# The Portable Extensible Toolkit for Scientific Computing

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University of Chicago

39th SPEEDUP Workshop on High-Performance Computing
ETH Zurich
Switzerland, September 6–7, 2010


# Outline

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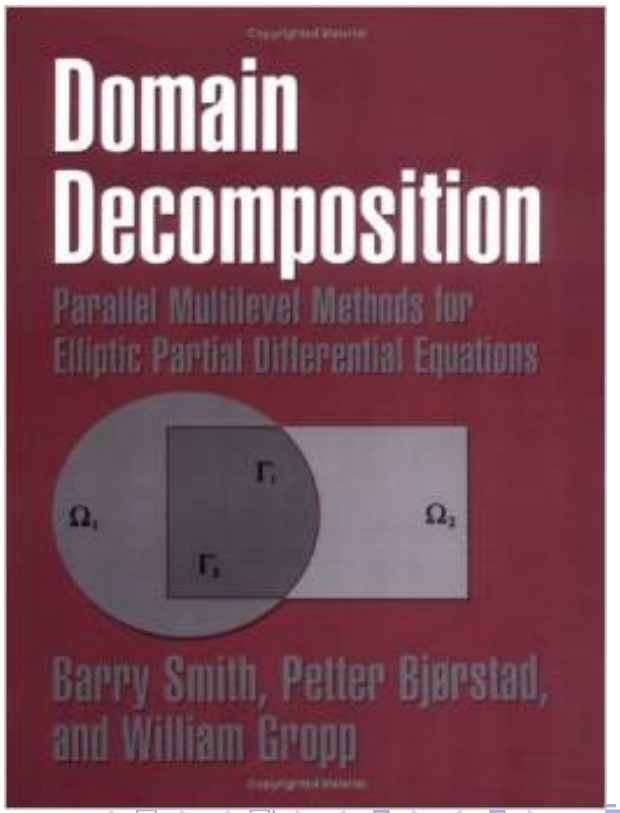
# How did PETSc Originate?

PETSc was developed as a Platform for Experimentation

We want to experiment with different

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



# 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

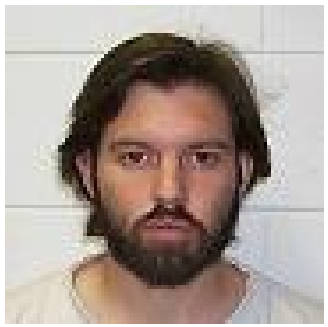
# The PETSc Team


Bill Gropp


Barry Smith


Satish Balay


Jed Brown


Matt Knepley


Lisandro Dalcin


Hong Zhang


Mark Adams


Toby Issac

# Outline

# Who Uses PETSc?

## Computational Scientists

- Earth Science
  - PyLith (CIG)
  - Underworld (Monash)
  - Magma Dynamics (LDEO, Columbia, Oxford)
- Subsurface Flow and Porous Media
  - STOMP (DOE)
  - PFLOTRAN (DOE)

# Who Uses PETSc?

## Computational Scientists

- CFD
  - Firedrake
  - Fluidity
  - OpenFOAM
  - freeCFD
  - OpenFVM
- MicroMagnetics
  - MagPar
- Fusion
  - XGC
  - BOUT++
  - NIMROD

# Who Uses PETSc?

## Algorithm Developers

- Iterative methods
  - Deflated GMRES
  - LGMRES
  - QCG
  - SpecEst
- Preconditioning researchers
  - Prometheus (Adams)
  - ParPre (Eijkhout)
  - FETI-DP (Klawonn and Rheinbach)

# Who Uses PETSc?

## Algorithm Developers

- Finite Elements
  - libMesh
  - MOOSE
  - PETSc-FEM
  - Deal II
  - OOFEM
- Other Solvers
  - Fast Multipole Method (PetFMM)
  - Radial Basis Function Interpolation (PetRBF)
  - Eigensolvers (SLEPc)
  - Optimization (TAO)

# 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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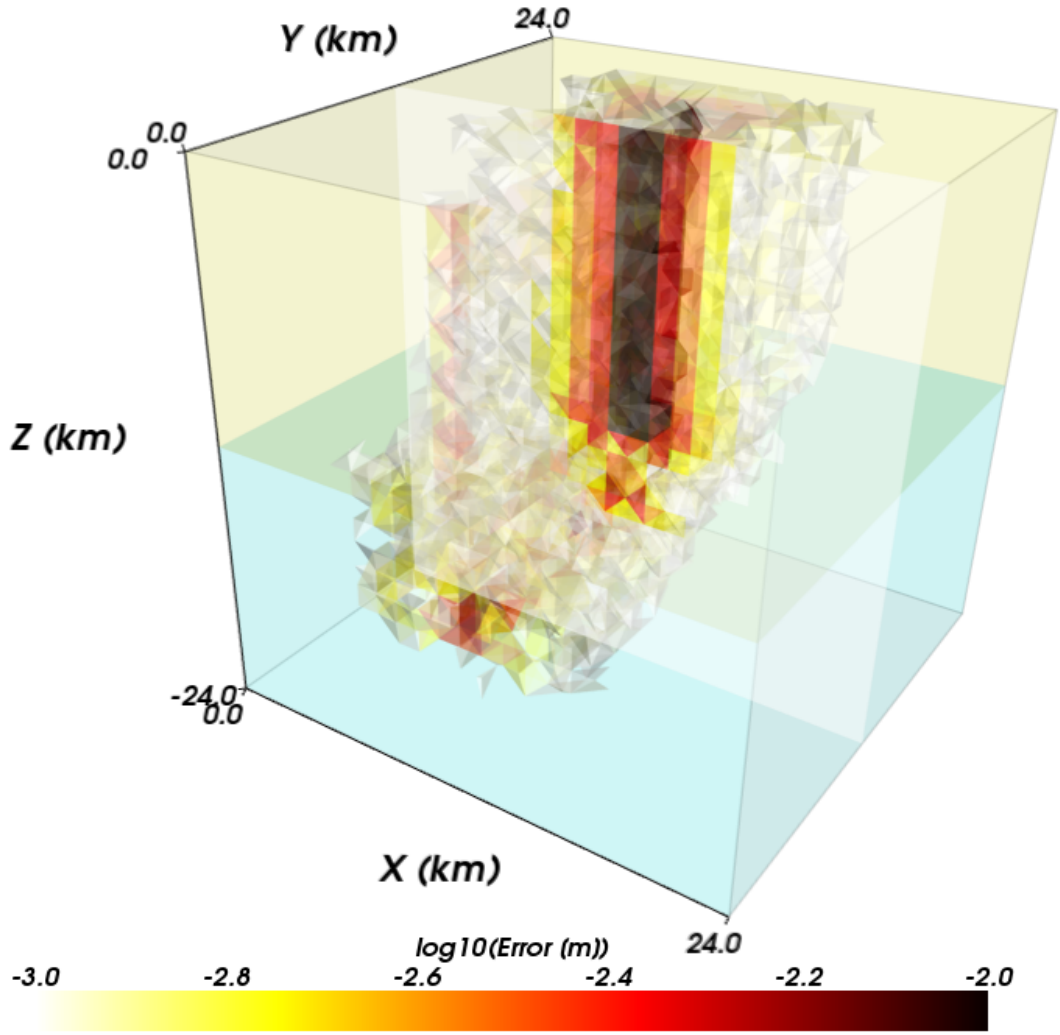
# PyLith

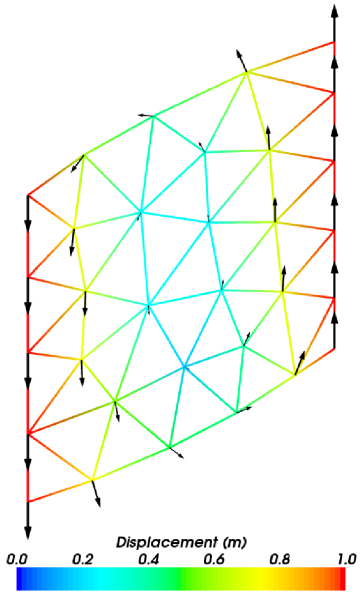
- Multiple problems
  - Dynamic rupture
  - Quasi-static relaxation
- Multiple models
  - Nonlinear visco-plastic
  - Finite deformation
  - Fault constitutive models
- Multiple meshes
  - 1D, 2D, 3D
  - Hex and tet meshes
- Parallel
  - PETSc solvers
  - DMPlex mesh management

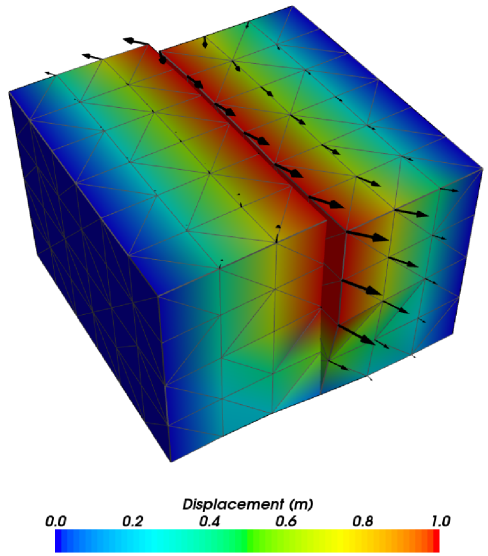



[a] Aagaard, Knepley, Williams

# Multiple Mesh Types

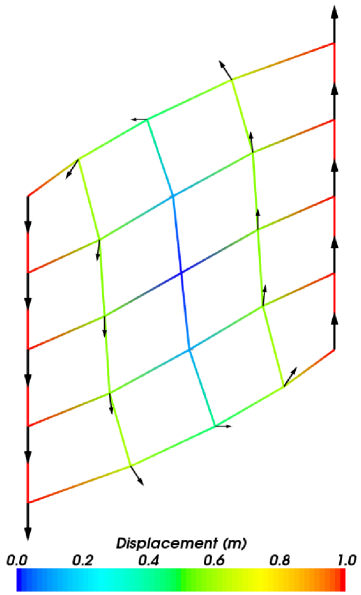
Triangular

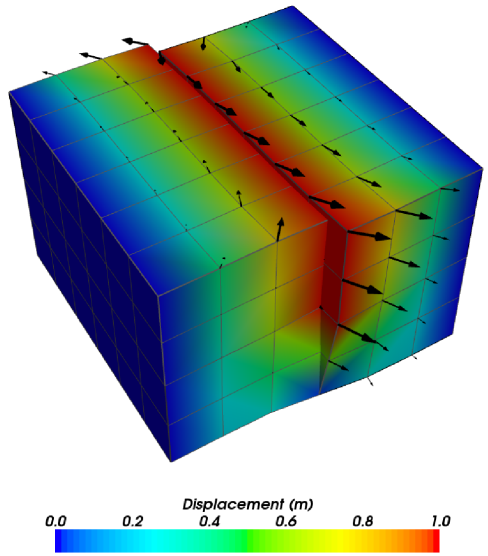



Tetrahedral

Rectangular

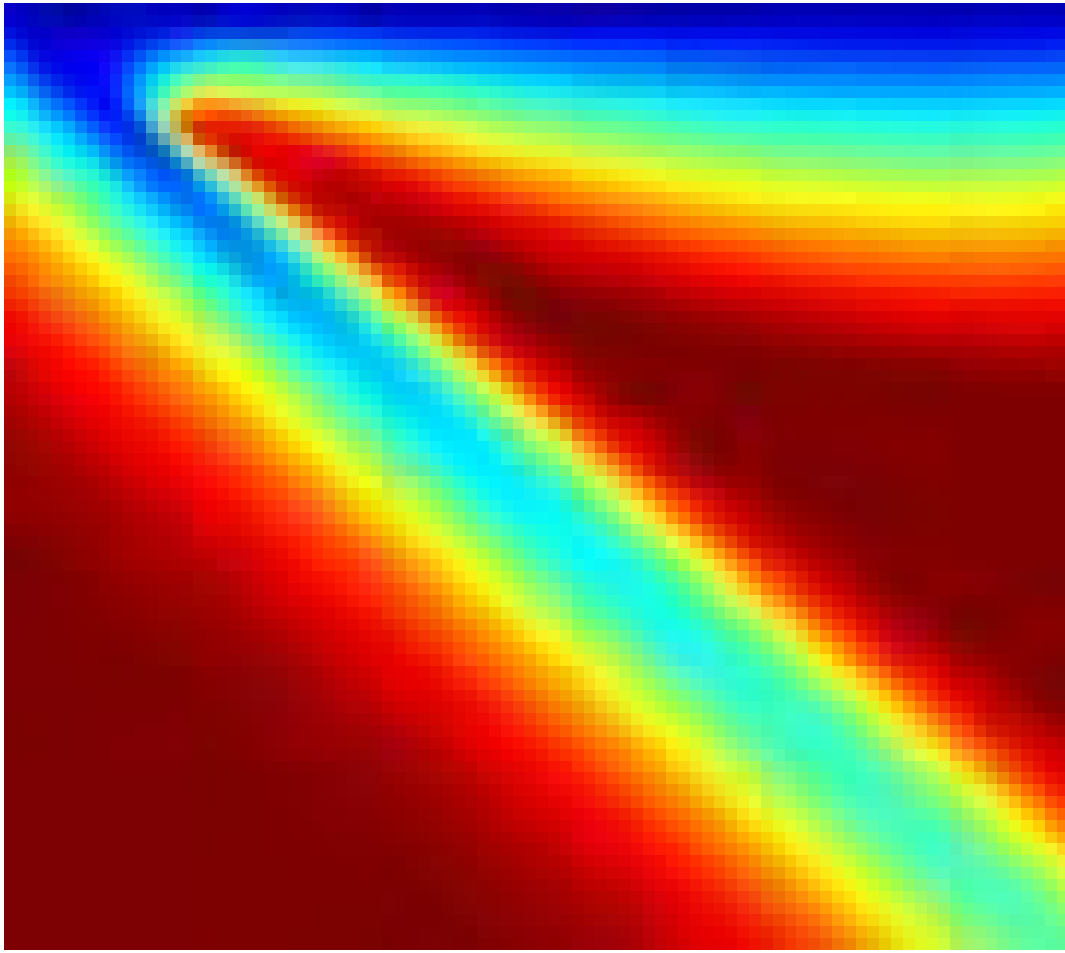



Hexahedral

# 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



[a] Katz, Speigelman

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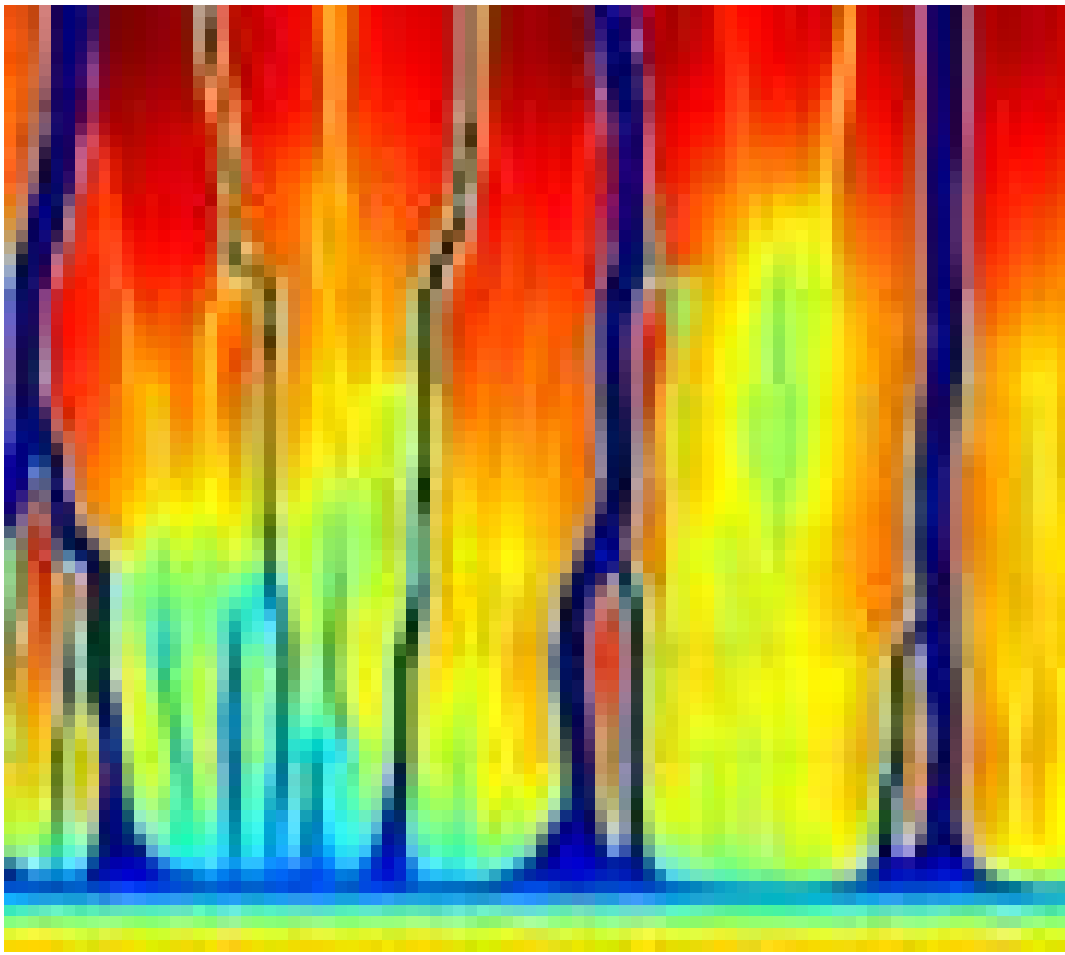
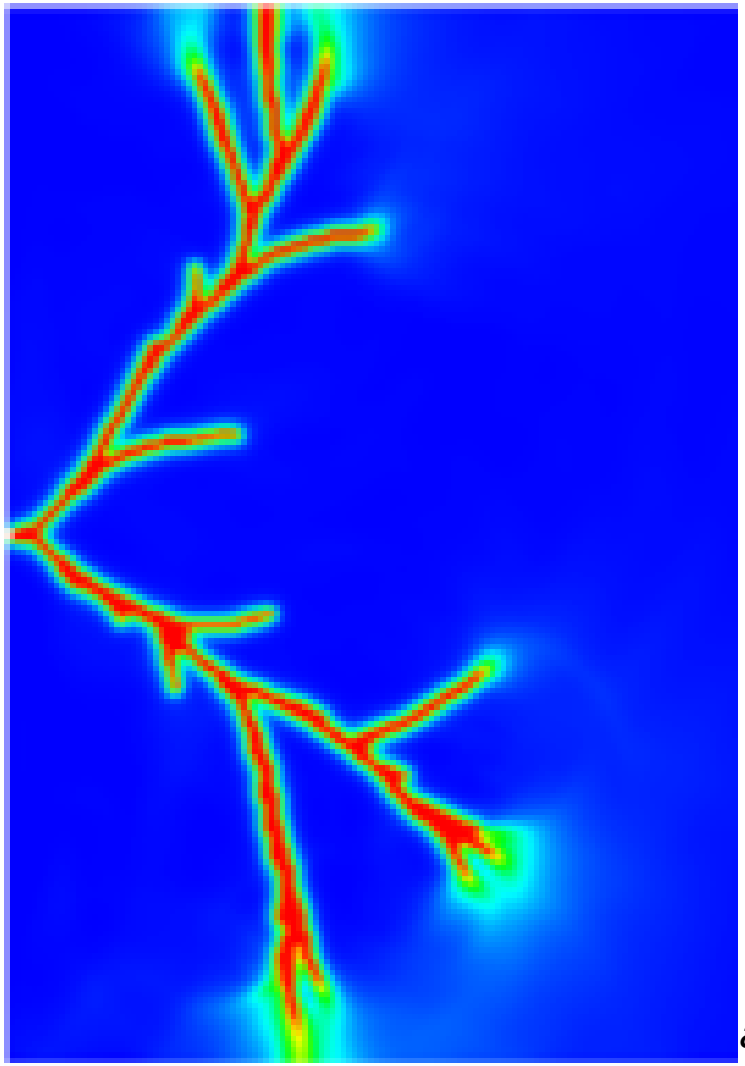


[a]Katz, Speigelman

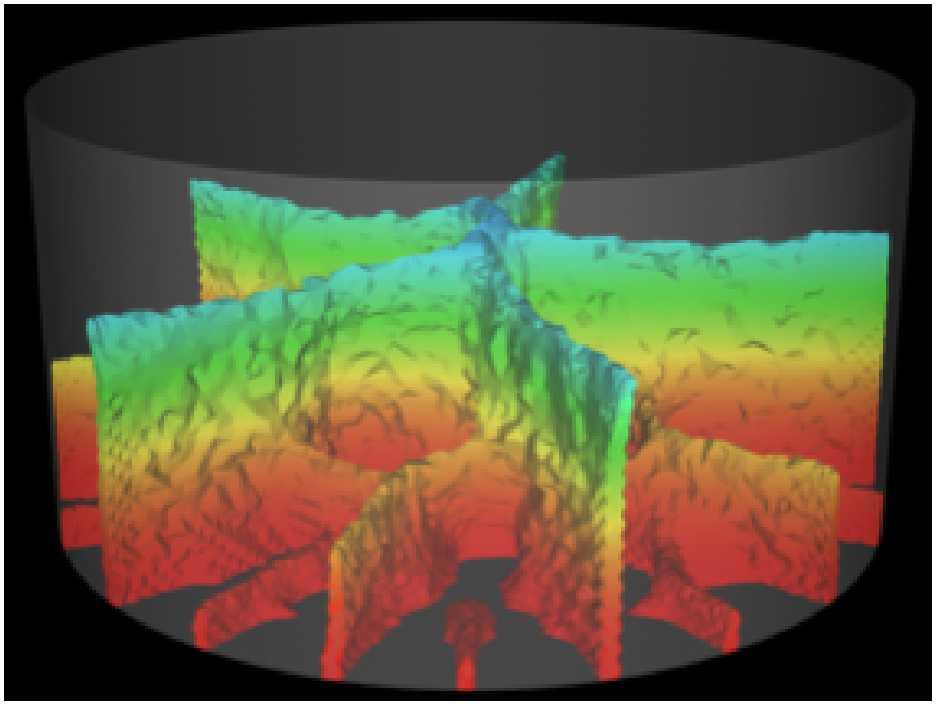
# Fracture Mechanics

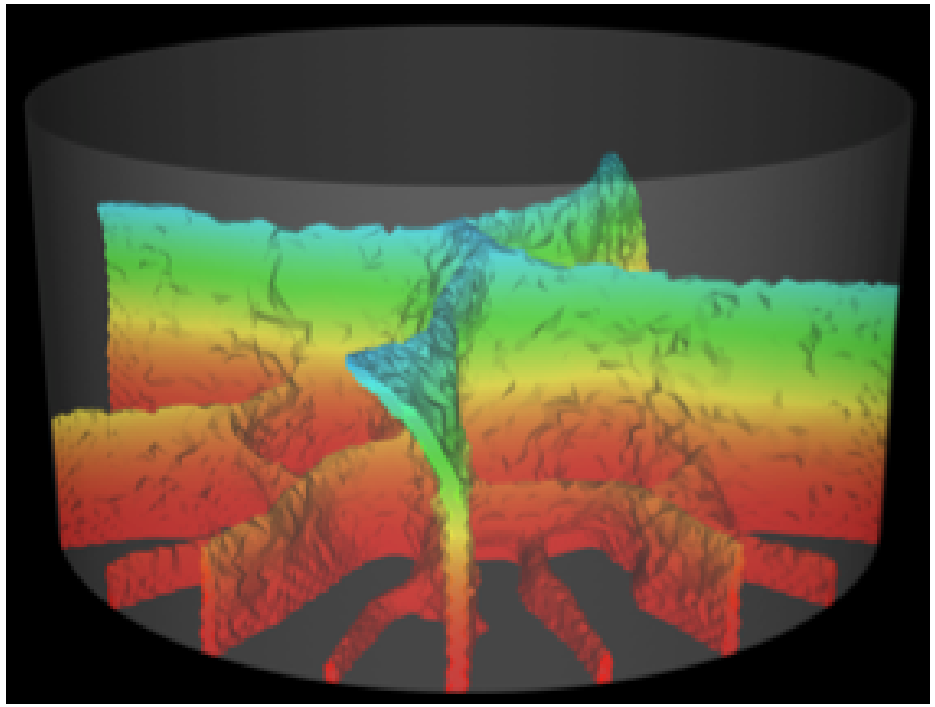
- Full variational formulation
  - Phase field
  - Linear or Quadratic penalty
- Uses TAO optimization
  - Necessary for linear penalty
  - Backtacking
- No prescribed cracks (movie)
  - Arbitrary crack geometry
  - Arbitrary intersections
- Multiple materials
  - Composite toughness



[a]Bourdin

# Fracture Mechanics



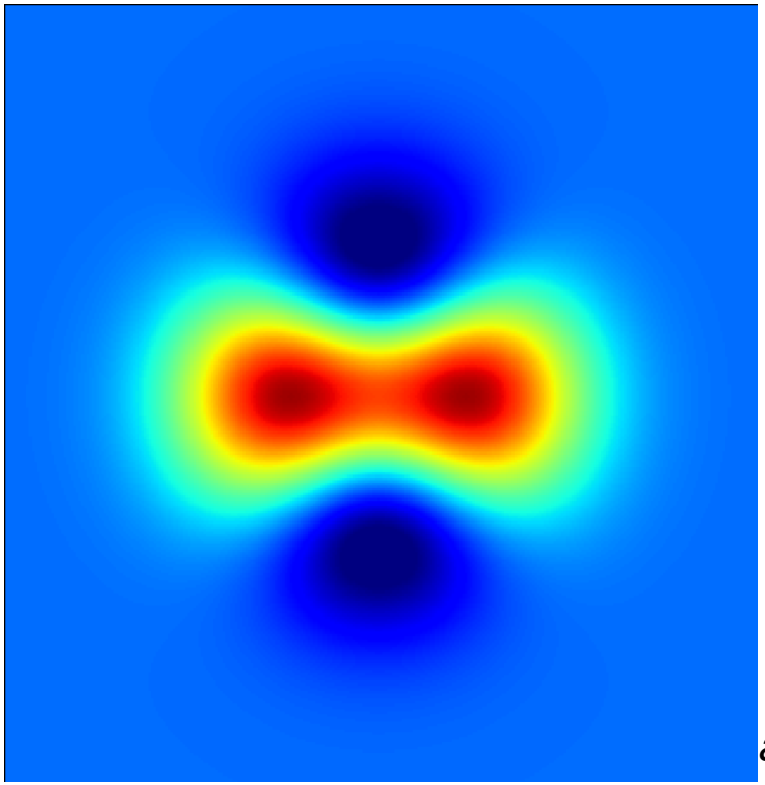


[1]

[1] Bourdin

# 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

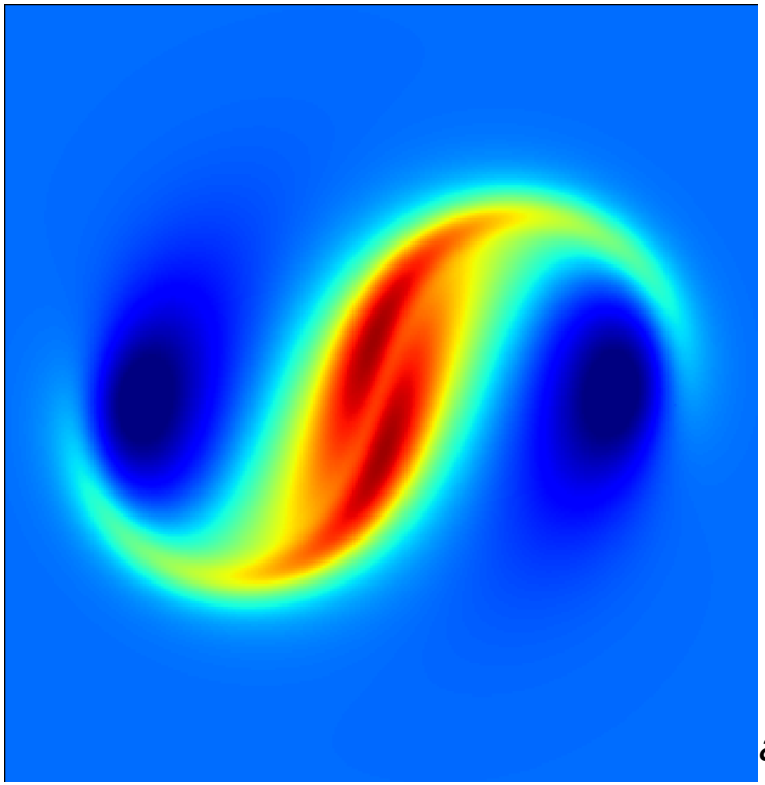


[a]Cruz, Yokota, Barba, Knepley

# Vortex Method

t = 100

- 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



[a]Cruz, 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
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  - Uses PETSc solvers
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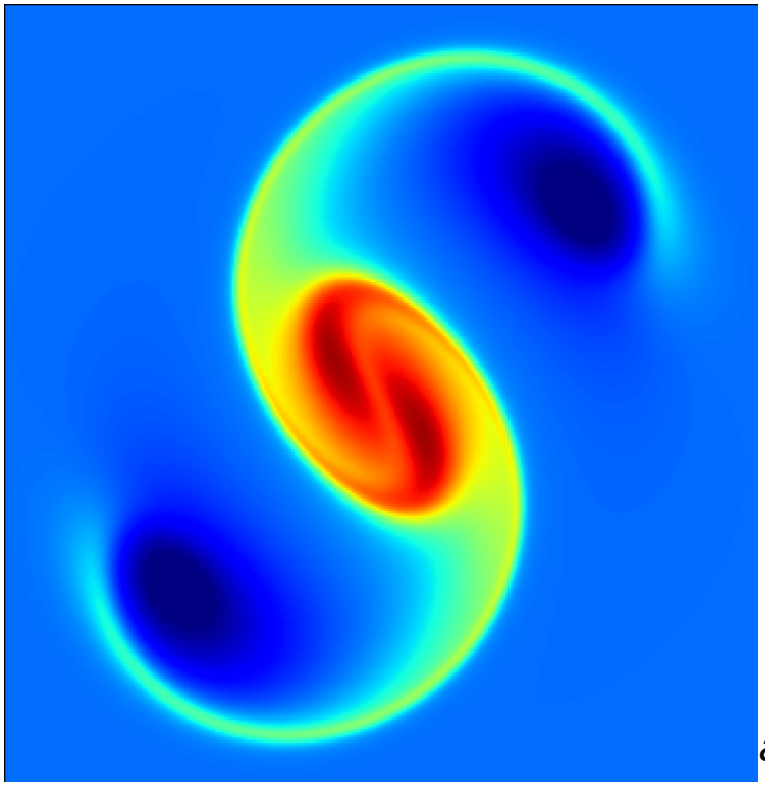
- Parallelism
  - MPI
  - GPU



[a]Cruz, 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
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  - Uses PETSc solvers
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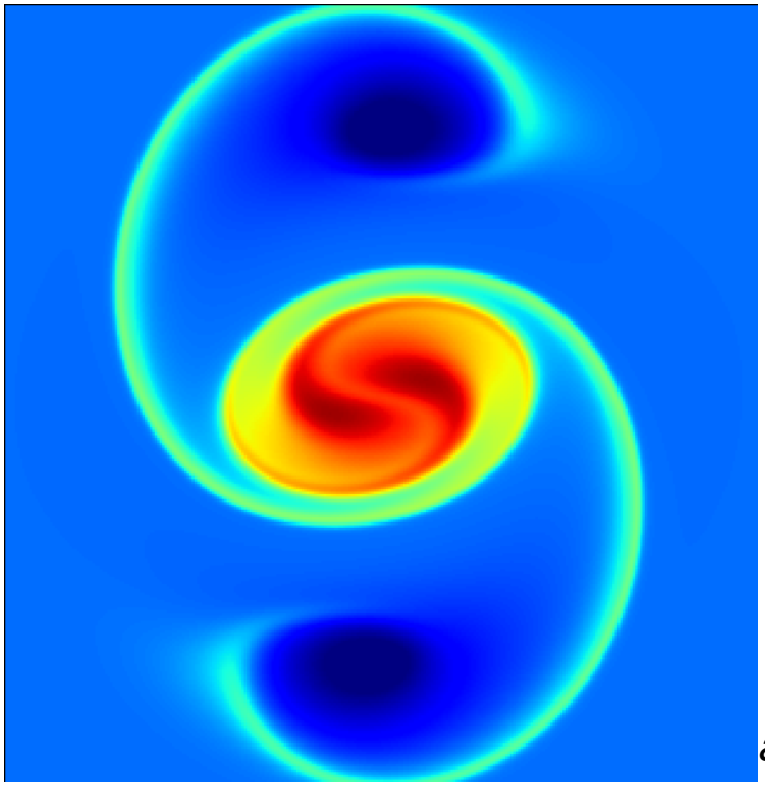
- Parallelism
  - MPI
  - GPU

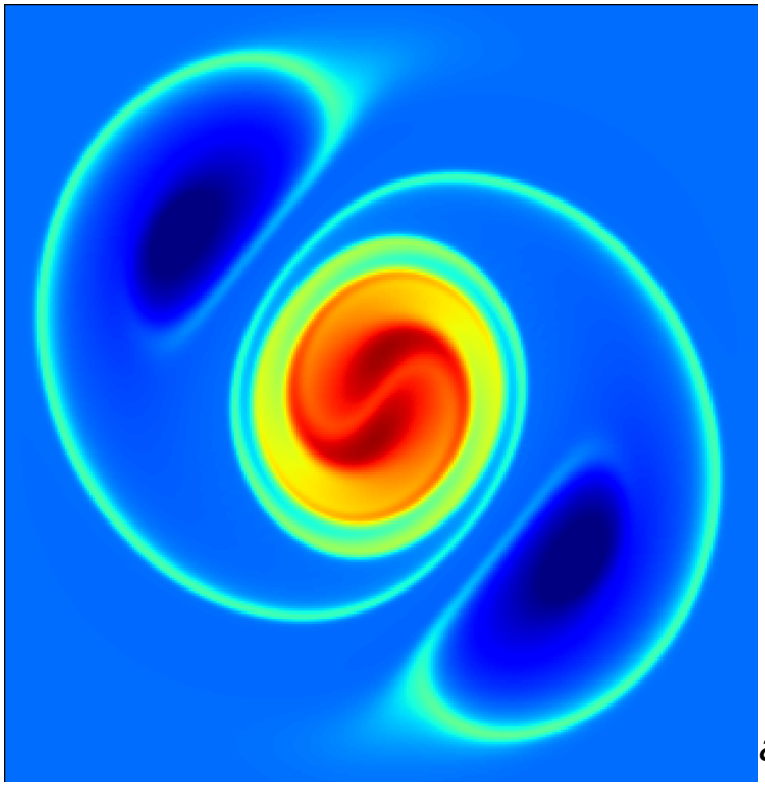


[a]Cruz, Yokota, Barba, Knepley

# 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
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU

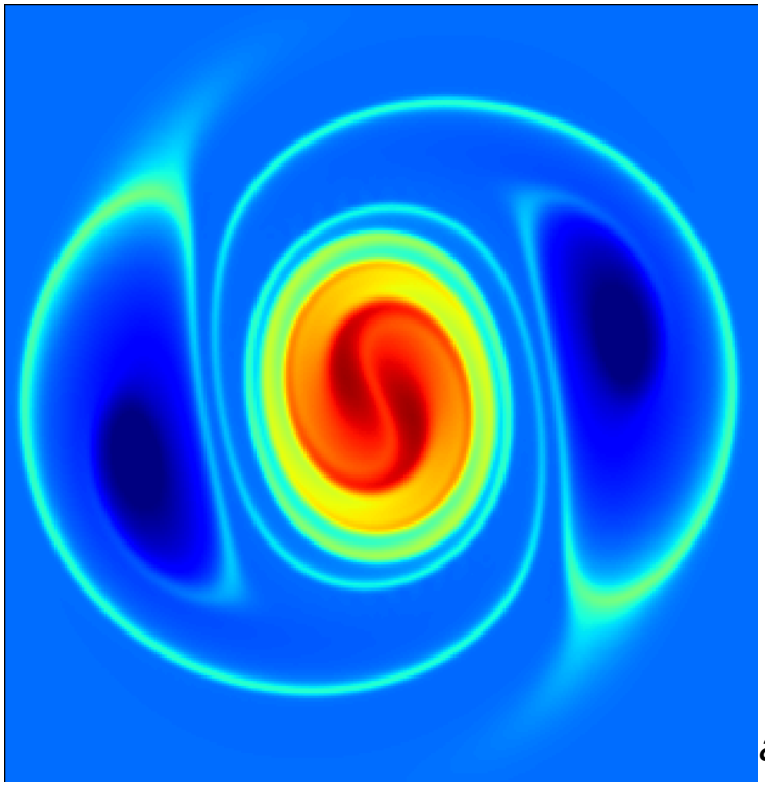


[a]Cruz, Yokota, Barba, Knepley

# 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
  - Uses PETSc solvers
  - Scalable preconditioner
- Parallelism
  - MPI
  - GPU



[a]Cruz, Yokota, Barba, Knepley

# Vortex Method

t = 600

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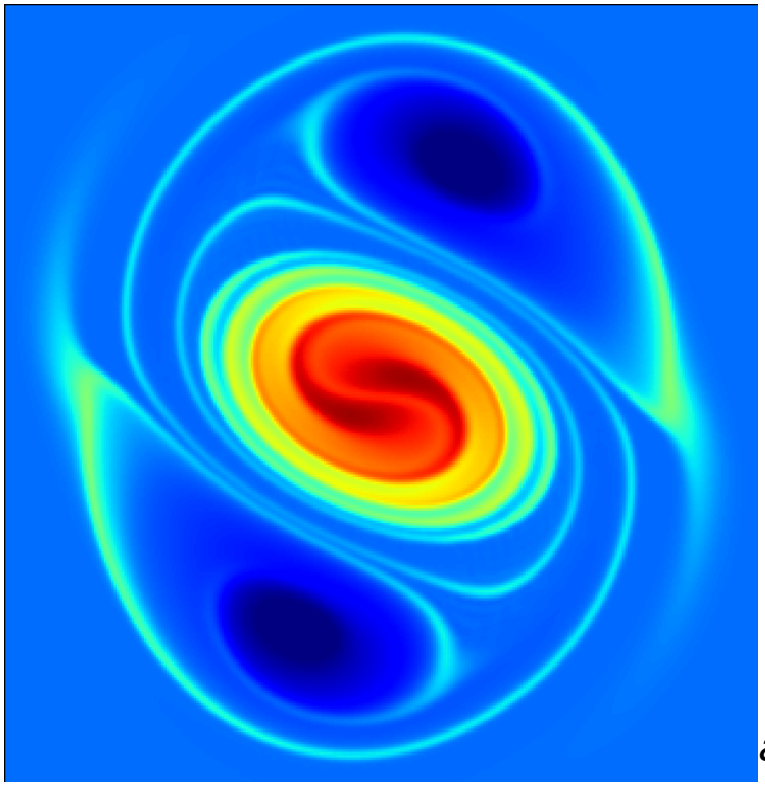

[a]Cruz, Yokota, Barba, Knepley

# Vortex Method

t = 700

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
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  - Variety of kernels
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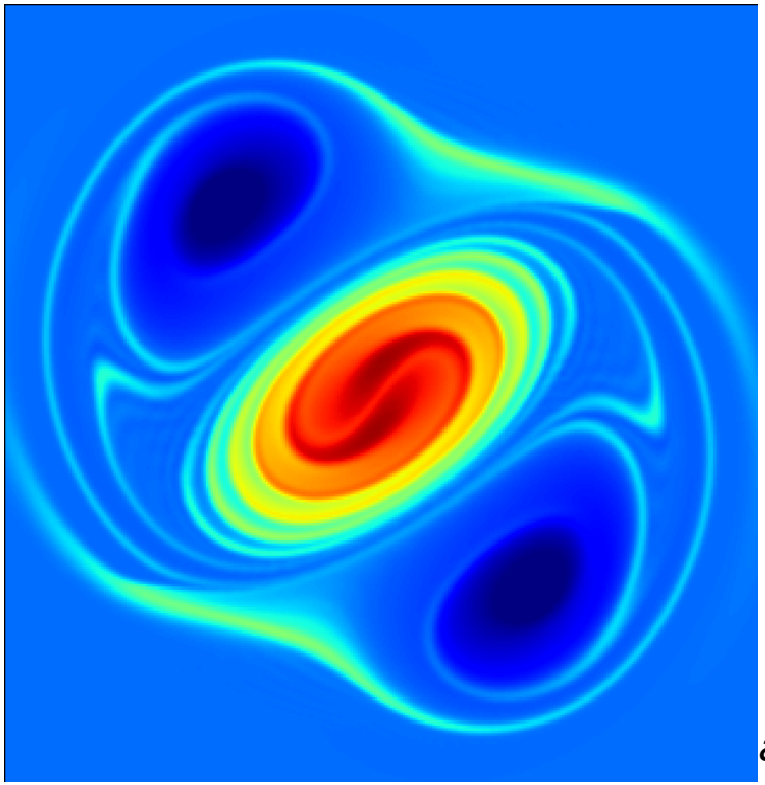

[a]Cruz, Yokota, Barba, Knepley

# Vortex Method
t = 800

- Incompressible Flow
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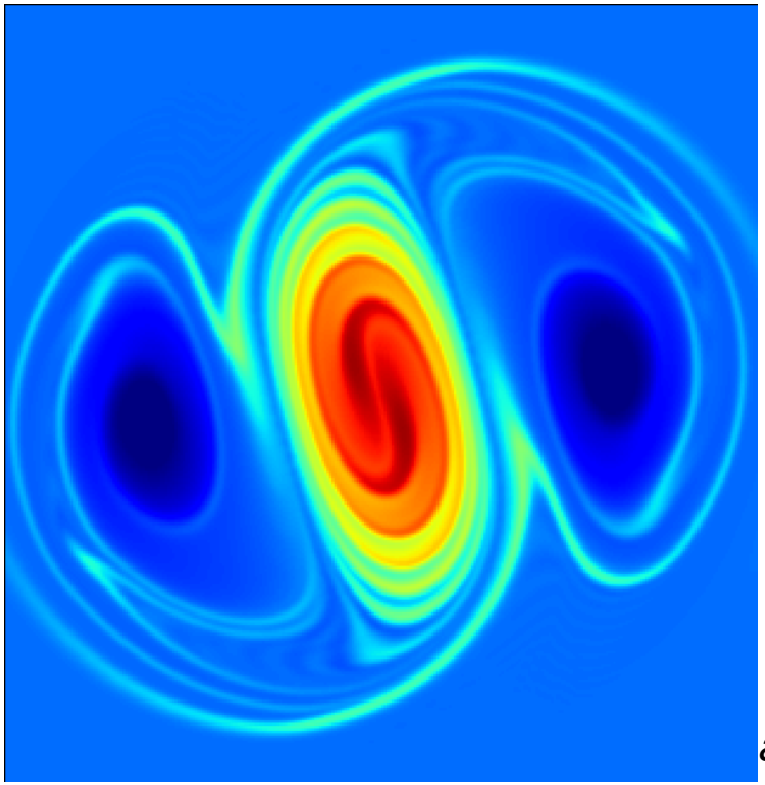
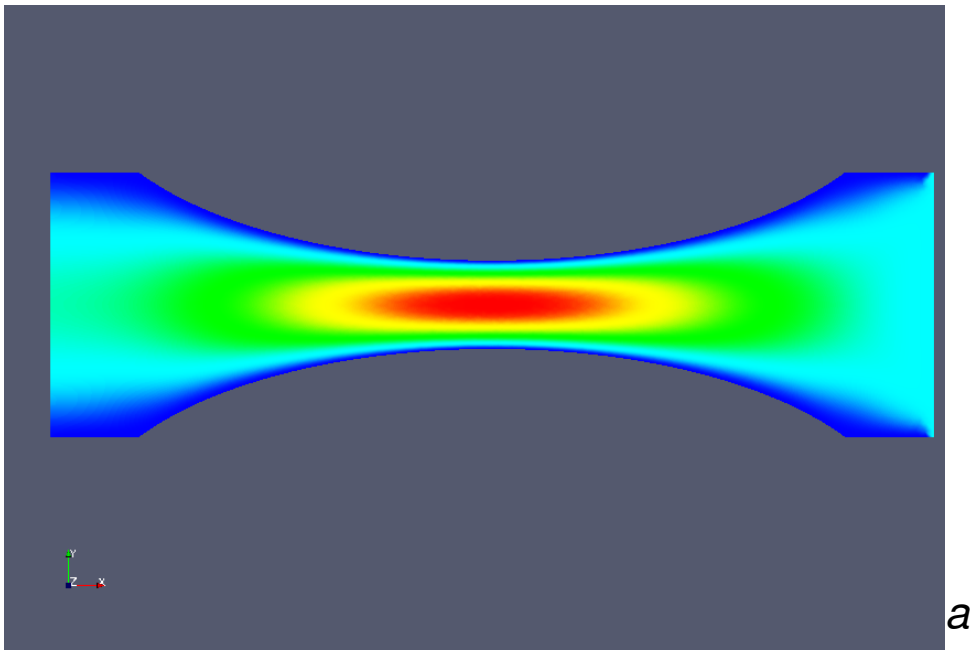


[a]Cruz, Yokota, Barba, Knepley

# FEniCS-Apps
## Rheagen

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



*a*

[a] Terrel

# FEniCS-Apps
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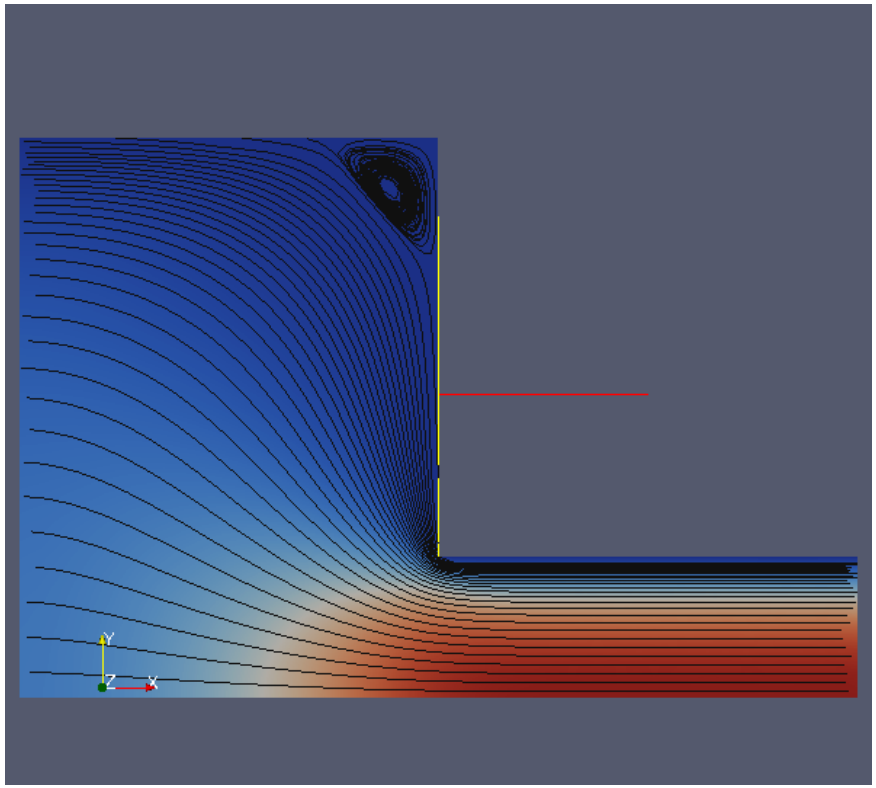
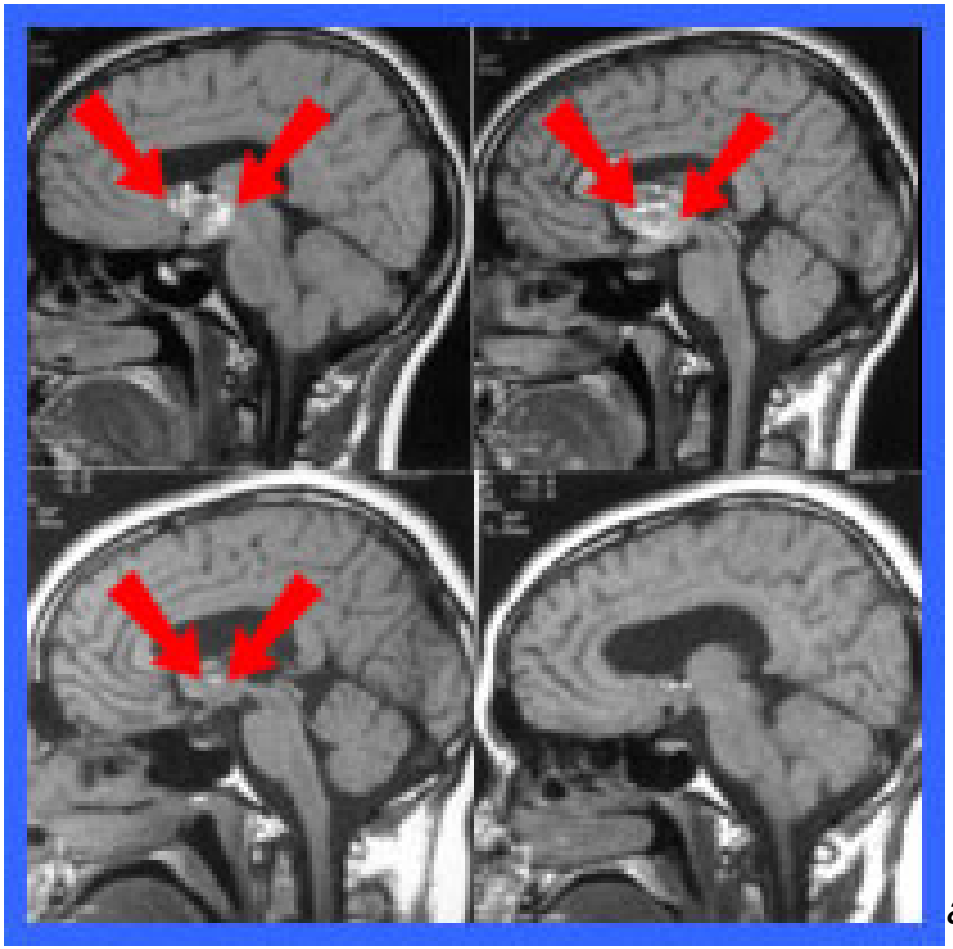


# Real-time Surgery

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



[a]

[a] Warfield, Ferrant, et.al.

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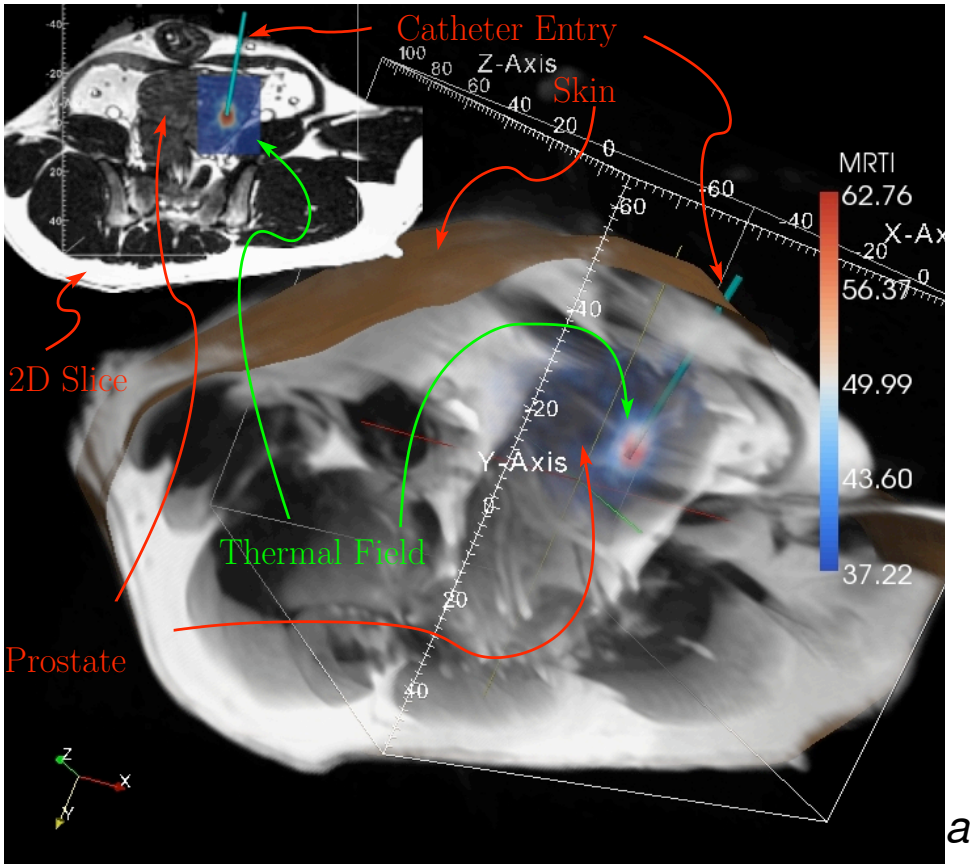


[a]

[a] Fuentes, Oden, et.al.

# 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

# 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`

# 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

# MultiPhysics Paradigm

## The **PCFieldSplit** interface

- extracts functions/operators corresponding to each physics
  - **VecScatter** and `MatGetSubMatrix()` 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.

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  - Generalizes `LocalToGlobal()` mapping
- is composable with ANY PETSc solver and preconditioner
  - This can be done recursively

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

# Solver Configuration: No New Code

ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Block-Jacobi (Exact)

```
-ksp_type gmres -pc_type fieldsplit -pc_fieldsplit_type additive
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Block-Jacobi (Inexact)

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type additive
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Gauss-Seidel (Inexact)

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type multiplicative
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Gauss-Seidel (Inexact)

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type multiplicative
 -pc_fieldsplit_0_fields 1 -pc_fieldsplit_1_fields 0
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Diagonal Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type diag
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type none
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Lower Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type lower
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type none
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Upper Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type upper
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type gamg
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type none
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Uzawa

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type upper
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
 -fieldsplit_pressure_ksp_type richardson
 -fieldsplit_pressure_ksp_max_its 1
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Full Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
 -fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### SIMPLE

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type lu
 -fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi
 -fieldsplit_pressure_inner_ksp_type preonly
  -fieldsplit_pressure_inner_pc_type jacobi
 -fieldsplit_pressure_upper_ksp_type preonly
  -fieldsplit_pressure_upper_pc_type jacobi
```

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

# Solver Configuration: No New Code

## ex62: $P_2/P_1$ Stokes Problem on Unstructured Mesh

### Least-Squares Commutator

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
-pc_fieldsplit_schur_precondition self
 -fieldsplit_velocity_ksp_type gmres -fieldsplit_velocity_pc_type lu
 -fieldsplit_pressure_ksp_rtol 1e-5 -fieldsplit_pressure_pc_type lsc
```

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

# Solver Configuration: No New Code

## ex31: $P_2/P_1$ Stokes Problem with Temperature on Unstructured Mesh

### Additive Schwarz + Full Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type additive
-pc_fieldsplit_0_fields 0,1 -pc_fieldsplit_1_fields 2
 -fieldsplit_0_ksp_type fgmres -fieldsplit_0_pc_type fieldsplit
 -fieldsplit_0_pc_fieldsplit_type schur
 -fieldsplit_0_pc_fieldsplit_schur_factorization_type full
   -fieldsplit_0_fieldsplit_velocity_ksp_type preonly
   -fieldsplit_0_fieldsplit_velocity_pc_type lu
   -fieldsplit_0_fieldsplit_pressure_ksp_rtol 1e-10
   -fieldsplit_0_fieldsplit_pressure_pc_type jacobi
 -fieldsplit_temperature_ksp_type preonly
 -fieldsplit_temperature_pc_type lu
```

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

# Solver Configuration: No New Code

ex31: $P_2/P_1$ Stokes Problem with Temperature on Unstructured Mesh

Upper Schur Comp. + Full Schur Comp. + Least-Squares Comm.

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_0_fields 0,1 -pc_fieldsplit_1_fields 2
-pc_fieldsplit_schur_factorization_type upper
 -fieldsplit_0_ksp_type fgmres -fieldsplit_0_pc_type fieldsplit
 -fieldsplit_0_pc_fieldsplit_type schur
 -fieldsplit_0_pc_fieldsplit_schur_factorization_type full
   -fieldsplit_0_fieldsplit_velocity_ksp_type preonly
   -fieldsplit_0_fieldsplit_velocity_pc_type lu
   -fieldsplit_0_fieldsplit_pressure_ksp_rtol 1e-10
   -fieldsplit_0_fieldsplit_pressure_pc_type jacobi
 -fieldsplit_temperature_ksp_type gmres
 -fieldsplit_temperature_pc_type lsc
```

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

# Outline

# Thrust

Thrust is a CUDA library of parallel algorithms

- Interface similar to C++ Standard Template Library
- Containers (`vector`) on both host and device
- Algorithms: `sort`, `reduce`, `scan`
- Freely available, part of PETSc configure (`-with-thrust-dir`)
- Included as part of CUDA 4.0 installation

# 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, 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

Preliminary Implementation of PETSc Using GPU,

Minden, Smith, Knepley, 2010

- 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 soon
--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

```
ex50 -da_vec_type seqcusp
  -da_mat_type aijcusp -mat_no_inode # Setup types
  -da_grid_x 100 -da_grid_y 100      # Set grid size
  -pc_type none -pc_mg_levels 1      # Setup solver
  -preload off -cuda_synchronize     # Setup run
  -log_summary
```

# Outline

# 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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- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

# 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

```
for(c = cells->begin(); c != cells->end(); ++c) {
  SectionRestrictClosure(coordinates, dm, c, &coords);
  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 */
      /* Linear term */
      /* Nonlinear term */
      elemVec[f] *= weight[q]*detJ;
    }
  }
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}
/* Aggregate updates */
```

# Integration

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      /* Linear term */
      /* Nonlinear term */
      elemVec[f] *= weight[q]*detJ;
    }
  }
  /* Update output vector*/
}
/* Aggregate updates */
```

# Integration

```
for(c = cells->begin(); c != cells->end(); ++c) {
  /* Compute cell geometry */
  SectionRestrictClosure(U, dm, c, &inputVec);
  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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}
/* Aggregate updates */
```

# Integration

```
for(c = cells->begin(); c != cells->end(); ++c) {
  /* Compute cell geometry */
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  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

```
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;
    }
  }
  /* Update output vector*/
}
/* Aggregate updates */
```

# Integration

```
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

```
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) {
      elemVec[f] += basis[q,f]*rhsFunc(realCoords);
      /* Linear term */
      /* Nonlinear term */
      elemVec[f] *= weight[q]*detJ;
    }
  }
  /* Update output vector*/
}
/* Aggregate updates */
```

# Integration

```
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

```
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 */
      /* 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];
          /* Update element matrix */
        /* Update element vector */
      }
      /* Nonlinear term */
      elemVec[f] *= weight[q]*detJ;
    }
  }
  /* Update output vector*/
```

# Integration

```
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 */
      /* 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;
    }
  }
  /* Update output vector*/
}
/* Aggregate updates */
```

# Integration

```
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

```
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 */
      elemVec[f] += basis[q,f]*lambda*exp(inputVec[f]);
      elemVec[f] *= weight[q]*detJ;
    }
  }
  /* Update output vector*/
}
/* Aggregate updates */
```

# Integration

```
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

```
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;
    }
  }
  SectionRealUpdate(locF, c, elemVec, ADD_VALUES);
}
/* Aggregate updates */
```

# Integration

```
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

```
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*/
}
DMLocalToGlobalBegin(dm, locF, INSERT_VALUES, F);
DMLocalToGlobalEnd(dm, locF, INSERT_VALUES, 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

# Why is PETSc cool?

PETSc gives you tools

to design and build

new Scientific Software

from simple pieces

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