

The Portable Extensible Toolkit for Scientific Computing

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Outline

- 1 What can PETSc do?
 - What is PETSc?
 - Who uses PETSc?
- 2 What's New in PETSc?
- 3 Conclusion

Outline

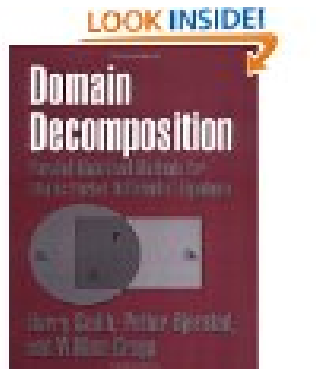
- 1 What can PETSc do?
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How did PETSc Originate?

PETSc was developed as a Platform for Experimentation

We want to experiment with different

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



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 XT5, BG/P, NVIDIA Tesla, Earth Simulator, Sun Blade
 - Loosely coupled systems, such as networks of workstations
 - IBM, Mac, Sun, 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, INL Reactor Program
 - National Science Foundation
 - CIG, CISE, Multidisciplinary Challenge Program

The PETSc Team



Bill Gropp



Barry Smith



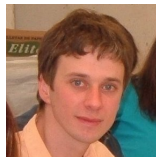
Satish Balay



Jed Brown



Matt Knepley



Lisandro Dalcin



Hong Zhang



Victor Eijkhout



Dmitry Karpeev

Outline

- 1 What can PETSc do?
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Who Uses PETSc?

- **Computational Scientists**
 - PyLith (CIG), Underworld (Monash), Magma Dynamics (LDEO, Columbia), PFLOTRAN (DOE)
- **Algorithm Developers**
 - Iterative methods and Preconditioning researchers
- **Package Developers**
 - SLEPc, TAO, DealII, PETSc-FEM, MagPar, PetFMM, PetRBF

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 **224,000** cores efficiently
 - UNIC on the IBM BG/P Intrepid at ANL
 - PFLOTRAN on the Cray XT5 Jaguar at ORNL
- PETSc applications have run at **22 Teraflops**
 - Kaushik on XT5
 - LANL PFLOTRAN code

What Can We Handle?

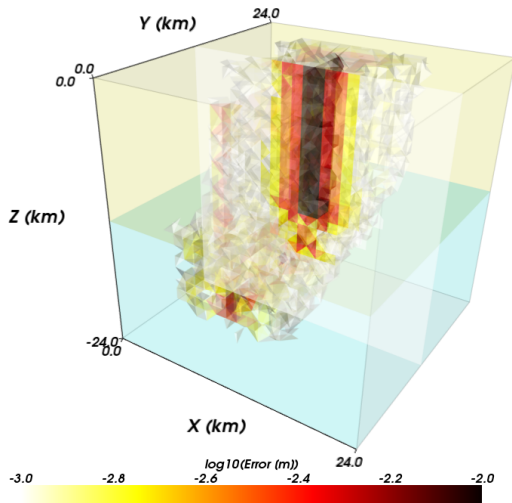
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PyLith

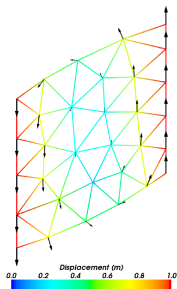
- Multiple problems
 - Dynamic rupture
 - Quasi-static relaxation
- Multiple models
 - Nonlinear visco-plastic
 - Finite deformation
 - Fault constitutive models
- Multiple meshes
 - 1D, 2D, 3D
 - Hex and tet meshes
- Parallel
 - PETSc solvers
 - Sieve mesh management



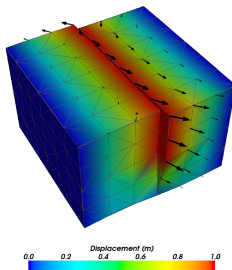
^aAagaard, Knepley, Williams

Multiple Mesh Types

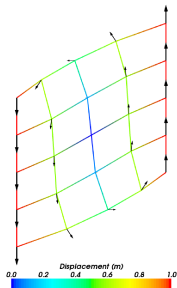
Triangular



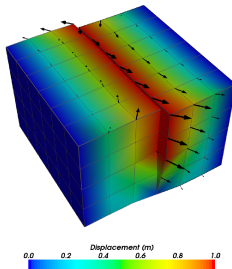
Tetrahedral



Rectangular

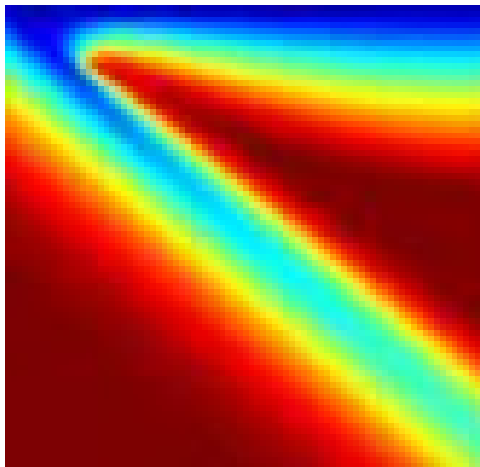


Hexahedral



Magma Dynamics

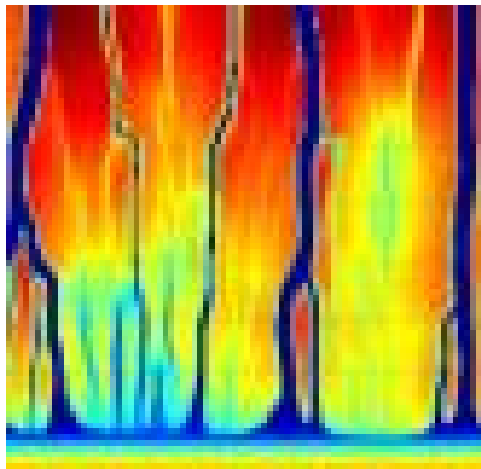
- Couples scales
 - Subduction
 - Magma Migration
- Physics
 - Incompressible fluid
 - Porous solid
 - Variable porosity
- Deforming matrix
 - Compaction pressure
- Code generation
 - FEniCS
- Multiphysics Preconditioning
 - PETSc FieldSplit



^aKatz, Spiegelman

Magma Dynamics

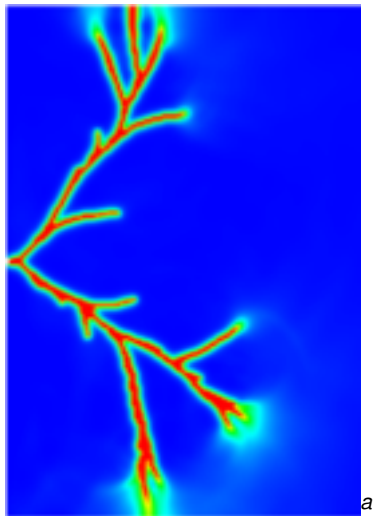
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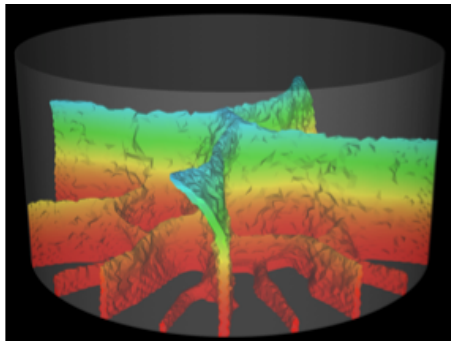
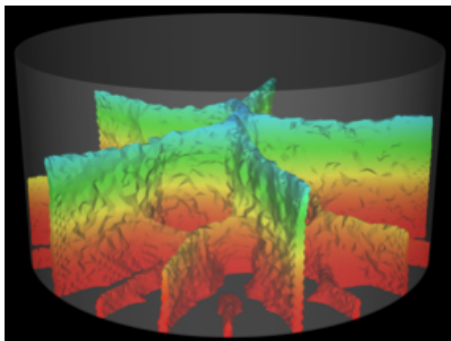
Fracture Mechanics

- Full variational formulation
 - Phase field
 - Linear or Quadratic penalty
- Uses TAO optimization
 - Necessary for linear penalty
 - Backtacking
- No prescribed cracks
 - Arbitrary crack geometry
 - Arbitrary intersections
- Multiple materials
 - Composite toughness



^aBourdin

Fracture Mechanics

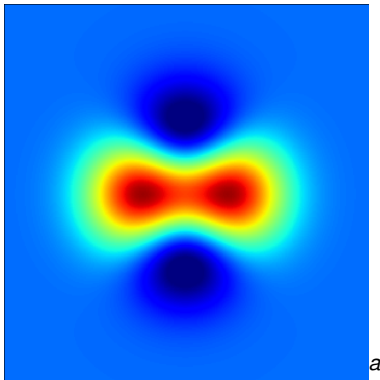


¹Bourdin

Vortex Method

$t = 000$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
 - Uses PETSc solvers
 - Scalable preconditioner
- Parallelism
 - MPI
 - GPU

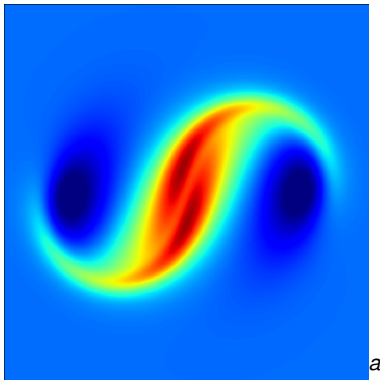


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 100$

- Incompressible Flow
 - Gaussian vortex blobs
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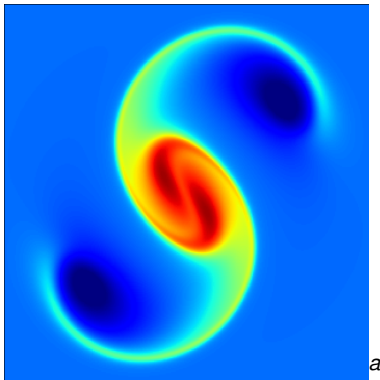


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 200$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
 - Uses PETSc solvers
 - Scalable preconditioner
- Parallelism
 - MPI
 - GPU

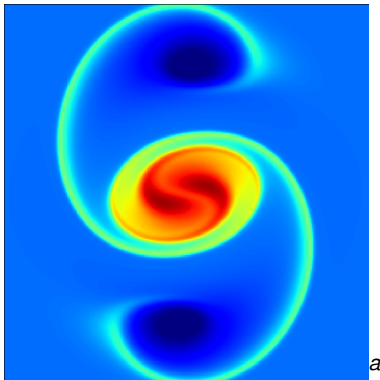


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 300$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
 - Uses PETSc solvers
 - Scalable preconditioner
- Parallelism
 - MPI
 - GPU

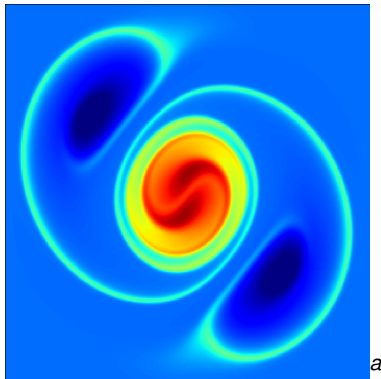


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 400$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
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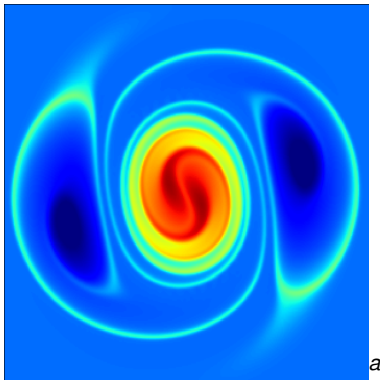


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 500$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
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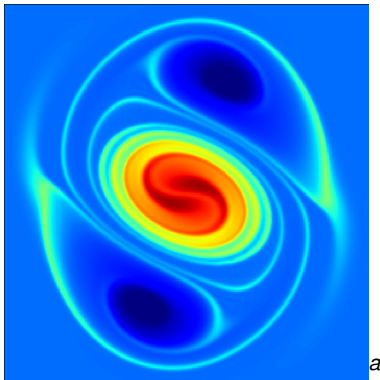


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 600$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
- PetRBF
 - Variety of RBFs
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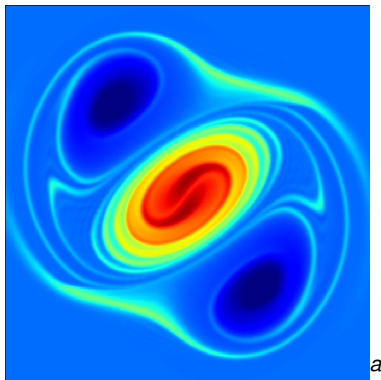


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 700$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
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 - Variety of RBFs
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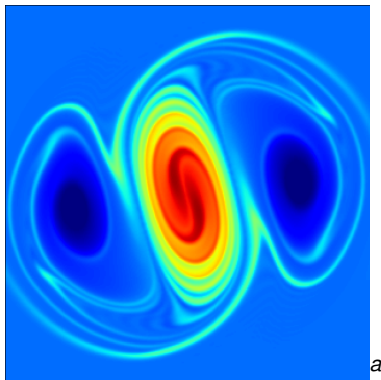


^aCruz, Yokota, Barba, Knepley

Vortex Method

$t = 800$

- Incompressible Flow
 - Gaussian vortex blobs
 - High Re
- PetFMM
 - 2D/3D domains
 - Automatic load balancing
 - Variety of kernels
 - Optimized with templates
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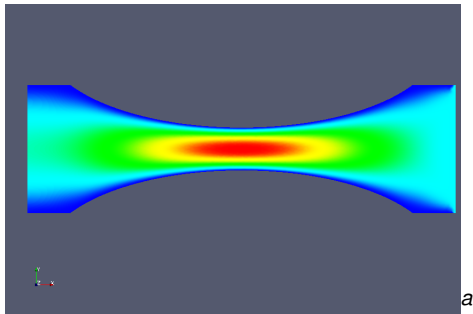


^aCruz, Yokota, Barba, Knepley

FEniCS-Apps

Rheagen

- Rheologies
 - Maxwell
 - Grade 2
 - Oldroyd-B
- Stabilization
 - DG
 - SUPG
 - EVSS
 - DEVSS
 - Macroelement
- Automation
 - FIAT (elements)
 - FFC (weak forms)

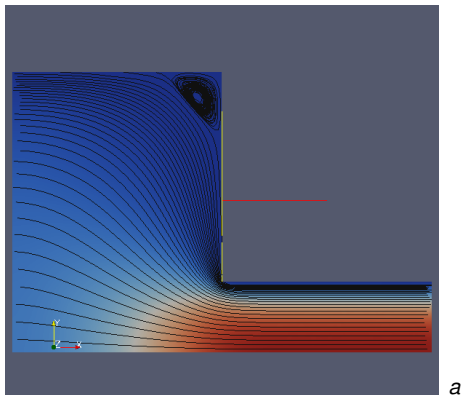


^aTerrel

FEniCS-Apps

Rheagen

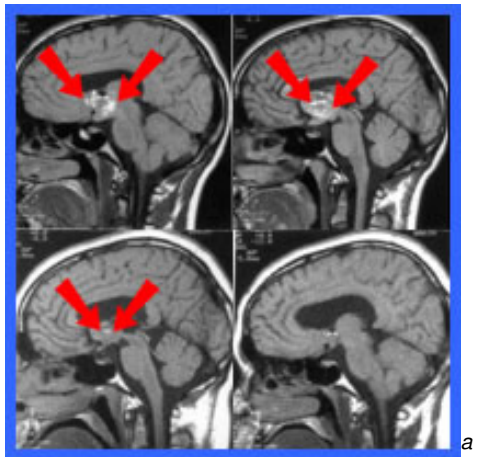
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^aTerrel

Real-time Surgery

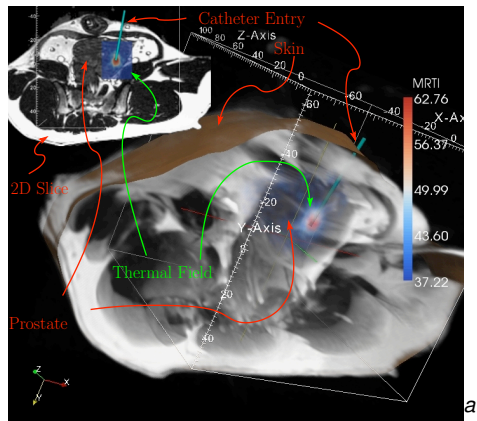
- Brain Surgery
 - Elastic deformation
 - Overlaid on MRI
 - Guides surgeon
- Laser Thermal Therapy
 - PDE constrained optimization
 - Per-patient calibration
 - Thermal inverse problem



^aWarfield, Ferrant, et.al.

Real-time Surgery

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^aFuentes, Oden, et.al.

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1 What can PETSc do?

2 What's New in PETSc?

- Python Bindings
- Physics-Based Preconditioning
- PETSc-GPU
- FEM

3 Conclusion

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2 What's New in PETSc?

- Python Bindings
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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

`petsc4py` 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

- Configure PETSc using `-download-petsc4py`
 - Can also use `-download-mpi4py`
- Downloaded to `externalpackages/petsc4py-version`
 - Demo code is here
- Installed into PETSc lib directory
- Add `$PETSC_DIR/$PETSC_ARCH/lib` to **PYTHONPATH**

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`

ex8.py

Setup

```
import sys, petsc4py
petsc4py.init(sys.argv)
from petsc4py import PETSc
import math

# Create the grid
da = PETSc.DA().create([-9], comm=PETSc.COMM_WORLD)
f = da.createGlobalVector()
x = f.duplicate()
J = da.getMatrix(PETSc.Mat.Type.AIJ);

# Create the solver
ts = PETSc.TS().create(PETSc.COMM_WORLD)
ts.setProblemType(PETSc.TS.ProblemType.NONLINEAR)
ts.setType(ts.Type.GL)

# Define the problem
ode = MyODE(da)
ts.setIFunction(ode.function, f)
ts.setIJacobian(ode.jacobian, J)
```

ex8.py

Residual

```
class MyODE:
    def function(self, ts, t, x, xdot, f):
        mx = da.getSizes()[0];          hx = 1.0/mx
        (xs, xm) = da.getCorners(); xs = xs[0]; xm = xm[0]
        xx      = da.createLocalVector()
        xxdot   = da.createLocalVector()
        da.globalToLocal(x, xx)
        da.globalToLocal(xdot, xxdot)
        dt = ts.getTimeStep()
        x0 = ts.getSolution()
        if xs == 0:      f[0]      = xx[0]/hx;          xs = 1;
        if xs+xm >= mx: f[mx-1] = xx[xm-(xs==1)]/hx;  xm = xm-(xs==1);
        for i in range(xs, xs+xm-1):
            f[i] = xxdot[i-xs+1]
                  + (2.0*xx[i-xs+1] - xx[i-xs] - xx[i-xs+2])/hx
                  - hx*math.exp(xx[i-xs+1])
        f.assemble()
```


ex8.py

Solving

```
ts.setTimeStep(0.1)
ts.setDuration(10, 1.0)
ts.setFromOptions()
x.set(1.0)
ts.solve(x)
```

Outline

2 What's New in PETSc?

- Python Bindings
- **Physics-Based Preconditioning**
- PETSc-GPU
- FEM

MultiPhysics Paradigm

The **PCFieldSplit** interface

- extracts functions/operators corresponding to each physics
 - **VecScatter** and `MatGetSubmatrices()` for efficiency
- assemble functions/operators over all physics
 - Generalizes `LocalToGlobal()` mapping
- is composable with **ANY** PETSc solver and preconditioner
 - This can be done recursively

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FieldSplit provides the **buildings blocks** for multiphysics preconditioning.

MultiPhysics Paradigm

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Notice that this works in exactly the same manner as

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

Preconditioning

Several varieties of preconditioners can be supported:

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

which only require actions of individual operator blocks

Notice also that we may have any combination of

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

since we have access to an algebraic interface

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit  
-pc_field_split_type  
-fieldsplit_0_pc_type ml  
-fieldsplit_0_ksp_type preonly
```

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit  
-pc_field_split_type additive  
-fieldsplit_0_pc_type ml  
-fieldsplit_0_ksp_type preonly  
-fieldsplit_1_pc_type jacobi  
-fieldsplit_1_ksp_type preonly
```

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & I \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit  
-pc_field_split_type multiplicative  
-fieldsplit_0_pc_type ml  
-fieldsplit_0_ksp_type preonly  
-fieldsplit_1_pc_type jacobi  
-fieldsplit_1_ksp_type preonly
```

$$\begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
-pc_fieldsplit_schur_factorization_type diag
```

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & -\hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit  
-pc_field_split_type schur  
-fieldsplit_0_pc_type ml  
-fieldsplit_0_ksp_type preonly  
-fieldsplit_1_pc_type none  
-fieldsplit_1_ksp_type minres  
-pc_fieldsplit_schur_factorization_type lower
```

$$\begin{pmatrix} \hat{A} & 0 \\ B^T & \hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit  
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-fieldsplit_0_ksp_type preonly  
-fieldsplit_1_pc_type none  
-fieldsplit_1_ksp_type minres  
-pc_fieldsplit_schur_factorization_type upper
```

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S} \end{pmatrix}$$

Stokes Example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-pc_fieldsplit_schur_factorization_type full
```

$$\begin{pmatrix} I & 0 \\ B^T A^{-1} & I \end{pmatrix} \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix} \begin{pmatrix} I & A^{-1} B \\ 0 & I \end{pmatrix}$$

Outline

- 2 What's New in PETSc?
 - Python Bindings
 - Physics-Based Preconditioning
 - **PETSc-GPU**
 - FEM

Thrust

Thrust is a CUDA library of parallel algorithms

- Interface similar to C++ Standard Template Library
- Containers (`vector`, `list`, `map`) on both host and device
- Algorithms: `sort`, `reduce`, `scan`
- Freely available, and part of PETSc configure
(`-with-thrust-dir`)

Cusp

Cusp is a CUDA library for sparse linear algebra and graph computations

- Builds on data structures in Thrust
- Provides sparse matrices in several formats (CSR, Hybrid)
- Includes some preliminary preconditioners (Jacobi, SA-AMG)
- Freely available, and part of PETSc configure (`-with-cusp-dir`)

VECCUDA

Strategy: Define a new **Vec** implementation

- Uses Thrust for data storage and operations on GPU
- Supports full PETSc **Vec** interface
- Inherits PETSc scalar type
- Can be activated at runtime, `-vec_type cuda`
- PETSc provides memory coherence mechanism

Memory Coherence

PETSc Objects now hold a coherence flag

PETSC_CUDA_UNALLOCATED	No allocation on the GPU
PETSC_CUDA_GPU	Values on GPU are current
PETSC_CUDA_CPU	Values on CPU are current
PETSC_CUDA_BOTH	Values on both are current

Table: Flags used to indicate the memory state of a PETSc CUDA **Vec** object.

MATAIJCUDA

Also define new **Mat** implementations

- Uses Cusp for data storage and operations on GPU
- Supports full PETSc **Mat** interface, some ops on CPU
- Can be activated at runtime, `-mat_type aijcuda`
- Notice that parallel matvec necessitates off-GPU data transfer

Solvers

Solvers come for **Free**

- All linear algebra types work with solvers
- Entire solve can take place on the GPU
 - Only communicate scalars back to CPU
- GPU communication cost could be amortized over several solves
- Preconditioners are a problem
 - Cusp has a promising AMG

Installation

PETSc only needs

```
# Turn on CUDA
--with-cuda
# Specify the CUDA compiler
--with-cudac='nvcc -m64'
# Indicate the location of packages
# --download-* will also work
--with-thrust-dir=/PETSc3/multicore/thrust
--with-cusp-dir=/PETSc3/multicore/cusp
# Can also use double precision
--with-precision=single
```

Example

Driven Cavity Velocity-Vorticity with Multigrid

```
ex19 -da_vec_type seqcuda
      -da_mat_type aijcuda -mat_no_inode # Setup types
      -da_grid_x 100 -da_grid_y 100     # Set grid size
      -pc_type none -dmmg_nlevels 1     # Setup solver
      -preload off -cuda_synchronize   # Setup run
      -log_summary
```

Outline

2 What's New in PETSc?

- Python Bindings
- Physics-Based Preconditioning
- PETSc-GPU
- **FEM**

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)

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Generic FEM

Can formulate assembly independent of

- spatial dimension
- element shape
- finite element (discretization)
- weak form (using FEniCS)

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
    /* Compute cell geometry */
    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Linear term */
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
        }
    }
    /* Update output vector*/
}
/* Aggregate updates */
```

Integration

```

cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
    coords = mesh->restrict(coordinates, c);
    v0, J, invJ, detJ = computeGeometry(coords);
    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
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```


Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
    /* Compute cell geometry */
    inputVec = mesh->restrict(U, c);
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Linear term */
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
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```

Integration

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for(c = cells->begin(); c != cells->end(); ++c) {
    /* Compute cell geometry */
    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        realCoords = J*refCoords[q] + v0;
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Linear term */
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
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    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            elemVec[f] += basis[q,f]*rhsFunc(realCoords);
            /* Linear term */
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
        }
    }
    /* Update output vector*/
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    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Transform J */
            for(d = 0; d < dim; ++d)
                for(e = 0; e < dim; ++e)
                    tDerReal[d] += invJ[e,d]*basisDer[q,f,e];
            for(g = 0; g < numBasisFuncs; ++g) {
                for(d = 0; d < dim; ++d)
                    for(e = 0; e < dim; ++e)
                        bDerReal[d] += invJ[e,d]*basisDer[q,g,e];
            }
        }
    }
}

```

Integration

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    /* Retrieve values from input vector */
    for(q = 0; q < numQuadPoints; ++q) {
        /* Transform coordinates */
        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Transform J */
            for(g = 0; g < numBasisFuncs; ++g) {
                for(d = 0; d < dim; ++d)
                    elemMat[f,g] += tDerReal[d]*bDerReal[d];
                elemVec[f] += elemMat[f,g]*inputVec[g];
            }
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
```


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        for(f = 0; f < numBasisFuncs; ++f) {
            /* Constant term */
            /* Linear term */
            elemVec[f] += basis[q,f]*lambda*exp(inputVec[f])
            elemVec[f] *= weight[q]*detJ;
        }
    }
    /* Update output vector*/
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/* Aggregate updates */
```

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            /* Constant term */
            /* Linear term */
            /* Nonlinear term */
            elemVec[f] *= weight[q]*detJ;
        }
    }
    mesh->updateAdd(F, c, elemVec);
}
/* Aggregate updates */
```

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        }
    }
    /* Update output vector*/
}
Distribution<Mesh>::completeSection(mesh, F);
```

GPU

Preliminary system for FEM integration on a GPU

- High order is basically done by others
- Low order much more prevalent in applications
- Use PyCUDA and Mako to generate kernels
- Nearly 100GF on a GTX 285

Outline

- 1 What can PETSc do?
- 2 What's New in PETSc?
- 3 Conclusion**

Why is PETSc cool?

PETSc gives you tools
to design and build
new Scientific Software
from simple pieces

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