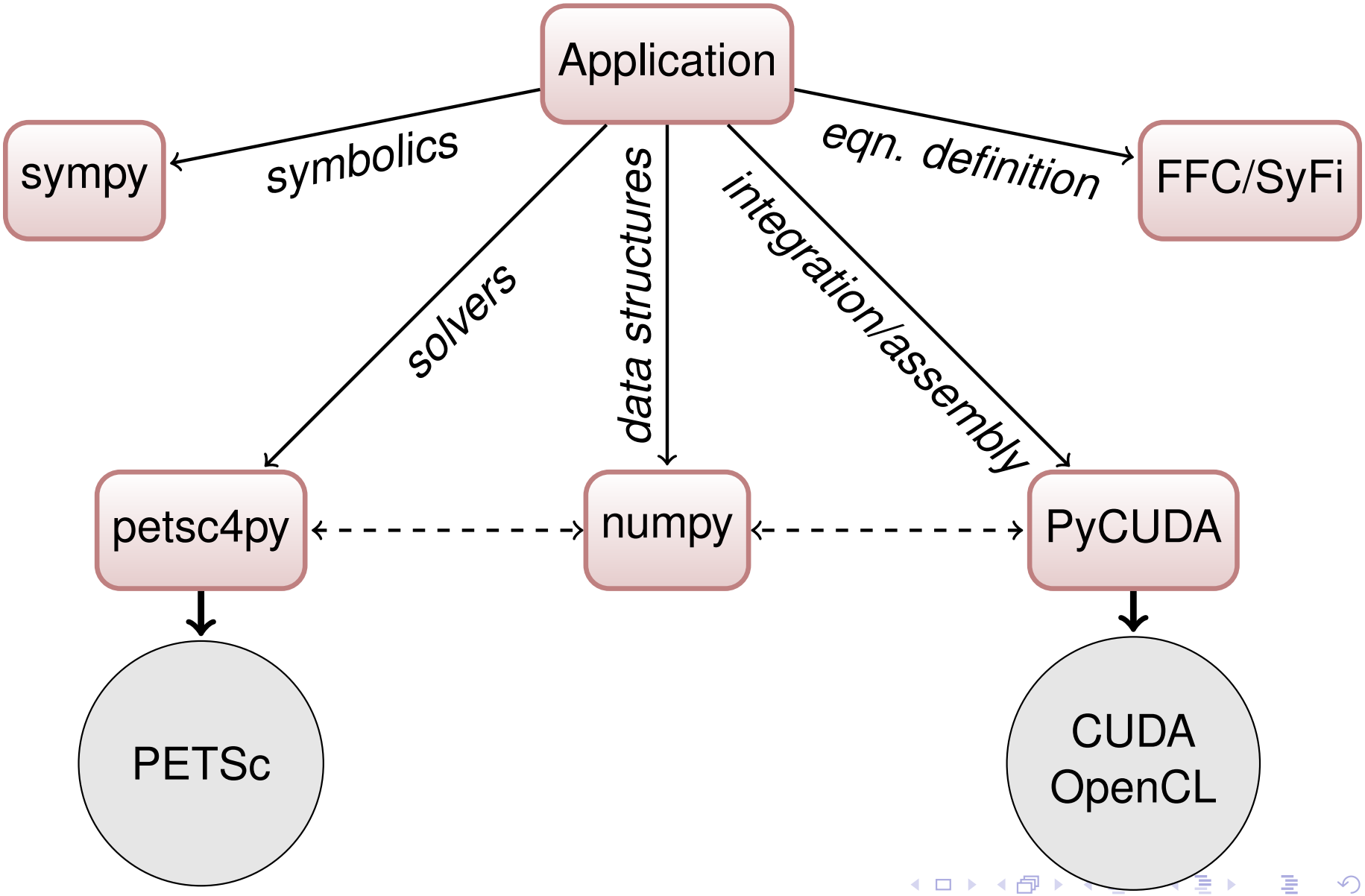
New Model for Scientific Software

Simplifying Parallelization of Scientific Codes by a Function-Centric Approach in Python

Jon K. Nilsen, Xing Cai, Bjorn Hoyland, and Hans Petter Langtangen

- **Python** at the application level
- **numpy** for data structures
- **petsc4py** for linear algebra and solvers
- **PyCUDA** for integration (physics) and assembly

New Model for Scientific Software



What is Missing from this Scheme?

- Unstructured graph traversal
  - Iteration over cells in FEM
    - Use a copy via numpy, use a kernel via Queue
  - (Transitive) Closure of a vertex
    - Use a visitor and copy via numpy
  - Depth First Search
    - Hell if I know
- Logic in computation
  - Limiters in FV methods
    - Can sometimes use tricks for branchless logic
  - Flux Corrected Transport for shock capturing
    - Maybe use WENO schemes which can be branchless
  - Boundary conditions
    - Restrict branching to PETSc C numbering and assembly calls
- **Audience???**

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Outline

Location and Retrieval

"Where's the Tarball"

- Version Control
  - Mercurial, Git, Subversion
- Hosting
  - BitBucket, GitHub, Launchpad
- Community involvement
  - arXiv, PubMed

Distributed Version Control

- CVS/SVN manage a single repository
  - Versioned data
  - Local copy for modification and checkin
- Mercurial manages many repositories
  - Identified by URLs
  - No one *Master*
- Repositories communicate by ChangeSets
  - Use `push` and `pull` to move changesets
  - Can move arbitrary changes with *patch queues*

Project Workflow

Figure: Single Repository

Project Workflow

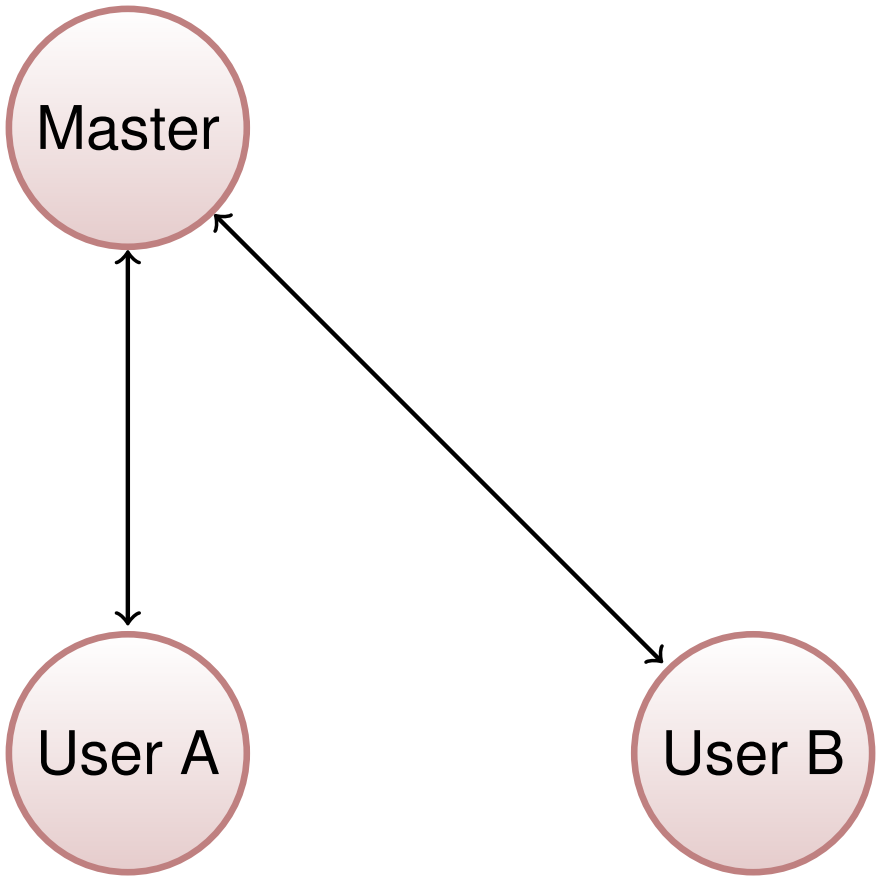

Figure: Master Repository with User Clones

Project Workflow

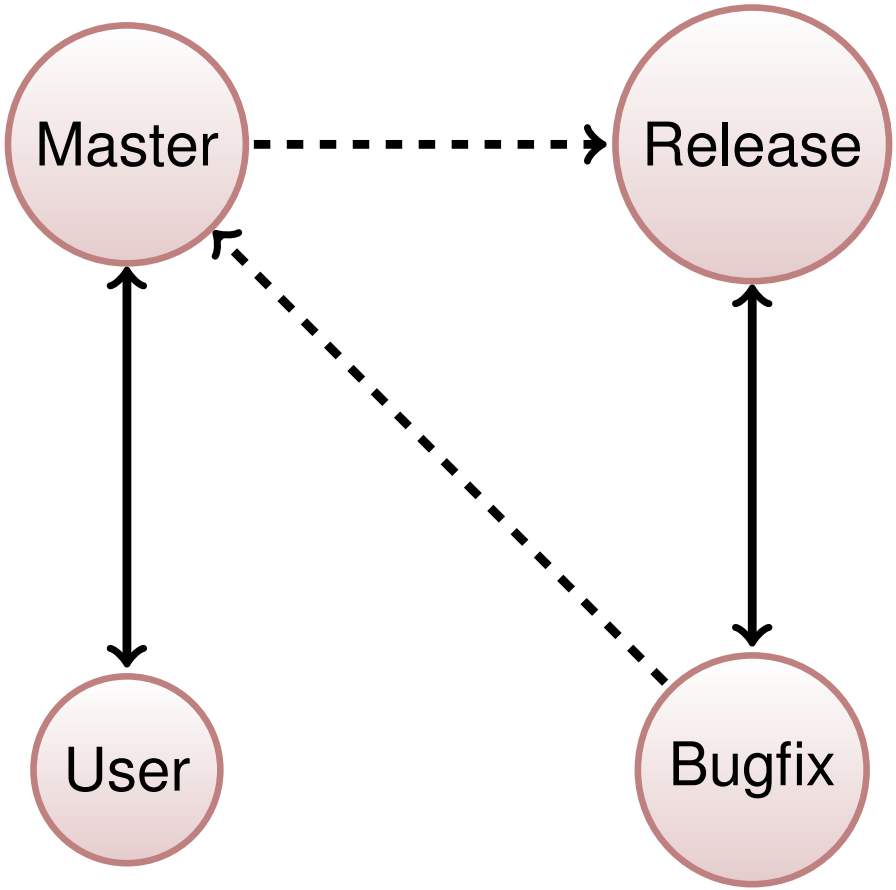

Figure: Project with Release and Bugfix Repositories

Outline

Configuration and Build

"It won't run on my iPhone"

- Portability
  - PETSc BuildSystem, autoconf
- Dependencies
  - Does this work with UnsupportedGradStudentAMG?
- Configurable build
  - Build must integrate with the configuration system
  - CMake, SCons

BuildSystem

Provides tools for Configuration and Build

- Dependency tracking and analysis
- Package management and hierarchy
- Library of standard tests
- Standard build rules
- Automatic package build and integration

http://petsc.cs.iit.edu/petsc/BuildSystem
http://petsc.cs.iit.edu/petsc/SimpleConfigure

Configure
Modules

`BuildSystem.config.base` configures a specific functionality

- Entry points:
  - `setupHelp()`
  - `setupDependencies()`
  - `configure()`
- Builtin capabilities:
  - Preprocessing, compilation, linking, running
  - Manages languages
  - Checks for executables
- Output types:
  - Define, typedef, or prototype
  - Make macro or rule
  - Substitution (old-style)

Configure
Framework

`BuildSystem.config.framework` manages the configure run

- Manages configure modules
  - Dependencies with DAG, `require()`
  - Options table
  - Initialization, run, cleanup
- Outputs
  - Configure headers and log
  - Make variable and rules
  - Pickled configure tree

Configure
Third Party Packages

`BuildSystem.config.package` manages other packages

- `BuildSystem/config/packages/*` examples (MPI, FIAT, etc.)
- Standard location and install hooks
- Standard header and library tests
- Uniform interface for parameter retrieval
- Special support for GNU packages

Configure
Build Integration

A module can declare a dependency using:

```
fw        = self.framework
self.mpi = fw.require('config.packages.MPI', self)
```

so that MPI is configured before `self`. Information is retrieved during `configure()`:

```
if self.mpi.found:
  include.extend(self.mpi.include)
  libs.extend(self.mpi.lib)
```

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```

Configure
Build Integration

A build system can acquire the information using:

```
class ConfigReader(script.Script):
  def __init__(self):
    import RDict
    argDB = RDict.RDict(None, None, 0, 0)
    argDB.saveFilename = os.path.join('path','RDict.db')
    argDB.load()
    script.Script.__init__(self, argDB = argDB)
    return

  def getMPIModule(self):
    self.setup()
    fw  = self.loadConfigure()
    mpi = fw.require('config.packages.MPI', None)
    return mpi
```

Make

GNU Make automates a package build

- Has a single predicate, older-than
- Executes shell code for actions
- PETSc has support for
  - configuration integration
  - automatic compilation
- Alternatives
  - SCons
  - CMake

builder

Simple replacement for GNU make

- Excellent configure integration
- User-defined predicates
- Dependency analysis and tracking
- Python actions
- Support for test execution

builder
Two Interfaces

The simple interface handles the entire build:

```
./config/builder.py
```

A more flexible front end allows finer control:

```
./config/builder2.py help [command]
./config/builder2.py clean
./config/builder2.py stubs fortran
./config/builder2.py build [src/snes/interface/snesj.c]
./config/builder2.py check [src/snes/examples/tutorials/ex10.c]
```

Testing

"They are identical in the eyeball norm"

- Unit tests
  - cppUnit
- Regression tests
  - buildbot
- Benchmarks
  - Cigma

Outline

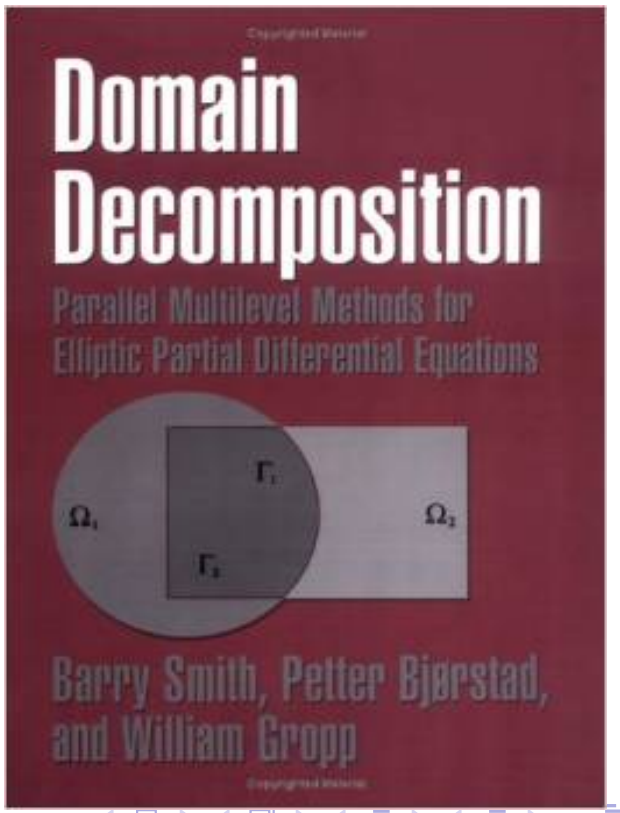
Outline

How did PETSc Originate?

PETSc was developed as a Platform for Experimentation

We want to experiment with different

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



The Role of PETSc

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

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

— Barry Smith

Advice from Bill Gropp

You want to think about how you decompose your data structures, how you think about them globally. [...] If you were building a house, you'd start with a set of blueprints that give you a picture of what the whole house looks like. You wouldn't start with a bunch of tiles and say. "Well I'll put this tile down on the ground, and then I'll find a tile to go next to it." But all too many people try to build their parallel programs by creating the smallest possible tiles and then trying to have the structure of their code emerge from the chaos of all these little pieces. You have to have an organizing principle if you're going to survive making your code parallel.

(http://www.rce-cast.com/Podcast/rce-28-mpich2.html)

What is PETSc?

A freely available and supported research code for the parallel solution of nonlinear algebraic equations

Free

- Download from http://www.mcs.anl.gov/petsc
- Free for everyone, including industrial users

Supported

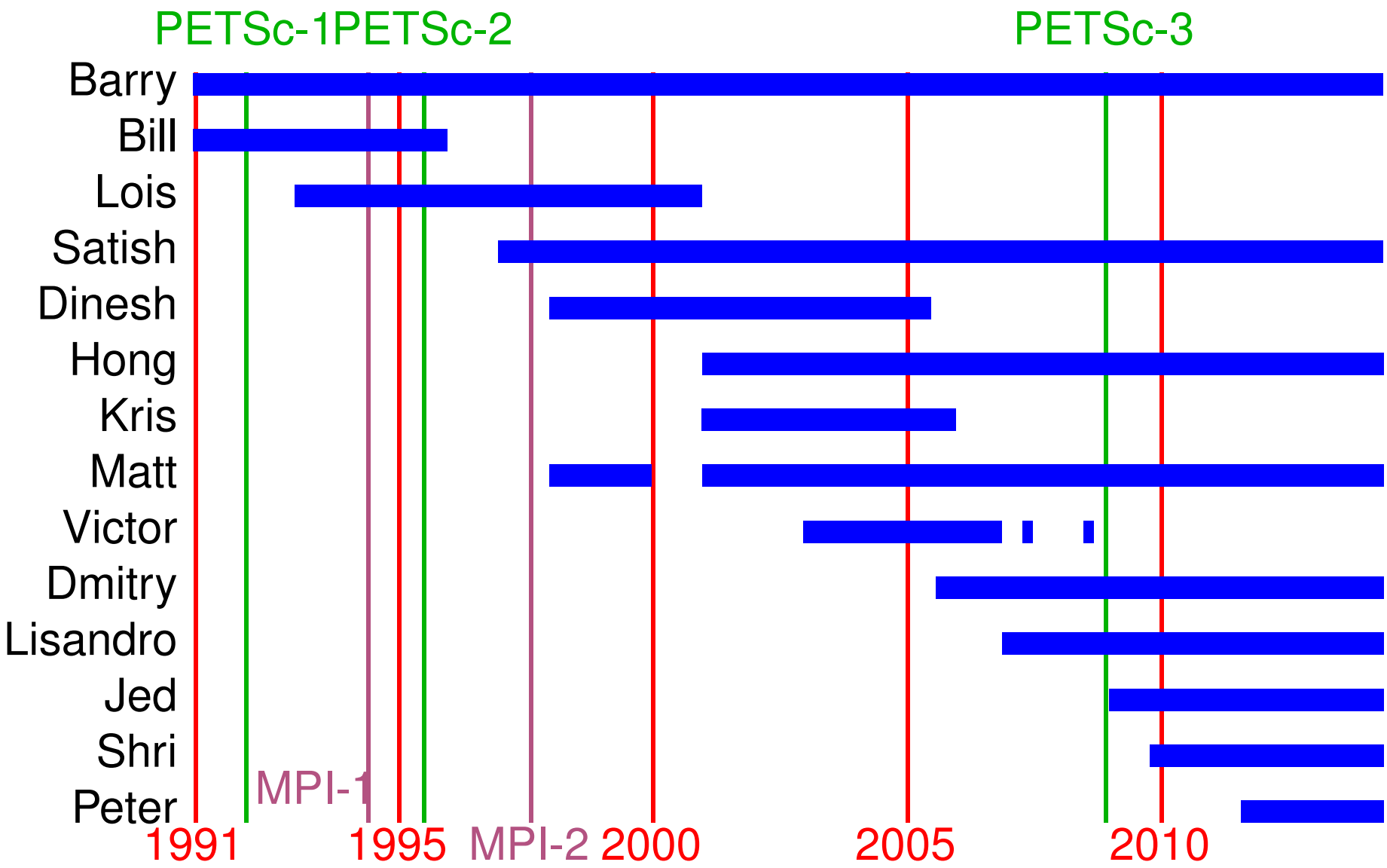
- Hyperlinked manual, examples, and manual pages for all routines
- Hundreds of tutorial-style examples
- Support via email: petsc-maint@mcs.anl.gov

Usable from C, C++, Fortran 77/90, Matlab, Julia, and Python

What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems
    - Cray XT6, BG/Q, NVIDIA Fermi, K Computer
  - Loosely coupled systems, such as networks of workstations
    - IBM, Mac, iPad/iPhone, PCs running Linux or Windows
- PETSc History
  - Begun September 1991
  - Over 60,000 downloads since 1995 (version 2)
  - Currently 400 per month
- PETSc Funding and Support
  - Department of Energy
    - SciDAC, MICS Program, AMR Program, INL Reactor Program
  - National Science Foundation
    - CIG, CISE, Multidisciplinary Challenge Program

Timeline


PETSc-1
PETSc-2
PETSc-3
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed
Shri
Peter
MPI-1
MPI-2
1991
1995
2000
2005
2010

What Can We Handle?

- PETSc has run implicit problems with over 500 billion unknowns
  - UNIC on BG/P and XT5
  - PFLOTRAN for flow in porous media
- PETSc has run on over 290,000 cores efficiently
  - UNIC on the IBM BG/P Jugene at Jülich
  - PFLOTRAN on the Cray XT5 Jaguar at ORNL
- PETSc applications have run at 23% of peak (600 Teraflops)
  - Jed Brown on NERSC Edison
  - HPGMG code

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petsc4py

petcs4py provides Python bindings for PETSc

- Provides ALL PETSc functionality in a Pythonic way
  - Logging using the Python `with` statement
- Can use Python callback functions
  - SNESSetFunction(), SNESSetJacobian()
- Manages all memory (creation/destruction)
- Visualization with matplotlib

petsc4py Installation

- Automatic
  - `pip install -install-options=-user petscp4y`
  - Uses `$PETSC_DIR` and `$PETSC_ARCH`
  - Installed into `$HOME/.local`
  - No additions to **PYTHONPATH**
- From Source
  - `virtualenv python-env`
  - `source ./python-env/bin/activate`
  - Now everything installs into your proxy Python environment
  - `hg clone https://petsc4py.googlecode.com/hg petsc4py-dev`
  - `ARCHFLAGS="-arch x86_64" python setup.py sdist`
  - `ARCHFLAGS="-arch x86_64" pip install dist/petsc4py-1.1.2.tar.gz`
  - **ARCHFLAGS** only necessary on Mac OSX

petsc4py Examples

- `externalpackages/petsc4py-1.1/demo/bratu2d/bratu2d.py`
  - Solves Bratu equation (SNES ex5) in 2D
  - Visualizes solution with matplotlib
- `src/ts/examples/tutorials/ex8.py`
  - Solves a 1D ODE for a diffusive process
  - Visualize solution using `-vec_view_draw`
  - Control timesteps with `-ts_max_steps`

Outline

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numpy

numpy is ideal for building Python data structures

- Supports multidimensional arrays
- Easily interfaces with C/C++ and Fortran
- High performance BLAS/LAPACK and functional operations
- Python 2 and 3 compatible
- Used by petsc4py to talk to PETSc

Outline

sympy

sympy is useful for symbolic manipulation

- Interacts with numpy
- Derivatives and integrals
- Series expansions
- Equation simplification
- Small and open source

sympy
Example of Series Transform

Create the shifted polynomial

$$\sum_{i=0}^{order} \frac{c_i}{i!}(x-a)^i$$

```
def constructShiftedPolynomial(order):
  from sympy import Symbol, collect, diff, limit
  from sympy import factorial as f
  c = [Symbol('c'+str(i)) for i in range(order)]
  g = sum([c[i]*(x-a)**i/f(i) for i in range(order)])
  # Convert to a monomial
  g = collect(g.expand(), x)
  return c, g
```

sympy
Example of Series Transform

Here is the shifted polynomial for order 5:

```
c0 - a*c1 + c2*a**2/2 - c3*a**3/6 + c4*a**4/24
+ x*(c1 - a*c2 + c3*a**2/2 - c4*a**3/6)
+ x**2*(c2/2 - a*c3/2 + c4*a**2/4)
+ x**3*(c3/6 - a*c4/6)
+ c4*x**4/24
```

sympy
Example of Series Transform

Construct matrix transform from

$$\sum_{i=0}^{order} \frac{c_i}{i!}(x-a)^i \qquad \text{to} \qquad \sum_{i=0}^{order} \frac{c_i}{i!}x^i$$

```
def constructTransformMatrix(order = 5):
  from sympy import diff, limit
  c, g = constructShiftedPolynomial(order, debug)
  M = []
  for o in range(order):
    exp = g.diff(x, o).limit(x, 0)
    M.append([exp.diff(c[p]) for p in range(order)])
  return M
```

sympy
Example of Series Transform

Here is the transform matrix M:

$$\begin{pmatrix} 1 & -a & \frac{a^2}{2} & -\frac{a^3}{6} & \frac{a^4}{24} \\ 0 & 1 & -a & \frac{a^2}{2} & -\frac{a^3}{6} \\ 0 & 0 & 1 & -a & \frac{a^2}{2} \\ 0 & 0 & 0 & 1 & -a \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Outline

PyCUDA and PyOpenCL

Python packages by Andreas Klöckner
for embedded GPU programming

- Handles unimportant details automatically
  - CUDA compile and caching of objects
  - Device initialization
  - Loading modules onto card
- Excellent Documentation & Tutorial
- Excellent platform for Metaprogramming
  - Only way to get portable performance
  - Road to FLAME-type reasoning about algorithms

Code Template

```
<%namespace name="pb" module="performanceBenchmarks"/>
${pb.globalMod(isGPU)} void kernel(${pb.gridSize(isGPU)} float *output) {
  ${pb.gridLoopStart(isGPU, load, store)}
  ${pb.threadLoopStart(isGPU, blockDimX)}
  float G[${dim*dim}] = {${','.join(['3.0']*(dim*dim))}};
  float K[${dim*dim}] = {${','.join(['3.0']*(dim*dim))}};
  float product       = 0.0;
  const int Ooffset   = gridIdx*${numThreads};

  // Contract G and K
% for n in range(numLocalElements):
%   for alpha in range(dim):
%     for beta in range(dim):
<%      gIdx = (n*dim + alpha)*dim + beta %>
<%      kIdx = alpha*dim + beta %>
  product += G[${gIdx}] * K[${kIdx}];
%     endfor
%   endfor
% endfor
  output[Ooffset+idx] = product;
  ${pb.threadLoopEnd(isGPU)}
  ${pb.gridLoopEnd(isGPU)}
  return;
```

Rendering a Template

We render code template into strings using a dictionary of inputs.

```
args = {'dim':                self.dim,
        'numLocalElements':   1,
        'numThreads':         self.threadBlockSize}
kernelTemplate = self.getKernelTemplate()
gpuCode = kernelTemplate.render(isGPU = True,  **args)
cpuCode = kernelTemplate.render(isGPU = False, **args)
```

GPU Source Code

```
__global__ void kernel( float *output) {
  const int        gridIdx = blockIdx.x + blockIdx.y*gridDim.x;
  const int        idx     = threadIdx.x + threadIdx.y*1; // This is (i,j)
  float G[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float K[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float product       = 0.0;
  const int Ooffset   = gridIdx*1;

  // Contract G and K
  product += G[0] * K[0];
  product += G[1] * K[1];
  product += G[2] * K[2];
  product += G[3] * K[3];
  product += G[4] * K[4];
  product += G[5] * K[5];
  product += G[6] * K[6];
  product += G[7] * K[7];
  product += G[8] * K[8];
  output[Ooffset+idx] = product;
  return;
}
```

CPU Source Code

```
void kernel(int numInvocations, float *output) {
  for(int gridIdx = 0; gridIdx < numInvocations; ++gridIdx) {
    for(int i = 0; i < 1; ++i) {
      for(int j = 0; j < 1; ++j) {
        const int  idx = i + j*1; // This is (i,j)
  float G[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float K[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float product       = 0.0;
  const int Ooffset   = gridIdx*1;

  // Contract G and K
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  product += G[5] * K[5];
  product += G[6] * K[6];
  product += G[7] * K[7];
  product += G[8] * K[8];
  output[Ooffset+idx] = product;
      }
    }
```

Creating a Module

CPU:

```
# Output kernel and C support code
self.outputKernelC(cpuCode)
self.writeMakefile()
out, err, status = self.executeShellCommand('make')
\end{minted}

\bigskip

GPU:
\begin{minted}{python}
from pycuda.compiler import SourceModule

mod = SourceModule(gpuCode)
self.kernel = mod.get_function('kernel')
self.kernelReport(self.kernel, 'kernel')
```

Executing a Module

```
import pycuda.driver as cuda
import pycuda.autoinit

blockDim = (self.dim, self.dim, 1)
start    = cuda.Event()
end      = cuda.Event()
grid     = self.calculateGrid(N, numLocalElements)
start.record()
for i in range(iters):
  self.kernel(cuda.Out(output),
              block = blockDim, grid = grid)
end.record()
end.synchronize()
gpuTimes.append(start.time_till(end)*1e-3/iters)
```

Outline

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

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

FIAT understands

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

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

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

FFC

FFC is a compiler for variational forms by Anders Logg.

Here is a mixed-form Poisson equation:

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

where

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

FFC
Mixed Poisson

```
shape = "triangle"

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

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

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

f = Function(DG0)
L = w*f*dx
```

FFC

Here is a discontinuous Galerkin formulation of the Poisson equation:

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

where

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

FFC
DG Poisson

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

Analytic Flexibility
Laplacian

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} \tag{1}$$

```
element = FiniteElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(grad(v), grad(u))*dx
```

Analytic Flexibility
Laplacian

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} \tag{1}$$

```
element = FiniteElement('Lagrange', tetrahedron, 1)
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u = TrialFunction(element)
a = inner(grad(v), grad(u))*dx
```

Analytic Flexibility
Linear Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{2}$$

```
element = VectorElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(sym(grad(v)), sym(grad(u)))*dx
```

Analytic Flexibility
Linear Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{2}$$

```
element = VectorElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(sym(grad(v)), sym(grad(u)))*dx
```

Analytic Flexibility
Full Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : C : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{3}$$

```
element  = VectorElement('Lagrange', tetrahedron, 1)
cElement = TensorElement('Lagrange', tetrahedron, 1,
                         (dim, dim, dim, dim))
v = TestFunction(element)
u = TrialFunction(element)
C = Coefficient(cElement)
i, j, k, l = indices(4)
a = sym(grad(v))[i,j]*C[i,j,k,l]*sym(grad(u))[k,l]*dx
```

Currently broken in FEniCS release

Analytic Flexibility
Full Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : C : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{3}$$

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a = sym(grad(v))[i,j]*C[i,j,k,l]*sym(grad(u))[k,l]*dx
```

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Analytic Flexibility
Full Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : C : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{3}$$

```
element  = VectorElement('Lagrange', tetrahedron, 1)
cElement = TensorElement('Lagrange', tetrahedron, 1,
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v = TestFunction(element)
u = TrialFunction(element)
C = Coefficient(cElement)
i, j, k, l = indices(4)
a = sym(grad(v))[i,j]*C[i,j,k,l]*sym(grad(u))[k,l]*dx
```

Currently broken in FEniCS release

Weak Form Processing

```
from ffc.analysis import analyze_forms
from ffc.compiler import compute_ir

parameters = ffc.default_parameters()
parameters['representation'] = 'tensor'
analysis = analyze_forms([a,L], {}, parameters)
ir = compute_ir(analysis, parameters)

a_K = ir[2][0]['AK'][0][0]
a_G = ir[2][0]['AK'][0][1]

K = a_K.A0.astype(numpy.float32)
G = a_G
```

Big Picture

- Usability is paramount
  - Need community by-in
  - Need complete workflow
- Leverage existing systems
  - Adoption is much easier with the familiar
  - arXiv, package managers